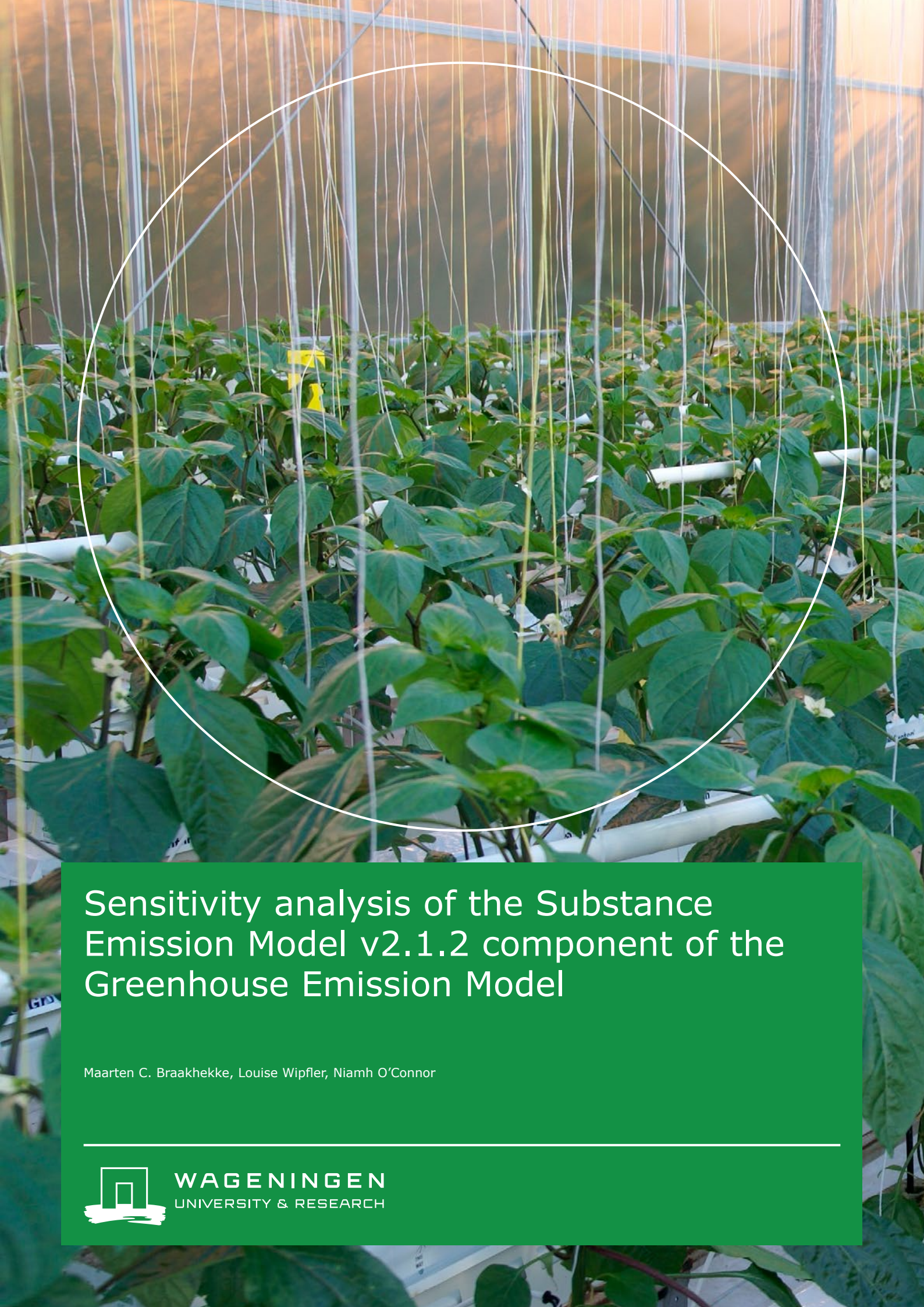

Sensitivity analysis of the Substance Emission Model v2.1.2 component of the Greenhouse Emission Model

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Sensitivity analysis of the Substance Emission Model v2.1.2 component of the Greenhouse Emission Model

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The substance emission model (SEM) simulates fate of plant protection products applied to crops grown in soilless cultures in greenhouses. It is part of the Greenhouse Emission Model used for regulatory risk assessment. This report presents a sensitivity analysis of SEM version 2.1.2 and is split into two parts. The first part of the report focuses on sensitivity of SEM predictions to the following (groups of) parameters: 1) the time step length of the numerical solution; 2) parameters defining partitioning processes in the cultivation part of the model; 3) saturated vapour pressure and solubility of the modelled substance; 4) deposition distribution of the applied substance; 5) degradation rate in the condensation water; 6) dissipation rate on the crop surface; 7) area fraction of the pots on tables. The second part of the report deals with sensitivity to the date of substance application. Results show that mass emitted from the greenhouse predicted by SEM (and hence the concentration in the receiving water course) is potentially highly sensitive to the application date. Based on these results we propose a procedure in which 12 GEM simulations for different application dates in each month of the year are performed. From the 12 concentration (PEC90) values resulting from these simulations the 90th percentile is determined, which is subsequently multiplied with a safety factor to avoid underestimation.

Keywords: soilless cultures, pesticides, emissions to surface water, greenhouse cultivation, model, sensitivity analysis, environmental risk assessment

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Summary

This report presents a sensitivity analysis of the Substance Emission Model (SEM), which simulates the fate of plant protection products applied to crops grown on soilless substrate in greenhouses. Together with the WaterStreamsModel (WSM) and the TOXSWA model, SEM is part of the Greenhouse Emission Model (GEM), which is used for aquatic risk assessment for plant protection products for soilless greenhouse cultivation in the Netherlands. This report describes the sensitivity of output of an updated version of SEM (version 2.1.2) to a selection of input parameters. The report is divided into two parts: the first part deals with the sensitivity to several parameters that are part of the scenario definition (i.e. cannot be modified by the user), as well as several substance properties. The second part focuses specifically on sensitivity to the selected date of application.

Sensitivity of SEM predictions to scenario parameters and selected substance properties
This part of the analysis focusses on the sensitivity of the predicted concentration in the drain water tank (serving as a proxy for the concentration of the discharged water) to seven (groups of) parameters. For each section the main conclusions are given below.

Time step length of the numerical solution. Based on comparing runs with the default time step length of 1 min. to results for runs with a time step length of 1 s, it was found that numerical errors can cause substantial underestimation of the concentration in the drain water tank. However, these errors occur directly after application, when the concentrations in the drain water tank are still low and are negligible by the time the peak concentration in the drain water tank occurs. Hence these errors are not expected to be relevant in practical applications of GEM.

Partitioning into materials in the cultivation tank. Based on the sorption coefficients for dimethamorph, it was found that partitioning into slabs and roots had the strongest effect on the concentration in the drain water tank as compared to other materials. For the foil and pipes the effect was negligible. Increasing the sorption coefficients for slabs, foil, and pipes, by a factor 10 led to a reduction of 35% of the maximum concentration, relative to a situation without sorption. Simulations with varying strength of partitioning into the roots show that this process has the potential to drastically reduce concentrations in the drain water tank.

Saturated vapor pressure and solubility. The substance properties saturated vapor pressure and solubility were found to have a potentially strong effect on predicted concentrations. This effect varied with the season and selected growth medium (substrate slabs or pots). The varying sensitivity of the predicted concentration in the drain water tank to saturated vapor pressure and solubility between summer and winter is related to the entry of substance via the condensation water into the recirculation water.

Deposition distribution of applied substance. The fraction of the applied dose deposited on the slabs and troughs shows a strong positive relationship to the concentration in the drain water tank because this fraction of the dose is directly added to the recirculation water. The fraction deposited on the roof has a small positive effect, depending on solubility and saturated vapor pressure. For substances with non-negligible saturated vapour pressure and solubility, the fraction deposited on the crop has for most part a negative relationship with the concentration in the drain water tank, owing to the loss off substance by dissipation on the crop surface, simulated in SEM.

Degradation in condensation water. A half-life of 0.1 d in the condensation water resulted in a reduction of 81% and 43% in summer and winter, respectively, compared to a half-life of 1000 d. The different sensitivities for winter and summer are explained by differences between residence time in the condensation water and temperature in the greenhouse.

Dissipation on crop surface. A half-life of 0.1 d on the crop surface resulted in a reduction of 85% and 83% in summer and winter, respectively, compared to a half-life of 1000 d.

Area fraction of pots on tables. A larger pots area fraction results in a lower concentration in the drain water tank, due to the lower amount of substance deposited on the tables and dissolved in the recirculation water during irrigation.

Sensitivity to the application date

This part of the analysis focusses on the sensitivity of the predicted emission from the greenhouse to the date of application. Predicted Exposure Concentrations (PECs) calculated with the GEM-soilless tool are sensitive to the date of substance application. This date is chosen by the user and may be anywhere in the application window supplied by the registrant, which may cover the entire year. This represents substantial uncertainty regarding the calculated PECs. In view of the required robust outcomes in the regulatory context, a procedure is needed to deal with this variability. At the same time, the outcomes of the exposure assessment should be sufficiently protective.

A sensitivity analysis was performed to quantify the sensitivity of GEM predictions to application date for 100 selected assessments that cover a wide range of possible input options in GEM for soilless cultivation. For each assessment, 365 simulations were performed with varying application date; one for each day of the year. For each simulation the 50th and 90th percentile (PEC50 and PEC90) of the annual concentration maxima of the discharged water were determined. These serve as a proxy for the concentration in the ditch, which is the endpoint variable of GEM. Subsequently, we determined the 90th percentile of the PEC90 and PEC50 over the 365 simulations with different application dates. Additionally, we analysed the effect of performing fewer than 365 simulations by determining the 90th percentile of the PEC50 and PEC90 values for a subsample of the of PEC90 and PEC50 values.

It was found that the application date has potentially a very large effect on the PEC90 and PEC50—up to several orders of magnitude. However, this sensitivity varied strongly between assessments. It was further found that underestimation of the 90th percentile of the PEC90 and PEC50 becomes stronger when fewer simulations with different application dates are performed. Again, this varied strongly between assessments.

Based on these outcomes we propose the following procedure for the exposure assessment:

- Perform 12 simulations with different application dates, one for every month of the year on a fixed date
- For each simulation, determine the 90th temporal percentile of the calculated annual PECs (PEC90), this is considered to be the 90th overall percentile
- Determine the 90th percentile of the PEC90 of these 12 runs
- Multiply the 90th percentile of the PEC90 by a safety factor determined by the half-life in recirculation water (DT50) and scenario of the WaterStreamsModel (WSM) as indicated in the following table:

	DT50 < 50 d	**DT50 ≥ 50 d**
WSM scenario number ≠ 40	1.5	1.2
WSM scenario number = 40	5	1.2

Samenvatting

In dit rapport wordt een gevoeligheidsanalyse van het Substance Emission Model (SEM) gepresenteerd. Dit model simuleert het gedrag van gewasbeschermingsmiddelen die worden gebruikt in kassen voor gewassen op substraatteelt. Samen met het WaterStromenModel (WSM) en het TOXSWA model is SEM onderdeel van het Greenhouse Emission Model (GEM) dat wordt gebruikt voor aquatische risicobeoordeling van gewasbeschermingsmiddelen binnen de substraatteelt in kassen in Nederland. Dit rapport behandelt de gevoeligheid van de uitvoer van een vernieuwde versie van SEM (versie 2.1.2) voor een selectie aan invoerparameters. Het rapport is in twee onderdelen verdeeld. Het eerste deel behandelt de gevoeligheid voor een aantal parameters die onderdeel zijn van de scenariodefinitie (m.a.w. die niet gewijzigd kunnen worden door de gebruiker van GEM), en enkele stofeigenschappen. Het tweede deel richt zich specifiek op gevoeligheid voor de geselecteerde datum van toediening van de gesimuleerde stof.

Gevoeligheid voor scenarioparameters en enkele stofeigenschappen
Dit deel van de analyse richt zich op de gevoeligheid van de berekende concentratie in de drainwatertank (welke dient als proxy voor de concentratie van het geloosde water) voor zeven (groepen van) parameters. De concentratie in de drainwatertank is een proxy voor de concentratie in het geloosde water. Hieronder worden voor elk onderdeel de hoofdconclusies gegeven.

Tijdstaplengte van de numerieke oplossing. Door resultaten van een simulatie met de standaard tijdstaplengte van 1 min te vergelijken met die van een simulatie met een tijdstaplengte van 1 s kan geconcludeerd worden dat numerieke fouten als gevolg van een grote tijdstap tot substantiële onderschatting van de concentratie in de drainwatertank leiden. Deze fouten zijn echter het grootst kort na de toediening van het middel als de concentratie in deze tank nog laag is, en nemen snel af in de tijd. De piekconcentratie in de drainwatertank vindt substantieel later plaats. Op dit tijdstip is de onderschatting verwaarloosbaar. Deze fouten zijn daarom naar verwachting niet relevant in praktische toepassingen van GEM.

Sorptie aan materialen in de teelttank. Op basis van sorptiecoëfficiënten voor dimethamorph kan geconcludeerd worden dat sorptie aan het materiaal van de substraatmatten en aan plantenwortels de sterkste invloed heeft op de concentratie in de drainwatertank ten opzichte van andere materialen. Voor het folie om de substraatmatten en toe- en afvoerbuizen was het effect van sorptie verwaarloosbaar. Verhoging van de sorptiecoëfficiënten voor substraatmatten, folie een buizen met een factor 10 leidde tot 35% reductie van de maximum concentratie ten opzichte van een simulatie zonder sorptie. Simulaties met verschillende parametrisaties voor sorptie aan wortels tonen aan dat dit proces potentieel de concentraties in de drainwatertank sterk kan verlagen.

Verzadigde dampdruk en oplosbaarheid. Verzadigde dampdruk en oplosbaarheid kunnen grote invloed uitoefenen op de berekende concentraties in het drainwater. Dit effect verschilde tussen seizoenen van toediening en het teeltmedium (substraatmatten of potten). De verschillen in gevoeligheid tussen winter en zomer kunnen verklaard worden door de verschillen in de aanvoer van de stof naar het recirulatiewater via het condensatiewater.

Verdeling van de depositie van de toegediende stof. De fractie van de toegediende stof die terecht komt op de substraatmatten en in de goten heeft een sterke positieve relatie met de concentratie in de drainwatertank. Dit komt doordat deze fractie direct wordt toegevoegd aan het recirculatiewater. Verhoging van de fractie die terecht komt op de beglazing van de kas heeft een licht positief effect op de concentratie, welke afhankelijk is van de oplosbaarheid en de verzadigde dampdruk van de toegediende stof. De fractie die terecht komt op het gewas heeft veelal een negatieve relatie met de concentratie in de drainwatertank. Dit wordt verklaard door het verlies van de stof op het gewas zoals berekend in SEM.

Afbraak in het condensatiewater. Een halfwaardetijd van 0,1 d in het condensatiewater resulteerde in een reductie van 81% en 43% ten opzicht van een halfwaardetijd van 1000 d, voor zomer, respectievelijk winter. Deze verschillen in gevoeligheid voor winter en zomer hebben te maken met verschillen in verblijftijd in het condensatiewater en de temperatuur in de kas.

Dissipatie op het gewasoppervlak. Een halfwaardetijd van 0,1 d op het gewas resulteerde in een reductie van 85% en 83% ten opzichte van een halfwaardetijd van 1000 d, voor zomer respectievelijk winter.

Bedekkingsgraad van de potten op de tafels. Een hogere bedekkingsgraad van de potten op de tafels resulteerde in een lagere concentratie in de drainwatertank, hetgeen wordt verklaard door een lagere hoeveelheid stof die terecht komt op de tafels, en daarmee een lagere hoeveelheid die oplost in het recirculatiewater ten tijde van irrigatie.

Gevoeligheid voor datum van toediening

Dit deel van het rapport richt zich op de gevoeligheid van de berekende emissie uit de kas voor de toedieningsdatum. De berekende blootstellingsconcentratie (Predicted Environmental Concentration; PEC) is gevoelig voor de datum waarop het middel wordt toegediend. Deze datum wordt gekozen door de gebruiker en kan op elke dag in de periode van toediening zijn die de gebruiker heeft opgegeven. Deze periode kan het gehele jaar beslaan. Dit is een substantiële bron van onzekerheid van de PEC's berekend door GEM. Omdat een robuuste voorspelling van de concentratie noodzakelijk is voor de risicobeoordeling, is een aanpak nodig om met deze onzekerheid om te gaan. De PEC's die uit deze aanpak volgen moeten bovendien voldoende beschermend zijn.

Een analyse is uitgevoerd om de gevoeligheid van GEM voor de toedieningsdatum te bepalen voor 100 verschillende "assessments" (GEM runs), welke een brede range van verschillende input mogelijkheden voor GEM substraat bestrijken. Voor elke van deze 100 assessments zijn 365 simulaties uitgevoerd met verschillende toedieningsdatums—één voor elke dag van het jaar. Voor elke simulatie is het 50ste en 90ste percentiel van de jaarlijkse maxima van de emissieconcentraties bepaald (PEC50 en PEC90). Deze variabele dient als benadering van voor de concentratie in de sloot, wat de relevante uitvoer van GEM is. Vervolgens is het 90ste percentiel bepaald van de PEC50- en PEC90-waarden, zowel voor de gehele populatie (365) en voor een reeks trekkingen met variërende steekproefgrootte. Hierdoor kan het effect van het uitvoeren van minder simulaties op de onzekerheid op de PEC50 en PEC90 waarden bepaald worden.

De resultaten bevestigen dat de toedieningsdatum een substantieel effect kan hebben op de PEC50 en PEC90. Een verschuiving van enkele dagen kan leiden tot meerdere orden van grootte verschil in de berekende PEC's. Deze gevoeligheid varieert echter sterk tussen verschillende assessments. De resultaten laten verder zien dat de potentiële onderschatting van de PEC50 en PEC90 groter wordt naarmate er minder simulaties met verschillende toedieningsdatauitgevoerd worden. Ook dit varieert echter sterk tussen de verschillende assessments.

Op basis van deze uitkomsten wordt de volgende procedure voor de risicobeoordeling voorgesteld:

- Voer 12 simulaties uit voor 12 toedieningsdatums voor elke maand van het jaar op een vaste dag
- Bepaal voor elke simulatie de PEC90: het 90ste percentiel van de jaarlijkse concentratie maxima
- Bepaal het 90ste percentiel van de 12 PEC90-waarden
- Vermenigvuldig het 90ste percentiel van de PEC90 met een veiligheidsfactor waarvan de waarde bepaald wordt door de halfwaardetijd (DT50) in het recirculatiewater en het scenario van het WaterStromenModel (WSM) volgende de onderstaande tabel:

	DT50 < 50 d	**DT50 ≥ 50 d**
WSM scenarionummer ≠ 40	1.5	1.2
WSM scenarionummer = 40	5	1.2

Abbreviations

PPP	Plant Protection Product
SEM	Substance Emission Model
GEM	Greenhouse Emission Model
WSM	WaterStreamsModel
RCF	Root Concentration Factor
SVP	Saturated Vapor Pressure
LVM	Low Volume Mister
PEC	Predicted Environmental Concentration

1 General introduction

The substance emission model (SEM) simulates the fate of plant protection products (PPPs) applied to crops grown in greenhouses on soilless cultivation (van der Linden et al., 2015). SEM is part of the greenhouse emission model (GEM), which is used for performing scenario simulations as part of aquatic exposure assessment of PPPs in the Netherlands, as well as the European Union (Boesten et al., 2020; van der Linden et al., 2015; Wipfler et al., 2023). In this context, the main task of SEM is to simulate emission of PPP resulting from water discharge to a ditch assumed adjacent to the greenhouse. The discharged water fluxes, as well as several other water fluxes in the greenhouse, are calculated by the WaterStreamsModel (WSM), and serve as input to SEM (Boesten et al., 2020). The discharged PPP mass fluxes calculated by SEM are subsequently used by the aquatic fate model TOXSWA to simulate the fate in the ditch and determine the predicted environmental concentration (PEC).
Note that SEM calculates PPP emission only for crops grown on soilless media (e.g. stonewool slabs or pots). Emission from PPP applied in soil-bound cultivation are calculated by the PEARL model (Wipfler et al., 2014).

In a comprehensive review of the concepts implemented in SEM1.1.1 (part of GEM3.3.2), Boesten et al. (2019) identified a number of shortcomings and proposed modifications to solve these. These improvements were implemented, resulting in SEM2.1.2, which will be incorporated in a new version of GEM. This report presents an analysis of the sensitivity of SEM2.1.2 predictions to a number of model inputs. Such a sensitivity analysis is useful to help understand the behaviour of the model and elucidate the results, identify potential weaknesses, and pinpoint key parameters that most strongly influence predictions.

The sensitivity analysis is divided into two parts. The first, presented is more general and deals with the time step length used in the numerical solution, a number of properties of the simulated substance, and several parameters which are part of the scenario for soilless cultivation (i.e. they are not set by the user). The second part focuses specifically on the sensitivity to the date on which a substance is applied. Discharge mass fluxes predicted by SEM are known to be highly sensitive to the timing of application. At the same time, this parameter is not part of GEM scenarios (i.e. it must be specified by the user), nor is there any guidance on which date to select. This inherent uncertainty related to application date requires a special procedure in the risk assessment in order to obtain robust and protective results, and thus warrants a more in-depth analysis. Based on the analysis a procedure is being proposed on how to deal with the sensitivity to the application date in the exposure assessment of PPPs.

2 SEM model description

Only a general description of SEM is given here. For a full description the reader is referred to Boesten et al. (2020).

In Dutch greenhouses, water cycles through a series of cyclically connected tanks, referred to as "recirculation water". Irrigation surplus is collected, filtered, disinfected, and ultimately reused—a mandatory practice in the Netherlands. Moreover, transpired or evaporated water which condenses on the glass roof and walls is collected and also reused. However, the system is not fully closed. To prevent that sodium concentrations rise above levels harmful to the crop, water must be periodically discharged and replaced from an external source. Additionally, water used for rinsing the filters may also be discharged. These discharge fluxes lead to emission of plant protection products from the greenhouse which are the main endpoint of a SEM simulation. The emitted mass per hour is calculated and subsequently used by the surface water fate model TOXSWA to simulated the fate in the receiving ditch.

SEM runs in one of six possible model configurations, which are defined by the type of growth medium used for cultivation and the method of substance application. For the growth medium type, slabs (e.g. stonewool) and pots can be selected, and the corresponding model configurations are denoted by SEM-S and SEM-P, respectively. Crops grown on slabs are irrigated via drip tubes running into the slab material, while crops grown in pots are assumed to be positioned on tables that are periodically flooded with water.

Substance is administered in one of several ways: (i) with nutrient solution via the drip irrigation tubes (for slabs; SEM-Sd) or irrigation water flooded on the tables (for pots; SEM-Pi), (ii) by spraying (SEM-Ss/SEM-Ps), (iii) or with a low volume mister (LVM; SEM-Sl/SEM-Pl). Applications of different types may occur within one simulation. With the combination of growth medium and application type, six different model configurations can be distinguished (Table 2.1). The following two sections give a more detailed description of the processes in the recirculation water and other locations.

Table 2.1 *Overview of the different configurations of the SEM model.*

Model configuration	Growth medium	Application type
SEM-Sd	Substrate slabs	Drip irrigation
SEM-Ss		Spraying
SEM-Sl		LVM
SEM-Pi	Pots	Irrigation water
SEM-Ps		Spraying
SEM-Pl		LVM

2.1 Substance in the recirculation water

In SEM, the recirculation water is simulated as a series of connected tanks, as depicted in Figure 2.1. Here "tank" refers to a reservoir of water, which may or may not be an actual tank. Loss of water from the recirculation water system may occur by crop uptake (cultivation tank), leakage (cultivation tank), and discharge (waste water tank). Input occurs into the mixing tank (from an external source) and the clean water tank (from condensation water). The cultivation tank represents the water stored either in the substrate slabs (SEM-S) or on the tables carrying the pots (SEM-P) and includes also the water in the irrigation and drainage tubes in the cultivation compartment. Note that in the latter case, the irrigation events are not explicitly simulated; water is assumed to flow continuously, as with growth medium type slabs. (However, substance deposited on dry tables between irrigation events is explicitly simulated, see

below). For substrate type slabs (SEM-S), the cultivation tank is divided into two sub-tanks. Substance uptake by roots is only considered for the first sub-tank (in the water flow direction). The water fluxes between the tanks are calculated from outputs of WSM. Additionally, WSM provides greenhouse air temperatures, which affects the rates of several fate processes. In the latest GEM version there are 32 possible (water flow) scenarios for the WSM model.

Substance can enter the recirculation water in three places: (1) the mixing tank, as part of an application with the nutrient solution (SEM-Sd/SEM-Pi); (2) the cultivation tank, either deposited on the slabs or troughs during a spraying or LVM application (SEM-Ss/SEM-Sl), or when substance on the dry tables dissolves during irrigation of the tables (SEM-Pl); (3) the clean water tank, by flow from the condensation water on the roof and walls of the greenhouse. Several of these fluxes are described in more detail in the next section. Loss of substance from the recirculation water occurs due to the above-mentioned water loss fluxes, as well as due to degradation and plant uptake. For growth medium type slabs, partitioning of substance onto slab material, surrounding foil, and the walls of transport pipes, as well as into plant roots may occur in the cultivation tank. This retards flow of substance to the drain water tank.

2.2 Substance in other locations

During application with the nutrient solution, all applied substance is added to the mixing tank; hence locations other than the recirculation water tanks are not considered in SEM. For spray or LVM applications, on the other hand, applied substance is assumed to be deposited onto several surfaces: floor (SEM-S only), roof, crop, pots (SEM-P only), dry tables (SEM-P only), slabs, and troughs (SEM-S only). Additionally, for LVM application, part of the applied dose remains in the greenhouse air. Substance deposited onto the slabs and troughs for SEM-S, is added to the water of the cultivation tank. For SEM-P, it is assumed that the tables are dry (i.e. not flooded) during application, and for one day thereafter. Substance deposited on the dry tables may volatilize to the greenhouse air; the remaining substance is added to the cultivation water tank after one day. Substance may also volatilize from the crop, floor, roof, and pots. Substance in the greenhouse air can partition into the condensation water on the glass roof and walls, from where it can flow to the recirculation water. Substance deposited on the roof can also dissolve into the condensation water directly, without first volatilizing. Substance located on the soil surface of the pots may be transported downward into the soil material. Upward transport within the pots (and subsequent volatilization) is also possible. Degradation of substance can occur on the crop surface, in the pots, and in condensation water.

2.3 SEM input

As part of a risk assessment with GEM, the user must provide the following inputs:
- Substance properties (e.g. degradation half-life, solubility)
- Crop type (selected from 60 possible crops)
- Nutrient emission reference period (2015–2017, 2018–2020, 2021–2023, or 2024–2027)
- Filter rinsing water option (discharge or reuse)
- Application types (nutrient solution, spraying, LVM), dates and dosage

The WSM scenario is parameterized based on the selected crop, nutrient emission reference period, and filter water option. The selected crop is translated to one of four reference crop types which have different parametrizations. The nutrient emission reference period determines the maximum annual discharge volume. For each of the 32 combinations of reference crop, filter water option, and nutrient emission reference period, a WSM parametrization was derived that satisfies that annual discharge limit. The selected crop also determines the growth medium type in SEM (slabs or pots), which, together with the application type, determines the distribution of applied substance over various locations as described in section 2.4.

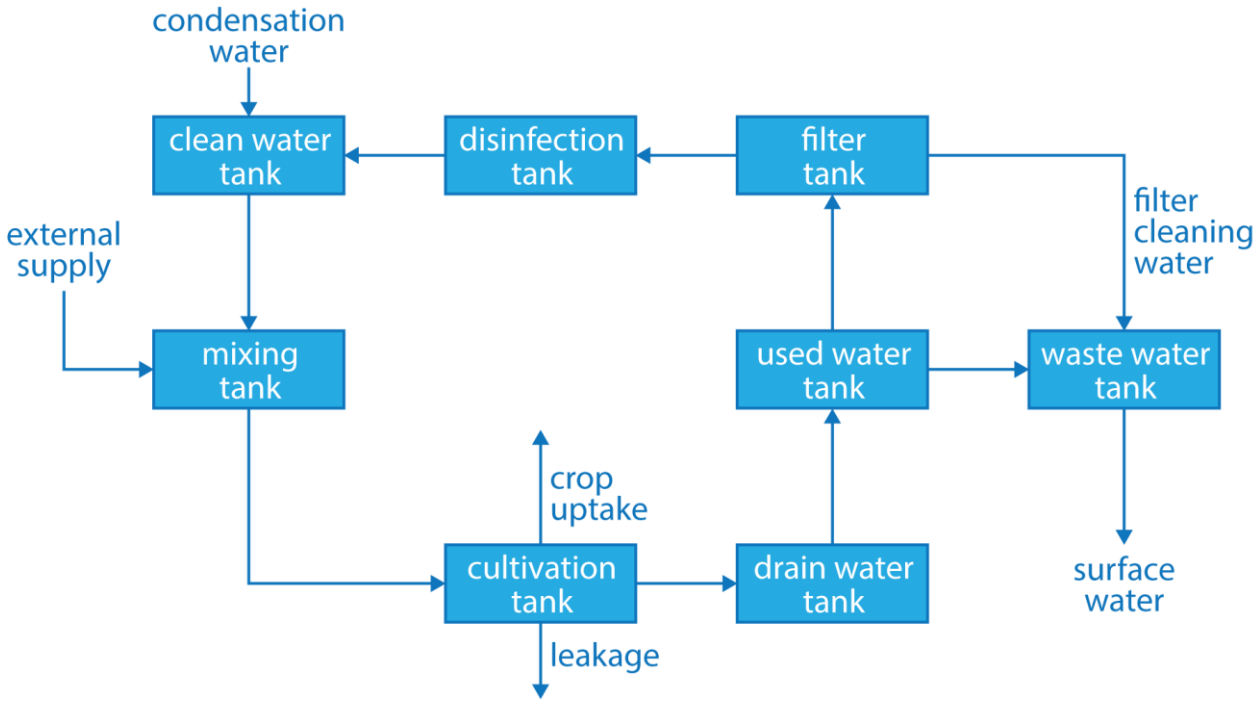

Figure 2.1 *Overview depicting the tanks in the recirculation water system and water flows in GEM for soilless cultivation.*

2.4 Factors influencing emission to surface water

The immediate factors determining substance emission to surface water are water discharge fluxes and concentration in the waste water tank. The latter is generally close to the concentration of the water flowing out of the cultivation tank. On the whole, the concentration in the waste water tank is the result from the input of substance into and processing (mainly degradation and partitioning) within the recirculation water.

With regard to substance input into the recirculation water system, it is relevant to note that for spray and LVM applications there are two routes: direct, by deposition on the troughs and slabs (SEM-S) or on the tables (SEM-P), or indirect, via the condensation water.

The discharge fluxes calculated by WSM are in the form of relatively short events, separated by periods without discharge. The temporal pattern of the discharges differs greatly between the different WSM scenarios.

Sensitivity of SEM predictions to scenario parameters and selected substance properties

3 Introduction

In this part of the report we present an analysis of the sensitivity SEM predictions to selected input parameters. We focus on the following aspects:

- Time step length of the numerical solution (chapter 4)
- Partitioning into materials in cultivation tank (chapter 5)
- Saturated vapor pressure and solubility (chapter 6)
- Distribution of applied substance (chapter 7)
- Degradation in condensation water (chapter 8)
- Dissipation on crop surface (chapter 9)
- Area fraction of pots on tables (chapter 10)

With regard to the time step length, the main objective is to analyse the effect of numerical errors on the SEM predicted emitted PPP masses. For the other aspects, the objective is to verify and understand the impact of selected fate processes as simulated by SEM on the predicted concentration in the recirculation water.

For the sake of consistency, all analyses were based on a single base simulation setup (parametrization listed in Annex 1), with only the relevant parameters changed. When applicable, parameters were kept at the default values used in GEM, as reported in (Boesten et al., 2020). Furthermore, a base set of substance properties was defined in line with recommendations on default properties as reported in (Wipfler et al., 2015b).
As discussed in section 2.4, the emitted mass from a greenhouse as predicted by SEM is the combined result of the concentration in the in the waste water tank and discharge water fluxes predicted by WSM (used as input by SEM). The discharge water fluxes may be highly variable in time, which results in similar variability of the predicted substance fluxes. Moreover, the temporal patterns differ substantially between WSM scenarios. Therefore, we focused on the predicted concentration in the drain water tank as response variable for the sensitivity analysis, being a proxy for the (sensitivity of) expected discharged mass fluxes. In the flow direction of the recirculation water, this tank receives water and substance from the cultivation tank and encapsulates all relevant processes. In case of a discharge event, the water coming from the drain water tank is discharged to the surface water (via the waste water tank). For consistency, a single WSM scenario was used for all analyses, viz. scenario 12, corresponding to reference crop rose, nutrient emission reference period 2018-2020, and discharge of filter water. This scenario has a relatively high discharge frequency, resulting in a high flow in the recirculation water. In practice we expect that the choice of WSM scenario has little effect on the concentration in the drainage tank.

4 Time step length of the numerical solution

4.1 Introduction

The mass conservation equations in SEM are solved using an explicit numerical scheme. The underlying assumption of this approach is that the fluxes between various reservoirs are constant during a single time step. This introduces a numerical error proportional with the length of the time step (default 1 minute). These numerical errors are larger when the fluxes are large compared to the size of the donor reservoir. Here we analyse these errors for the concentration in the drain water tank in relation to the time step length.

4.2 Methods

Simulations were performed using a time step length of 1 minute (the default) and 1 second for four combinations of growth medium type and application type: slabs + drip (SEM-Sd), slabs + spraying (SEM-Ss), pots + irrigation (SEM-Pi), pots + spraying (SEM-Ps). In all simulations the default substance was used and the simulation period was 1-Jan-2000 to 31-Jan-2000 with application on the first day.
We calculate the relative difference of the concentration in the drain water tank for the simulations with a time step length of 1 minute and 1 second, where the latter is taken as baseline (given its higher accuracy).

4.3 Results

Figure 2 shows the relative difference in predicted drain water tank concentration between the two simulations with two time step lengths for the first 24 h after application. For all setups, a 1 minute time step length result in an underestimated concentration in the drainage tank compared to a 1 second time step length. In the first minutes directly after application the underestimation is 100%, meaning that the 1-minute concentration is zero, while the 1-second concentration is non-zero. This is because with a shorter time step length an earlier "arrival" of substance to the drainage tank can be simulated. The SEM-Ps model setup (pots + spraying) shows the strongest underestimation, while for SEM-Ss (slabs + spraying) the underestimation is lowest. The relative underestimation quickly decreases with time, and is less than 1% after 20h for all model setups. It should be noted that, at the time of the peak concentration, the relative underestimation is negligible because this occurs much later than the period depicted in Figure 2. SEM-Pi shows the earliest peak at approximately 83 hours. Hence, the underestimation is not relevant in the context of risk assessment, since here the focus is on the maximum concentration.

4.4 Conclusions

A considerable relative underestimation of the concentration in the drain water tank can occur with a time step length of 1 minute (the default), as compared to a simulation with a time step length of 1 s. However, these errors affect mostly concentrations shortly (~10 h) after application, while the peak typically occurs much later. Therefore, we expect that these errors have a minor impact on the final mass emitted to surface water and consequently the concentration in the receiving water course.

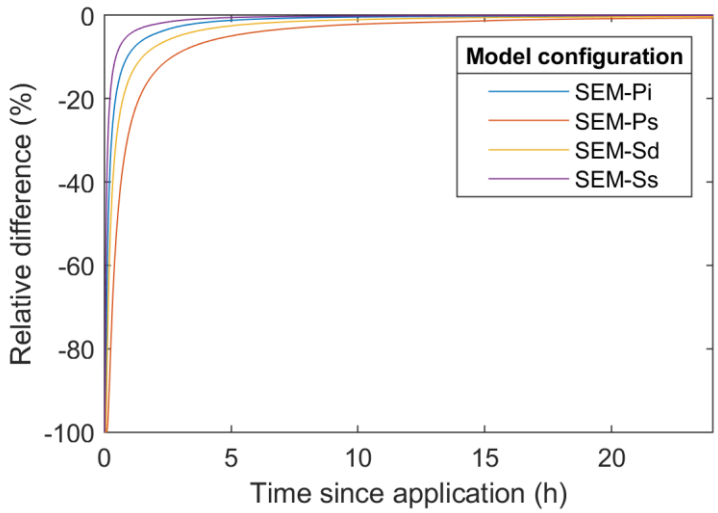

Figure 3.1 *Effect of time step length on predicted concentration, in the first 24 hr after application in drain water tank for the four tested model configurations. The graph shows the relative difference of the predicted concentration with 1 minute time step length compared to with a 1 second time step length. Negative values indicate underestimation.*

5 Partitioning processes

5.1 Introduction

For growth medium type slabs, several partitioning processes are simulated in the cultivation tank. Equilibrium sorption of substance is considered to substrate slabs, foil surrounding the slabs, and to three types of pipes (polyethylene irrigation and capillary tubes and PVC transport pipes). Additionally, partitioning into plant roots in the substrate is considered. These processes reduce the concentration in the liquid phase, thereby decreasing the flow to the drain water tank. Thus, these processes will reduce peak concentrations in discharged water.

The partitioning is simulated as an equilibrium process. For the slabs, foil, and pipes, sorption is parameterized by sorption coefficients and the mass of these materials in the cultivation tank. Partitioning into roots is determined by mass of wet roots and the root concentration factor (RCF), which is a non-linear function of the octanol-water partitioning coefficient (K_{OW}). The sorption coefficients and K_{OW} are substance-specific parameters.

Three aspects of these partitioning processes were analysed with regard to the concentration in the drain water tank:

1. Effect of the different materials
2. Sorption strength for slabs, foil, and pipes
3. Effect of the strength of partitioning into roots

5.2 Methods

All three analyses used slabs for growth medium type and spraying was used for application type (SEM-Ss). Simulations ran for the period 1–31 January 2000, with application occurring on the first day. Sorption to slabs, foil, and pipes was controlled by varying the respective sorption coefficients for these materials. For the base values we used values for dimethomorph, derived by Boesten and Matser (2017) (see Annex 1).

The substance property determining partitioning into roots is the octanol-water partitioning coefficient (K_{OW}). However, this parameter was not varied to assess the impact of partitioning to roots, since it is also used in SEM to determine the plant uptake, which is not included in this analysis. To allow for an independent assessment, partitioning into roots was controlled by varying the mass of wet roots. All other substance properties were equal to the default values listed in Annex 1.

5.2.1 Effect of individual materials

The contribution of substrate slabs, foil, pipes, and roots was analysed in six simulations (Table 5.1). The impact of sorption to the three different types of pipes (polyethylene irrigation and capillary pipes and PVC transport pipes) was analysed as a group, i.e. in one simulation. Partitioning into roots was controlled by using the mass of wet roots, using either 0 or 9500 kg (the default value; Boesten et al., 2020).

Table 5.1 *Parameter values used in the simulations for analysing the effect of partitioning of individual materials. PE tubes refers to polyethylene capillary and irrigation tubes. Partitioning into roots was varied by means of the mass of wet roots, see section 5.2. The non-zero values for the sorption coefficients are measurements for dimethamorph taken from Boesten and Matser (2017).*

Simulation	Sorption coefficient (L kg^{-1})				Mass of wet roots (kg)
	Slabs	Foil	PVC tubes	PE tubes	
No partitioning	0	0	0	0	0
Foil only	0	0.0675	0	0	0
Pipes only	0	0	0.0475	0.075	0
Roots only	0	0	0	0	9500
Slabs only	1	0	0	0	0
All materials	1	0.675	0.0475	0.075	9500

5.2.2 Sorption strength of slabs, foil, and pipes

The effect of strength of sorption to slabs, foil, and pipes was analysed by means of a scaling factor multiplied with the base values of the sorption coefficients for dimethomorph for these materials (Table 5.3). A scaling factor of 1 refers to the base values, a scaling factor of zero indicates no sorption. Partitioning to roots was not modified and the base value was used in all simulations shown in Table 5.3.

Table 5.2 *Sorption coefficients (L kg-1) used in the 6 simulations for analysing the strength of sorption to slabs, foil, and pipes. PE tubes refers to polyethylene capillary and irrigation tubes. Partitioning into roots was kept at the default value.*

Scaling factor	Slabs	Foil	PVC tubes	PE tubes
0	0	0	0	0
0.1	0.1	0.0675	0.00475	0.0075
0.5	0.5	0.3375	0.02375	0.0375
1	1	0.675	0.0475	0.075
2	2	1.35	0.095	0.15
10	10	6.75	0.475	0.75

5.2.3 Partitioning into roots

The effect of the strength of partitioning into roots was analysed with a set of simulations intended to represent different values of the octanol-water partitioning coefficient, which in turn determines the root concentration factor (RCF). The K_{OW} values were selected based on the range of values for substances analysed by Wipfler et al. (2015a) in the GEM impact analysis. From the population of reported values we selected the highest and lowest K_{OW} value and the 95% percentile (Figure 5.1). Additionally, a simulation with the default K_{OW} value of 100 was performed. For reasons discussed in section 5.2, the desired partitioning into roots was achieved by multiplying the mass of wet roots with scaling factor based on the RCF change relative to the default value instead of varying the K_{OW}. The derivation of the mass of wet roots and the associated scaling factor is given in Table 5.3.

Table 5.3 *K_{OW} values and related RCF and mass of wet roots used in the simulations to analyze the effect of partitioning into roots. Note that only the mass of wet roots was changed in the simulations, in order to mimic the effect of varying K_{OW}.*

log-K_{OW} (-)	K_{OW} (-)	RCF (m^3 kg^{-1})	Scaling factor (-)	Mass wet roots (kg)
-1.51	0.0308	0.00082	0.44	4180
2.00	100	0.00187	1	9500
5.12	132000	0.26531	142	1349855
6.37	2360000	2.43567	1304.5	12392655

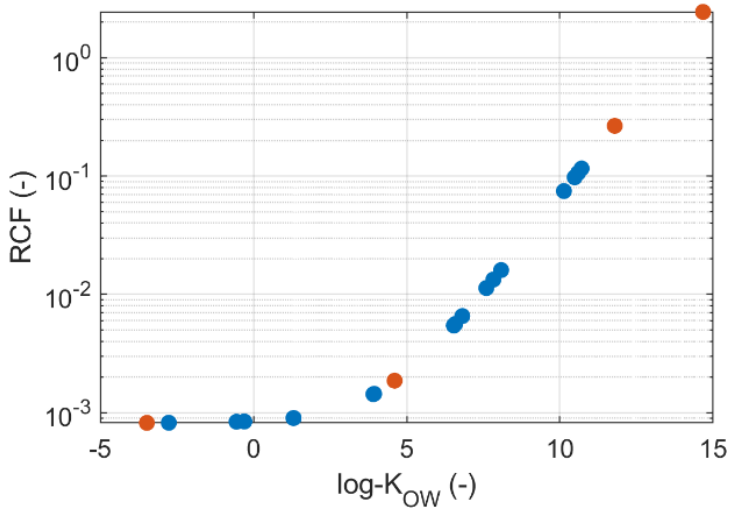

Figure 5.1 *Root Concentration Factor (RCF) as a function of log-K_{OW} for each of the substances of in Wipfler et al. (2015a). Shown in red are the values as given in Table 5.3 and used in the analysis.*

5.3 Results

5.3.1 Effect of individual materials

Figure 5.2 depicts the simulated concentration in the drain water tank for the six simulations to analyse the effect of individual materials with regard to partitioning. The predicted concentration for sorption to pipes and for sorption to foil simulations is virtually identical to that for the simulation without sorption (reduction of 0.11% and 0.04% of the maximum concentration, respectively). Hence the effect of these materials is negligible for dimethomorph. Sorption to slabs and to roots have a larger effect, causing a reduction of 4.9% and 4.5% of the maximum concentration compared to the simulation without sorption.

5.3.2 Sorption strength of slabs, foil, and pipes

Figure 5.3 depicts simulated concentration in the drain water tank for the six simulations to analyse the effect of sorption strength for slabs, foil, and pipes as indicated in Table 5.2. For the selected scaling factors the relationship between the (maximum) concentration and the sorption coefficients is approximately linear. Sorption coefficients 10 times higher than the base values cause a reduction of approximately 35% compared to a situation without sorption (scaling factor 0).

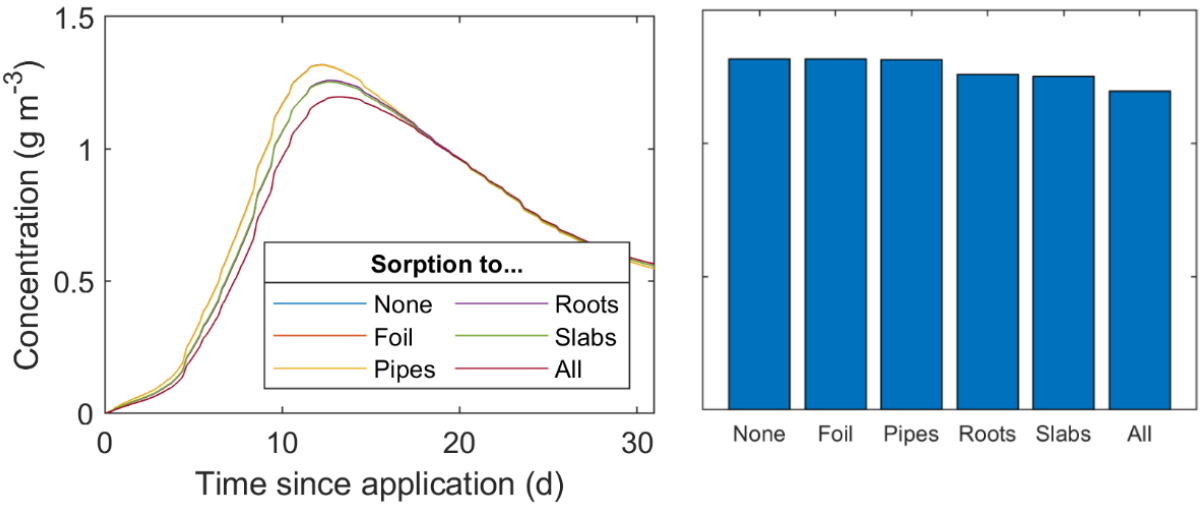

Figure 5.2 *Effect of partitioning into various materials on concentration in drain water tank. Left: concentration vs time after application; right: maximum concentration.*

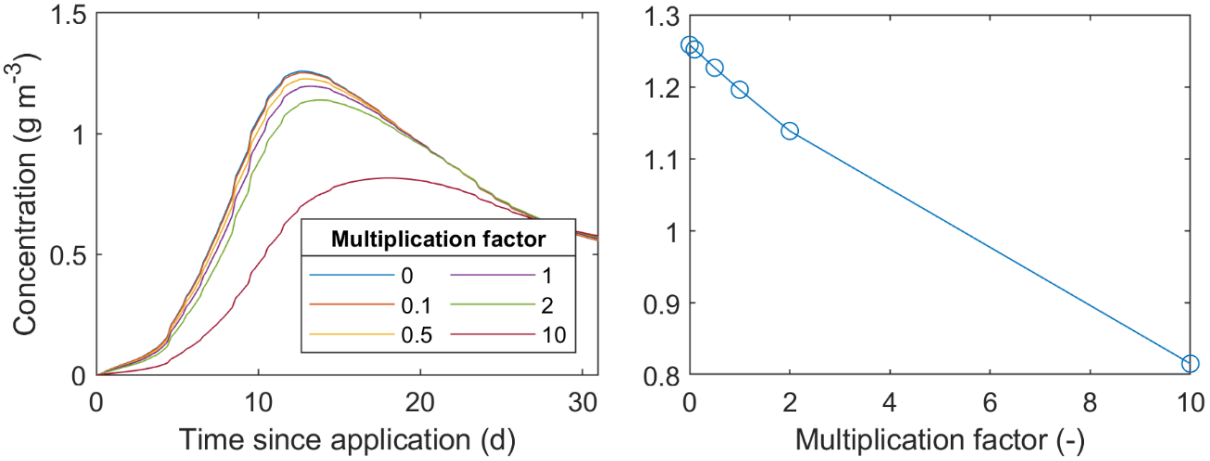

Figure 5.3 *Effect of sorption strength on concentration in drainage tank. Left: concentration vs time; right: maximum concentration in drain water tank vs multiplication factor, i.e. scaling factor. Base sorption coefficients (multiplication factor 1) are valid for dimethomorph. Zero indicates that sorption is not simulated.*

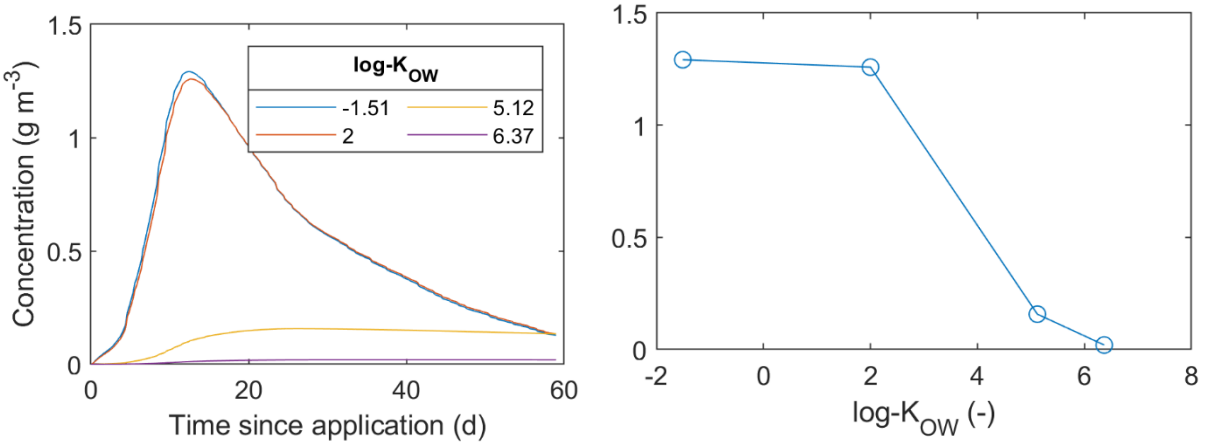

Figure 5.4 *Effect of partitioning to roots on concentration in drainage tank. Left: concentration vs time for different log-K_{OW} values; right: maximum concentration in drain water tank vs log-K_{OW}.*

5.3.3 Partitioning into roots

Figure 5.4 depicts simulated concentration in the drain water tank for the four simulations to analyse the effect of the strength of partitioning into roots. At low log-K_{OW} values, sensitivity to a change of log-K_{OW} is relatively low. Above log-K_{OW} 2 however, sensitivity increases. This behaviour is explained by the non-linear relationship between the root concentration factor (RCF) and log-K_{OW} used in SEM (Figure 5.1). For substances with high log-K_{OW} values, partitioning into roots substantially reduces concentration in the drain water tank: increasing the log-K_{OW} from 2 to 6.37 results in a 98% reduction of the concentration.

5.4 Conclusions

Of the materials for which partitioning is simulated in SEM, slabs and roots had the strongest effect on the concentration in the drain water tank, using sorption coefficients for dimethomorph. For the foil and pipes the effect was negligible. Increasing the sorption coefficients for slabs, foil, and pipes, by a factor 10 led to a reduction of 35% of the maximum concentration, relative to a situation without sorption. However, for this simulation the sorption coefficient for the slab material was 10 L kg^{-1}. Such a value is very unlikely for any substance (J. Boesten, pers. comm.). Simulations with varying strength of partitioning into the roots show that this process has the potential to drastically reduce concentrations in the drain water tank. This occurs for very high—but not impossible—K_{OW} values.

6 Saturated vapor pressure and solubility

6.1 Introduction

In this section we analyse the combined sensitivity of SEM to saturated vapor pressure (SVP) and solubility, in relation to growth medium type and application date. In SEM, substance deposited on the floor, crop, roof, and dry tables during spraying or LVM applications can volatilize to the greenhouse air. This flux is controlled by the saturated vapor pressure (SVP), which determines the maximum simulated concentration of a substance in the air. Similarly, solubility determines the maximum simulated concentration of a substance in water. This is relevant for dissolution of substance into the condensation water from the roof or greenhouse air. Together, SVP and solubility determine the input of substance into the recirculation water via the condensation water, which is potentially an important route for emission to surface water. For growth medium pots, however, volatilization also reduces the amount of substance present on the tables when irrigation occurs. The date of application is relevant in two ways. First, higher temperatures in summer increase both volatilization and dissolution. Second, condensation water flow to the recirculation water is higher in winter due to the larger temperature difference with the outside air.

6.2 Methods

A factorial analysis was performed focusing on SVP and solubility, as well as growth medium type and application time. The substance was applied via spraying. The result of the analysis is expected to be marginally impacted by whether the substance is applied via spraying or via LVM. Five combinations of SVP and solubility values were investigated (Table 6.1). These values were taken from selected (anonymized) substances analysed by Wipfler et al 2015a. All other substance properties were as listed in Annex 1. Simulations were performed for growth medium type pots and slabs, and for application date in summer (1 July) and in winter (1 January). Hence, the full factorial analysis comprised 20 (5 x 2 x 2) runs. Simulations ran for 3 months in 2000, starting on the date of application.

Table 6.1 *Saturated vapor pressure and solubility values of the five analyzed substances.*

Substance	Properties	Saturated Vapor Pressure (Pa)	Solubility (mg L^{-1})
A	High SVP - High Solubility	0.00166	600
B	High SVP - Low Solubility	0.0011	0.121
C	Low SVP - High Solubility	4.0×10^{-10}	613
D	Low SVP - Low Solubility	6.3×10^{-12}	0.88
E	High SVP – Mid Solubility	0.00048	100

6.3 Results

Figure 6.1 shows the maximum concentration in the drain water tank for the 20 simulations with varying SVP and solubility, growth medium type, and application date. For substrate type slabs (right hand side plots in Figure 6.1), substances A (high SVP and solubility) and E (high SVP, intermediate solubility) have the highest maximum concentration, for both application dates. Substances, B, C, and D have a similar, much lower, maximum concentration. These differences are explained by variation of substance input into the recirculation water via condensation water. For substances B, C, D, this flux is low due to either low SVP, low solubility, or both. Hence, for these substances, the concentration in the drain water tank is determined mainly by the direct input by deposition on slabs and troughs—which is a constant fraction of the application

dose. For substances A and E, however, the route via condensation water is significant, leading to a much higher concentrations, with E slightly lower due to a lower solubility. The maximum concentration for substance A and E is higher in winter than summer. Apparently, the higher condensation water flux in winter outweigh the lower volatilization and dissolution rates due to lower temperatures.
For growth medium type pots (left hand side plots in Figure 6.1), the situation is somewhat more complicated. For substance B (high SVP, low solubility) maximum concentration in the drain water tank is low. Substances A and E have higher concentration with substantial differences between winter and summer. Substances C and D have very similar concentrations with virtually no difference between winter and summer. As with substrate slabs, the high concentrations for substances A and E, as well as the differences between winter and summer, are explained by input into the recirculation water via condensation water. For substances C (low SVP, high solubility) and D (low SVP, low solubility) a substantial amount is present on the tables by the time irrigation occurs, due to the low volatilization rate, resulting in a high input in the recirculation water. For substance B, both entry routes to the recirculation water are small. The high SVP causes quick volatilization from the tables, hence little substance remains on the tables by the time irrigation occurs. On the other hand, the low solubility slows dissolution into the condensation water, causing the substance to remain in the air.

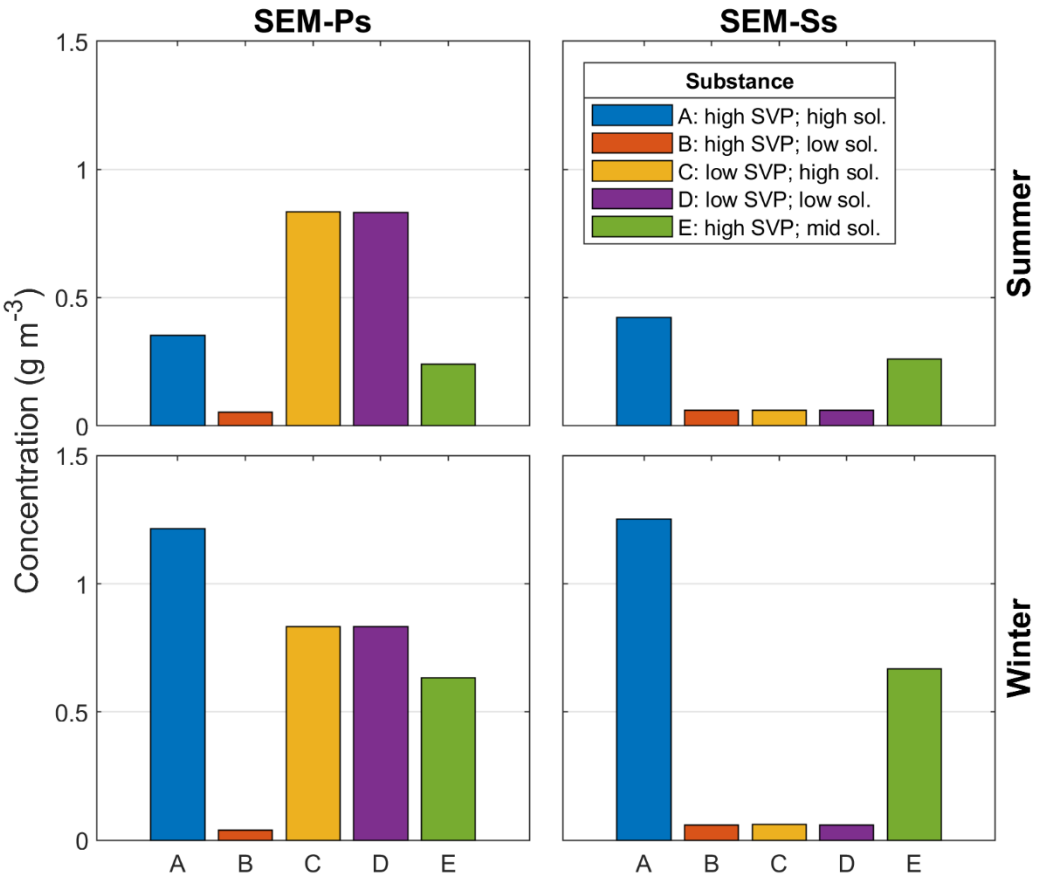

Figure 6.1 *Effect of saturated vapor pressure (SVP) and solubility on the maximum concentration in the drainage tank. Results are shown for pots (left) and slabs (right) and application in summer (1 July; top) and in winter (1 January; bottom).*

6.4 Conclusions

The varying sensitivity of the predicted concentration in the drain water tank to SVP and solubility between summer and winter is related to the entry of substance into the recirculation water. High SVP and solubility simulate relatively high concentrations due to substance entering the recirculation water via the condensation water. This route is more important in winter, due to higher condensation water fluxes. For growth medium type pots, dissolution of substance deposited on the tables during irrigation represents an additional entry route. This route is stimulated by a low SVP, which prevents substance from volatilizing to the greenhouse air.

7 Deposition distribution of applied substance

7.1 Introduction

With growth medium type slabs, substance applied by spraying is distributed over five surfaces: crop, roof, floor, slabs, and troughs. From the crop, roof, and floor, volatilization to the greenhouse air occurs. Additionally, substance on the roof can dissolve directly into the condensation water. On the crop surface also dissipation occurs, leading to loss of substance. Substance deposited on the slabs and troughs directly enters the recirculation water. Thus, the distribution of substance over the five surfaces has potentially a great impact on concentration in the recirculation water. In GEM the fractions defining this distribution depends the growth medium and application type and cannot be altered by the user. Using SEM in standalone, however, altering the fractions is possible. In this section we analyse the effect of varying the fractions defining the distribution of applied substance over the different surfaces in SEM-Ss (growth medium type slabs, application type spraying) on the predicted concentration in the drain water tank, in relation to saturated vapor pressure (SVP) and solubility.

7.2 Methods

Three sets of simulations were performed to analyse the sensitivity of SEM-Ss to the distribution fractions, focusing on three surfaces: (i) roof, (ii) crop, and (iii) slabs + troughs. The latter two were combined since they are functionally identical. The sum of the deposition fractions must by definition be equal to 1. Therefore, for troughs + slabs and roof changes in fraction were balanced by an opposite change in the fraction deposited on the crop. For the crop, fraction changes were balanced by the fraction deposited on the floor. Additionally, runs were performed with the default fractions used in GEM (labelled "control"). Table 6.2 lists the fractions for the eight dose distributions that were analysed. Furthermore, five combinations of SVP and solubility were considered (see section 6.2); other substance properties are as listed in Annex 1. Hence the total factorial analysis comprised 40 (8 x 5) simulations. The substance was applied by spraying on 1 January 2000. Simulation ran from 1 January to 31 March 2000, with application on the first day.

Note that LVM application is not considered here since we expect the results to be similar to spraying application.

Table 6.2 *Deposition fractions (%) used in the simulations to analyse the sensitivity to distribution of the applied dose. "Control" refers the default fractions used in GEM for growth medium type slabs and application type spraying (SEM-Ss).*

		Crop	Roof	Slabs	Troughs	Floor
Control		39.4	0.100	1.00	0.300	59.2
Slabs + troughs	Zero	40.7	0.100	0.00	0.00	59.2
	High	38.1	0.100	2.00	0.600	59.2
Roof	Low	39.5	0.0500	1.00	0.300	59.2
	High	39.3	0.200	1.00	0.300	59.2
Crop	Zero	0.00	0.100	1.00	0.300	98.6
	Low	19.7	0.100	1.00	0.300	78.9
	High	98.6	0.100	1.00	0.300	0.00

7.3 Results

7.3.1 Slabs and troughs

Figure 6.2a depicts the relative effect of changes in the combined fraction deposited on slabs and troughs on the maximum concentration in the drain water tank, as compared to the control. The black asterisk (∗) indicates the reference situation, i.e. the default fractions used in GEM which is 1.3%. Within the range of 0 to 2.6%, sensitivity to this fraction is high for substances B, C, and, D, showing approximately 1:1 relationship. For substances A and E the response is almost negligible. This difference is explained by the potential of a substance for entering the recirculation water via the condensation water. For substances B, C, and D, this flux is low, due to either low SVP, solubility, or both. Therefore, entrance to the recirculation water occurs predominantly via deposition on the slabs and troughs, thus these substances are sensitive to the amount deposited there. For substances A and E, the flux to condensation water is high, hence substance enters the recirculation water also if direct input is low.

7.3.2 Roof

Response of the concentration in the drain water tank to a change of the roof deposition fraction is in general low, as compared to the slabs and troughs (Figure 6.2). This is presumably explained by the low overall fraction that is deposited on the roof (0.05–0.2%). Response for substance C (low SVP, high solubility) is notably higher than for the other substances, with a maximum increase of 1.5% for a doubling of the fraction relative to the control. For this substance, volatilization is low, hence little substance volatilizes to the greenhouse air. On the other hand, solubility is high for substance C, which means that substance deposited on the roof, can easily dissolve into the condensation water, resulting in a stronger sensitivity to the fraction deposited there. The other substances have either a low solubility (substances B and D), impeding flow to the condensation water regardless of the source, or both a high SVP and high or intermediate solubility (substances A and E), meaning that substance can easily enter the condensation water from any surface.

7.3.3 Crop

Response to the fraction deposited on the crop shows a quite different pattern compared to that for slabs + troughs and roof (Figure 6.2c). For substances B, C, and D, the response is very small. Above a fraction of 20%, there is a negative response for substances A and E, i.e. an increase in fraction results in a lower concentration in the drain water tank. This can be explained by the fact that we balanced the change in fraction deposited on the crop by an opposite change in the fraction deposited on the floor. Substance can volatilize from both surfaces but on the crop also dissipation occurs, causing a loss. This is, however, not relevant for substances B, C, and D, since for these substances flow to the condensation water is blocked by a low SVP, solubility, or both.

Interestingly, below a fraction of 20%, there is a *positive* relationship between the deposition fraction and the concentration in the drain water tank. The precise cause is difficult to determine but this is presumably related to differences in volatilization for the crop and floor.

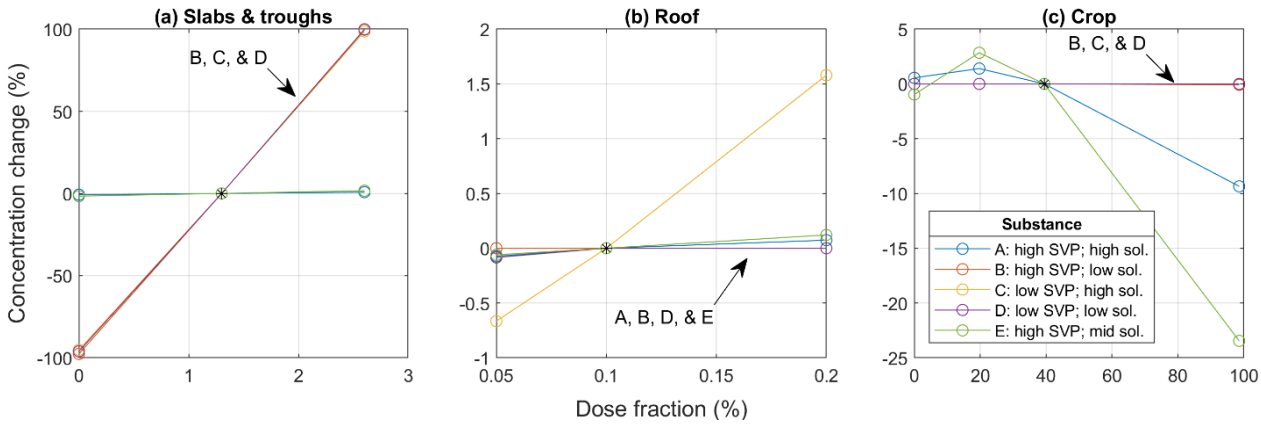

Figure 6.2 *Effect of changing the fraction of the applied dose deposited on crop surface, slabs and troughs, and roof on the maximum concentration in the drainage tank for the five analysed substances. The y-axis indicates the change of the maximum concentration relative to the control situation (indicated by the ∗ marker), defined by the default fractions used in GEM (see Table 6.2).*

7.4 Conclusions

The fraction of the applied dose deposited on the slabs and troughs shows a strong positive relationship to the concentration in the drain water tank for substances with low SVP and/or solubility. This is as expected, given that this substance is directly added to the recirculation water. The fraction deposited on the roof has, in the analysed range (0.05–0.2%), a small positive effect, most importantly for a substance with a high solubility but low SVP. For substances with mid to high SVP and solubility, the fraction deposited on the crop has generally a negative relationship with the concentration in the drain water tank, owing to the loss off substance by dissipation on the crop surface, simulated in SEM.

8 Degradation in condensation water

8.1 Introduction

Degradation in the condensation water, due to e.g. hydrolysis or microbial degradation, reduces the amount of substance entering the recirculation water from this reservoir. This is relevant in situations when the residence time of the substance in the condensation water is high. The degradation rate of a substance is expected to have a lower impact in winter than in summer, for two reasons. First, the flow of condensation water is higher in winter due to the larger temperature difference with the outside air, which reduces the residence time of substance in the condensation water. Second, degradation rates increase with temperature. In this section we analyse the sensitivity of SEM-Ss to the degradation half-life for the condensation water in relation to the timing of application.

8.2 Methods

The impact of four half-lives (DT50) in the condensation water on the concentration in the drain water tank were tested: 0.1, 1, 10, and 1000 d. With a half-life value of 1000 d, effectively no degradation occurs. Additionally, runs were performed with application in winter (1 January) and in summer (1 July). Substance properties are as listed in Annex 1. Slabs and spraying were used for growth medium and application type, respectively (SEM-Ss). The simulation period was 3 months in year 2000, starting from the date of application.

8.3 Results

As expected, an increase in DT50, corresponding to a lower degradation rate coefficient, results in a higher substance concentration in the drain water tank (Figure 8.1). Compared to a DT50 value of 1000 d, a value of 0.1 d results in a reduction of 81% in summer and 43% in winter. The difference in sensitivity between summer and winter is explained by the residence time in the condensation water, which is higher in summer. Moreover, overall concentrations are lower in summer due to the higher temperatures enhancing degradation in general.

8.4 Conclusions

A half-life of 0.1 d in the condensation water resulted in a reduction of 81% and 43% in summer and winter, respectively, compared to a half-life of 1000 d (approximately zero degradation). The different sensitivities for winter and summer are explained by differences between residence time in the condensation water and temperature in the greenhouse.

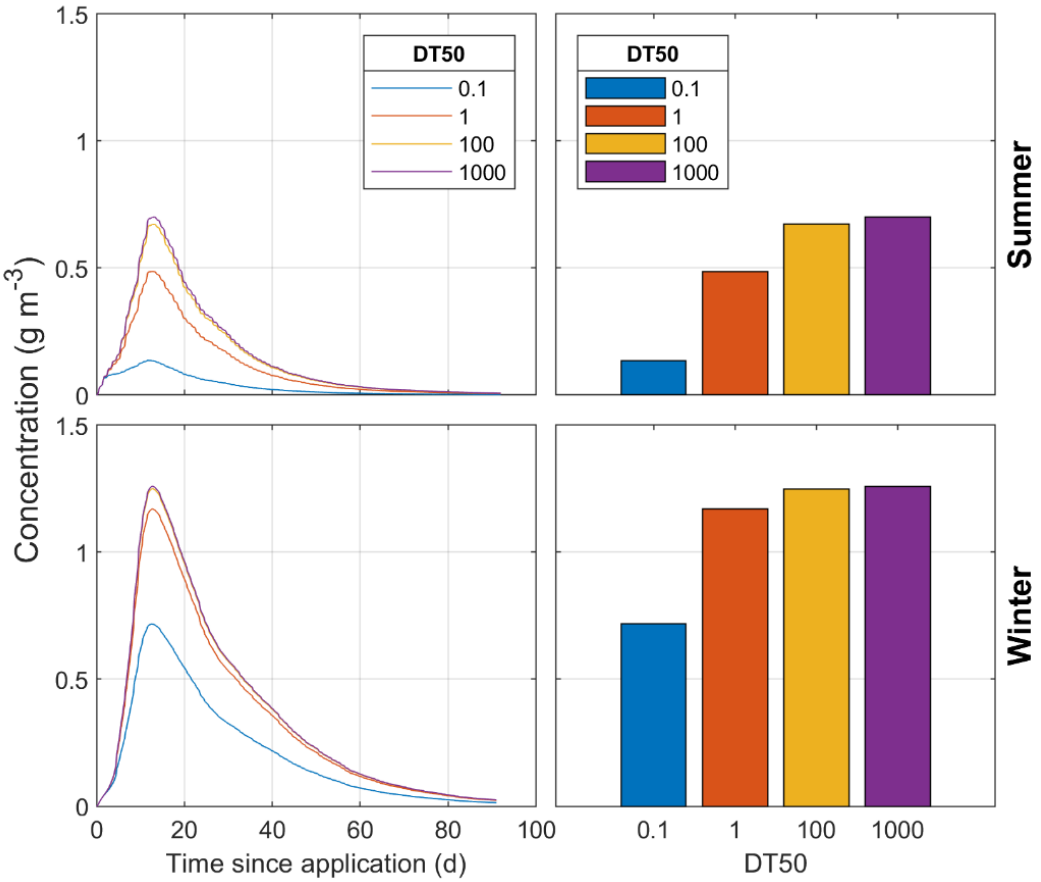

Figure 8.1 *Effect of changing the DT50 for degradation in the condensation water on the maximum concentration in the drain tank. Results are shown for application in summer (1 July; top) and in winter (1 January; bottom). Dissipation on the crop surface.*

9 Dissipation on the crop surface

9.1 Introduction

Dissipation on the crop surface causes a loss of substance from the greenhouse. This is relevant for substances that can potentially enter the recirculation water via the condensation water by volatilization to the greenhouse air and subsequent dissolution into the condensation water.

9.2 Methods

Four half-lives (DT50) for dissipation on the crop surface were tested: 0.1, 1, 10, and 1000 d. With a half-life value of 1000 d, effectively no degradation occurs. Additionally, runs were performed with application in winter (1 January) and in summer (1 July). Substances properties are as listed in Annex 1. Slabs and spraying were used for growth medium and application type, respectively. The simulation period was 3 months in year 2000, starting from the date of application.

9.3 Results

The DT50 for dissipation on the crop surface has a clear effect on the concentration in the drain water tank (Figure 9.1). Compared to a DT50 value of 1000 d (approximately zero degradation), a value of 0.1 d results in a reduction of 85% in summer and 83% in winter. The response to DT50 is very similar for both application dates. However, the overall concentrations are lower in summer due to the effect of higher temperatures on degradation in general.

9.4 Conclusions

A half-life of 0.1 d on the crop surface resulted in a reduction of 85% and 83% in summer and winter, respectively, compared to a half-life of 1000 d (approximately zero degradation). The slightly higher sensitivity for summer is explained by the a higher temperature in the greenhouse during this time.

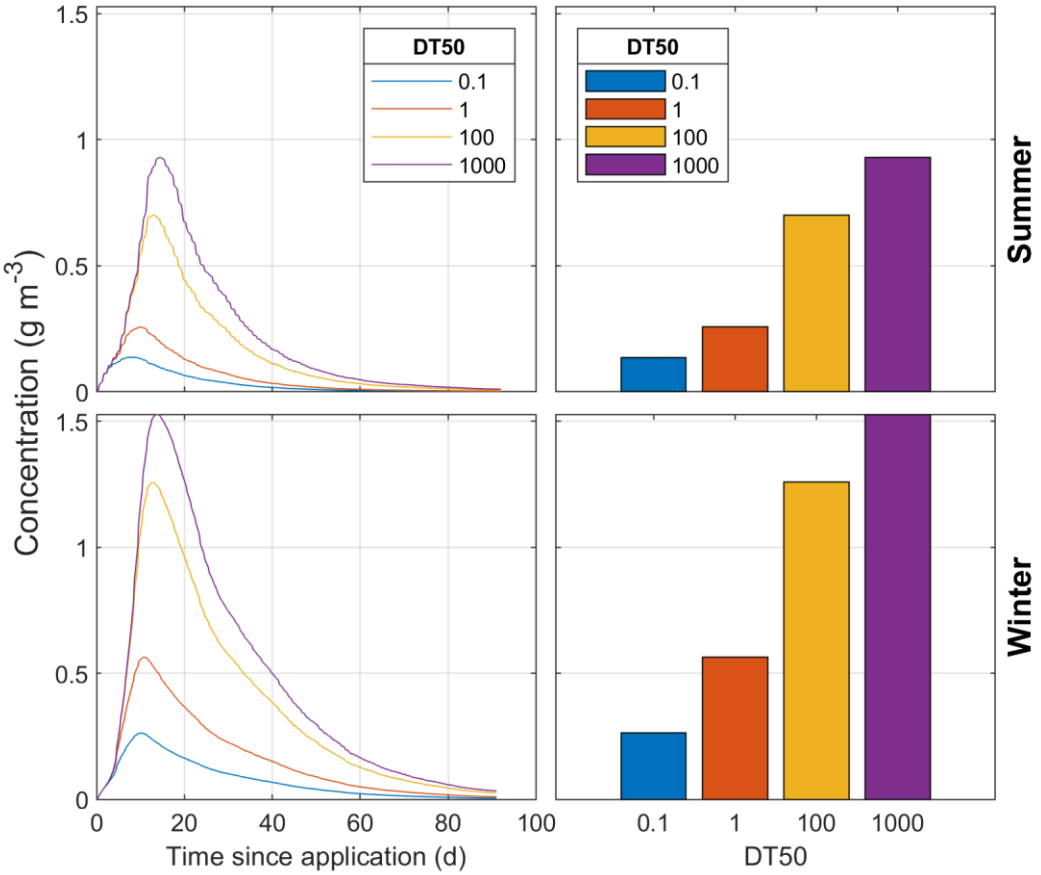

Figure 9.1 *Effect of changing the DT50 on the crop surface on the maximum concentration in the drain water tank. Results are shown for application in summer (1 July; top) and in winter (1 January; bottom).*

10 Area fraction of pots on tables

10.1 Introduction

For growth medium type pots (SEM-P), part of the substance applied by spraying or LVM is deposited on the pots and tables. This deposition is further divided over the pots and the table based on the pots area fraction. Substance deposited on the pots may diffuse into the soil material, where it can be lost due to degradation. It may also volatilize to the greenhouse air, provided that the concentration gradient is sufficient. The tables are assumed to be dry at the time of application, hence substance deposited there may volatilize to the greenhouse air. After 1 d, irrigation occurs and any substance remaining on the table is added to the recirculation water.

In general, substance deposited on the tables will more quickly enter the recirculation water, given the potential of the pots to absorb and degrade substance. In this section we analyse the sensitivity of SEM-P to the distribution of applied substance over the pots and tables, as controlled by the pots fraction. In GEM, this parameter is set at 30% and cannot be altered by the user.

10.2 Methods

Simulations were performed for three pots fractions: 10, 30, and 72%. Additionally, we investigated three combinations of saturated vapor pressure (SVP) and solubility, corresponding to substances A (high SVP and solubility), C (high SVP, low solubility), and D (low SVP, low solubility) discussed in section 6.2. Other substance properties are as listed in Annex 1. Finally, two application dates were simulated, summer (1 July) and winter (1 January). Application type was spraying. The simulation period was 3 months in 2000, starting from the date of application.

10.3 Results

Figure 10.1 depicts the results of the simulations. As expected, a negative relation between the pots fraction and concentration in the drain water tank exists, caused by the tendency of the pots to absorb and degrade substance. Substances C (low SVP, high solubility), and D (low SVP and solubility) show a stronger sensitivity than substance A (high SVP and solubility). Also, substance A has a stronger sensitivity in summer. A probable explanation for this difference is that for substance A substantial volatilization to the greenhouse air from the pots surface occurs, which can enter the recirculation water via the condensation water. For substances C and D, this route is negligible, hence dissolution during irrigation of the tables is the dominant route to the recirculation water.

10.4 Conclusions

A larger pots area fraction results in a lower concentration in the drain water tank, since this will result in less substance deposited on the tables during spraying application and dissolved in the recirculation water during irrigation. This effect is stronger for substances that have a low SVP and/or solubility, which prevents entry in the recirculation water via the condensation water.

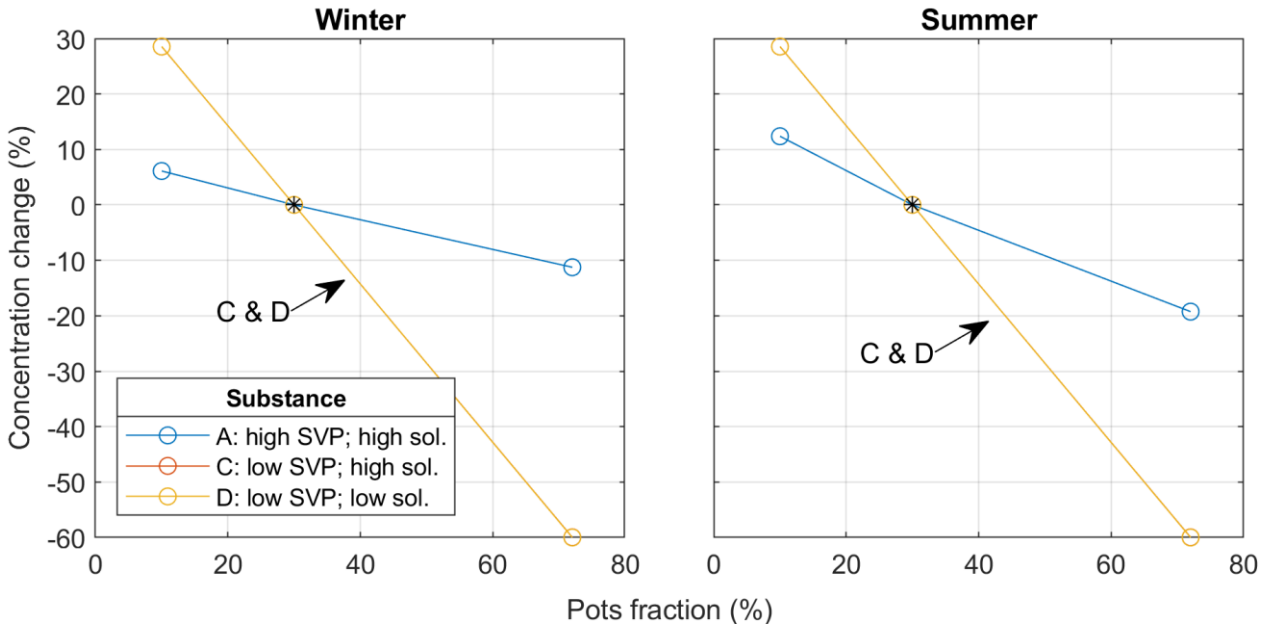

Figure 10.1 *Effect of changing the area fraction of pots on the maximum concentration in the drainage tank for application in winter and summer and three analysed substances. The Y-axis shows the change in maximum concentration relative to the control pots fraction (30%, indicated by the ∗ marker).*

Sensitivity to the application date

11 Introduction

Predicted Environmental Concentrations (PECs) calculated with GEM-soilless scenarios are sensitive to the application date. Requests for registration of products used in soilless cultivation are generally not restricted to a specific period within a year, they mostly cover application over the entire year. In view of the required robust outcomes in the regulatory context, a procedure is needed to cope with this variability and to get robust PECs to be used in the risk assessment.

GEM-soilless simulates pesticide concentrations in surface water due to emissions from soilless cultivations in greenhouses. Discharge of water from the greenhouse occurs as relatively short events and may be one of wo types:

a. discharge because sodium concentration exceeds a threshold level
b. discharge of water used for rinsing of filters.

Concentrations in the recirculation water in the greenhouse usually decrease rapidly after application due to discharge, but also due to a range of other processes, such as transformation and uptake by the crop. As a result, concentrations in discharge water are highly sensitive to the timing of pesticide application, relative to the timing of discharge events. This sensitivity depends also on various parameters, including pesticide properties and method of application.

Since the timing of application is a decision by the grower, it is difficult to predict. Hence, multiple simulations with different application dates are needed to obtain a robust estimate of the PEC. Ideally, such an ensemble would consist of 365 simulations—one for every day of the year. However, this requires considerable computation time, and is generally not needed to obtain reliable estimates. The current approach to risk assessment applied by the Ctgb is to run a GEM simulation for every month in the application window. Thus, in case potential application period covers the entire year, 12 evenly distributed application windows are needed. Subsequently, the application date resulting in the highest PEC is selected and two additional runs are performed with application one week before and one week after that date. Then, the maximum PEC is selected[1]. The SAFE instrument was developed to support this procedure (Berg et al., 2019).

Recently, additional soilless cultivation scenarios and updated concepts were developed and implemented in GEM (Boesten et al., 2020). It is yet unknown (i) what is the sensitivity of the GEM model to the application timing and (ii) what should be the procedure for assessing the PEC for these new scenarios.

The aim of this part is to quantify the sensitivity of pesticide outflow to application timing for a range of representative assessments. This is done by comparing the 90th percentile[2] of the outcomes of the 365 runs with those from a smaller sub-set of these runs, with the rationale that the sub-set should preferable be small to limit computational requirements (e.g. each month or each week), but should not lead to underestimation of the PEC50 or PEC90. A second aim is to develop a robust estimate of the 90th percentile PEC for the window of application.

[1] (https://www.ctgb.nl/documenten/instructies-gewasbeschermingsmiddelen/2018/01/18/selecteren-van-het-toepassingstijdstip-in-gem).

[2] The application timing reflects the behaviour of the grower. The 90th percentile is considered to be an approximation of a realistic worst case behaviour.

12 Methodology

12.1 Definitions used

Assessment: this is the combination of crop/scenario, substance and application technique.

PEC: Predicted Environmental Concentration: this is the annual maximum of the concentration in discharged water. As GEM runs for 7 years, each run has 7 PECs.

PEC50: the 50th percentile of the PECs of one run.

PEC90: the 90th percentile of the PECs of one run.

12.2 Approach

Model representation. A sensitivity analyses requires a large number of model simulations. E.g. to assess the impact on the application date on the PEC for one assessment only already 365 runs are needed. To save simulation time a simplified representation of the fate in the simulation ditch is assumed: Analysis showed that the annual maximum mass flux emitted to the surface water together with the 10 day maximum mass flux are good proxies for the maximum concentrations in the receiving water course for situations with high flow velocities and low flow velocities, respectively. We will use these two proxies in the analyses. We refer to Annex 2 for further detail on the analysis.

One annual application. The analysis is confined to assessments with one annual application only. It can statistically be demonstrated that for assessment with multiple annual applications the model outcomes will be more robust than for one annual application. Hence, the outcomes of the assessment based on one annual application can also be used for other assessments.

Temporal percentile. Furthermore, the analysis was done for the 50th percentile PEC (PEC50) and the 90th percentile PEC (PEC90) based on the annual maxima of the seven years. The first is the temporal percentile which is currently adopted for the Dutch registration procedure, the latter is the temporal percentile adopted for the EU.

Percentile taken from all application timings. In the current procedures used by the Ctgb, the maximum PEC is taken from all application timings. In the analysis we decided to use the 90th percentile of the application timings. This is considered a more robust estimate and allows to leave out outliers. Moreover, it seems inconsistent to use a 50th or 90th percentile over the years (i.e. a probabilistic approach) in combination with a 100th percentile for the application date.

Quantification of sensitivity. Focus of the analysis is on the relative difference between the 'true' values, being all runs with application timings from the 1st of January to the 31st of December and a selection of runs. This difference is quantified by (i) the relative deviation from the best estimate, (ii) the multiplication factor needed to get the same PEC value from this estimate. The exact calculation method is explained below.

12.3 GEM-soilless assessments: selection of representative combinations

In Boesten et al. (2020) a set of 32 scenarios was developed for the WSM model for different choices of:
- Crop type. There are 4 model crop types, i.e. sweet pepper, pot-plant, tomato and rose
- Annual discharge limit, related to the maximum annual nitrate emission over the period 2015-2027. Four emission periods are considered. 2015-17; 2018-20; 2021-24; 2025-27.
- Either discharging or reusing of filter rinsing water

A simulation is further defined by growth medium, method of pesticide application, application date and dose, substance properties. The following model input parameters are considered most relevant for the sensitivity assessment:
- Scenario of the WaterStreamsModel. We decided to only consider scenarios from 2018 onwards, i.e. 24 scenarios). The numbers that represent each of the WaterStreamsModel runs are given in Annex 3.
- Application method: application by spraying, LVM, or with nutrient solution
- Growth medium: pots or slabs
- Substance properties:
  - Saturated vapour pressure
  - Water solubility
  - Transformation rate in the recirculation water
  - Sorption coefficients
  - Crop uptake factor

As it was considered infeasible to do a full factorial analysis for all of the parameters above a further selection was made. The reasoning for reducing the number of combinations in the analysis is given below:
- LVM and spraying only differ conceptually in the direct deposition on the floor, the roof and the crop. It is expected that this has a small impact on the interaction with the discharge frequencies. This hypothesis is checked by doing a small number of runs with spray application and compare the differences in relative deviation from the best estimate.
- Crop uptake and transformation have the same impact on the concentration in the recirculation water. We hypothesize that by selecting a substance with a high degradation rate and a high uptake factor, and a substance with a low degradation rate and no uptake both extremes in substance properties are covered.
- For application with the nutrient solution the model is not expected to be sensitive to the volatilization and solubility. This means that for this type of application these parameters do not need to be taken into account in the analysis.
- Sorption has the most impact for application with the nutrient solution, for the other application methods this substance property is of less importance. As sorption to roots is dominant to other processes, this is considered as representative for the impact of sorption on the sensitivity to the application date.
- For spraying or LVM application, pesticide may enter the recirculation water via direct deposition on slabs or on the tables, or via the collection of condensation water from the roof. Based on earlier analysis two types of substances can be distinguished (Boesten et al., 2020): A for which the route via the condensation water is relevant and B for which it is not (as direct deposition is dominant for these type of substances). For substances with $P_{sat} > 10^{-5}$ Pa and $c_{w,sol} > 1$ mg/L the contribution from the recirculation water is expected to be significant. In the analysis two representative substances will be used, one for the situation in which contribution from the condensation water is significant and one for the situation in which contribution from the condensation water is not significant.

This resulted in the selection of four model substances (see Annex 4 for details):
- Substance A: a model substance with high vapour pressure and high solubility. The degradation is the recirculation water is very low (1000 d). Also sorption is low.
- Substance B: a model substance similar to substance A, but with low vapour pressure and low solubility.
- Substance C: a model substance similar to substance A, but with high sorption to the roots.
- Substance D: a model substance similar to substance A, but with a high degradation rate (1 d) and high plant uptake (plant uptake factor of 1).

This resulted in the following list of assessments (i.e. model input combinations). Applied mass is 1 kg/ha for all assessments:

Table 12.1 *Simulations carried out for the analysis.*

Slabs/pots	Application method	WaterStreams scenarios	Substances	Number of assessments
Slabs	With nutrient solution	All scenarios for crops grown on slabs (18)	C and D	32
Slabs	LVM	All scenarios for crops grown on slabs (18)	A and B	32
Slabs	Spraying	Only scenario 16	A and B	2
Pots	With nutrient solution	All scenarios for crops grown in pots (6)	C and D	12
Pots	LVM	All scenarios for crops grown in pots (6)	A and B	12
Pots	Spraying	Only scenario 14	A and B	12

12.4 Setup of sets of runs with different application dates

For each GEM assessment setup, 365 runs with varying application dates were performed, each yielding daily average substance outflow due to discharge. The results were then processed as follows; for each of the 365 simulations:

1. Calculate 10-day moving averages of the daily substance outflow
2. Determine the annual maximum of both the daily outflow and the 10-day moving average, for each of the 7 simulation years (2000–2006)
3. Calculate median (50th percentile; PEC50) and the 90th percentile (PEC90) over the 7 annual maxima for both the daily outflow and the 10-day moving average
4. Calculate the 90th percentile of the 365 PEC50 and PEC90 values

12.5 Effect of number of simulations with different application dates

The above-described PEC50 and PEC90 based on 365 simulations are considered to be their best estimates. We analyzed the error introduced by doing fewer simulations by calculating the PEC50 and PEC90 based on subsamples from the 365 simulations. The deviation of a PEC value based on a subsample with N simulations (q^N) from the true value based on 365 simulations (q^{365}) is quantified as: 1) the relative deviation from the true value: $(q^N - q^{365})/q^{365}$; and 2) the multiplication factor required to obtain the true value: q^{365}/q^N.

Analysis was carried out for the following subsample sizes: 12, 15, 18, 20, 24, 30, 36, 40, 45, and 60. It can be expected that results of two SEM simulations are more similar if their application dates are closer together. In this sense the statistics may be seen as auto-correlated in terms of the application date. Therefore, the selected application dates were evenly spread out over the year to ensure minimal dependence. For a given value of N, there are approximately M_N=365/N ways to select N evenly spread out dates. For example, for N=52, i.e. approximately one date every week, there are M_{52}=7 sets of application dates—one for every day of the week. Similarly, for N=12 (approximately monthly), there are M_{12}≈30 possible sets of application dates. The results will vary, dependent on which of the M_N sets is analyzed. For each value of N analyzed, the statistics were calculated over all possible M_N sets. In further analysis focused on underestimation of the PECs, for a given value of N, we calculated the 10th percentile of the M_N PEC50 and PEC90 values.

13 Results

13.1 Sensitivity of substance outflow to application date

Figure 13.1 shows the annual maximum daily mass outflow versus each application date for two example assessments. For many assessments the annual maximum of substance outflow is very sensitive to application date. In some cases differences of multiple orders or magnitude are observed. A number of assessments show a clear seasonal trend, but for most assessments this is not the case. Other assessments have extended periods in which application timings result in negligble outflow, interspersed by peaks or longer periods in which application leads to higher outflow maxima. A smaller number of assessments have a relatively small sensitivity to application date. It is further notable that for many assessments the year 2003 has substantially higher outflow than the other simulation years. This is explained by the fact that year 2003 had an extremely hot and dry summer, which results in higher crop evaporation and thus a higher discharge volume. The PEC90 shows to be more stable than the PEC50.

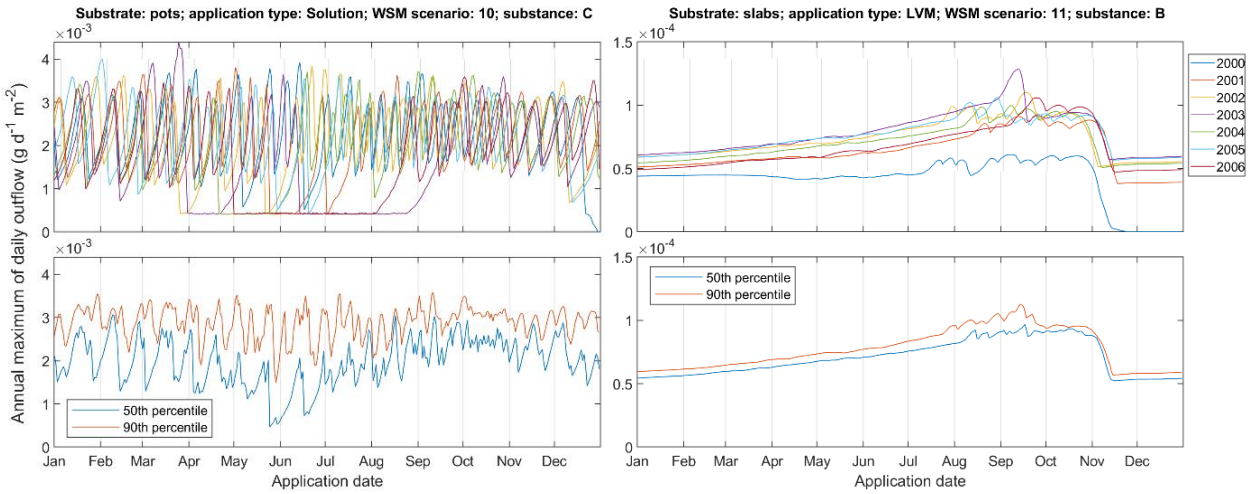

Figure 13.1 *Annual maximum of daily substance outflow versus application date for two SEM assessments. The top graphs show the annual maximum for all years; the bottom graphs show the 50th and 90th percentile over the annual maxima. Note that the individual lines are not time series of a single model outcome but summarize results from SEM simulations for 365 application dates. Further note that the proposed endpoints of the assessments are the 90th percentiles taken from the lines in the bottom graphs.*

13.2 Effect of number of simulations on percentile estimates

In this section first the underestimation of percentile estimates relative to the true values based on 365 simulations is discussed and then some remarks are made regarding the multiplication factors. The multiplication factors (see section 12.5) are reported in full detail in the supporting csv files. These files provide for each of the assessments the multiplication factors that correspond to the subsample sizes: 12, 15, 18, 20, 24, 30, 36, 40, 45, and 60, for the PEC50 and PEC90.

Relative underestimation

Figure 13 shows an example of how the uncertainty of the percentile estimate depends on the number of simulations with different application dates. As expected, the uncertainty of the percentile estimates decreases with increasing number of simulations with different application dates. However, the decrease is in general not monotonous: frequently an increase in spread is observed when moving to a larger subsample size (c.f. top graph of Figure 13.1, N=30 and N=36). A possible explanation for this behaviour is that discharge events simulated by WSM often occur predominantly with certain frequencies. The same frequencies occur in the relationship between maximum discharge and application date. If the subsample size results in sets of application dates with similar frequency, this may result in interference with some of the M_N sets capturing mainly the peaks, while other sets capture mainly the minima, resulting in greater overall spread.

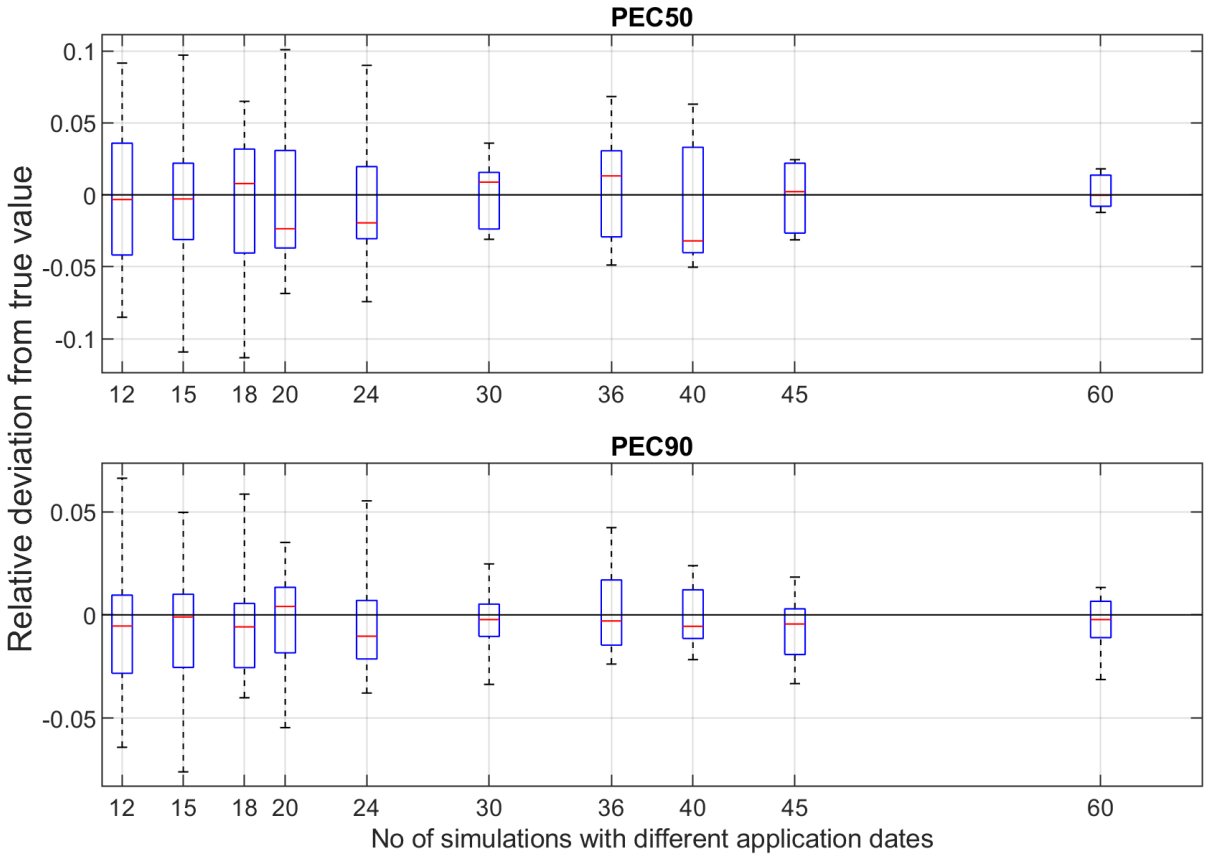

Figure 13.2 *Effect of the number of simulations on the uncertainty of percentile estimates of daily outflow for one SEM assessment setup (substrate: pots; application type: solution; substance C; WSM scenario 10). For different number of simulations (N; x-axis) the deviation of the 90th percentile over the N simulations, relative to the true value based on 365 simulations is shown (y-axis). The boxplots indicate the spread resulting from the different ways N evenly spread out dates can be selected. The top and bottom graphs show results for the 50th (PEC50) and 90th percentile (PEC90) of the 7 annual maxima, respectively.*

The uncertainty is in general smaller for the PEC90 than for the PEC50, particularly for setups where overall uncertainty is large. Furthermore, for the majority of the simulations, uncertainty is also smaller for 10-day average of daily outflow than for daily average. There are strong differences between assessments, both with regard to the overall uncertainty, as well as to the relationship with the number of simulations. Since underestimation of the annual outflow maxima is more undesirable than overestimation, we focus on the former in the remainder of this section. Specifically, we look at the 10th percentile of all PEC values for each value of *N*.

Figure 13.3 shows the distribution of the 90th percentile of the relative underestimation over the 100 assessments, for different values of *N*. The large majority of the assessments has less than 10% underestimation, even with only 12 simulations—independent of the choice for PEC50 or PEC90 percentile and daily or 10-day average outflow. However, for a small number of assessments, large underestimation occurs.

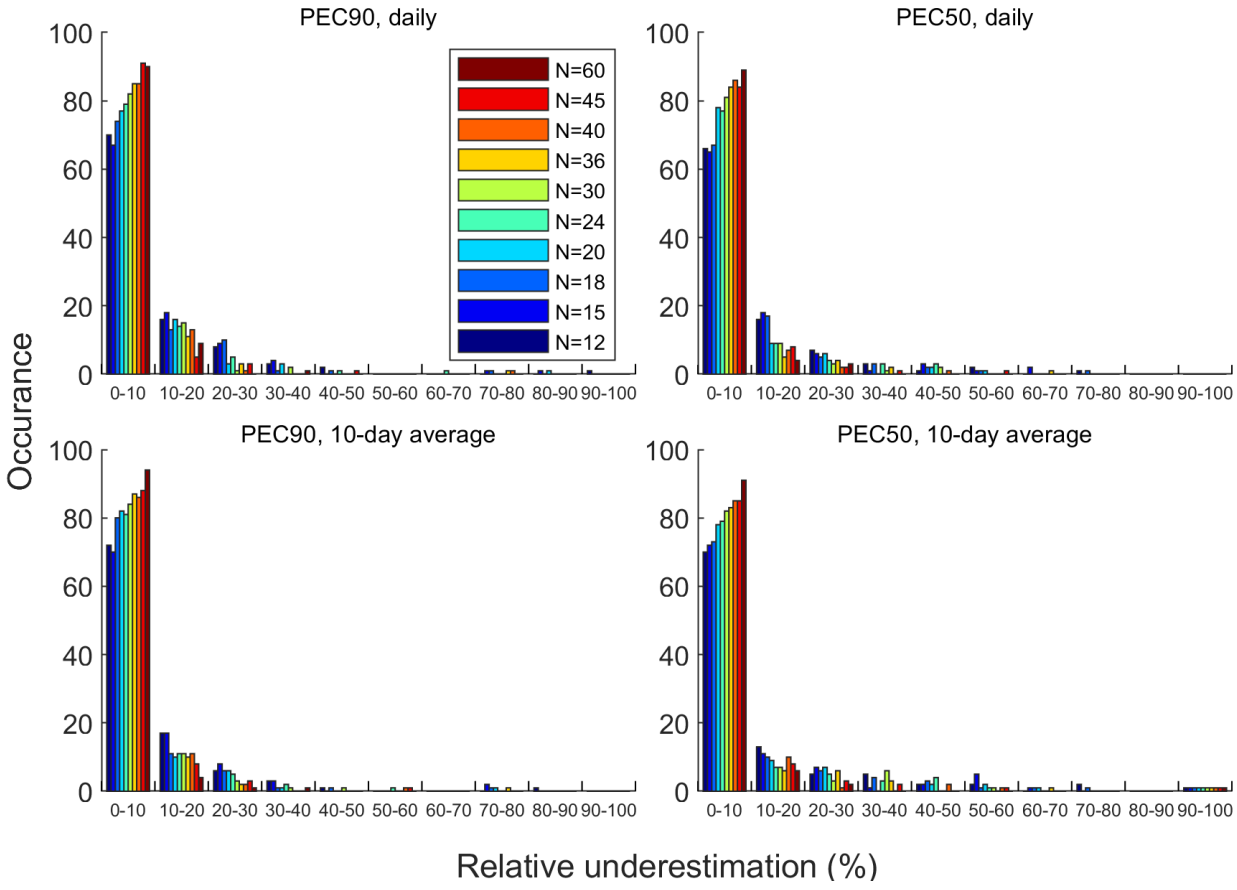

Figure 13.3 *Distribution of the 90th percentile relative underestimation of the 90th percentile over all applications for the 50th and 90th percentile over the annual maxima and for daily and 10-day average outflow, i.e. PEC50 and PEC90. For each SEM setup and value of N, the 90th percentile of the relative underestimation was calculated over all possible sets (i.e. the 10th percentile). The histograms show the distribution over the 100 SEM setups.*

Of all factors that vary over the 100 assessments, only the substance type has a distinguishable effect on the uncertainty of the percentile estimates, with substance D having in general stronger underestimation than the other substances. This substance is characterized by a high disappearance from the recirculation water due to a high degradation rate and plant uptake factor. As a result, it is more sensitive to the timing of application relative to that of discharge.

Multiplication factors

We also calculated the multiplication factors, following the definitions as explained in section 12.5. The multiplication factor represents the factor that is needed to multiply the PEC50 or PEC90 to cover the (90th percentile) error that might occur due to taking N<365. Multiplication factors were calculated for the annual max and the 10-day average concentration. A summary of the calculated multiplication factors for N=12 is given in Table 13.1. We refer to the supporting data files for the multiplication factors of all assessments and sub-sets.

Table 13.1 *Number of multiplication factors per multiplication factor range, for N=12 (each month).*

Multiplication factor range	Number of assessments in range (PEC50)		Number of assessments in range (PEC90)	
	Annual max	10-day average	annual max	10-day average
1−1.2	85	86	90	93
1.2−1.5	10	8	8	5
1.5−4.5	1	5	1	2[a]
>4.5	0	0	1[b]	0
Total	96[c]	99[c]	100	100

a Multiplication factors 1.6 & 4.0.

b Multiplication factor 5.0.

c for several assessments no multiplication factor could be determined because the true PEC values were (approximately) zero.

For PEC90, 90 (daily) and 93 (10-day average) out of the 100 assessments have a multiplication factors below 1.2. For all assessments except two the multiplication factor is smaller than 1.5. The two exceptions are both for substance D and with WSM scenarios 36 and 40, of which the latter has highest factor, 5. The multiplication factors are generally higher for PEC50, with 1 (daily) and 5 (10-average) assessments having factors between 1.2 and 1.5. All of these have either substance D or WSM scenario 40.

13.3 Difference between spraying and LVM applications

Contrary to our assumption, spraying and LVM do not always behave similarly in terms of the relative underestimation, as shown in Figure 13.4. For the four situations that were used to assess the representativity of LVM applications for spray applications (WSM file 14 and 16, for substance A and B) the combination of file 16 and substance B shows an underestimation of the relative error when using LVM instead of spray application up to 4 times the relative error. For the other three situations the relative error is more or less the same or lower. The relative error for WSM scenario 16, substance B is still within the range of the 10% error as shown in Figure 13.4. Therefore, to quantify the sensitivity of the PEC50 and PEC90 to application timing and to develop a robust estimate, the range of assessment combinations should be sufficient.

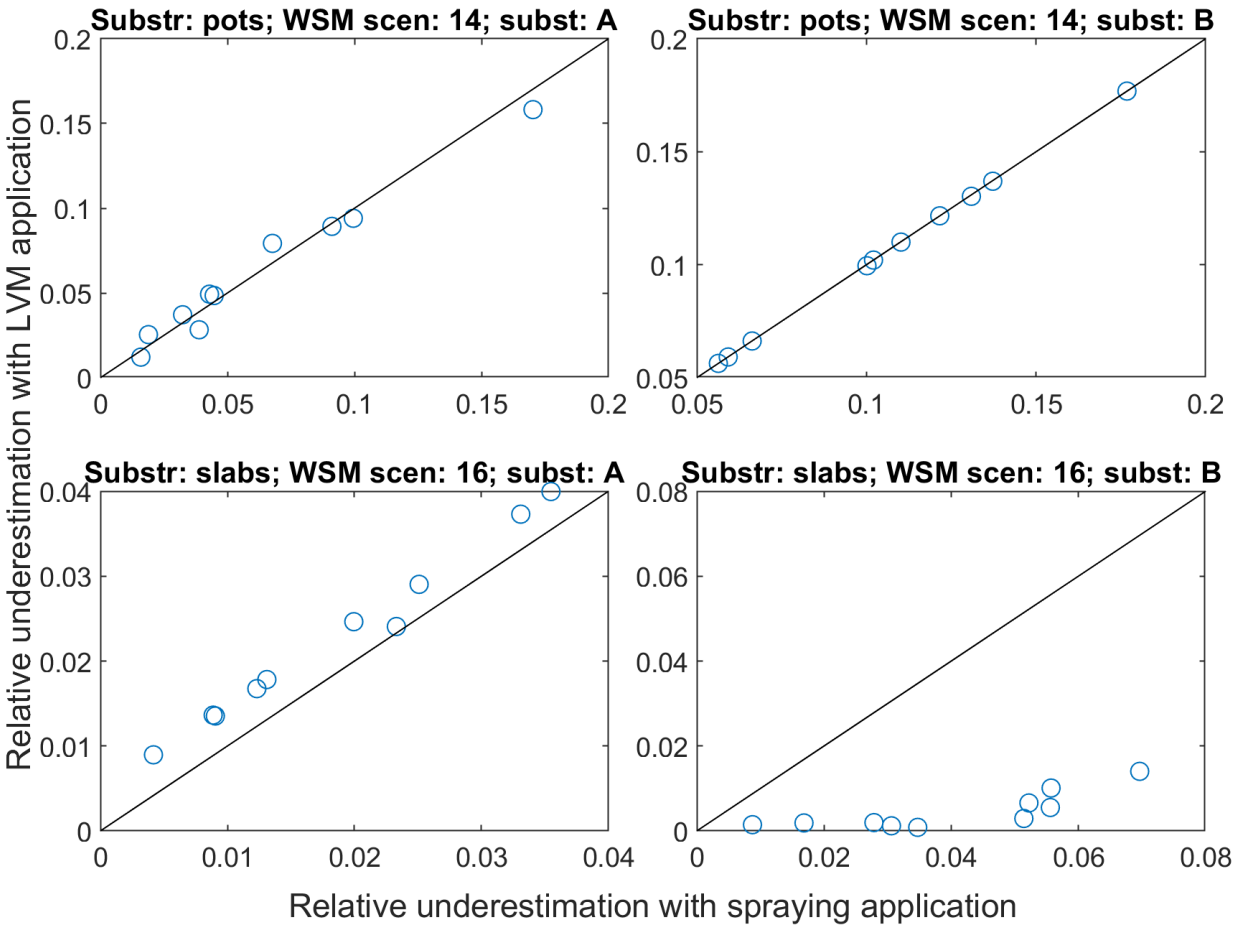

Figure 13.4 *Difference between spraying and LVM with respect to the relative underestimation for the PEC90 for the daily average outflow. The graphs show the maximum relative underestimation at different values of N for four sets of assessments.*

14 Conclusions on the sensitivity to the application timing

We found that there are strong differences between assessments, both with regard to the sensitivity of outflow to the application date, as well as to the number of simulations needed to obtain a reliable estimate. The highest uncertainties were found for substance D, due to its fast disappearance from the recirculation water. However, these high uncertainties were only found in certain combinations with other factors. Furthermore, no other factors in the assessment setup had an unequivocal effect on the uncertainty. This shows that the uncertainty is determined by a combination of factors.

With 12 simulations, the 90th percentile underestimation of the PEC50 and PEC90 is less than 10% for more than 70% of the assessments. Specifically for the PEC90 of daily outflow, underestimations were generally lower. Strong underestimations occur for specific combinations of assessment setup and number of simulations. One assessments stands out due to a very high uncertainty (substrate: pots, application type: nutrient solution, WSM scenario: 40, substance: D).

For 95 out of 100 assessments, the multiplication factors to cover the error with 12 simulations are mostly (95%) less than 1.2. The 5 assessments with higher multiplication factors are all for substance D. The highest multiplication factor (for the assessments mentioned above) is 5.

Remark: Note that the sensitivity to the application date does not only occur for GEM-soilless cultivations. Also the procedure which was recently developed by EFSA to deal with the considerable sensitivity to the application date (FOCUS repair, European Food Safety Authority (EFSA) et al., 2020). Surface water systems are rather dynamic and hence are very sensitive to e.g. discharge events, much more than groundwater systems. At the same time the GEM model only runs for 7 years, which makes the sensitivity to discharge events even larger.

15 Considerations regarding the temporal percentile

The sensitivity analysis was done for the 50th percentile PEC (PEC50) and the 90th percentile PEC (PEC90) of the annual maximum concentrations. The first is the temporal percentile which is adopted for the Dutch registration procedure, while the latter is the temporal percentile adopted for the exposure assessment in the EU (with GEM version 3.3.2).

For the updated concepts that were implemented in te latest GEM version the temporal percentiles need to be reconsidered. The rationale for selection of the temporal percentile is given hereafter.
It is common practice in the EU and in the Netherlands to address the 90th overall percentile of concentrations in the area of use (which is considered to be 'realistic worst case'). Translating this to soilless grown crops in the Netherlands, this would imply the 90th percentile concentration due to pesticide uses in Dutch greenhouses, with no distinction between type of crops.

As differences in concentration are considered to be mostly due to grower practices, van der Linden et al. (2015) decided to go for a realistic worst case behaviour and translated this to annual discharge volumes. All other aspects that drive variability in the concentrations were considered of minor importance or it was decided to take median practices or median situations (e.g. the type of ditch).

In Boesten et al. (2020), the WSM scenarios were developed as depicted in the table in Annex 3. These scenarios assume grower practices that for the entire simulation period of 7 years comply with legislative constraints to reduce emissions ("Activity Decree"; Activiteitenbesluit, 2017). This can be considered as a median behavior, i.e. most growers are expected to comply with the Activity Decree. Note that this differs from van der Linden et al. (2015) as they assume that the 90th percentile grower complies with the Activity Decree, and hence, 10 percent of the growers do not comply with the Activity Decree.
Given that the behavior of the 'model' grower is more or less equal to the average behavior of the growers in the Netherlands it can be justified (although not based on quantitative data) that this could be combined with a 90th temporal percentile, i.e. selection of the 'realistic worst case' concentration of an median behavior of a Dutch grower.
Note that the 90th percentile has the advantage of more robust assessment outcomes with respect to the application date.

16 Recommendations for exposure assessment

16.1 Safety factors

The risk assessment procedure should give results that are robust and safe, i.e. covering a realistic worst case situation. For the robustness it is sufficient to indicate fixed dates to be used in the risk assessment, which are within the application window on the label. Since performing a large number of simulations is impractical, we propose to maintain the current practice at the Ctgb of performing 12 simulations with monthly intervals on the 15th of the month. To avoid underestimation of the PEC90 we advise to introduce a safety factor, multiplied with the PEC90. As discussed in section 13.2, with 12 simulations, the multiplication factor is lower than 1.2 for most assessments. The exceptions are assessments with either substance D, WSM scenario 40, or both. These two elements may be incorporated in choosing the safety factors. With regard to substance D, the high uncertainty is related to the fast decline rate in the recirculation water, caused by a low half-life in the recirculation water (1 d). In practise, few substances have such low half-lives. Wipfler et al. (2016) carried out an impact analyses into 23 frequently used substances. Most of these substances have a half-life of 1000 d. Only 2 of these had a half-life in the recirculation water <50 d; 1 had a half-life <1 d.
In summary, we propose the following exposure assessment procedure as to achieve a robust PEC90 for a realistic worst case scenario:

- Perform 12 simulations with application occurring every month of the year on a fixed date
- For each simulation, determine the 90th temporal percentile of the calculated annual PECs (PEC90), this is considered to be the 90th overall percentile
- Determine the 90th percentile of the PEC90 of these 12 runs
- Multiply the 90th percentile of the PEC90 by a safety factor determined by the half-life in recirculation water (DT50) and water stream scenario as indicated below:

	DT50 < 50 d	**DT50 ≥ 50 d**
WSM scenario ≠ 40	1.5	1.2
WSM scenario = 40	5	1.2

16.2 Assessments with multiple applications per year

GEM allows application schemes with multiple applications per year. For example, a grower may have multiple crop cycles per year, with each crop cycle having one or more applications. In such situations an analysis of the sensitivity to application date may be carried out in a similar fashion. The selected application dates then refer to the first application in the year and the other applications are placed relative to the first, according to the annual application scheme. This may result in a situation where some applications are shifted to the following simulation year. For the last year of the GEM simulation period (2000−2006) these applications would not occur, which is undesirable. We propose to solve this by "wrapping" these applications to the start of the simulation period. Hence, applications shifted to 2007 would be moved to 2000, on the same date. We advise to modify the SAFE tool (Berg et al., 2019) to incorporate these changes.

Supplemental information

Supplemental information to this report is available online at: https://doi.org/10.4121/6c61effc-9d0c-4246-8a22-ad7618f4f278.

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Annex 1 Default parameters values used in parameter sensitivity analysis

Table A1.1 *General parameters. Note that the characteristic of the pots are only relevant for SEM-P.*

Parameter and units	Value
Bulk density of soil in pots (kg m^{-3})	1000
Porosity of soil in pots (-)	0.6
Organic matter fraction of soil in pots (-)	0.1
Area fraction of pots on tables (-)	0.3
Leaf area index (-)	4
Time step length (s)	60
Application dose (kg)	1

Table A1.2 *Substance parameters.*

Parameter and units	Value
Degradation	
Half-life in greenhouse recirculation water at reference temperature (d)	1000
Reference temperature for half-life in greenhouse recirculation water (C)	25
Half-life of substance in disinfection tank at reference temperature (d)	1000
Reference temperature for half-life in disinfection tank (C)	25
Half-life of substance in condensation water at reference temperature (d)	100
Reference temperature for half-life in condensation water (C)	25
Molar activation energy in recirculation water, condensation water, and disinfection tank (kJ mol^{-1})	65.4
Sorption	
Half-life of substance on the crop surface (d)	10
Half-life of substance in the soil in pots (d)	118
Half-life of substance on greenhouse floor (d)	100
Equilibrium sorption coefficient to organic matter in pots (L kg^{-1})	131
Equilibrium sorption coefficient for substrate slabs (L kg^{-1})	0
Equilibrium sorption coefficient for foil around substrate slabs (L kg^{-1})	0
Equilibrium sorption coefficient for PVC transport tubes (L kg^{-1})	0
Equilibrium sorption coefficient for PE irrigation tubes (L kg^{-1})	0
Equilibrium sorption coefficient for PE capillary tubes (L.kg^{-1})	0
Other	
Molar mass (g mol^{-1})	255.7
Octanol-Water partitioning coefficient (-)	3.71
End of pipe removal fraction (-)	0
Diffusion coefficient in air at reference temperature (m^2 d^{-1})	0.43
Diffusion coefficient in water at reference temperature (m^2 d^{-1})	4.3×10^{-5}
Reference temperature for diffusion (C)	20
Saturated vapour pressure at reference temperature (Pa)	4×10^{-10}
Reference temperature for saturated vapour pressure (C)	20
Molar enthalpy of vaporisation (kJ mol^{-1})	95
Solubility in water at reference temperature (mg L^{-1})	613
Reference temperature for solubility (C)	20
Molar enthalpy of dissolution (kJ mol^{-1})	27

Annex 2 Relation between GEM emissions and surface water concentrations

To limit the required computation time, the sensitivity analysis was carried out on the outputs of the Substance Emission Model (SEM), rather than the simulated concentrations by TOXSWA. SEM calculates half-hourly discharge fluxes of substance, which serve as input for TOXSWA. The concentrations in the ditch resulting from these fluxes are smoothed due to the volume of water already present. Therefore the half-hourly fluxes are presumably considerably more variable in time and therefore not a good proxy for the concentration in the ditch water. The appropriate time-scale is dependent on the residence time of the water in the ditch. Here we present analysis of the ditch hydrology in order to derive the appropriate averaging time of the substance fluxes for the sensitivity analysis.

In addition to substance concentrations, TOXSWA simulates water depth over time for a 100 m long ditch based on prescribed water input fluxes from upstream and due to discharge from greenhouse with an area of 1 ha. Unless there is a discharge from the greenhouse the flow velocities and water depth are relatively constant within one day. When no pre-existing substance is present in the ditch, the peak substance concentration after a discharge is equal to the emitted mass divided by the water volume at the time of the ditch. If a significant amount of substance is present at the time of discharge the situation is more complex. This may occur when multiple discharge emissions occur in close succession.

Figure A2.1 shows that the upstream water fluxes for the ditch of the GEM scenario are highly variable in time, including periods with negligible flow. This is confirmed by cumulative frequency distribution of the fluxes (Figure A2.2): approximately 25% of the days are characterized by low flow.

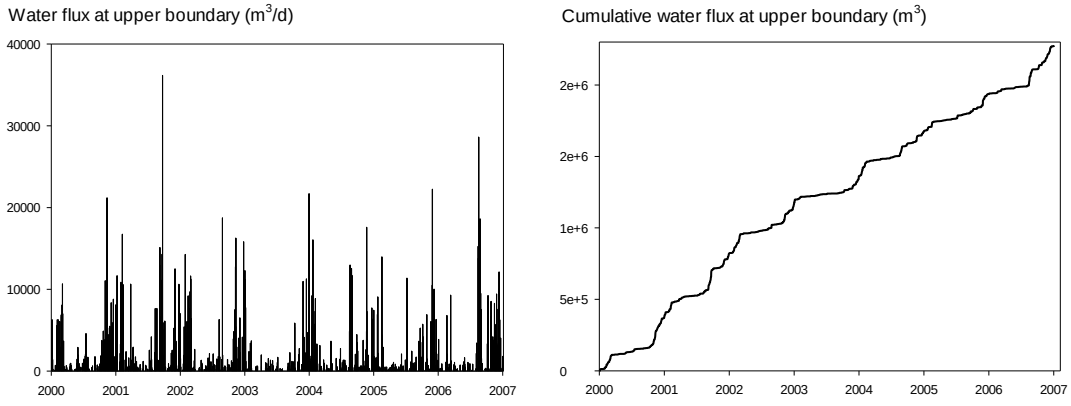

Figure A2.1 *Upstream water fluxes for the ditch of the GEM scenario. Left: daily fluxes; right cumulative fluxes.*

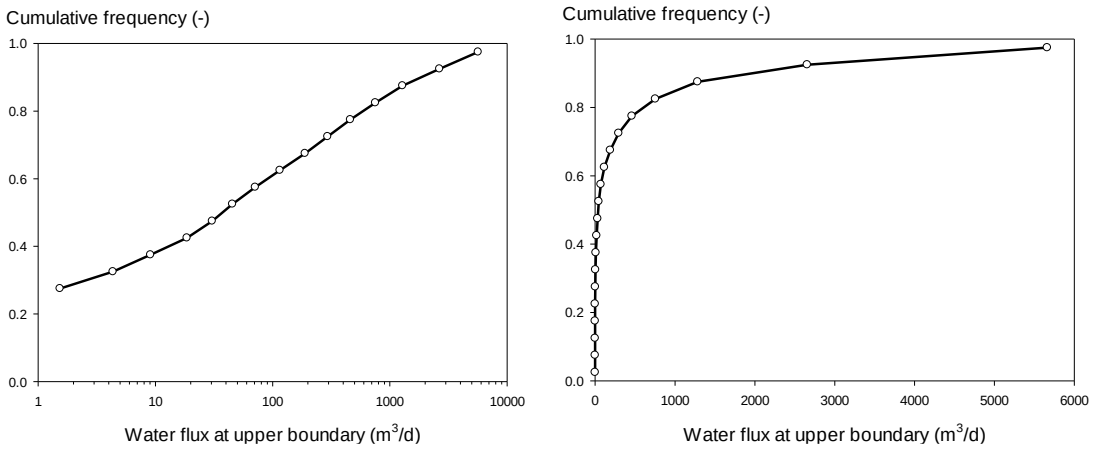

Figure A2.2 *Cumulative frequency distribution of the upstream fluxes for the ditch of the GEM scenario. Left: log-scale; right: linear scale.*

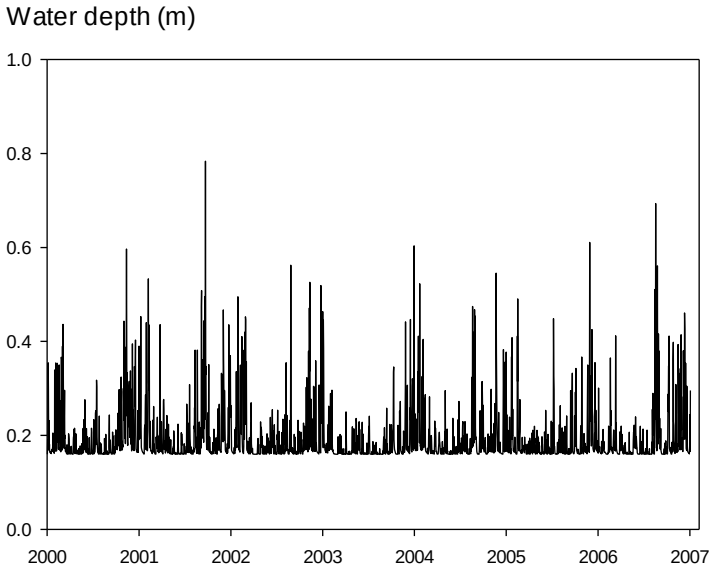

Figure A2.3 *Water depth in the GEM ditch simulated by TOXSWA. Greenhouse discharge fluxes were taken from a GEM3.3.2 scenario (crop: rose; nutrient emission reference period: 2015-2017; filter water option: re-use).*

The water depths calculated by TOXWA (Figure A2.3) show similarly high variability ranging between 16 and 80 cm. The residence time of the water in the ditch may be estimated as the ratio of the water volume (derived from the water depth) and the input water fluxes (Figure A2.4). Again, variability is very high, with values from a fraction of a day up to 100,000 days. The right graph shows that periods of ~1 week in with low residence times can occur in spring and summer.

Figure A2.5 shows the cumulative frequency distribution of the residence times for daily and 10-day averages. For the daily averages the median residence time is approximately 1 d. For the 10-day averages, residence times are much lower because the probability of a day with high flow occurring in a 10-day period is relatively high.

Analysis of the discharge for several WSM scenarios shows that water volumes discharged are generally small compared to the volume of the ditch, which means that the emitted mass will be substantially diluted. Hence, the focus of the analysis should be on emitted mass flux, rather than the concentration of the discharge water. Based on the frequency distribution of the residence times we conclude that it is sufficient to analyze the daily and 10-day average discharged substance mass. Daily masses capture the annual peaks

when emissions are sufficiently spread out in time that accumulation is not relevant. The 10-day average masses can capture the situation where the concentration in the ditch is influenced by multiple successive emissions. Periods longer than 10 days do not need to be considered because most generally almost all water will have been replaced after this time.

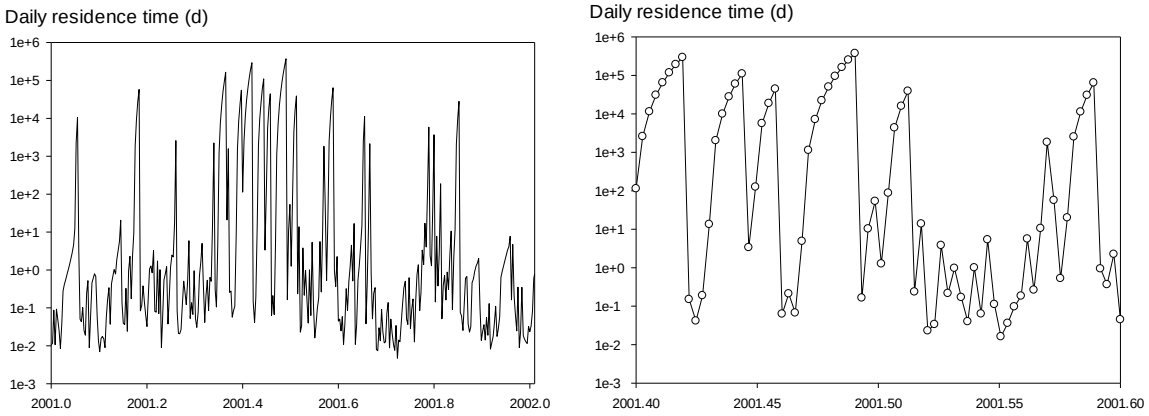

Figure A2.4 *Residence times for 2001 simulated by TOXSWA for the GEM ditch. Greenhouse discharge fluxes were taken from a GEM3.3.2 scenario (crop: rose; nutrient emission reference period: 2015-2017; filter water option: re-use). Left daily mean residence times; right 10-day averages (calculated as the ratio of average fluxes and average volumes). The residence times are calculated for the first segment in the ditch (the water depths and fluxes of the other segments are virtually the same).*

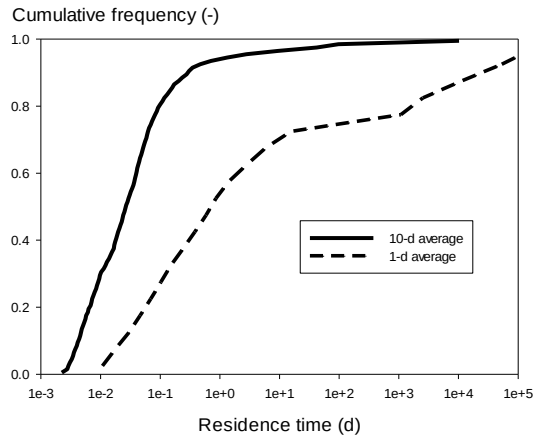

Figure A2.5 *Cumulative frequency distribution of residence times simulated by TOXSWA for the GEM ditch. Greenhouse discharge fluxes were taken from a GEM3.3.2 scenario (crop: rose; nutrient emission reference period: 2015-2017; filter water option: re-use).*

Annex 3 WaterStreamModel scenarios

Table A3.1 *Specification of the water stream scenarios (scenario numbers used in the analysis).*

	Discharge filter water				Reuse filter water			
Nutrient emission reference period	**Sweet pepper**	**Potplant (ficus)**	**Tomato**	**Rose**	**Sweet pepper**	**Potplant (ficus)**	**Tomato**	**Rose**
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

Annex 4 Substance properties

Table A4.1 *Values of properties for the substances included in the analysis. Values set in bold deviate substantially from those of the other substances. Note that, depending on the assessment, parameters some properties are not used.*

Parameter	A	B	C	D
Molar Mass (g mol^{-1})	250	250	250	250
Half-life in greenhouse water (d)	1000	1000	1000	**1**
Reference temperature for transformation in recirculation water (°C)	25	25	25	25
Half-life in disinfection tank (d)	1000	1000	1000	1000
Reference temperature for transformation in disinfection tank (°C)	25	25	25	25
Molar activation energy in recirculation water (kJ mol^{-1})	65.4	65.4	65.4	65.4
Octanol-Water partitioning coefficient (-)	0.01	0.01	**3.16E+06**	0.01
End of pipe removal fraction (-)	0	0	0	0
Reference temperature for diffusion (°C)	20	20	20	20
Reference diffusion coefficient in air (m^2 d^{-1})	0.43	0.43	0.43	0.43
Diffusion coefficient in water at reference temperature (m^2 d^{-1})	0.43	0.43	0.43	0.43
Saturated vapour pressure (Pa)	0.001	**6.30E-12**	0.001	0.001
Molar enthalpy of vaporisation (kJ mol^{-1})	95	95	95	95
Reference temperature for saturated vapour pressure (°C)	20	20	20	20
Solubility in water at reference temperature (mg L^{-1})	1000	**0.88**	1000	1000
Molar enthalpy of dissolution (kJ mol^{-1})	27	27	27	27
Reference temperature for solubility (°C)	25	25	25	25
Half-life at crop surface (d)	10	10	10	10
Half-life in pots (d)	1000	1000	1000	1000
Half-life on the greenhouse floor (d)	100	100	100	100
Half-life of substance in condensation water at reference temperature (d)	1000	1000	1000	1000
Reference temperature for transformation in condensation water (°C)	25	25	25	25
Equilibrium sorption coefficient for substrate (L kg^{-1})	100	100	100	100
Sorption coefficient to organic matter in pots (L kg^{-1})	100	100	100	100
Equilibrium sorption coefficient for foil around substrate mats (L kg^{-1})	0	0	0	0
Equilibrium sorption coefficient for PVC transport tubes (L kg^{-1})	0	0	0	0
Equilibrium sorption coefficient for PE irrigation tubes (L kg^{-1})	0	0	0	0
Equilibrium sorption coefficient for PE capillary tubes (L kg^{-1})	0	0	0	0
Coefficient for uptake by plant (-)	0	0	0	**1**

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