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Modelling dynamic pesticide amounts in multiple environmental compartments at landscape scales in ALMaSS

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Abstract

A dynamic model of the pesticide amount at a landscape scale (10 km x 10 km with the finest spatial resolution of 1 m^2) is implemented in the ALMaSS (Animal, Landscape and Man Simulation System) framework. The spatial resolution can be configured, allowing the user to control how detailed the simulation should be according to the specific needs. Three application types, spray, seed coating treatment and granular, can be applied through the pesticide engine according to the management plan of crops in ALMaSS. A drift model is implemented for the spray application to include the effect on adjacent unsprayed areas. After applying a pesticide, the pesticide module controls transfer amongst different environmental compartments and follows the fate of up to ten different pesticides simultaneously. It enables ALMaSS to be used for complex risk assessment through impact studies of pesticides on many species, including pollinators.

Introduction

The fate of pesticides, when used in agricultural situations, will determine the pattern of environmental contamination. Prediction of contamination is important for evaluating environmental scenarios as part of risk or impact assessment, for example, predicting pesticide residues on crops. The fate also determines the environmental concentrations to which organisms are exposed in environmental and even human risk assessment.

Some models for the determination of pesticide fate are very detailed. For example, the PEARL model (https://www.pesticidemodels.eu/pearl/home) is used to evaluate the leaching of pesticides into water bodies and their persistence in soil. PEARL describes the fate of pesticides in the plant-soil system, which is coupled to the hydrological model SWAP (Soil Water Atmosphere Plant). It calculates changes in pesticide concentrations in different compartments as affected by various physical and chemical processes. Models such as PEARL simulate dynamics at a point location with high precision. They are often used to model physicochemical processes when environmental fate is the focus of the study. In other cases, the prediction of environmental pesticide concentrations forms part of a larger evaluation, such as predicting the pesticide impact on organisms moving through a landscape. In these cases, the precision of the fate model is of less importance than the accuracy and often calculation time must be reduced to make the model tractable. This is particularly the case when the simulation aims to assess a higher organisational level (e.g. population) when the precise exposure of individuals is not critical.

The pesticide fate model built into ALMaSS (Animal, Landscape and Man Simulation System) (Topping et al. 2003, Topping 2022) falls into the latter category of fate models. The purpose here is to predict changing amounts of pesticides over a large area (e.g. 10 km x 10 km), but at a detailed scale, typically 1 m^2. Similarly, the model generally runs over many years (e.g. 30 years) with a fine temporal resolution of one day. The model may be used to calculate pesticide amounts in map form as an output, but is more typically used to drive effect models, for example, evaluating pesticide policy's impact on beetles (Ziółkowska et al. 2022). These models can cover many organisms and types of behaviour and have been used to simulate pesticide effects on non-target arthropods, birds and mammals (e.g. Topping et al. (2005), Dalkvist et al. (2009), Topping et al. (2014), Mayer et al. (2020)).

The pesticide fate model, used in ALMaSS up to 2022, considered the pesticide amount in one compartment only, i.e. only a total environmental amount. However, to align ALMaSS better with current approaches in pesticide risk assessment, a more detailed model is needed. The original ALMaSS pesticide model was dubbed ToxImpact and was introduced for modelling pesticide effects in skylarks (Topping et al. 2005). This model considered the spraying pattern of a pesticide which determined the environmental amount, which then decayed following a fixed rate (DT_{50}). In this model, drift could be calculated as part of the application procedure using constants for an arbitrary compound selected from the FOCUS software commonly used for risk assessment (FOCUS 2001). Further refinements were introduced in the form of temperature variable decay rates by Ziółkowska (Ziółkowska et al. 2022), but the model still only considered a single amount.

The 'blueprint' for the current model was laid down as a feature wish by EFSA Panel on Plant Protection Products and their Residues (PPR) (Residues (PPR) 2015), with the wish to create separate, but linked vegetation and soil compartments. This expansion of the model was further developed to include amounts of pesticides inside plants and differentiation between plant parts to support the evaluation of pesticide impacts on pollinators (Duan et al. 2022). This paper describes the implementation of the new model to fulfil these feature wishes.

Methods

The pesticide engine of ALMaSS includes consideration of both the application (spray, seed coating treatment and granules treatment) and the fate of the pesticide. These are explained in Pesticide Application and Pesticide Fate, respectively.

The pesticide module has different levels of complexity depending on which model of the module is used. The simplest model considers only a single compartment for the pesticide. We call this model the 1-compartment model. For a more complex version, we consider whether the pesticide is on the plant canopy or the soil, so we split the pesticide between these two compartments. We refer to this version as the 2-compartment model. In this case, we also consider the rain wash-off from the canopy to the soil. The 3-compartment model is an even more complex model in which we consider an additional compartment inside the plant. It is the amount of pesticide in this 'in plant' compartment, that is used to calculate the pesticide concentration in the pollen and nectar. It is simply given by the amount of pesticide divided by the green biomass times a pollen (or nectar) specific partition coefficient.

In the 2- and 3-compartment models, the pesticide can be transferred between the different compartments as described in Pesticide Transfer. Building on the 3-compartment model, another level of complexity is added if seed coating is turned on. The seed coat adds another compartment and enables additional transfer, effectively resulting in a 4-compartment model.

In practice, a pesticide map is added for each of the compartments per pesticide (compartment maps). The compartment maps can have the same resolution as the landscape or coarser. It is currently possible to consider up to 10 different pesticides simultaneously and they will each have a unique set of compartment maps. ALMaSS takes many parameters as inputs for the pesticide module, with parameter settings applied through a configuration file. These parameters are listed in Model Parameters.

Examples of usage demonstrates the models by showing the pesticide amount as a function of time under certain conditions.

Pesticide Application

In ALMaSS, pesticides can be applied in three ways: sprays, granules and seed coating. The model used for sprayed pesticides is the most complicated of the three since it can consider the drift caused by the wind and the division of the pesticide between the plant canopy and the soil. On the contrary, the granular application is assumed not to experience drift and only be applied to the soil compartment map, based on the application rate. For seed coating, the pesticide will be added to the seed coating compartment map at the time of sowing and will, from that time on, be able to decay and be transferred to the other compartments, as explained in Pesticide Transfer.

The spatial resolution of the landscape in ALMaSS is 1 m^2. At default, all the pesticide maps use the same resolution as the landscape with the possibility of using coarser resolutions. All three pesticide application events, spraying, granules or seed coating are managed by adding them to an event queue, which is then executed once per day when the weather allows. Each event includes information on the pesticide type, application rate and the landscape element that the pesticide should be applied to, typically a field. The pesticide is applied to the pesticide map(s) by looping over the cells in a bounding-box rectangle around the treated polygon, where the pesticide should be applied. Each cell is then checked to see whether it is inside the sprayed polygon. If the cell is inside, the pesticide amount is first added to a temporary map (the twin map), which has the same dimensions as the compartment maps. Before continuing, the need for a border correction is checked for in case the size of the pesticide map extends beyond the boundary of the actual landscape. If yes, the pesticide amount in the temporary map is reduced according to the size of the area beyond the boundary of the actual landscape. After this is done, the three types of applications are handled differently. Based on the temporary map, the pesticide is applied to the soil compartment map for granule application or to the seed coating compartment map for seed coating treatment.

For pesticide spray, the drift caused by wind is considered before it is transferred to the compartment maps. Only the wind direction is considered in the model, without the inclusion of the impact of the wind speed. Four wind directions (South, North, East and West) are used. Drift inclusion is done by choosing a drift vector at the beginning of the simulation. The drift vector is used to diffuse the pesticide in the temporary map to its surrounding cells, especially along the wind direction. In ALMaSS, we assume that drift happens up to 10 m along the wind direction and 1 m for the upwind direction and the two directions perpendicular to the wind direction. This assumption is supported by the studies in Destain et al. (2011) which compare drift measurements with a detailed simulation of the spray cone. To form the drift vector the results from Stallinga et al. (2014) and Stallinga et al. 2016 are used, which provided the ground deposit from a single nozzle 1 m upwind and 10 m downwind for two different forward speeds (7.2 and 14.4 km/h) and 17 different nozzles. However, these data could not be used directly and needed to be processed in the following way:

First, the downwind ground deposit is fitted to a power function $y = Ax^B$ where x is the distance from the nozzle and y is the pesticide proportion of the application rate. The fit is not performed over the whole range of the data, but only from x_1 to x_2. Whereas x_2 is always set to the last measurement point ($x_2 = 9.75$ m), x_1 is chosen such that a good fit is obtained. It, therefore, varies from $x_1 = 1.25$ m to $x_1 = 2.75$ m. For ALMaSS, we want to know the drift in increments of 1 m starting from -1 m to 10 m in the downwind direction as well as ±1 m perpendicular to the wind direction around the spraying point. For the cells 1 m upwind and perpendicular to the wind direction, we use the measurement point at $x = -0.75$ m, whereas for downwind (positive) x-values, the power function fit is used when available; otherwise, the average of the logarithm of the two surrounding measurement points are used:

The amount at $x = 0$ m is then the amount that has not drifted, so 100% of the applied amount minus the sum of the upwind drift and three times the downwind drift to also consider the amount that goes perpendicular to the wind direction. This assures that the intended amount of pesticide is spread in the landscape. An example of the original data, the fit and the derived drift vector for a BCPC-F/M nozzle with a forward speed of 14.4 km/h is shown in Fig. 1.

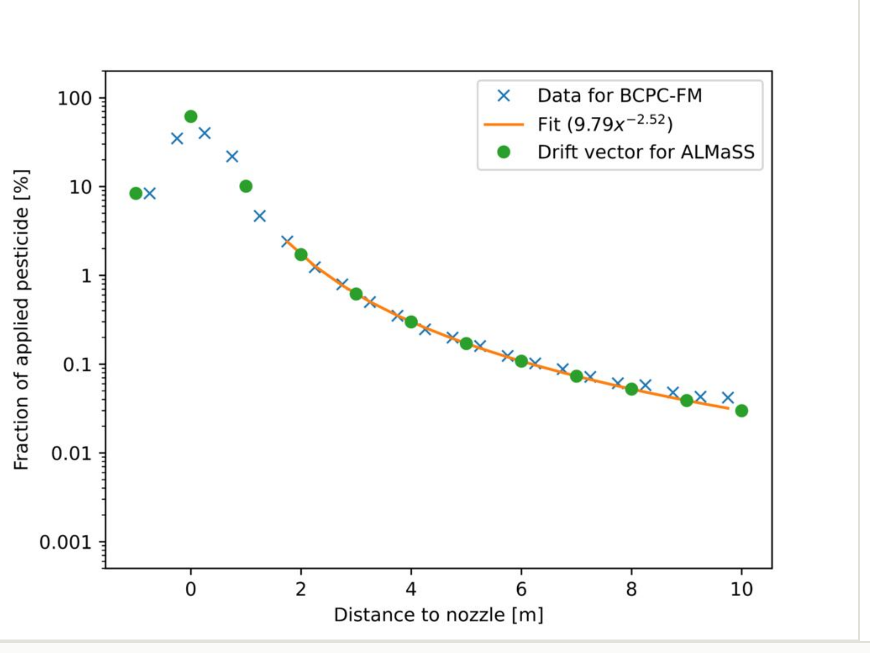

Figure 1. doi

Ground deposit data for BCPC-F/M nozzle at a forward speed of 14.4 km/h (blue crosses) (Stallinga et al. 2014, Stallinga et al. 2016) fitted with a power function (orange line) together with the derived drift vector to be used in ALMaSS (green points). Note that the amount at -1 m is also used for the two cells perpendicular to the wind direction.

Fig. 2 and Fig. 3 shows the derived drift vectors for all the different nozzles at a forward speed of 7.2 and 14.4 km/h, respectively. For both speeds, at a distance to the nozzle of 1 m, the fraction of applied pesticide varies by roughly one order of magnitude and, at 10 m, it varies almost by two orders of magnitude.

Pesticide drift measurements are often not done per nozzle, but instead, as the accumulated drifted amount outside the spraying area as in, for example, the study done by Rautmann et al. (2001). Fig. 4 shows the accumulated drifted amount of pesticide for the different nozzles at a forward speed of 14.4 km/h, as well as the Rautmann result which is given by $f = 2.7705x^{-0.9787}$ where f is the fraction of the applied pesticide and x is distance from the sprayed area in metres.

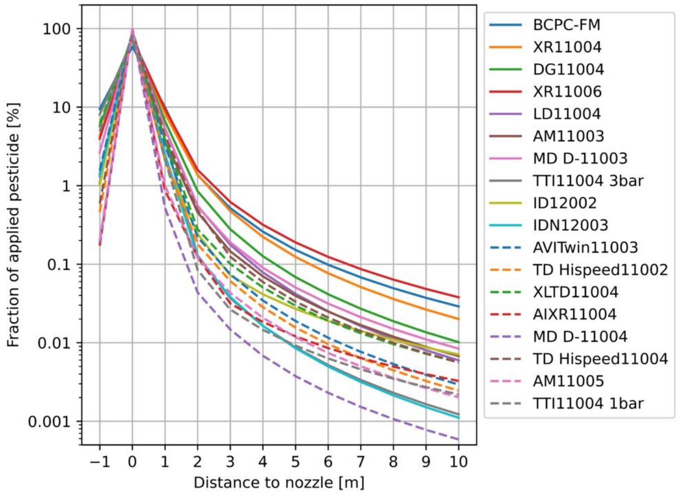

Figure 2. doi

Drift vectors for different nozzles at a forward speed of 7.2 km/h. The distance is measured along the wind direction. Note that the amount at -1 m is also used for the two cells perpendicular to the wind direction.

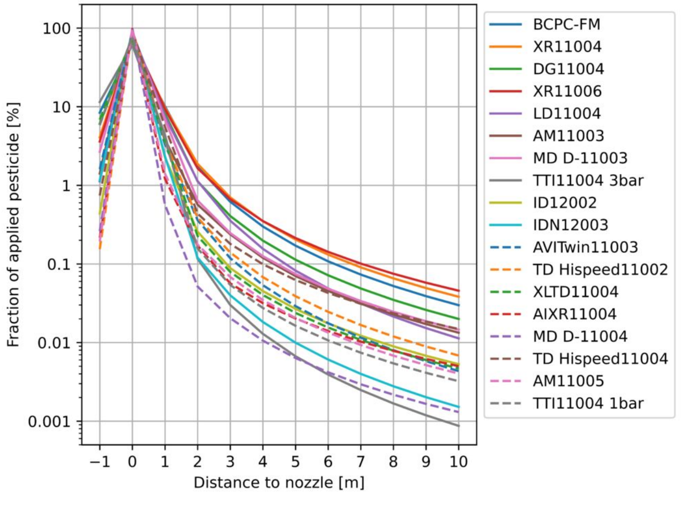

Figure 3. doi

Drift vectors for different nozzles at a forward speed of 14.4 km/h. The distance is measured along the wind direction. Note that the amount at -1 m is also used for the two cells perpendicular to the wind direction.

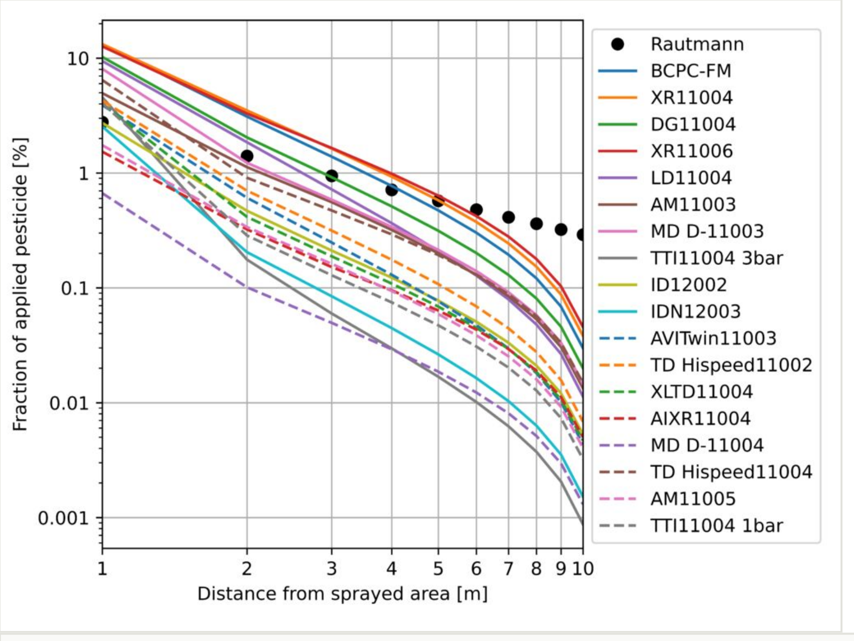

Figure 4. doi

The accumulated drifted amount of pesticide outside the field (in the wind direction) for the different nozzles at a forward speed of 14.4 km/h compared to the result of Rautmann et al. (2001).

Fig. 5 shows the pesticide distribution on and outside of a rectangular field with a width of 18 m immediately after the spraying, on a day with a westerly wind. In this case, the drift for the BCPC-F/M nozzle with a forward speed of 14.4 km/h is used. The figure shows that, upwind to the left side of the field, the drift only reaches 1 m (pink column) and the rest of the area is unaffected (white columns). Inside the field, the pesticide amount gradually increases from left to right until it reaches 100% (yellow columns) before decreasing to around 92% for the last 1 m (turquoise column). On the right side of the field, the amount of pesticide follows the BCPC-F/M distribution in Fig. 4, gradually decreasing from around 13% to 0%. Please note that the pink colour scales are not linear.

The last step of the spraying is distributing the pesticide between the different compartments. In the 1-compartment model, the whole amount is simply applied to the same map. For the 2- and 3-compartment model, it is shared between the plant canopy and soil compartments by using Beer's Law (EFSA 2017) to calculate the canopy cover. According to this law, the fraction of the surface covered by the crop is given by:

$$\mathrm{SC} = 1 - e^{-\kappa \mathrm{LAI}}$$

where LAI is the leaf area index and κ is the extinction coefficient for diffuse solar radiation which has a default value of 0.6, but can be specified in the configuration file. The fraction of the pesticide added to the plant canopy is then given by SC.

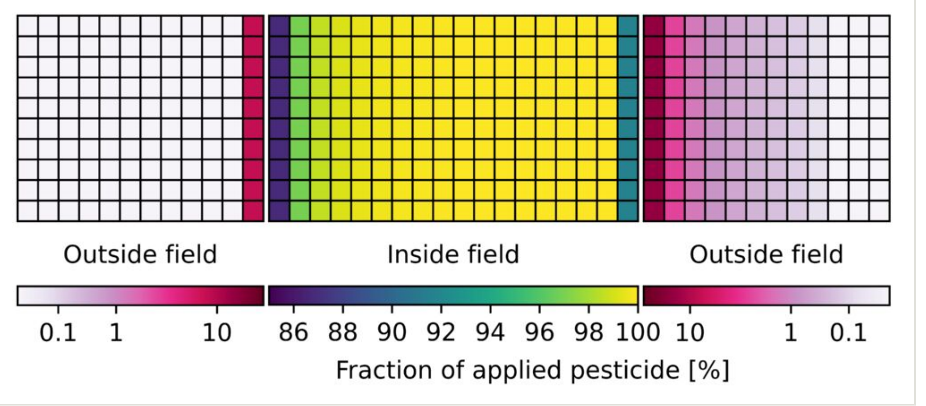

Figure 5. doi

Pesticide distribution on landscape after drift using a BCPC-F/M nozzle with a forward speed of 14.4 km/h. Each square is 1 m x 1 m and the sprayed field is the 18 columns in the middle with the purple-green-yellow gradient.

Pesticide Fate

The pesticides are assumed to undergo a first-order decay every day. Therefore, the remaining fraction of pesticide after one day is given by:

$$f = 10^{\frac{\log_{10}(0.5)}{t_{\frac{1}{2}}(T)}}$$

where $t_{\frac{1}{2}}(T)$ is the temperature-dependent half-life, which is given by:

$$t_{\frac{1}{2}}(T) = t_{\frac{1}{2}}(20) \cdot e^{0.094779 \cdot (20 - T)}$$

where $t_{\frac{1}{2}}(20)$ is the half-life at 20°C and T is the average temperature on the given day. The half-life can vary for different pesticides and compartments. They can, therefore, be specified in the configuration file, but have a default value of 10 days. The daily fraction remaining is calculated for each pesticide and compartment once daily to account for the temperature dependence.

The decay of the pesticides is then calculated by looping over all the cells and multiplying the current amount in each cell by the daily fraction remaining. A flag is set to true as soon as a pesticide has been applied. During the decay process, the remaining amount of pesticide is checked against a user-defined threshold for infinitesimally small values and the cell value is set to zero. To prevent running the computationally heavy loop over all the cells when there is nothing to decay if all cells are zero, the application flag is unset and the decay process is no longer run.

The amount of pesticide in the plant compartments (plant canopy and in plant) can also decrease or be completely removed due to a number of farm management events like harvesting or plouging. Note that this does not affect the soil compartment or the only compartment in the 1-compartment model. The amount of pesticide in the 'in plant' compartment is also decreasing when the green biomass transform to dead biomass. In this way, we are just considering the amount of pesticide in the living part of the plant since it is only this part that will be able to transfer into the pollen and nectar.

Pesticide Transfer

The pesticides are transferred between the different compartments when the multiple-compartment models are used. A sketch of the transfer can be seen in Figure 6. In the case of the 2-compartment model, the only transfer mechanism is rain wash-off, which transfers part of the pesticide from the plant canopy to the soil as indicated by the blue arrow. The rain wash-off depends on the daily gross precipitation in mm. To implement this, the leaf area index (LAI) and surface cover (SC) is used to calculate the intercepted precipitation given by Prochnow et al. (2012):

$$P_i = a \cdot \mathrm{LAI}\left(1 - \frac{1}{1 + \frac{\mathrm{SC} \cdot P}{a \cdot \mathrm{LAI}}}\right)$$

where P is the gross precipitation and a is an empirical coefficient set to 0.25 mm/day for agricultural crops. The proportion of the pesticide that is washed off because of gross precipitation P is then given by:

$$R_w = w \cdot \mathrm{SC} \cdot (P - P_i)$$

where:

$$w = 0.0016 \cdot S^{0.3832}$$

is the wash-off factor (EFSA 2012), that is dependent on the water solubility of the pesticide, S, which is set to a default value of 10000 mg/l unless another value is given in the configuration file.

In the case of the 3-compartment model, several transfer mechanisms are considered in addition to the rain wash-off. This is indicated by the green and brown arrows in Fig. 6. Part of the pesticide amount is absorbed from the plant canopy and the soil into the plant. In the case that seed coating is used, two additional mechanisms of transfer are considered, from the seed coating to the soil and into the plant. This is indicated by the orange arrows.

The transfer between the seed coating and soil compartment is simply calculated by multiplying the pesticide amount with a rate $R_{\mathrm{seed}\to\mathrm{soil}}$, such that the amount in each cell goes from $x_{\mathrm{seed,old}}$ to $x_{\mathrm{seed,new}}$ in the seed coating compartment and from $x_{\mathrm{soil,old}}$ to $x_{\mathrm{soil,new}}$ in the soil compartment:

$$x_{\mathrm{seed,new}} = x_{\mathrm{seed,old}} - x_{\mathrm{seed,old}} R_{\mathrm{seed}\to\mathrm{soil}}$$

$$x_{\mathrm{soil,new}} = x_{\mathrm{soil,old}} + x_{\mathrm{seed,old}} R_{\mathrm{seed}\to\mathrm{soil}}$$

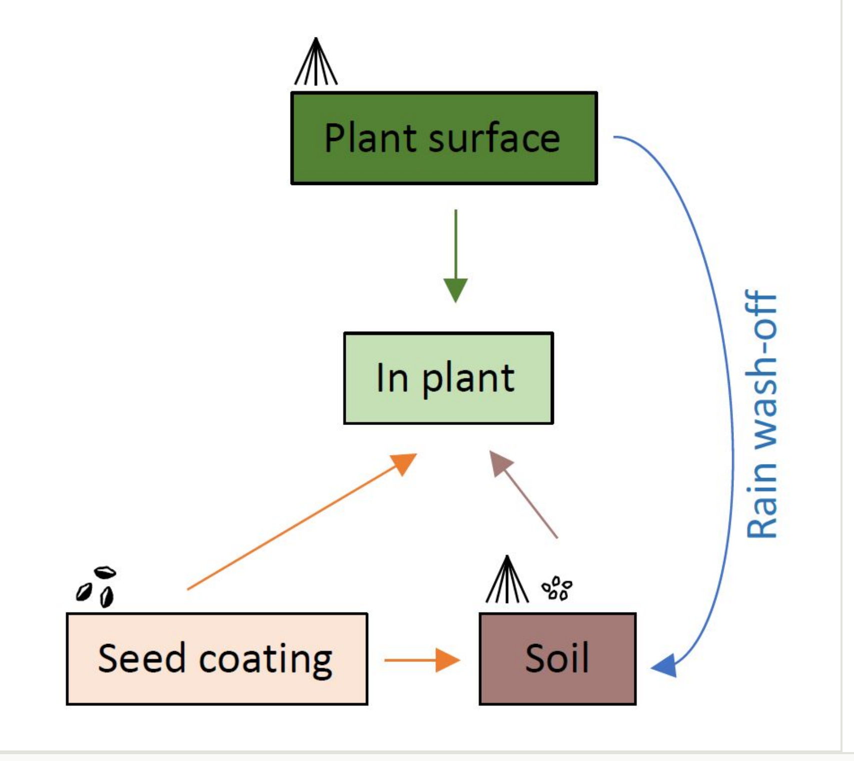

Figure 6. doi

Diagram of transfer between different pesticide compartments. The 2-compartment model includes the dark green and brown compartments, whereas the 3-compartment model also includes the light green one. The 4-compartment model furthermore includes the orange box. Small symbols indicate how the compartments can be supplied with pesticide through the application: spray, granular and seed coating.

For the three types of transfer into the plant, the transfer is depending on the green biomass of the plant m_{green} with the assumption that a large plant absorbs more than a small plant so:

$$x_{\mathrm{f,new}} = x_{\mathrm{f,old}} - x_{\mathrm{f,old}} R_{\mathrm{f \to in\ plant}} m_{\mathrm{green}}$$

$$x_{\mathrm{in\ plant,new}} = x_{\mathrm{in\ plant,old}} + x_{\mathrm{f,old}} R_{\mathrm{f \to in\ plant}} m_{\mathrm{green}}$$

where f stands for one of the three compartments (plant surface, seed coating or soil) from which the pesticide is transferred. The transfer rates are given in the configuration file and the default value for all rates is set to 10%. The green biomass m_{green} is given in kg/m^2. The order of the transfers is: plant canopy to inside the plant, soil to inside the plant and seed coating to inside the plant and to the soil.

Model Parameters

In Table 1, the model parameters, which are used to control the simulation, are listed. Table 2 shows a list of the different nozzle types that can be chosen.

Table 1.

Model parameters controlled in the configuration files for ALMaSS.

Parameter	Default value
GENERAL	
Number of pesticides (1-10)	1
Pesticide water solubility (for each pesticide)	10,000 mg/l
Pesticide half-life (for each pesticide and each compartment: soil, plant canopy, plant and seed coating)	10 days
Transfer rate (for each of the transfers: soil to plant, plant canopy to plant, seed coating to plant, seed coating to soil)	10%
Pesticide amount (for each pesticide)	1
Partition coefficient (for pollen and nectar)	0.01
SPRAYING	
Driving slow (true or false)	false
Nozzle type (0-17)	0

Table 2.

List of nozzle types.

Number	Nozzle type
0	BCPC-F/M
1	XR11004
2	DG11004
3	XR11006
4	LD11004
5	AM11003
6	MD D-11003
7	TTI11004 3bar
8	ID12002
9	IDN12003
10	AVITwin11003
11	TD Hispeed11002
12	XLTD11004

Number	Nozzle type
13	AIXR11004
14	MD D-11004
15	TD Hispeed11004
16	AM11005
17	TTI11004 1bar

Optimisation

The pesticide code is very computationally intensive both with regard to CPU time and memory consumption. To decrease both time and memory use, it is possible to decrease the resolution of the pesticide maps to, for example, a 4 m^2 or 16 m^2 grid instead of the 1 m^2 resolution of the landscape.

Another way to run the code quicker is to use several CPU cores in parallel. The loop over the cells in the pesticide map can be done in parallel for both the decay and transfer methods, which are some of the most time-consuming parts of the code. This is possible because the cells are independent of each other.

Examples of usage

These examples are designed to show that the pesticide behaviour works as described, but do not purport to show a real case. An example of the decay and transfer of the pesticide between the different compartments is shown in Fig. 7. The default values for the half-life, water solubility and transfer rates are used. The figure shows the amount of pesticide in mg/m^2 in a field with winter rape, which is fully sprayed. Note that the default transfer rates have been set at relatively high values to produce a clear pattern; hence, all pesticide transfers quickly from canopy and soil to 'in plant'. Slower transfer and degradation rates would result in higher pesticide amounts in different compartments for longer.

At the time of spraying (4 April), most of the pesticide is sprayed on the plant canopy (blue). However, the pesticide is quickly transferred to the soil (orange) due to the rain wash-off and the plant starts absorbing the pesticide both from the soil and the canopy, which increases the amount inside the plant (green).

The stack of the three compartments is seen to match the curve for the 1-compartment model (black dashed line) until day 154 (3 June) after which the stack decreases quicker. This is caused by the transformation of green biomass to dead biomass starting this day, which decreases the amount of pesticide in the 'in plant' compartment as explained in Pesticide Fate. Note the curves only match in this example because the half-lives are kept the same for all compartments; this is unrealistic, but is shown to confirm that the transfers work correctly.

Fig. 8 shows the pesticide amount in an area which is first applied with seed coating (brown) and then alternately sprayed pesticide and seed coating in a total of six applications over three years. The figure shows a case where the pesticide from the seed coating has barely decayed before the sprayed pesticide is applied.

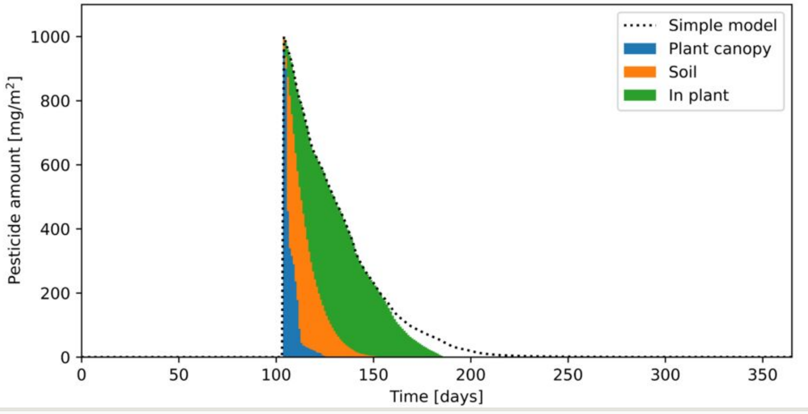

Figure 7. doi

Pesticide amount as a function of time in the different compartments in an area, which is fully sprayed on 4 April (day 104). The 3-compartment model is used. Note that the assumed pesticide amount in the simple 1-compartment model is not affected by the degradation of the plant as explained in the main text.

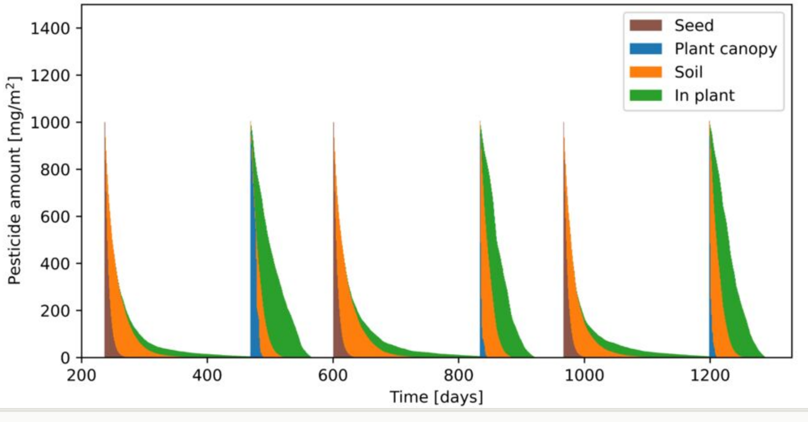

Figure 8. doi

Pesticide amount as a function of time in the different compartments in an area where seed coating and sprayed pesticides are applied alternately. The 4-compartment model is used.

Fig. 9 shows an example of the pesticide amount in the different compartments when applying a granular pesticide instead of spraying it. The main difference is that there is no pesticide on the plant canopy, but otherwise, the transfer occurs in the same way as for the sprayed pesticide.

Fig. 10 demonstrates that the framework is able to keep track of several pesticides at the same time. In this case, the first pesticide (PPP1) is sprayed on 4 April and the second (PPP2) on 18 April.

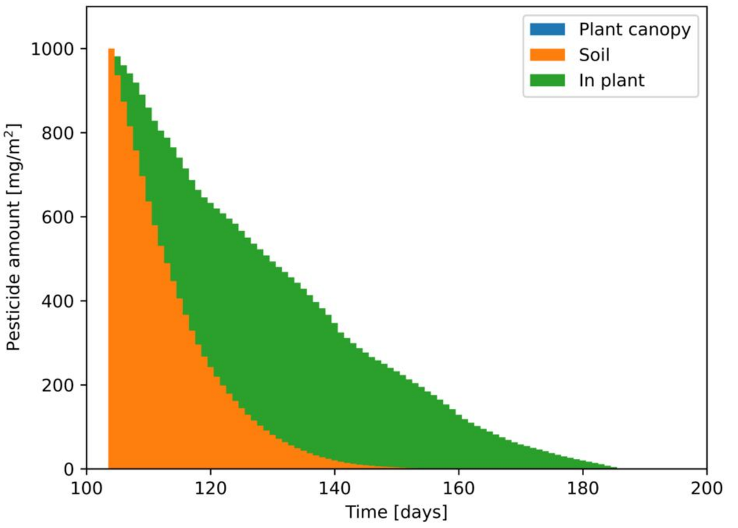

Figure 9. doi

Pesticide amount as a function of time in the different compartments in an area where a granular pesticide is applied on 4 April (day 104). The 3-comparment model is used, but there is no pesticide on the plant canopy.

Fig. 11 demonstrates the effect of the half-life of the pesticide. The decay in the 1-compartment model is shown for a half-life of 5, 7.5, 10 and 12.5 days, respectively. The expected behaviour with a faster decay with a lower half-life is observed. The small wiggles in the curves are caused by the temperature-dependence of the half-life as explained in Pesticide Fate.

Fig. 12 demonstrates the effect of the water solubility of the pesticide. The decay in the 2-compartment model is shown for water solubility of 1, 5, 10 and 15 g/l, respectively. The bumpy distributions are caused by the rain wash-off, which depends on the daily precipitation, as explained in Pesticide Transfer.

Discussion

The way pesticides are handled in ALMaSS is not a one-to-one replica of reality. That is, however, not the goal and would not be computationally feasible. The implementation merely aims to cover the main exposure routes that would impact the numerous organisms simulated in ALMaSS.

The drift which occurs when the pesticide is sprayed was the most complicated part to implement. The main challenge is that most of the available data on drift is not directly applicable to the simulation. The studies from, for example, Rautmann and Ganzelmeier (Rautmann et al. 1995, Rautmann et al. 2001), investigated the total drift outside the field after having sprayed a whole field. They assume that the field is broad enough that pesticides sprayed at one side will lead to negligible drift on the opposite side. However, in ALMaSS, we have complex field geometries (e.g. very narrow stretches of field), so we are interested in knowing the drift caused by spraying on a single square metre to not overestimate the drift outside those parts. Here the studies on drift from a single nozzle by Stallinga et al. (2016) are more applicable. Using their results, we can calculate the drift up to 10 m away from the spraying point in the wind direction. In reality, the drift can go further, but the effect is deemed very small and would require additional computing power, as well as an uncertain estimate of the amount deposited due to the missing data above 10 m. The effect of only applying the drift up to 10 m is seen in Figure 4 where the distribution drops off at the end. This figure also shows the results from Rautmann (Rautmann et al. 2001), which has a less steep slope. However, a paper by Butler Ellis et al. (2017) shows that the slope of the drift distribution varies significantly between different studies; for example, the Fera PS2022 result (Anon. 2010) has a similar slope to that which we obtained here.

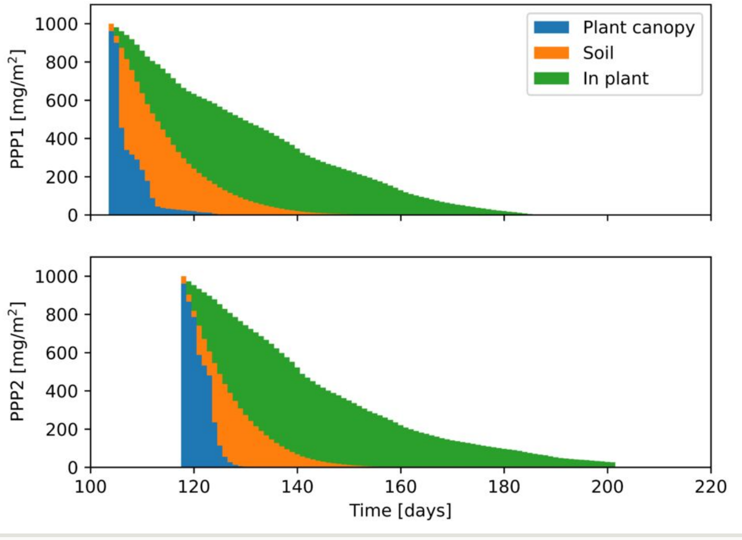

Figure 10. doi

Pesticide amount for two different pesticides (PPP1 and PPP2) as a function of time in the different compartments in an area, which is fully sprayed with PPP1 on 4 April (day 104) and PPP2 on 18 April (day 118). The 3-compartment model is used.

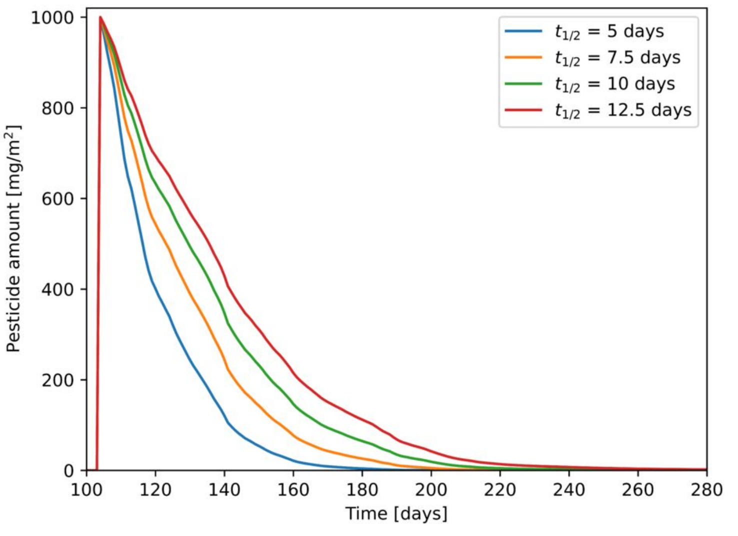

Figure 11. doi

Pesticide amount as a function of time for different half-life assumptions in an area, which is fully sprayed on 4 April (day 104). The 1-compartment model is used.

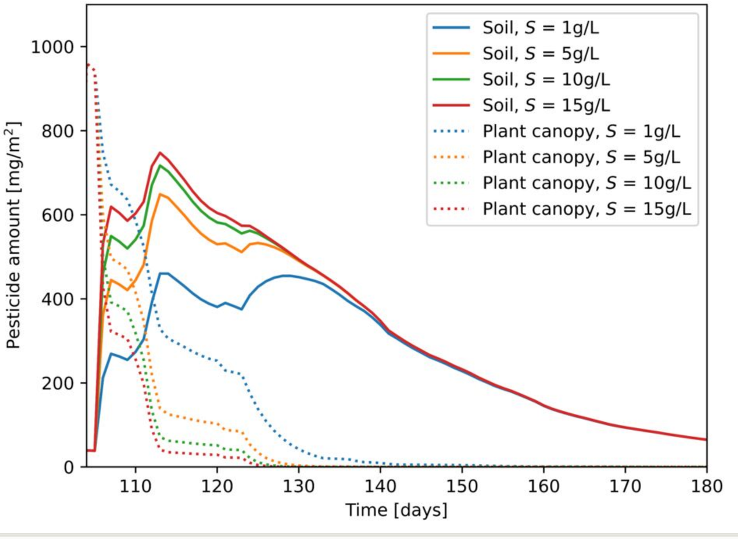

Figure 12. doi

Pesticide amount as a function of time for different water solubility assumptions in an area, which is fully sprayed on 4 April (day 104). The 2-compartment model is used.

There are also more general considerations related to the assumptions in the current model. The drift is caused by the wind, which, at low speeds, is variable in direction and strength, but in the ALMaSS simulation, the main drift is only dependent on the wind in that the drift is applied in the average wind direction of the day (in four directions). Future extensions could consider variations in wind direction during the day and include wind speed in the calculation. This might have an effect on which habitats surrounding a field receive drift. However, the range for the wind speed is limited since the farmers are typically not supposed to spray pesticides unless the wind speed is less than 5 m/s, hence the change in drift distance will be minimal.

Another assumption used for the drift is that the drift at a point in time mainly occurs with the wind direction. This assumption is based on the results from Destain et al. (2011) showing that a simulation which only assumes a drift of around 0.5 m perpendicular and opposite to the wind direction for each nozzle gives a good description of the measured drift, so the assumption of only 1 m drift perpendicular and opposite to the wind direction should hold. Since we do not have any measurements of the drift perpendicular to the wind direction, we have assumed that it is the same as the amount going upwind, even though it is probably a bit more. This could be altered in future versions if this proves to be an important simplification.

This model considers what happens to the pesticide when it is portioned between soil and vegetation, but other factors can be important in the field. One important, but missing mechanism for pesticide mass transport is runoff. Runoff describes the removal of pesticides from the soil caused by water flow; since ALMaSS does not currently simulate surface water, it would be complicated to include this effect. It might be possible to include this in the future, but it would require implementing an ALMaSS surface water model, which has not been explored so far.

There are also simplifications regarding environmental decay. The temperature-dependent half-life given in Pesticide Fate stems from decay in soil and is, therefore, strictly speaking, only valid for the soil compartment. It is, however, also used for the other compartments, with different parameters, since it is the best estimate we have at the moment. In future versions, it might be possible to implement a solar radiation-dependent half-life for the plant canopy or another suitable model, if available.

Conclusions

We have demonstrated that the pesticide module in ALMaSS can apply pesticides to the landscape in the form of sprays, granules and seed coating. For sprayed pesticides, the model takes into account the drift caused by the wind, as well as the division of the pesticide between the plant canopy and the soil by using Beer's Law. Furthermore, the pesticides can be transferred between different compartments, for example, from leaf surface by rain wash-off or absorption.

The ALMaSS pesticide module is highly configurable and has several levels of complexity. It can be used as a relatively simple model with only one compartment if the precise division of the pesticides is not deemed important for a particular simulation. However, in some cases, for example, for honeybees, it might be important to model the fractions of the pesticides that enter the pollen and nectar. The more complex 3- and 4-compartment models can be used in such a case. However, it requires detailed calibration data such that the pesticide half-lives, transfer rates and partition coefficients can be determined for a given pesticide. These data will preferably include residue measurements in soil, plant, pollen and nectar several times after the pesticide application. If such data are not available, worst-case estimates would have to be used.

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