Fate, Transport, and Effects of Glyphosate on Population Dynamics of Non-Target Organisms in Agricultural Settings: A Simulation Study

Mwema Felix*, Alice Sharp, and Niels Holst

Abstract— *Agriculture is the backbone of many countries. This sector has been challenged by the increasing number of pests including weeds. Chemicals such as herbicides are therefore used for weed control. One of such herbicides is glyphosate. The use of herbicides has however been associated with the population decline of non-target organisms like frogs. In this study, fate, transport, and effects of glyphosate on population dynamics of frogs (Crinia insignifera) were simulated using an object-oriented model known as PestTox. Two scenarios were simulated; the agricultural field and the receiving water body (stream or pond) were separated by buffer zones of 30 m and 0 m. The simulation was done using weather conditions of Pathumthani province (Thailand) for the year 2012. Results show that if the field is not surrounded by a buffer zone of at least 30 m, spray drifts and runoffs could transfer glyphosate off the field edge to the receiving waterbody, potentially killing all tadpoles only if glyphosate concentrations are sufficiently high. Results indicate that buffer zones should be used around the fields to reduce spray drifts and runoffs which in turn could help to maintain the healthy population of frogs and other non-target organisms. This study has potential limitations. First, the study used secondary data from various sources. Second, numerous processes are based on analytical expressions/regressions from various pedoclimatical contexts. These may have influenced model estimates. However, the findings may be of interest to those involved in pesticide registration and monitoring.*

Keywords— **Ecological modeling, Object-oriented modeling, Population dynamics, Predictive modeling.**

1. INTRODUCTION

Agriculture is among the sectors that contribute to the national economy of many countries including Thailand. However, among other pests, weeds pose great threats for many crops as potentially could reduce crop yield by about 30%. For example, in year 2001-2003 about 10% of the global crop yield were lost due to weeds [1]. Of all the crops, maize and other field crops are highly affected by weeds such as *Imperata cylindrical* commonly found in West Africa [2] and Southeast Asia [3]. In an attempt to reduce loss of crop yields, globally, farmers use pesticides.

It is estimated that herbicides are the most widely used type of pesticides (50% of the global pesticides use) because they help to reduce tillage, thus, minimize human labour [4, 5]. However, the use of herbicides has been widely associated with the population decline of non-target organism such as amphibians (frogs) [6-9]. This could be due to the movements of herbicides from one point to another (fate and transport processes), example, through spray drift, washoff, and runoff [10]. Herbicides contamination could be one of many factors that could be responsible for the population decline of amphibians [11, 12].

Practically, it could be difficult to study the effect of a herbicide to the true population of frogs in the environment because of the complexity of the ecosystem processes involved. In this study, fate, transport, and effects of glyphosate on population dynamics of *C. insignifera* [13] were therefore simulated using object-oriented modeling paradigm. The aim was to establish and inform about the potential effects and impact of glyphosate on population dynamics of amphibians in an agricultural settings. This species of frogs was the selected non-target organisms because its toxicity data (48 h LC_{50}) for glyphosate (Roundup®) was readily available for simulating mortality rates of its four growth development stages (i.e. eggs, tadpoles, froglets, and adults). In addition to that, this species could be found in either subtropical or tropical environment and wetlands [14], conditions assumed to be similar to the conditions in Thailand. Glyphosate was selected because it is widely used for weed control in Thailand [15-17] and many other parts of the world. Also, maize was selected as the study crop because it is one of the main crops grown in Thailand [18] and many other parts of the world, for example Tanzania where it is a staple food.

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2. MATERIALS AND METHODS

2.1 Model Adoption and Specifications

PestTox model [19] was developed by modifying PestLCI models [20, 21]. This model is an objected-oriented and open source (other software used are also open source i.e. Universal Simulator 2, Qt development environment, Notepad++, Boost libraries, and R for statistical computing). Being an open source, it means that its codes can be extended and reused by other modelers/users [22, 23] depending on the objective, scope, and structure of the intended studies [24]. PestTox model is programmed in standard C++ language and it is provided as a plug-in in Universal Simulator 2 [19]. Sensitivity analysis of the model estimates due to variation of the model inputs was modeled using Latin Hypercube Sampling (LHS) method with random numbers drawn from uniform statistical distribution [25].

PestLCI models were designed to estimate pesticides emissions to air, surface water, and ground water as aggregated fractions (amount). These estimated emissions are then used as inputs on USEtox for further toxicity assessments in the context of LCA [26]. Modifications were necessary to make use of the advantage of the object-oriented modeling paradigm and to add crop model, weather model, fate and transport model, frog population dynamics model, and simulation time steps [19]. In addition to that, washoff process from the crop/leaf surfaces was included in the PestTox model (this process was initially not included in PestLCI models). Universal Simulator 2 program [25] was used to simulate the results by reading the Extensible Markup Language (XML) or box files which were prepared using Notepad++. The XML and box files were used for model specifications as well as for database especially for climatic data (temperature and rainfall).

2.2 Case Study

The study assumed that the agricultural field is 100 x 100 m and it is located in Pathumthani Province, Thailand at 14.02° N [27, 28]. The field and the receiving water body (2 m wide, 1 m deep, and 10 m long) are separated by a buffer zone of 0 m (scenario 1) and 30 m (scenario 2) (Fig. 1). For scenario 1; when the buffer zone is 0 m, it means that the receiving water body is right at the field edge. At the beginning of the simulation (before spraying), the assumption was that 1,000 tadpoles were present in the receiving water body. Glyphosate was sprayed twice (on 14/3/2012 and 28/3/2012) before sowing of maize at a rate of 1,500 g a.i/ha [29] using conventional boom sprayer and that the field was later prepared under conventional tillage. Due to different tillage practices, the first application was to kill all standing grasses, followed by conventional tillage, and the second application was to kill any potential remaining grasses/weeds before sowing of maize seeds. Maize was thereafter sown on 04/4/2012. *C. insignifera*, a species native to Australia [13] was the selected non-target organisms. The model was run at a one day time step for 250 steps using weather data for Pathumthani province for the year 2012 [30] (Fig. 2). Model description, weather data, and other files such as *pesticide-scenarios-bufferzone.box* and *scenarios-*bufferzone.*box* files are provided in the dedicated input folder of the source code after installing the model (e.g. C:\Dev\UniSim2\input\PestTox\). This model is hosted permanently on GitHub on https://github.com/NielsHolst/UniSim2/releases. Alternatively, these files may be obtained from the corresponding author. Data used to simulate results are provided in Table A. Refer to Felix et al. [19] on how to install and run PestTox model. After the installation, refer to the Universal Simulator 2 explained book (http://www.ecolmod.org) to install and build the source code (developer version). Locate PestTox folder, load and run *pesticide-scenarios-bufferzone.box* and *scenarios-bufferzone.box* files.

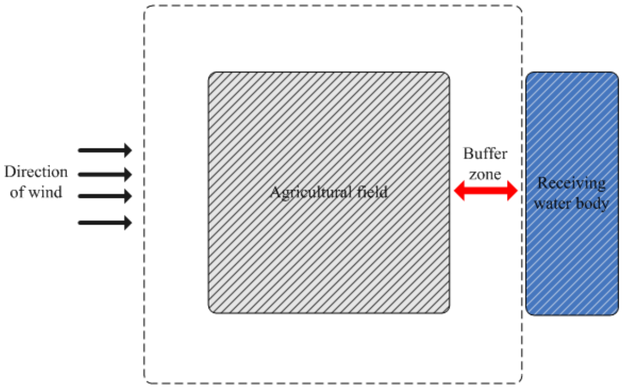

Fig. 1. Field layout (with buffer zone and the receiving water body).

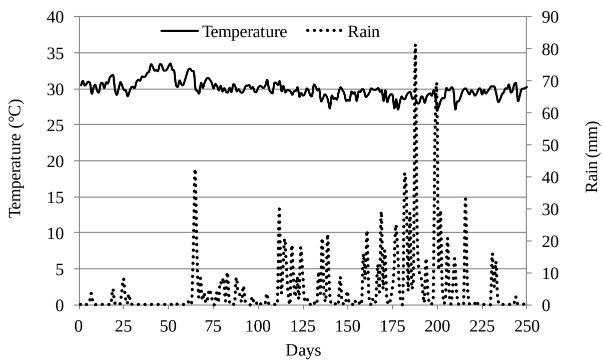

Fig. 2. Pathumthani Province weather data [30]. Note: Day 0 means before simulation starts, and day 1, 2, 3, ... 250 are simulation days starting from 13/03/2012.

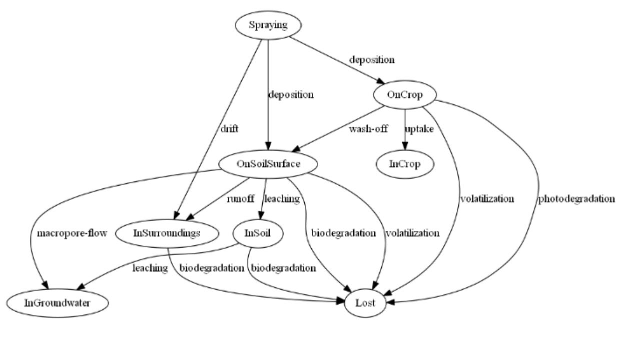

Fig. 3. Potential pesticides distribution after spraying.

The study assumed that fate and transport pathways in the environment would be as shown in Fig. 3. Two types of distributions are considered: primary and secondary. Primary distribution occurs at the time of spraying (application). This includes soil deposition, crop deposition, and spray drifts. Secondary distribution includes processes that remove glyphosate from the soil, crop surfaces, and surface waters. Macropore flow, runoff, leaching, biodegradation, and volatilization are the competing processes that remove glyphosate from the topsoil. Washoff, uptake, volatilization, and photodegradation are the competing processes that remove glyphosate from the crop surfaces while biodegradation removes glyphosate from the surface water. Also, the study assumed that the buffer zone is covered with vegetation; hence resistance is created against the runoff [31].

3. RESULTS AND DISCUSSION

3.1 Primary Distribution

Primary distribution occurs at the time of application. This distribution includes spray drifts, crop deposition, and soil deposition. Spray drift is the movement of pesticides/herbicides due to wind off the field edge to non target sites such as receiving water body (streams or ponds) or other crops that need no spraying at that time. This study assumed that spray drift is deposited in the receiving water body where frogs live (Fig. 1). Results show that when the field is surrounded by the buffer zone of 0 m and 30 m, spray drifts that reaches the receiving water body (non target site) was estimated at 281 g a.i/ha and 1.82×10^{-10} g a.i/ha respectively. For scenario 1, there is no buffer zone; therefore, all the spray drifts are assumed to be deposited on the receiving water body. Ideally, spray drifts decreases off field edge as the distance from the edge of the field increases. Also, soil deposition was estimated at 1,219 g a.i/ha and about 1,500 g a.i/ha when the field is surrounded by the buffer zone of 0 m and 30 m respectively. It should be noted that, in this study, crop deposition was zero because glyphosate was applied before the crop was sown. This is to say that, for other types of pesticides, if spraying is done on standing crops, then there would be some crop depositions.

3.2 Secondary Distribution

The study assumed that macropore flow, runoff, biodegradation, and volatilization are the main competing processing that remove glyphosate from the topsoil. Fig. 4 shows two highest peaks for each scenario. These two peaks correspond to the days of application. The first highest peak corresponds to the first application and the second highest peak corresponds to the second application. Results show that all glyphosate applied was removed completely by the competing processes within 25 days (Fig. 4) after the first application. This finding could mean that the glyphosate that is deposited on the topsoil could stay there for a short time before it is removed from the topsoil by the competing processes such as macropore flow, runoff, biodegradation, and volatilization. The finding suggests that glyphosate do not stay longer in the environment. However, other studies in the literature, have reported a half life of glyphosate ranging from 2-197 days depending on the conditions [32-35].

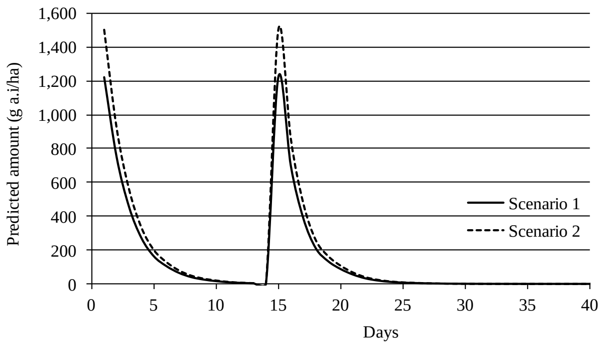

Fig. 4. Predicted amount of glyphosate on the topsoil.

Of all the competing processes, the study assumed that runoff is responsible for transferring glyphosate from the topsoil to the receiving water body that is located near the field when there is rainfall [36] (Fig. 1). Eventually, glyphosate contained in the runoff water is transferred into the receiving water body. Frogs living in this water body are therefore exposed to glyphosate in this way. Also, the study assumed that biodegradation is the main process that removes glyphosate in the water body. Furthermore, the study assumed that when the runoff water is higher than the receiving water body capacity, water in the receiving stream or pond is replaced by the incoming water i.e. here the study assumed that the current predicted glyphosate concentration in the water is equal to the glyphosate concentration of the incoming runoff water.

Results show that for scenario 1, the highest predicted glyphosate concentration in the receiving water body was estimated at 14 mg a.i/L while for scenario 2 was estimated at 7.0×10^{-5} mg a.i/L. For scenario 1, the predicted amount of glyphosate in the receiving water body is about 19% of the glyphosate applied (about 281 g a.i/ha – mostly from spray drifts). For scenario 2, the predicted amount of glyphosate is negligible. This means that when buffer zone is not used (scenario 1), the predicted glyphosate concentration in the receiving water body is very high compared to when the buffer zone of 30 m is used mainly due to spray drifts that could have otherwise be minimal if buffer zones were placed (Fig. 5). The finding is however in agreement with Dunn et al. [37] who reported that 10 m and 30 m buffer zones reduced 52% and 78% of the pesticides in runoff respectively. With this finding, it means that, for scenario 1, potential exposure of frogs to glyphosate in the receiving water body is higher than for scenario 2 (when buffer zone is used).

Results suggest that when buffer zone is not used (scenario 1), the mortality on eggs and tadpoles was very high especially within the first few days following the glyphosate application (Fig. 6). Mortality on eggs and tadpoles reached 93% at the time of application and then dropped to 86%, 75%, 59%, and 41% for the duration of four days following the application. After that, mortality was negligible. Around this time, the predicted concentration of glyphosate in the receiving water body was very low (Fig. 5). This is because at the time of application, glyphosate concentration was very high and then the concentration decreased with time. For scenario 2, mortalities of eggs and tadpoles were negligible (Fig. 7). For scenario 1 (when buffer zone is not used), high predicted glyphosate concentration (Fig. 5) caused high predicted glyphosate-induced mortality within the first few days following the application thus potentially killing all tadpoles that were present in the receiving water body.

Also, for scenario 2 (when buffer zone of 30 m was used), most tadpoles survive and grow to adults (Fig. 8): mainly due to low glyphosate concentrations predicted in the receiving water body (Fig. 5). Also, for scenario 2, Fig. 8 shows that around day 100 of the simulation, population of *C. insignifera* increases significantly. This is because of the growth/population modeling dynamics of the frog population as well as low glyphosate concentration predicted in the receiving water body (Fig. 5). This led to the predicted low glyphosate-induced mortality rates. Eventually, at around 100 day of the simulation (Fig. 8) eggs and tadpoles that were present in the receiving water body develop to froglets and adults. Furthermore, results of the sensitivity analysis suggest that tadpole could be the critical stage of frogs' development (Fig. 9 and Fig. 10). The development time (duration of tadpoles) were varied uniformly between 60-120 days using Hypercube Sampling (LHS) method [25]. Results suggest that the longer tadpoles took to develop to froglets, the population of eggs, tadpoles, froglets, and adults decreases (Fig. 9 and Fig. 10). This means that, when there is an exposure (i.e. if glyphosate concentrations are sufficiently high) and if the tadpoles took longer to develop, population of frogs could be at risk of declining.

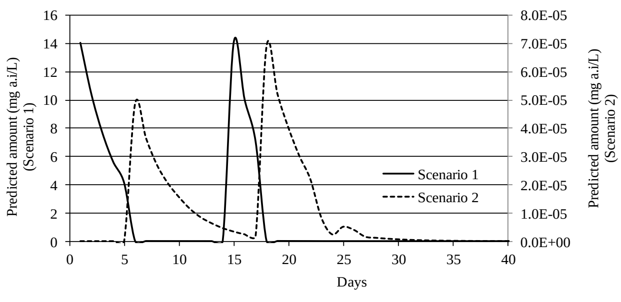

Fig. 5. Predicted amount of glyphosate in the receiving water body.

In connection to this study, most parts of the country (Thailand) have canals commonly known as *khlong*. These *khlong* are connected to small ponds, streams, lakes, and rivers; environments needed for the life cycle of amphibians. More often, these canals surround the agricultural fields in close proximity; therefore, there is a probability of glyphosate contamination into these canals by spray drifts, direct contamination, or through runoff. Since water bodies in small ponds, streams, rivers, and lakes have been polluted by various kinds of pesticides [15] due to spray drifts, direct contamination, runoff from the sprayed agricultural fields, etc., according to the findings of this study, there is a possibility that probably species of amphibians in glyphosate contaminated streams or ponds could be at risk of declining population. Therefore, it is important that farmers and other users of pesticides/herbicides to follow good agricultural practices when working with pesticides/herbicides to minimize potential damages to frogs and the environment at large. Lastly, this study contributes to the seventh Millennium Development Goal; to ensure environmental sustainability.

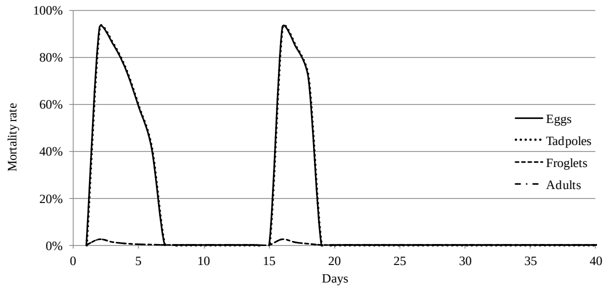

Fig. 6. Predicted glyphosate-induced mortality rates (scenario 1).

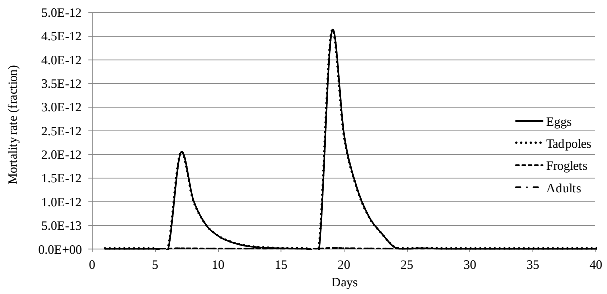

Fig. 7. Predicted glyphosate-induced mortality rates (scenario 2).

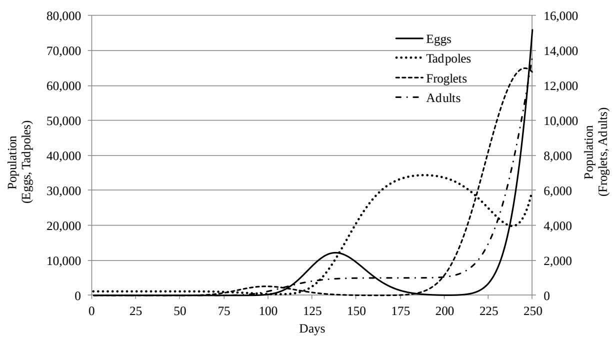

Fig. 8. Predicted population dynamics of frogs (scenario 2).

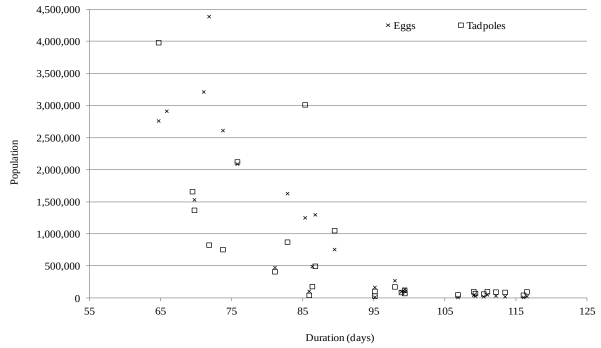

Fig. 9. Sensitivity of eggs and tadpoles population dynamics to changes in duration it takes for tadpoles to develop.

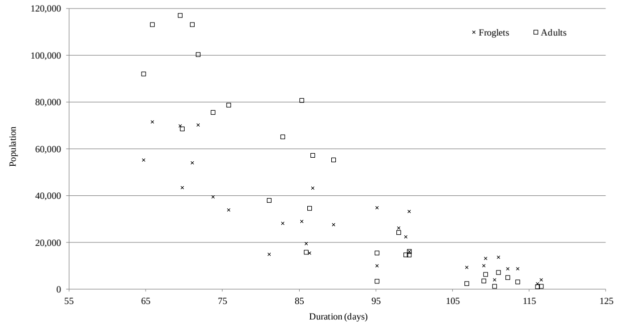

Fig. 10. Sensitivity of froglets and adults population dynamics to changes in duration it takes for tadpoles to develop.

4. CONCLUSION

In this study, the PestTox model was used to simulate fate, transport, and effects of glyphosate on population dynamics of frogs (*Crinia insignifera*) in an agricultural setting. Two scenarios were simulated i.e. the agricultural field and the receiving water body (stream or pond) were separated by buffer zones of 30 m and 0 m using the year 2012 weather conditions of Pathumthani province, Thailand. Results suggest that runoff from the agricultural field to the receiving water body increases if the field is not surrounded by a buffer zone of at least 30 m. Also, results suggest that spray drifts off-field edge to the receiving water body is higher if the field is not surrounded by a buffer zone of at least 30 m. This could lead to potential glyphosate contamination in the receiving water body which could potentially kill all tadpoles that are present in the receiving water body if the concentration of glyphosate is sufficiently high. Eventually, this could potentially affect the population dynamics of frogs present in that receiving water body. In conclusion, the study recommends that pesticide/herbicide users or farmers use recommended buffer zones around their fields to reduce the potential risk. This study has potential limitations. First, the study used secondary data from various sources. Second, numerous processes are based on analytical expressions/regressions from various pedoclimatical contexts. These may have influenced model estimates. However, the findings may be of interest to those involved in pesticide registration and monitoring.

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APPENDIX

Table A. Simulation data

Parameter	Value	Description	Reference
General data			
steps	250 days	Maximum simulation steps	User defined
initialDateTime	13/03/2012, 13/03/2013	First day of the simulation	User defined
timestep	1 day	Time step during simulation	User defined
timeunit	day	Time unit	User defined

Parameter	Value	Description	Reference
iterations	30 iterations	Number of iterations for sensitivity analysis	User defined
		Field data	
area	10,000 m^2	Area of the whole field	User defined
wbz	0 m, 30 m	Width of the buffer zone	User defined
x	0 m, 30 m	Distance off field edge	User defined
latitude	14.02° N	Latitude of the study area (Pathumthani Province, Thailand)	[27, 28]
S	0.18	Slope fraction of the field	[38]
T_f	1	Tillage factor	[21]
		Crop data	
sowingDate	04/04	Day of sowing (04/04/2012 and 04/04/2013)	User defined
seeds	1	Fraction of seeds sown	User defined
T0	10 °C	Threshold temperature for maize development. Varies from 5°C [39] to 10 °C [40, 41]	[40, 41]
f_i	leafDevelopment 0.25, tillering 0.50, stemElongation 0.70, and senescence 0.90	Crop deposition fractions for cereals	[42]
duration	leafDevelopment 87, tillering 282, stemElongation 657, and senescence 1,518	Degree day values for maize development (leaf development, tillering, stem elongation, and senescence)	[40]
leafType	Waxy	Cuticle characteristics similar to that of citrus leaves	[21]
a_1	18.1851%	Regression constants	[43]
a_2	0.5553%		
b_1	1.0701 m^{-1}		
b_2	0.0871 m^{-1}		
		Pesticide data	
applicationDate	14/03, 28/03	Day of application; 14/03 (app1), 28/03 (app2)	User defined
concentration	480 g a.i/L	Concentration of the active ingredient, based on application dose of 1,500 g a.i/ha [29]	[29]
rate	3.125 L/ha	Application rate, based on application dose of 1,500 g a.i/ha [29]	[29]
VP	2.45x10^{-5} Pa	Vapour pressure	[32]
T_{refVP}	25°C	Reference temperature at which vapour pressure was	[32]

Parameter	Value	Description	Reference
		measured	
MW	169.07 g/mol	Molar mass of the pesticide	[33, 44]
MV	96.61 cm^3/mol	Molecular volume of the pesticide (density 1.75 g/cm^3 [45]	User defined
T_{ref}	25°C	Reference temperature at which the half-life time of pesticide was determined in the soil	User defined
Q_{10}	2.58	Increase in biodegradation rate per 10 °C	[46]
kOH	79x10^{-12} cm^3/molecules/h	Overall OH• oxidation rate constant	[21]
pK_a	0.8	First acid dissociation constant of glyphosate	[47, 48]
K_{oc}	20,100 L/kg	Organic carbon-water partitioning coefficient	[33]
P_{sol}	11.5 g/L	Solubility of the pesticide at 25°C	[32]
DT_{50}	3 days	Soil half-life (parent material); varies from 3-174 days [32], 2-197 days [33, 34], 3-130 days [35] and 47 days [49]	[32-35]
DT_{50}	4.5 days	Half-life in water (parent material); varies from few days to 91 days [33], 4.5 days [50], 7-10 weeks in natural water [51]	[50]
		Weather data	
T_{air}	Read from the weather file	Average air temperature (°C)	[30]
P	Read from the weather file	Daily rainfall (mm)	[30]
$t_{p,event}$	3 h	Number of hours precipitation occurs on a rainy day	[52]
		Soil data	
f_{oc}	0.2	Fraction of organic carbon in the topsoil	[53]
ρ_b	1.365 kg/L	Soil bulk density (average, Thailand)	[54]
f_{sand}	0.1043	Fraction of sand in the soil	[29]
f_{silt}	0.3114	Fraction of silt in the soil	[29]
f_{clay}	0.5849	Fraction of clay in the soil	[29]
f_{om}	0.1	Fraction of organic matter in the topsoil	[55]
pH	5	pH of the soil; can range between 4-7 [29, 38, 56]	[29]

Parameter	Value	Description	Reference
f_a	0.25	Fraction of air in the soil	User defined
f_w	0.25	Fraction of water in the soil	User defined
f_s	0.5	Fraction of soil solids in the soil	User defined
		Frog data	
initial	1,000 tadpoles	Initial number of tadpoles	User defined
duration	14 days	Longevity of eggs	User defined
duration	90 days	Longevity of tadpoles. It takes about three to five months [57, 58]	[57, 58]
duration	21 days	Longevity of froglets	User defined
duration	365 days	Longevity of adults	User defined
duration	21 days	Days after entering adult stage that eggs will be laid	User defined
eggsPerFemale	70 eggs	Number of eggs laid per female frog, varies between 66-268 eggs	[57, 58]
LC_{50}	4.8 mg a.i/L	Egg stage (48 h); assumed based on LC_{50} for tadpole stage	User defined
LC_{50}	4.8 mg a.i/L	Tadpole stage (48 h); converted from 3.6 mg a.e/L	[59]
LC_{50}	69 mg a.i/L	Froglet stage (48 h); converted from 51.8 mg a.e/L	[59]
LC_{50}	65.9 mg a.i/L	Adult stage (48 h); converted from 49.4 mg a.e/L	[59]
sexRatio	0.5	Proportion of female frogs in the population	[60]
slope	2.341 volume/amount	Sigmoidal function	[61]