Supporting information for: Simulating the ~~BeePop+ model~~ effects of pesticides on honey bee (*Apis mellifera* L.) colonies with BeePop+

The purpose of this supporting information is to provide details on the pesticide component of the BeePop+ model. This information describes how the model estimates effects and exposures of simulated pesticides.

1. Accounting for pesticide exposures to individual honey bees

Exposure routes for bees differ based on application type. In the model, bees foraging in a field treated with a pesticide through foliar spray could potentially be exposed to the pesticide through direct spray (contact exposure) as well through consuming contaminated food. For honey bees foraging in fields treated with a pesticide through direct application to soil (*e.g.,* drip irrigation), or through seed treatments, direct spray onto bees is not expected. For these application methods, pesticide exposure through consumption of residues in nectar and pollen are expected to be the dominant routes. Foraging honey bees may also be exposed to pesticides via contact with dust from seed treatments or via consumption of water from surface water, puddles, dew droplet formation on leaves and guttation fluid; however, those routes will be implemented in a future version of the model. The parameters included in this paper are defined in **Table S1**.

Table S1. Parameter descriptions

Parameter symbol	Description	Units
AR	Single application rate.	lb a.i./A
$C_{grass(t)}$	Pesticide concentration in grass at time t. Used as a surrogate to estimate pesticide concentrations in pollen and nectar when chemical-specific empirical data for pollen and nectar are not available.	µg a.i./g
$C_{nectar(t)}$	Pesticide concentration in nectar at time t. Dependent upon application rate and method.	µg a.i./g
$C_{pollen(t)}$	Pesticide concentration in pollen at time t. Dependent upon application rate and method.	µg a.i./g
C_{soil}	Pesticide concentration in soil.	µg a.i./g
d	Soil depth.	cm
$D_{contact(t)}$	Pesticide dose received at time t by forager bees through direct spray.	µg a.i./bee
$D_{diet(t)}$	Pesticide dose received at time t through diet.	µg a.i./bee
$D_{nectar(t)}$	Pesticide dose received at time t through consumption of contaminated nectar.	µg a.i./bee
$D_{pollen(t)}$	Pesticide dose received at time t through consumption of contaminated pollen.	µg a.i./bee
f_{oc}	Fraction of organic carbon in soil	none
IR_{nectar}	Daily intake rate of nectar by individual bee. Varies by type of bee.	g/day
IR_{pollen}	Daily intake rate of pollen by individual bee. Varies by type of bee.	g/day
K_{oc}	Soil organic carbon-water partitioning coefficient	L/kg-oc

LD_{50}	Median lethal dose (*i.e.,* pesticide dose resulting in mortality to 50% of exposed bees).	µg a.i./bee
$T_{oral(larva)}$	Tolerance of individual honey bee larva receiving oral pesticide dose.	µg a.i./bee
$T_{oral(adult)}$	Tolerance of individual honey bee adult receiving oral pesticide dose.	µg a.i./bee
$T_{contact(adult)}$	Tolerance of individual honey bee adult receiving contact pesticide dose.	µg a.i./bee
TSCF	Transpiration stream concentration factor.	none
$t_{1/2(foliage)}$	Foliar dissipation half-life.	days
$t_{1/2(soil)}$	Aerobic soil metabolism half-life.	days
θ	Soil-water content by volume.	cm^3/cm^3
ρ	Soil bulk density.	$g\text{-}dw/cm^3$

Estimating contact exposure to individual bees

Contact exposure to pesticides was assessed for forager bees following foliar spray applications. Contact exposure was considered on the day of application (*i.e.,* on non-application days, $D_{contact(t)}=0$). For each bee a dose was randomly selected from a lognormal distribution where the mean was the application rate times the normalized mean measured residue on bees and an assumed standard deviation of 20% (which was varied in the sensitivity analyses). The mean value used, 0.89 µg a.i./bee per lb a.i./A, was based on *Phacelia* field trials (Koch and Weisser 1997) where residues on bees were quantified directly after being sprayed.

For in-hive bees, it was assumed that contact exposure was negligible relative to the oral exposure they would receive from consuming contaminated nectar and pollen collected from treated fields. For soil applications and seed treatments, contact exposure is not assessed.

Estimating dietary exposure to individual bees

As depicted in **Equation 1**, dietary doses are calculated by multiplying food intake rates (IRpollen and IRnectar) by concentrations in pollen and nectar. Methods for estimating pesticide concentrations in pollen and nectar ($C_{pollen(t)}$ and $C_{nectar(t)}$) differ by application method, with different approaches for foliar spray, soil applications and seed treatments. Also described below are the food intake rates for different bees.

Equation 1. $D_{diet(t)}=C_{pollen(t)}*IR_{pollen}+C_{nectar(t)}*IR_{nectar}$

Table S2. Nectar and pollen consumption rates for individual bees by different castes and ages (USEPA 2012)**.**

Life stage	Caste or task in hive	Average age (in days)	Nectar (IRnectar; mg/day)	Pollen (IRpollen; mg/day)
Larval	Worker	1	0	0
		2	0	0
		3	0	0
		4	60	1.8
		5	120	3.6

	Drone	6+	130	3.6
	Queen	1	0	0
		2	0	0
		3	0	0
		4+	0	0
Adult	Worker (cell cleaning and capping)	0-10	60	6.65
	Worker (brood and queen tending, nurse bees)	6 to 17	140	9.6
	Worker (comb building, cleaning and food handling)	11 to 18	60	1.7
	Worker (foraging for pollen)	>18	43.5	0.041
	Worker (foraging for nectar)	>18	292	0.041
	Drone	>10	235	0.0002
	Queen (laying 1500 eggs/day)	Entire lifestage	0	0

Estimating pesticide concentrations for foliar sprays

Pesticide concentrations on food items are calculated by considering initial residue concentrations on food items at the time of application and the effect of the dissipation of the pesticide, as defined by the dissipation half-life. The initial residue on grass ($C_{grass(t=0)}$) was assumed to follow a lognormal distribution, with a mean of 84.8 µg a.i./g (normalized to 1 lb a.i./A) and a standard deviation of 60.3 (Fletcher *et al.* 1994). The initial residue value was multiplied by the application rate of the pesticide to derive the pesticide concentration in pollen and nectar at time 0 (*i.e.,* $C_{pollen(t=0)}$ and $C_{nectar(t=0)}$). In modeling exposures over multiple days, it was necessary to account for dissipation of pesticide residues over time. Pesticide concentrations in pollen and nectar at different times were calculated using **Equations 2 and 3**. Foliar dissipation half-life values ($t_{1/2(foliage)}$) are obtained from the literature or from registrant submitted studies. A default value of 35 days is generally used when no pesticide-specific data are available (Willis and McDowell 1987).

Equation 2. $C_{pollen(t)}=C_{nectar(t)}==C_{grass(t)}=C_{grass(t=0)}*e^{-kt}$

Equation 3. $k=ln(0.5)/t_{1/2}$

Estimating pesticide concentrations for soil applications

Pesticide concentrations in pollen and nectar of crops growing in treated soil can be estimated using **Equation 4**, based on a model published by Briggs et al. (1982 and 1983) and modified by Ryan et al. (1988). This equation depends upon the K_{ow} and K_{oc} of a chemical as well as basic soil properties. For the fraction of organic carbon in soil (f_{oc}), a default value of 0.01 is used. A value of 1.5 g-dw/cm^3 is selected to represent bulk density (ρ). Soil water content (θ) is set to 0.2 cm^3/cm^3 (all these parameters were

varied in the sensitivity analyses). Note that if K_{oc} is not available or appropriate for a chemical, the K_d can be used by replacing the following portion of **Equation 4**: K_{oc} * f_{oc}. The Transpiration Stream Concentration Factor (TSCF) was calculated based on the Log K_{ow} of the assessed pesticide (**Equation 5**).

Equation 4. $C_{pollen(t)}=C_{nectar(t)}=C_{soil(t)}*[10^{(0.95*LogKow-2.05)}+0.82]*TSCF*[\rho/(\vartheta+\rho*Koc*foc)]$

Equation 5. $TSCF = -0.0648 * (LogKow)^2 * 0.241 * LogKow + 0.5822$

As depicted in **Equation 6**, the pesticide concentration in soil at time t can be estimated by dividing the application rate (which was converted to kg a.i./ha by multiplying by 1.12) by the soil depth (d, in cm). A default, depth of 15 cm (equivalent to 6 inches) was used. Degradation of the pesticide in soil was also accounted for using **Equation 4**, where the half-life value was the chemical-specific aerobic soil metabolism half-life ($t_{1/2(soil)}$, in days). This approach assumes no loss of the pesticide from soil via leaching, runoff or volatilization. These assumptions could be reduced by using $C_{soil(t)}$ values that are estimated by a runoff model.

Equation 6. $C_{soil(t)}=[(AR*1.12)/d]*e^{-kt}$

Estimating pesticide concentrations for seed treatments

For seed treatments, the estimated pesticide concentration in pollen and nectar of treated crops is 1 µg a.i./g. This is based on EPPO's (European Plant Protection Organization) screening value (EPPO 2010). If the seed concentration is constant regardless of seed treatment then this is an insensitive parameter.

Input of empirical residues in pollen and in nectar

If empirically based data are available to quantify concentrations of a pesticide of interest in pollen and in nectar, the values can be input into the model directly to represent $C_{pollen(t)}$ and $C_{nectar(t)}$ on a given simulation day.

2. Estimating pollen and nectar loads (model parameters) and proportion of foragers

Since the colony model assigns the same nectar and pollen loads to all individual bees, mean estimates of pollen and nectar loads across foragers are needed as input parameters. Values vary in the literature. For pollen, mean loads range 15-35 mg. For nectar, mean loads range 22-51 mg/bee (**Table S3**). The central estimates of the available data, *i.e.*, 26 mg pollen/bee and 45 mg nectar/bee (Winston 1987) are used to represent the default parameters.

Table S3. Mean pollen and nectar loads per bee in the literature.

Resource	Value (mg/bee)	Comments	Source
Pollen	15	Estimated from Figure 2	Eckert et al 1994
	26	Author reported that pollen load is 20% of body weight. Value calculated assuming body weight of 128 mg/bee.	Winston 1987

	31	Authors reported 24% of body weight. Value calculated assuming body weight of 128 mg/bee. Mean body weight of test bees was 73 mg.	Feuerbacher et al. 2003
	35	Authors reported 27% of body weight. Value calculated assuming body weight of 128 mg/bee. Mean body weight of test bees was 73 mg.	Feuerbacher et al. 2003
Nectar	22	Authors reported 19.2 µL /bee for a large colony. Value was converted from volume to mass using density of sucrose solution with 30% sugar (*i.e.*, 1.127 g/cm^3).	Eckert et al 1994
	41	Authors reported 32% of body weight. Value calculated assuming body weight of 128 mg/bee. Mean body weight of test bees was 73 mg.	Feuerbacher et al. 2003
	45	Author reported that nectar load is 35% of body weight. Value calculated assuming body weight of 128 mg/bee.	Winston 1987
	51	Authors reported 40% of body weight. Value calculated assuming body weight of 128 mg/bee. Mean body weight of test bees was 73 mg.	Feuerbacher et al. 2003

The colony's import and consumption of pollen and nectar resources are simulated. In this simulation, the amount of incoming resources and the amount consumed by the colony each day is calculated. If more resources are brought in than needed for consumption, the extra amount is stored in the colony. If the amount needed exceeds the amount brought in, the deficit is made up by consuming stored resources. If the amount needed exceeds the amount available either from fresh forage or in stores, the colony dies. Using this approach, it appears the colony resource store quantities are highly sensitive to initial conditions and parameters such as number of foraging trips per day. A change of +/- 5% in some of these parameters can make the difference between a colony that dies and one that has resources continuing to grow year over year. In actual honeybee colonies, there are some mechanisms that influence the number of bees which are recruited to actually forage for resources. The hypothesis is that if we were able to implement such a mechanism, the sensitivity to initial conditions would decrease and the colony simulation could respond to current states in ways that are similar to actual honeybee colonies. Because only a portion of eligible foragers actually forage at a given time, the model user has the ability to simulate the proportion of active foragers. Model evaluations have indicated that approximately 30% active foragers is an appropriate parameter estimate to allow for colony survival and strength representative of empirical data (unexposed colonies).

3. Method for translating pesticide toxicity data into mortality of bees

To calculate the percent mortality to adults following field pollen, nectar and contact exposure as well as larvae to -in-hive dietary exposure, the model uses three separate dose-response relationships that are based on model inputs (*i.e.,* LD_{50} and slope). The percent reduction due to mortality is applied to the proportion of groups of individuals that do not have a tolerance threshold greater than the calculated dose. Tolerance thresholds are pre-determined upon initializing the model or when births occur by dividing each cohort into equal numbers of bees and assigning each a set tolerance threshold. Note that

the percent mortality predicted for different cohorts are different depending upon the age of exposure. For example, only foraging bees experience contact exposures. Also, hive bees and foraging bees receive different dietary exposures of pesticides. Therefore, input parameters include adult oral LD_{50} and slope; adult contact LD_{50} and slope; and larval oral LD_{50} and slope. LD_{50} values and associated slopes for adults and larvae are obtained from standard acute toxicity studies with honey bees (OECD test guidelines 213, 214 and 237).

The proportion of honeybees (p-hat) that do not survive a given exposure concentration (EEC) was calculated using probit analysis, a specialized type of regression for binomial outcomes that accounts for the sigmoidal nature of the survival curve. In this case, for each combination of pesticide exposure and honeybee age class, the outcome is survival of the honeybee or not. **Equation 7** was derived from **Equation 8.** The z term in this equation was based on the appropriate EEC, LD_{50} and slope to estimate the percent mortality for a cohort. For larvae, dietary EECs were recalculated for each day of the simulation. To assess mortality to larval cohorts, EECs were used in **Equation 7** with the larval oral LD_{50} and slope. For all adults, dietary-based EECs were used in combination with the adult oral LD_{50} and slope to estimate mortality to adult cohorts. Note that in-hive bees have different dietary exposures than forager bees due to differences in exposure concentrations and feeding rates (that can be attributed to different energetic requirements of their respective tasks). For forager bees, estimated exposures due to contact from foliar applications of pesticides were entered into **Equation 7** along with the contact-based LD_{50} and slope.

Equation 7. $z = slope * [log(EEC)-log(LD_{50})]$

Equation 8. $p\text{-}hat=[1/(2*pi)^{0.5}]*e^{-(z^2)/2}$

Equation 9. $LD_x=10^{(LogLD50+z/slope)}$

Where:
p-hat = proportion of honeybee mortality associated with an EEC
z = standard normal deviate, EEC = estimated environmental concentration (µg a.i./bee)
LD_{50} = median lethal dose (µg a.i./bee)
LD_x = lethal dose resulting in x% mortality to tested individuals (µg a.i./bee)
slope = describes the steepness of the dose-response curve used to derive the LD_{50}

Sublethal effects may also be considered by the model user. The model includes parameters that represent adult life span and foraging (*e.g.,* number of foraging trips). If available toxicity data suggest that a pesticide may have sublethal effects on these endpoints, the model user may choose to simulate these effects. This can be done by decreasing the adult life span or number of trips per forager. The model user can also decrease the percentage of possible foragers that are active.