

# SolBeePop<sub>ecotox</sub>

## Population model for solitary bees in agricultural landscapes with exposures and effects of pesticides

### TRACE documentation

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The documentation of the model SolBeePop<sub>ecotox</sub> presented here follows the TRACE (transparent and comprehensive ecological model) documentation (Schmolke et al. 2010; Grimm et al. 2014). The model description (Chapter 2) is organized according to the ODD (overview, design, and details) protocol (Grimm et al. 2006; Grimm et al. 2010; Grimm et al. 2020).

The model code (SolBeePop\_ecotox.nlogo), files referred to in this documentation as well as scripts used for model simulations and analysis are available on GitHub:

<https://github.com/SolBeePop/SolBeePop>

The TRACE documentation has been extended to include the exposure and effect extension of the original model (SolBeePop). Extensions applied for SolBeePop<sub>ecotox</sub> are presented in green font.

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# 1. CONCEPTUAL MODEL

## 1.1. Model objectives

Solitary bees summarize all bee species that share a non-social lifestyle, with each female producing and provisioning her own offspring. Solitary species make up the vast majority of described species (>75%) across bee families (Danforth et al. 2019). They share life history traits related to their solitary lifestyle which include the mass-provisioning of each offspring in a brood cell separating it from its siblings, and extended periods of dormancy of in-nest life stages. However, their traits related to nesting and foraging vary widely. Recently, solitary bees have moved increasingly into the focus of conservation of biodiversity in agricultural landscapes due to their importance for crop pollination provided by wild as well as managed populations. In the context of ecological risk assessments of pesticides, their interactions with crops imply a potential for the exposure to pesticides. We developed a population model for solitary bees. The objectives of the model include the following points:

- a) The model should capture a variety of solitary bee species, represented by the model species identified by Sgolastra et al. (2019) and Schmolke et al. (2021). Different bee species should be represented by varying inputs that define the numerical or categorical values of a set of traits previously identified (Schmolke et al. 2021).
- b) The representation of the full life cycle of solitary bees. Temporal aspects of co-occurrences of bee life cycle and exposures should be considered for later addition.
- c) Interactions with the environment that correspond to different exposure routes identified as important for solitary bees, including exposure via pollen and nectar as well as nesting materials.
- d) Capture exposure time series from the different exposure routes with the possibility to represent different pesticides (compounds).
- e) Effect representations should be possible to parameterize using (standard) laboratory-based toxicity studies.
- f) Provide the possibility to test mitigation scenarios, assess effects from different exposure routes separately and in combination and analyze interaction between traits, exposures and effects.
- g) Simulation of wild populations, populations managed for pollination and specific conditions of studies conducted in the context of higher-tier pesticide risk assessments.

Processes and details represented in the model should be general enough to represent a variety of solitary bee species and agricultural landscapes. Traits identified as important in the context of exposure and effects should be represented explicitly. For other aspects of bee ecology, assumptions should be applicable to all represented solitary bee species. Data on bee life history and ecology is derived from the scientific literature (see Appendix A). The conceptual model addresses the representation of solitary bee populations based on their ecological traits. For the extension of SolBeePop<sub>ecotox</sub>, exposures and effects are represented explicitly.

The conceptual model development following Pop-GUIDE (Raimondo et al. 2021) is described in the following. The conceptual diagrams shown throughout the step-wise development indicate the aspects included in the model. The conceptual model diagram presented in Figure 1 captures the final concept.

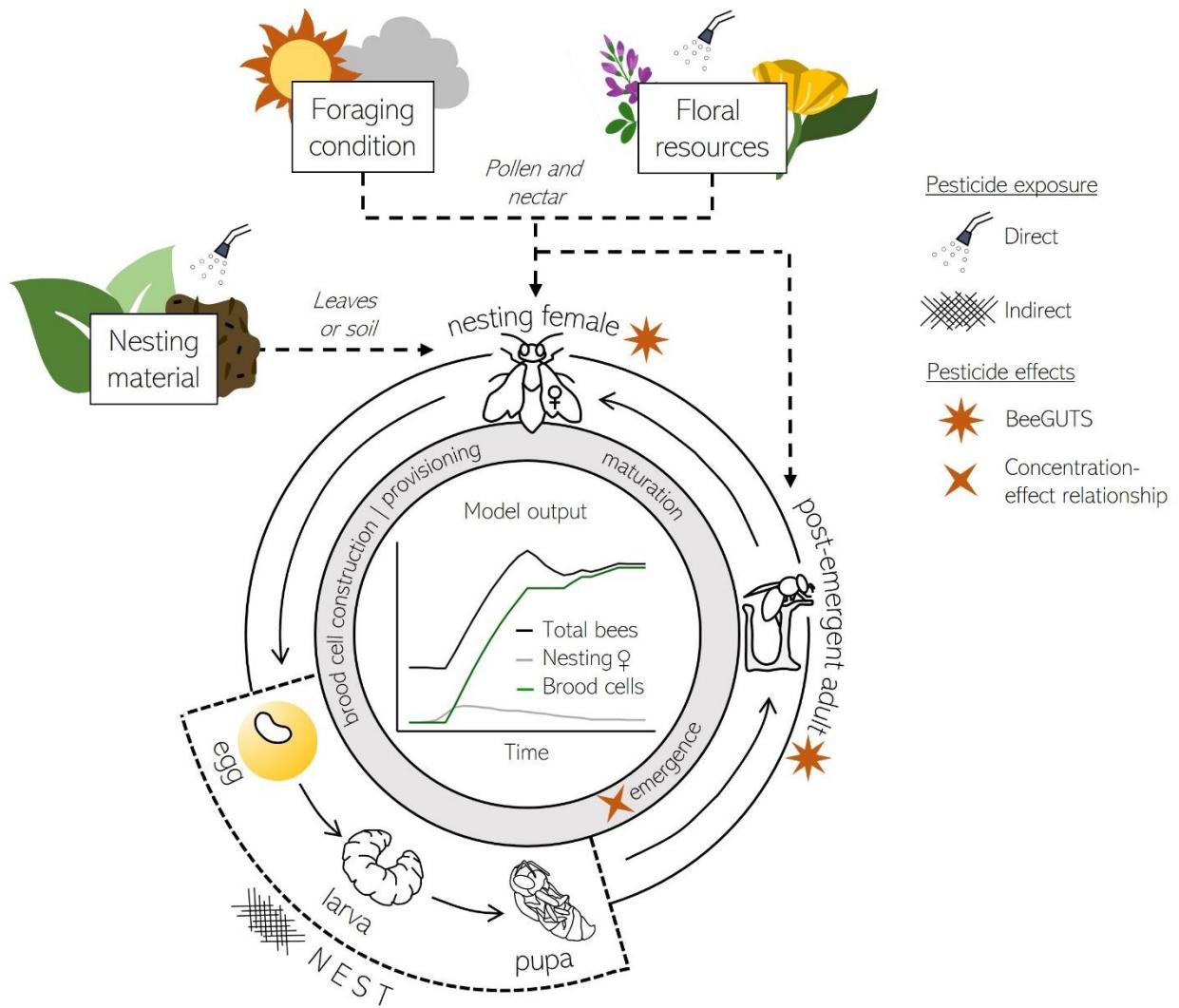


Figure 1. Graphical representation of the completed conceptual model with the representation of exposures and effects for SolBeePop<sub>ecotox</sub>.

## 1.2. Conceptual model for solitary bees

The conceptual model for solitary bee populations is developed by following Pop-GUIDE (Raimondo et al. 2021). The step-wise development explicitly states the decisions and assumptions that inform the model. The model is developed to represent the following model bee species: four species of *Osmia* spp. (*O. lignaria*, *O. cornifrons*, *O. cornuta*, *O. bicornis*), *Megachile rotundata*, *Nomia melanderi*, and *Eucera (Peponapis) pruinosa*. The model solitary bee species were chosen following the identification of potential surrogate species for pesticide risk assessments of solitary bees and included in a trait-based vulnerability analysis (Sgolastra et al. 2019; Schmolke et al. 2021). The species are important for crop pollination and have been investigated in empirical studies from which data can be used for model development and parameterization. The model species represent different nesting ecologies, and thus, may be considered as surrogate species for a wider range of species with comparable life history and nesting characteristics (traits). The representation of different nesting strategies is important in the context of pesticide risk assessment because they may be related to varying routes of exposure to pesticides. Like most solitary bees, adult females of the model species collect food provisions for each egg, and seal them in individual brood cells (Michener 2007; Danforth et al. 2019). All four species of *Osmia* nest above ground in existing cavities. The model *Osmia* species use soil or mud to cap each brood cell in sequence (Bosch et al. 2001). *M. rotundata* also uses above-ground existing cavities, but lines them with leaf pieces (Tasei and Masure 1978; Kemp and Bosch 2000; Gemmill-Herren and Strohm 2014). *N. melanderi* is a ground-nesting species, a trait it has in common with the majority of solitary bee species (Michener 2007; Danforth et al. 2019). Ground-nesting bees are hard to rear commercially. *N. melanderi* was chosen as model species for ground-nesting solitary bees because nesting aggregations are managed by farmers for alfalfa pollination in the Western USA (Sgolastra et al. 2019). The squash bee species, *E. pruinosa*, extends the representation of solitary ground-nesting bees (Schmolke et al. 2021). Squash bees are important pollinators of curcubit crops and are commonly found nesting close to pumpkin fields (Hurd et al. 1974; Julier and Roulston 2009), with potential of exposures to pesticides (Willis Chan et al. 2019a). The data available for the model development by species are summarized in species-specific data tables in Appendix A.

The life cycle representation corresponds to the simplest representation of solitary bees in the population model. In the following decision steps, the conceptual model is further developed, making assumptions in the model explicit following Pop-GUIDE (Raimondo et al. 2021). The questions and answers presented in the tables generally address population models developed in the context of chemical risk assessment and are not specifically tailored to bees. These decision steps expand on the decision steps for the development of conceptual population models for plants (Schmolke et al. 2017). The corresponding text paragraphs provide the explanation for the decisions taken, focusing specifically on the data availability and objectives of the conceptual model for solitary bees. Detailed processes, parameters and inputs included in the model will be defined in a separate model description. The model description will correspond to the implemented model. The conceptual model presented here focuses on the decision processes involved in the development of the model concept, emphasizing the assumptions taken during model development.

### 1.2.1. Life cycle representation

Solitary bees go through a distinct life cycle that is completed in a single year (univoltine species) or less than a year (multivoltine species). In a few species, some individuals may remain dormant for more than a year, resulting in the completion of the life cycle in multiple years (Michener 2007), a special case not represented in our model. After emergence from the nest, adult bees mate and feed on floral resources.

Females build nests and collect food for their offspring whereby each egg is deposited in a separate brood cell with a food provision. Larvae consume the food provision, and developing bees remain in the brood cell until emergence as adults. In univoltine species and in overwintering individuals of multivoltine species, usually either the bees overwinter in their last (non-feeding) larval stage (pre-pupa) or as adults after completing metamorphosis. Non-overwintering offspring in multivoltine species go through the development without an extended dormant stage, and emerge as adults from the nest during the same year as they were laid as eggs (Michener 2007; Bosch et al. 2008; Sgolastra et al. 2019). The life cycle can thus be represented by four life stages: adult (active), egg (inactive), larva (inactive, feeding), pre-pupa to pre-emergent adult (inactive) (Figure 2).

Males do not participate in nest building or provisioning of the offspring and have a short post-emergent life span in many species (Danforth et al. 2019). In the model, we assume that enough males are present in a population for successful mating. Post-emergent males are assumed not to contribute to the population dynamics, and are assumed to die shortly after emergence.

During offspring production by the nesting females, a particularity of the biology of Hymenoptera including all bees is considered in the model: sex is determined through fertilization whereby fertilized eggs will develop into females and unfertilized eggs into males. Whether an egg is fertilized or not is controlled by the egg laying bee. Males are smaller in many solitary bees, including our model species except *N. melanderi*, and require smaller food provisions. Accordingly, the sex ratio of a bee's offspring is not constant. These characteristics of bee biology will be further considered in the following decision steps.

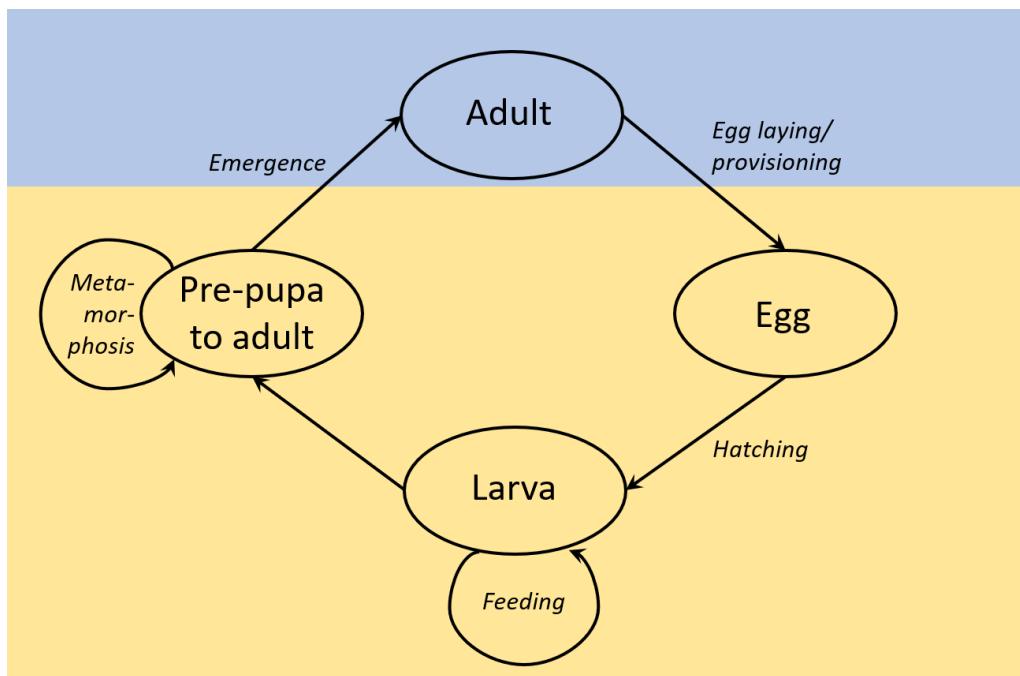


Figure 2. Generalized life cycle representation of solitary bees for the model. The stages from pre-pupa (5<sup>th</sup> larval instar after the larva ceased feeding) to adult prior to emergence from the nest are combined. Overwintering (dormancy) may occur either in pre-pupal or adult stage, dependent on species. In generations of bivoltine species that emerge the same year that they were laid as egg, the life cycle is completed without extended dormant phases in the development.

## 1.2.2. Life History Characteristics

### *Growth and development*

	Question	Yes	No
1	Is there sufficient information to represent growth continuously?	2	No additions to model concept
2	Is there sufficient information to represent growth physiologically?	3	Simple growth model maybe included (Von Bertalanffy, Gompertz, Logistic, other)
3	Is there sufficient information to represent the maturation process and fecundity through physiology?	Physiologically-based (DEB) including maturation and fecundity (next decision step can be skipped)	Wisconsin FB or similar

Growth of individuals is not represented explicitly in the model. The size (weight) of a pre-pupal bee and correspondingly its emergence weight is mostly determined by the provisioning size (Bosch et al. 2001; Bosch and Vicens 2006; Sedivy et al. 2011). Accordingly, adult size can be predicted from the provisioning size without explicit representation of larval growth. No growth occurs in adult bees.

Female pre-pupal or adult weight have been linked to emergence rate, i.e., survival to maturity (Bosch and Kemp 2004). However, mature female body weight is not consistently linked to fecundity (Bosch and Vicens 2006). Accordingly, variation in individual bee sizes (and growth) is not be represented explicitly. However, survival rates to emergence may be directly linked to provision size (see Section 3.4: Habitat characterization).

### *Maturation and reproduction*

	Question	Yes	No
1	Is there sufficient information to represent maturation dependent on body size/ mass/ energy reserves?	Maturation dependent on body size / mass/ energy reserves	Maturation dependent on age (constant or distribution)
2	Is there sufficient information to represent fecundity dependent on body size/ mass/ energy reserves or specific age?	Fecundity dependent on body-size/ mass/ energy reserves or age	Fecundity independent of size/ mass/ energy reserves or age (constant or distribution)

Solitary bees of the same species go through all immature life stages within the nest (Figure 2). Female bees start mating and nesting shortly after emergence. In univoltine species, emergence of adults is often synchronized, i.e., adults emerge within a few days in a given population, generally triggered by temperature (Mathewson 1968; Bosch and Kemp 2000; Pitts-Singer and Cane 2011; Schenk et al. 2018). Males often emerge a few days prior to females. In multivoltine species, emergence of mature adults in non-dormant generations occurs once the development is completed. Accordingly, the timing of

maturation and the onset of reproduction is not dependent on body size, mass or energy reserves of the individual, but dependent on external triggers once metamorphosis is complete (Section 1.2.4).

Female fecundity has not been reliably linked to body size (Bosch and Vicens 2006; Seidelmann et al. 2010). Rather, fecundity (total nests produced per female) is mainly determined by mature adult life span. In addition, the resource availability, particularly the availability of pollen and nectar influences the rate of nest provisioning, and accordingly, the total eggs produced per female during her life time (Goodell 2003). In species that build strings of brood cells in cavities, the first batch of brood cells contain female eggs, and the last batch male eggs, resulting in the earlier emergence of males (Hurd et al. 1974; Bosch et al. 2001; Pitts-Singer and Cane 2011). The ratio of female to male eggs produced may shift with the female bee's age: early in the season, more females are produced. Towards the end of the season (and the life-time of the female), she produces more male eggs (Torchio and Tepedino 1980; Bosch and Vicens 2005; Giejdasz et al. 2016). The shift in offspring sex ratio with increasing female age occurs in parallel with declining provisioning activity and provisioning sizes of female offspring. The shift related to female age has been mainly attributed to reduced foraging capacity (Tepedino and Torchio 1982a; Bosch and Vicens 2005).

In the model, we consider the decline in female eggs produced dependent on female age (Figure 3). The availability of floral resources impacts the rate of egg production (see Habitat Characterization).

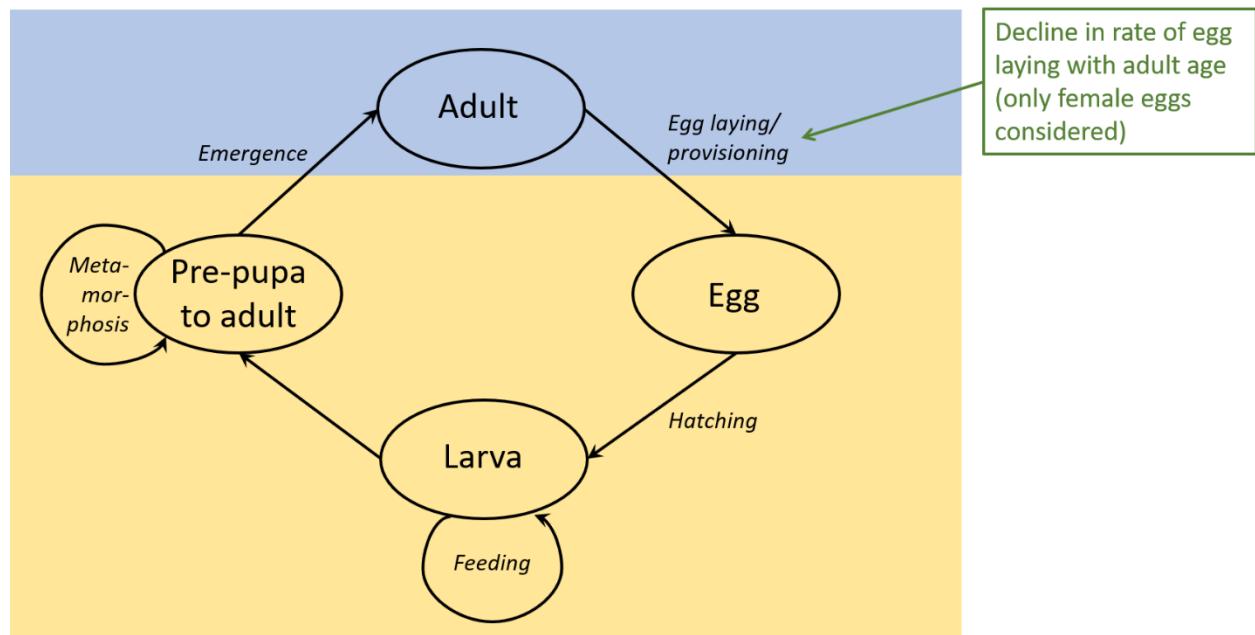


Figure 3. Rate of egg laying is declining with the age of the nesting female.

### 1.2.3. Population and Spatial Factors

#### *Population Status*

	Question	Yes	No
	Are data available to demonstrate that populations exhibit high variability between years, i.e. do the population dynamics considerably deviate from stability?	Include representative environmental variability in the model	Variation can be represented by demographic factors alone.
	Is the estimated species' overall abundance or population size very small?	Because small populations are more prone to stochastic extinctions, addition of stochasticity in life history representation (e.g., demographic rates) is important	Variation can be represented by demographic factors alone.

The population status of most unmanaged solitary bee populations is not available (Burkle et al. 2013; Goulson et al. 2015). Declines in bee diversity, abundance or pollination service have been shown in a few regionally-specific studies (Biesmeijer et al. 2006; Burkle et al. 2013; Carvalheiro et al. 2013). Population abundances may vary between years (Bischoff 2003; Franzén and Nilsson 2013), but available studies are limited to very few species, and do not reveal clear relationships with environmental factors. For the model, we assume that population sizes are large enough to exclude stochastic local extinction events.

#### *Density Dependence*

	Question	Yes	No
1	Do populations experience documented resource or space limitation?	2 *	5
2	Are the factors driving density dependence (e.g., spawning sites, food limitations) known?	3	Apply ceiling type density dependence
3	Are life stages affected differently by density effects?	4	Represent density dependence as mortality function (e.g., Ricker) of population abundance or biomass across all life stages

	<b>Question</b>	<b>Yes</b>	<b>No</b>
4	Does density dependence affect growth or fecundity?	Represent density dependence as a continuous function of affected endpoint relative to total or life-stage-specific abundance or biomass	Represent density dependence as mortality function (e.g., Ricker) of population abundance on affected life stage(s)
5	Are populations reported to experience Allee effects due to low densities?	Include Allee effect, e.g., as function linking fecundity to adult abundance	Density dependence does not need to be considered

\* Density dependence included in the model as optional process.

Density dependence refers to the causal relationship between population size and its growth rate, i.e., the size of the population itself causes the growth rate to change (Begon and Townsend 2021). Density-dependence results in the ‘regulation’ of a population through changes in birth, death or reproductive rates in the population with changes in density. Through processes such as intraspecific competition for a resource, density-dependent predation, parasitism or disease rates, density dependence can result in changes in growth rate in both directions (increase or decrease). Negative density dependence refers to processes resulting in the decrease in population growth rate with its size. In the following, possible processes that can lead to negative density dependence in solitary bees are addressed.

For solitary bees, negative density dependence has been discussed in the context of affecting the reproductive outputs of nesting females in a population due to intra- or inter-specific competition for food or nesting resources (Pitts-Singer and James 2008; Steffan-Dewenter and Schiele 2008; Pitts-Singer and Bosch 2010; Dainese et al. 2018) or parasitism rate in the brood (Wcislo 1984; Rosenheim 1990; Farzan 2018; Groulx and Forrest 2018).

#### ***Density-dependent brood parasitism rates***

Brood parasitism has been investigated as potentially related to nesting density in multiple solitary bee species. The reduction of brood parasitism has been suggested as a possible advantage of gregarious nesting (Wcislo 1984; Farzan 2018). However, the relationship between nest density (or size of artificial nest blocks) and parasitism rate across studies is inconclusive (Rosenheim 1990; Steffan-Dewenter and Schiele 2008), including findings of no correlation between nesting density and parasitism rate (Farzan 2018), decrease (Wcislo 1984), and increase in parasitism rate with increasing nesting density (Dainese et al. 2018; Groulx and Forrest 2018). While these studies cannot exclude that parasitism rates may be dependent on nesting densities of bee populations, no conclusion can be drawn that apply across populations of a species or across species (Danforth et al. 2019).

#### ***Competition for floral resources***

Pollen and nectar may become limited resources in cases of high numbers of foraging bees frequenting the same resource patch (e.g., a flowering crop field), resulting in nesting females being unable to provide adequate provisions for their brood (Pitts-Singer and James 2008). This situation can be created in experimental settings or in managed bee populations if high numbers of bees are released for crop pollination. Pitts-Singer and Bosch (2010) noted that in the US, a common practice (at the time) was to

release considerably higher numbers of *Megachile rotundata* for the purpose of alfalfa pollination than the recommended number per area (recommendation: release of 75,000-99,000 bees per hectare; current practice in the US: release of 100,000-150,000 bees/ha). Viable female brood produced by the released *M. rotundata* was generally considerably below replacement. Lower release rates in Canada (<75,000 bees/ha) correlated with the production of excess bees. Based on the hypothesis that the difference in reproductive rates were caused by intra-specific competition for floral resources, Pitts-Singer and Bosch (2010) conducted experiments in enclosures installed above flowering alfalfa fields in Utah, USA. Numbers of *M. rotundata* released per area of the enclosure were varied over a range of about one magnitude. The floral resource availability could not be quantified because the number of flowers varied considerably between enclosures of the same treatment within and between years. In the study, a negative correlation between brood cell production per released female and number of released bees could be established.

Peterson and Roitberg (2006) also conducted a study with *M. rotundata* in enclosures installed over flowering alfalfa fields in Alberta, Canada. In their study, the number of released bees was identical across enclosures but the number of alfalfa plants in the enclosures were reduced for the medium and low resource treatments. The average number of brood cells was significantly correlated with the treatment whereby the highest numbers of brood cells were produced in the highest floral resource treatment (no alfalfa plants removed from the enclosure). Brood cells producing viable offspring ranged between 70-74% independent of treatment. The offspring sex ratio was not correlated with treatment. In addition to increased numbers of total brood cells, the size of female offspring increased significantly with floral resource availability. The authors assumed that the floral resources were limited even in the highest resource treatment. The results were discussed in the context of impacts of floral resource limitation on reproductive output. The role of intra-specific competition (or population density) was not explicitly addressed in the article. Similar relationships were also found in enclosure experiments conducted with *Osmia pumila* (Goodell 2003) and *M. apicalis* (Kim 1999)

The impact of floral resource availability in field populations has also been indicated. For instance, (Dainese et al. 2018) found a significant relationship between floral resource availability in the landscape and total number of brood cells (across species) in trap nests. However, the effect size varied between years and season. In most landscape settings, floral resources may be limited spatially (landscape composition) and temporally (flowering phenology). Multiple pollinator species usually forage on the same flowering plant species (Wojcik et al. 2018; Danforth et al. 2019; Yourstone et al. 2021).

### **Competition for nest sites**

Suitable nesting sites can be seen as a limited resource in solitary bee populations as well. For instance, bees nesting in existing cavities may be limited in their reproductive rate by the availability of adequate cavities (Steffan-Dewenter and Schiele 2008; Dainese et al. 2018; Danforth et al. 2019). Ground-nesting bees generally require patches of bare soil for the construction of their nests, and may additionally have preferences for specific soil characteristics (Johansen et al. 1978; Cane 1991; Danforth et al. 2019). Cane (2008) documented the increasing number of *Nomia melanderi* in the Touchet Valley in Washington, USA, with increasing number and size of nesting beds managed by farmers for alfalfa pollination, suggesting that the total nesting area is limiting for the size of this managed bee population in a highly agricultural landscape.

In cavity-nesting bees, the number of nests and brood cells in provided nest boxes (or trap nests) can be assessed. Under these conditions, the number of brood cells is directly limited by the number (and size) of nest cavities provided. Dainese et al. (2018) could demonstrate that the higher the number of brood cells in trap nests, the lower the growth of the subsequent brood cell number in the same season.

Steffan-Dewenter and Schiele (2008) found that *O. bicornis* brood cell numbers in trap nests increased every year if trap nests were increased in size. These studies indicate that the availability of adequate cavities can be limiting to population growth. Direct aggression among nesting females has been observed in cavity-nesting bees, suggesting competition for nest sites (Danforth et al. 2019). In addition, cavity-nesting bees were found to be more common in fragmented urban habitats compared to non-urban and more natural habitats which could be explained by nesting cavities available in human structures (Danforth et al. 2019).

#### ***Representation of density dependence in the SolBeePop model***

From the literature addressing density dependence in solitary bees, it is suggested that bee populations are likely to be affected by density-dependent processes to some degree, probably varying considerably dependent on species, landscape and species community composition, and environmental factors such as weather. The studies reviewed suggest that density dependence is most likely to affect populations through bottom-up (competition for floral or nesting resources) rather than top-down (brood parasitism) processes. In addition, the resource limitation is assumed to affect the reproductive rates of females rather than survival rates of any life stage.

The limitation of floral resources is likely to vary considerably even within a flight season of a bee population. Temporal variation in floral resource availability and weather-dependent foraging are provided as input to the model and affect reproductive relationships. The model can address floral resource limitations but does not specifically address intra-specific competition for these resources. The estimation of the strength of intra-specific competition for floral resources would be challenging and would have to be considered to be temporally variable as well.

Thus, the intra-specific competition for nest sites is considered as the density-dependent process in the model. The available nesting space is used as proxy for density-dependent resource limitation. With decreasing nesting resources, the brood cell production rates of nesting females are assumed to decline. Because the population densities in natural populations leading to population regulation are not well known, the model can be run with and without density dependence.

#### ***Movement and Behavior***

	Question	Yes	No
1	Are aspects of the behavior <i>other than migration</i> affected by exposures?	2	4
2	Are data available to mechanistically/explicitly represent behaviors potentially affected by exposure?	Include explicit representation of identified behaviors	3
3	Can effects on behavior be linked to submodels (e.g., survival, growth, bioenergetics, fecundity)?	Represent effects on behavior as impacts on appropriate submodel	Categorical or qualitative impacts on behavior could be included to add realism

4	Do individuals migrate outside the action area?	Incorporate function of migration to represent time spent in action area; continue to 5	5
5	Within the action area, is dispersal of individuals important, and may interact with exposure?	Incorporate function of dispersal in the model	Dispersal does not need to be represented

Solitary bees are not migratory but spend their whole life cycle within a limited spatial range (up to a few km in radius, depending on species). Dispersal capacity as well as foraging range are assumed to be positively correlated with body size (Greenleaf et al. 2007; Bommarco Riccardo et al. 2010), but dispersal ranges of newly emerged adults are not reported. Dispersal rates may be dependent on resource availability at time of emergence (Bosch et al. 2008), but may be confounded with increased failure in nest establishment by females.

For the model, we apply the simplifying assumption that the newly emerged adults will nest in the same area where they emerged. Net losses to the breeding population due to dispersal are implicitly represented by failure to nest in the simulated area, i.e., survival rate of newly emerged females. Note that the assumption that no immigration occurs limits the capacity for population recovery in the model. This is a conservative assumption in the context of pesticide risk assessment because potential population-level effects of exposures of a population to a pesticide may not be buffered by non-exposed neighboring populations. The use of different habitat types within a populations' range is addressed in Habitat characterization. Other aspects of behavior are not available from the literature and are not represented in the model.

### Habitat characterization

	Question	Yes	No
1	Does the species occupy more than one habitat type that needs to be represented in the model (e.g., different exposures occurring in the habitats, and are data available to distinguish between habitats)?	2	No explicit representation of space in the model
2	Are data available to distinguish between habitats?	3	Spatially-implicit representation
3	Are spatially explicit interactions with the habitat defined?	Explicitly represent spatial distributions of habitat and/or exposure	Represent habitat(s) implicitly, e.g., along a single axis (e.g., location in the water column, stream section)

In solitary bees, adult females start nesting behavior within a few days or weeks after emergence from the nest (Hurd et al. 1974; Bosch et al. 2008; Pitts-Singer and Cane 2011). Suitable nest sites depend on species' nesting preferences. Some species prefer pre-existing cavities above ground, e.g., hollow sticks. Other species dig their own nest cavities in soil. Additional nesting material (mud, leaf pieces) may be

collected by the female to line individual brood cells or build separating walls (partitions) between cells (Cross and Bohart 1960; Hurd et al. 1974; Bosch et al. 2008; Pitts-Singer and Cane 2011). The resources provided to the offspring as nest provision consist of a combination of pollen and nectar (Klostermeyer et al. 1973; Michener 2007). Food sources other than pollen and nectar exploited by bees as food source (e.g., oils) are not explicitly considered in the model.

Many species may move between habitat types because nesting sites, nesting material and food resources may not be available within a single habitat type (Kremen et al. 2004; Greenleaf et al. 2007). The habitat types visited by a female bee, and the matrices the bee gets in contact with from these habitats may differ in their potential for pesticide exposure.

The distance between habitat types (nesting, nest material source and floral resource sites) have to occur within the foraging ranges of bees. Foraging ranges are assessed as maximum or average distances the bees were observed from their nest (Greenleaf et al. 2007; Zurbuchen et al. 2010). In some cases, maximum or average homing distances were available instead. Reported foraging distances of focal solitary bee species can provide inputs to the model to allow linking realistic landscape compositions to population-level outcomes in different bee species.

The available information about the bees' interactions with the habitats are limited to the foraging ranges of a bee and the matrices collected in the habitats. Depending on the species, bees may exploit a wide variety of flowers (polylectic species, including *O. lignaria*, *O. cornifrons*, *O. cornuta*, *O. bicornis*, *M. rotundata* and *N. melanderi*) while others are relying on pollen and nectar from a small range of plant species, often within the same taxonomic group (oligolectic, including *E. pruinosa*). Habitat requirements of oligolectic species may be narrower than for polylectic species. Beyond the floral preferences, detailed information on how different solitary bee species choose habitats and specific resources is not available.

We represent three distinct habitat types in the model: nesting site, nest material site, and floral resource site (Figure 3), corresponding to a partially explicit representation of the spatial relationship between these three distinct habitats. The representation of the habitat types makes it possible to represent exposures specific to these habitats in the future. We assume that the nest site habitat and the habitat used for collection of nest material will not change during a season, and are within short distance of each other, leading to a stable nest material collection time. The characteristics of the floral resource site may change over the active season of a bee, reflecting flowering times of different plants including mass-flowering crops. The floral resource site may change over time in pollen and nectar availability and distance to the nest site, both affecting the rate of provisioning of nests by females. We combine these floral resource site attributes into a single factor representing the floral resource quality. The floral resource quality can be defined on a daily basis.

In the model, the lower the floral resource site quality, the higher the foraging effort, corresponding to more time requirement to collect the same amount of food per day. In response to decreasing habitat quality, females in the model a) shift to a higher rate of male egg laying (Bosch and Vicens 2005), effectively reducing the female egg laying rate in the model; b) reduce provision sizes of female offspring, lowering the offspring's chance of survival to emergence (Tepedino and Torchio 1982b; Bosch and Kemp 2004; Bosch and Vicens 2006; Bosch 2008), and c) reduce the daily egg laying rate, further impacting female offspring production and life-time fecundity (Kim 1999; Goodell 2003; Peterson and Roitberg 2006b).

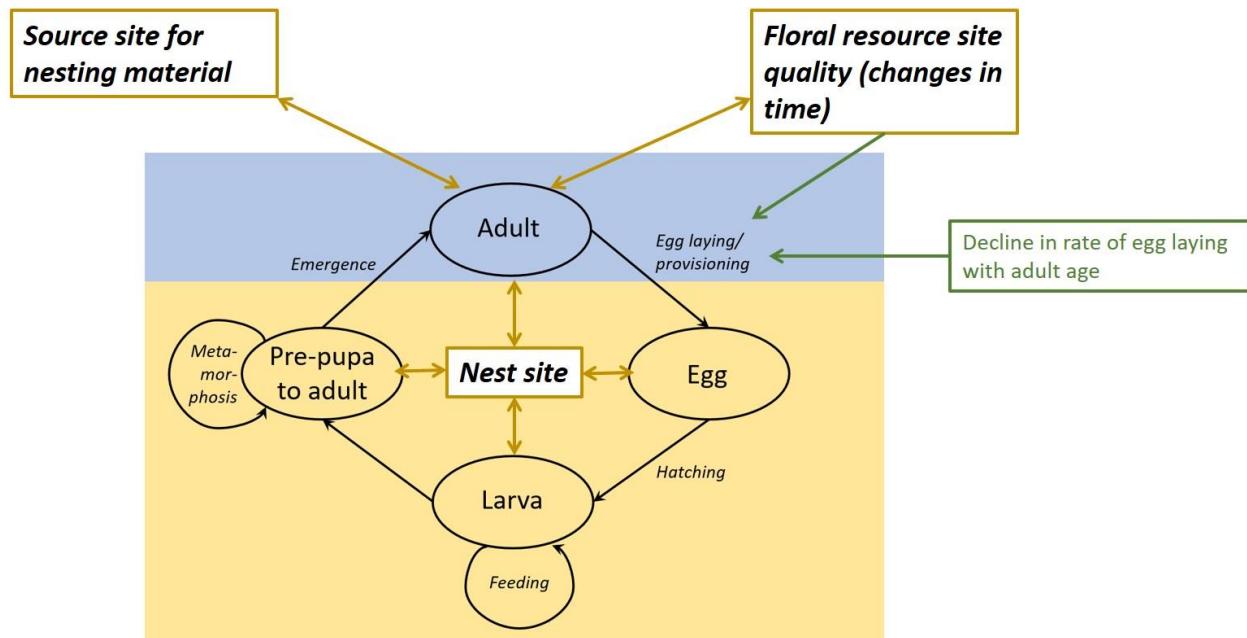


Figure 4. Representation of habitat types used by the solitary bees in the model.

#### 1.2.4. External Factors

##### Diet

	Question	Yes	No	Remarks
1	Is the species diet expected to be impacted by the chemical (based on mode of action or available data)?	2	No additions to model concept	Potential reduction in non-crop floral resources (from herbicides); no data available
2	Are data available to determine how the species' diet may be affected by the chemical exposure (e.g., dose-dependent food reduction)?	3	Categorical or qualitative impacts to diet could be included to add realism of indirect effect	

	<b>Question</b>	<b>Yes</b>	<b>No</b>	<b>Remarks</b>
3	Can effects on prey be represented as effects on vital rates (e.g., growth, survival)?	Include indirect effects mediated by diet as impacts on appropriate vital rate estimates to add precision	Categorical or qualitative impacts to diet could be included to add realism of indirect effect	

Floral resources provide most of any bee's diet (Michener 2007). Sugars in nectar are the main source of carbohydrates for both, adult bees and larvae. Pollen provides a bee's principal source of protein, and is consumed by larvae and post-emergent adults, particularly by reproductive females.

Food availability to bees may be impacted by herbicides, potentially reducing non-crop floral resources (Gabriel and Tscharntke 2007; Holzschuh et al. 2008; Potts et al. 2011). However, detailed data on the interaction of herbicide use and floral resources available to solitary bees are not available. In the current model, we will not consider indirect effects of pesticides on bees through reduction in food availability.

### *Other interspecific interactions*

	<b>Question</b>	<b>Yes</b>	<b>No</b>	<b>Remarks</b>
	Does the species have obligatory relationships with other species potentially affected by the chemical?	Include indirect effects mediated by obligatory relationship as impacts on appropriate submodel(s)	No additions to model concept	No. Excludes brood parasites. Assumes that plants providing resources are not affected by pesticide
	Are biota critical to habitat integrity potentially affected by the chemical stressor (e.g., cover from predators/herbivores)?	Consideration of inclusion if indicated that the species is strongly dependent on specific conditions that may be affected by the stressor	No additions to model concept	

The diet of solitary bee species can range from bees foraging on a large variety of plant species (polylectic species) to bees with strong preferences for pollen and nectar collection from a single or few plant taxa (oligolectic) (Michener 2007). Oligolecty is a form of obligatory relationship. This relationship will not be considered explicitly in the model because we assume that pesticide exposures do not affect food availability. In some cases, the crop itself represents the food source of oligoleptic species (for

instance, the squash bee *E. pruinosa*; Hurd et al. 1974). Cleptoparasitic species may be specialized in parasitizing the nests of a single or few non-parasitic bee species, but cleptoparasites are not addressed in the current model approach.

### **Abiotic factors**

Question	Yes	No
Are environmental conditions indicated to be important drivers of the population dynamics (e.g. temperature, precipitation, water depth, stream flow, flood events, habitat connectedness, etc.) and do those drivers differ between years or habitats of the species?	Dependence on environmental condition should be represented; Variation in across-year environmental conditions may be captured by stochasticity in the model	Species-specific environmental conditions do not need to be represented explicitly in the model
Is the species impacted by additional stressors not previously discussed that may interact with the chemical stressor?	Include relationships as impacts on appropriate submodel(s)	No additions to model concept
Is the species the subject of an existing management plan that may influence exposure probability or effects?	Include relevant management scenarios in model, as appropriate.	No additions to model concept

Emergence timing of adult bees after the dormant period is influenced by temperatures experienced by the dormant stage within the nest. Temperatures triggering emergences vary across species.

Temperature triggers are assumed to similarly affect the floral resources each species relies on, i.e., bee emergence is assumed to occur in synchrony with floral resource availability. If emergence of bees and floral resource availability are desynchronized, fitness losses of bees may result (Schenk et al. 2018 May 1). The model does not explicitly represent environmental triggers. Temporal mismatches between emergence and floral resource availability could be tested by simulating low floral resource site quality at time of bee emergence.

A decline in insect abundances in general (Hallmann et al. 2017) and bee abundances in particular (Biesmeijer et al. 2006; Winfree et al. 2009; Goulson et al. 2015) has been observed in many regions. Reasons for declines are attributed to land use changes, agricultural intensification (including the effects of pesticides) and habitat loss and fragmentation. While these drivers of bee declines are likely to affect many solitary bee species, the current model approach is developed with the future application to pesticide risk assessments. We will not represent interactions with other stressors explicitly. The impact of floral resource availability can be tested explicitly (see Habitat characterization).

## 1.2.5. Exposure impacts

### *Exposure and effects representation*

	Question	Yes	No
1	Do multiple exposure routes need to be considered, e.g., exposure via water in aquatic species, contact exposure, dietary exposure, exposure via nesting material?	2	3
2	Are separate sets of toxicity data available to inform the effects from each exposure route?	Represent each exposure route separately, and address questions 3 and following for each exposure route	Combine the exposures from the exposure routes for the effect representation; continue with 3
<b>Sublethal effects</b>			
7	Are data on sublethal effects available, e.g., effects on growth, reproductive rate, etc.?	8	Sublethal effects are not represented in the model
8	Can measured sublethal effects be linked with corresponding organism-level processes explicitly represented in the model, e.g., growth, maturation, reproduction, bioenergetics, etc.?	Sublethal effects represented affecting the corresponding organism-level process	9
9	Can sublethal effects be expressed as reduction in survival and/or reproductive rates?	'Translate' sublethal effects to lethal effects and/or impacts on fecundity	Sublethal effects are not represented in the model

Solitary bees may be exposed to pesticides via different exposure routes: a) oral (dietary) exposure of adult bees through residues in nectar or pollen, b) contact exposure of adult bees visiting a crop or adjacent area during treatment or contact with exposed plant material or soil, c) combined oral and contact exposure of larvae in the nest through their food provisioning (consisting of pollen and nectar collected by the mother bee) and exposed nesting material and/or soil in which the nesting cavity is built (Sgolastra et al. 2019). In the model, we will consider these exposure routes explicitly, assuming potentially different exposure patterns of food and nesting resources, respectively. In Figure 5, we depict the exposures specific to the habitats used by the bees in the model. Note that the floral resource sites are defined as crop (potentially treated) and non-crop (untreated) resources. The floral resource input includes the daily resolution of pesticide residue concentrations in crop nectar and pollen as well as the nesting material or matrix (dependent on species, the residues on leaves used for brood cell lining are characterized if leaf-cutting bees are simulated, soil/mud used for partitions in Osmia or soil in below-ground nesting bees). Currently, only one nest site and one source site for nesting material (if applicable) are assumed.

In the following, the exposure routes are conceptualized reflecting the data availability of effects: a) oral exposures of active adults, b) contact exposures of active adults, and c) exposures to in-nest life stages

(see Pop-GUIDE questions below for each exposure route). Standard toxicity studies with honey bees assess the effects of these three distinct exposures whereby acute and chronic toxicity of adult exposure is assessed in two separate trials, contact exposure is assessed from a single exposure (with acute effects) and larva are exposed over their entire life stage through combined oral and contact exposure.

Lethal effects are simulated using a toxicokinetic-toxicodynamic model for adult bees (BeeGUTS) and a dose-response relationship for in-nest life stages (Baas et al. 2022). For the implementation of effects, the model will rely on data from honey bee toxicity studies. Where available, effect data for the model species (*Osmia bicornis*, *O. cornifrons*, *O. cornuta*, *O. lignaria*, *Megachile rotundata*, *Nomia melanderi*, *Eucera pruinosa*) may be used. Sublethal effects are not considered in the current concept. Sublethal effects may be recorded during honey bee toxicity studies (U.S. Environmental Protection Agency 2016) but are not consistently available across compound. In addition, the translation of the recorded sublethal effects (e.g., deformities of bees emerging from the larval chronic study, proboscis extension reflex or locomotor activity adult studies) into effects relevant for long-term survival or nesting efficiency in solitary bees remain unresolved.

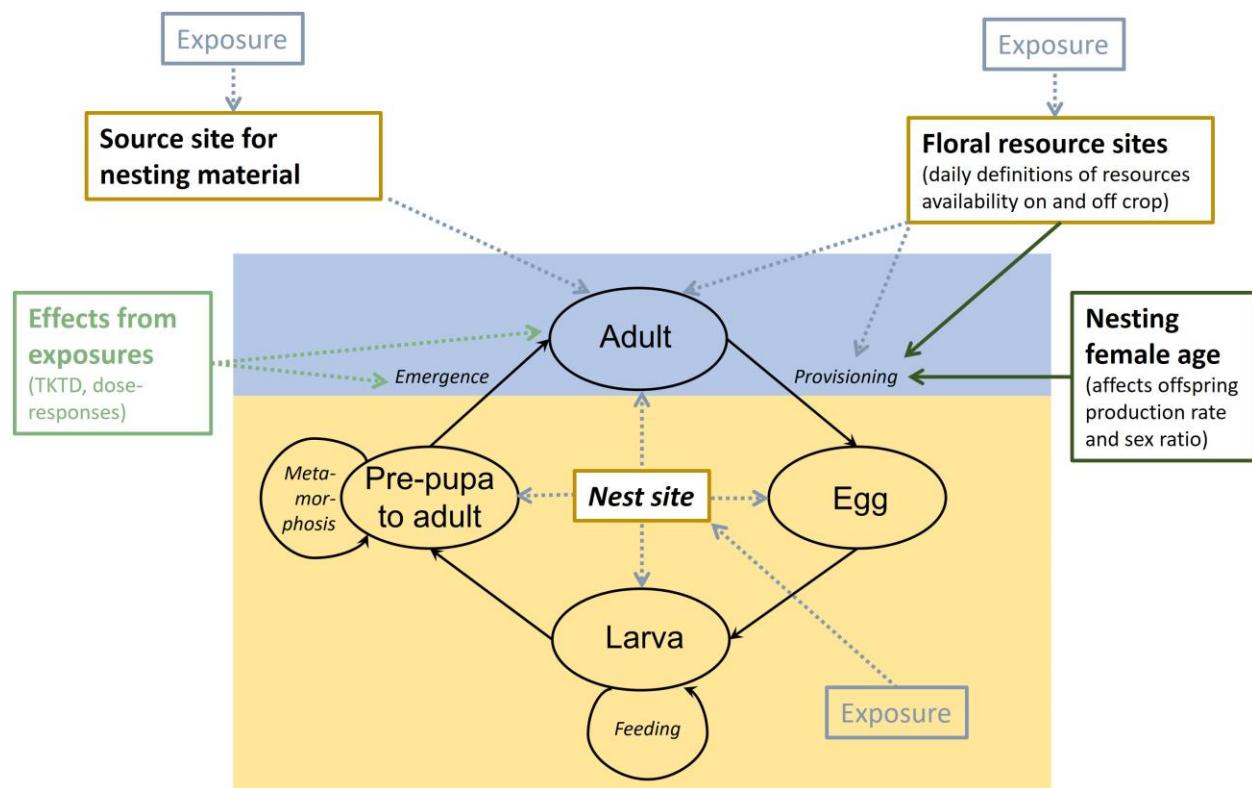


Figure 5. The model concept including exposure routes and life stages affected by the simulated lethal effects. Exposures from the different exposure routes will be additive on the individual level. Adults can be affected through contact and dietary exposures (considered separately). For in-nest life stages, exposures from contact and diet are not distinguished and effects are considered at time of emergence only.

*a) Oral exposures of active adults*

	Question	Yes	No
3	Are lethal effects measures available?	4	7
4	Can the available study data be used to fit / apply a time-variable effects model, e.g. toxicokinetic-toxicodynamic model (TKTD / GUTS)?	Represent effects of time-variable exposures based on all study data; continue with 7 [see Table 1]	Represent effects as dose-response functions or effects thresholds (e.g., NOEC, LC <sub>x</sub> ); continue with 5
5	Are lethal effects endpoints available from studies with different durations, e.g., acute and chronic studies?	6	7
6	Are exposures occurring / represented exclusively as temporally limited pulses (<duration of acute studies)?	Use data from acute (short-term) toxicity study data for the representation of effects; continue with 7	Use effects from chronic study data, and apply it to time-averaged exposures, or represent acute and chronic effects separately; continue with 7

Exposure to and effects from pesticides of actively flying bees (after emergence from the nest) will only be considered for females. Bee males do not contribute to nesting, and in the model species, are generally short-lived after their emergence from the nest. During their post-emergent life span, males may be exposed to pesticides through consumption of nectar or direct exposure to overspray. Lethal effects on bee males would only have an effect on bee populations if they would result in limited mating opportunities of females. This is a very unlikely scenario because males generally emerge prior to the females and remain at nesting sites to mate with newly emerging females. Mating limitation is not considered in the model. In addition, toxicity data are typically available for female bees (honey bees and other species). Accordingly, exposure and effects to males are not considered in the model.

For post-emergent females, oral exposure can occur due to consumption of exposed nectar or pollen. Female *O. cornifrons* and *N. melanderi* were reported to consume nectar and pollen throughout their life time (Taniguchi 1956; Cane 2016; Cane et al. 2017). Data on nectar and pollen consumption rates for solitary bees are not generally available (with one notable exception the number of pollen grains found in a bee's digestive tract reported in *N. melanderi* (Cane et al. 2017)). Nectar and pollen consumption rates may be based on estimates derived from honey bee data (Sgolastra et al. 2019). The residue mass (or concentration) in the consumed nectar and pollen directly corresponds to the bee exposure.

In addition to foraging for its own consumption, a nesting female collects nectar and pollen for provisioning brood cells. Although nectar is transported internally in the bee's crop (stomach), it is assumed that nectar collected for brood cell provisioning does not contribute to the exposure of the nesting bee. The crop is assumed to be inert and the uptake of toxicants is assumed to occur only once the nectar is released to the midgut and digested by the bee (Baas et al. 2022). In the model species, pollen is transported on the outside of the body in specialized hair (scope) on the abdomen or legs.

Thus, it is assumed that no oral exposure occurs from pollen collected for provisions either. In the species (e.g., *Hylaeus* sp.) that transport pollen for the provisions internally (Michener 2007; Danforth et al. 2019), the assumption that the crop is inert would apply (as for nectar collected for brood provisions) but we do not currently explicitly address these species with the model. In addition, we assume that potential oral exposure from other sources are negligible and are not included in the model. Water collection is common in honey bees, but has not been described in solitary bees (Kopit and Pitts-Singer 2018; Sgolastra et al. 2019). Accidental ingestion of water, soil or plant material during collection and nest construction cannot be excluded but no data on quantities or potential adverse effects are known (Kopit and Pitts-Singer 2018).

The sum of daily exposures from nectar and pollen (for own consumption) corresponds to the assumed daily oral exposure of an adult female bee. The effects from oral exposure are simulated applying a toxicokinetic-toxicodynamic model for survival that was adapted for honey bees (BeeGUTS; (Baas et al. 2022)). Effects simulated with BeeGUTS are based on combined oral and contact exposures (see next section).

### *b) Contact exposures of active adults*

	Question	Yes	No
3	Are lethal effects measures available?	4	7
4	Can the available study data be used to fit / apply a time-variable effects model, e.g. toxicokinetic-toxicodynamic model (TKTD / GUTS)?	Represent effects of time-variable exposures based on all study data; continue with 7 [see Table 1]	Represent effects as dose-response functions or effects thresholds (e.g., NOEC, LC <sub>x</sub> ); continue with 5
5	Are lethal effects endpoints available from studies with different durations, e.g., acute and chronic studies?	6	7
6	Are exposures occurring / represented exclusively as temporally limited pulses ( $\leq$ duration of acute studies)?	Use data from acute (short-term) toxicity study data for the representation of effects; continue with 7	Use effects from chronic study data, and apply it to time-averaged exposures, or represent acute and chronic effects separately; continue with 7

As for oral exposures and effects to adult bees, only female bees are considered. Post-emergent females can come in contact with pesticides through different matrices, particularly once they start nesting. If a bee is foraging in crop during treatment, she may be exposed to direct overspray. In case of a spray application occurring on a given day in the model, it will be assumed that each simulated bee foraging on crop will be exposed via this route whereby the probability of exposure corresponds to the % foraging on crop that day. The exposure concentration directly corresponds to the concentration in the application (and to the acute contact standard toxicity studies conducted with honey bees).

Potentially exposed matrices that a post-emergent female may come in contact with include contaminated soil, pollen, flowers and other plant surfaces or water in treated areas (Kopit and Pitts-Singer 2018; Sgolastra et al. 2019). Water foraging has not been observed in solitary bees and accordingly, water is not considered in the model as separate exposure route. Contact exposure to plant surfaces during nectar and pollen foraging is considered negligible as well as contact exposure to pollen transported on the exterior of the body. In most solitary bees species including the model species, pollen is transported dry (not mixed with nectar like in honey bees) in specialized hair (scopa) on the outside of the body (Danforth et al. 2019; Sgolastra et al. 2019). For the purpose of the model, it is assumed that above-ground cavities used for nesting (e.g., by *Osmia* and *Megachile*) are not a relevant route of exposure.

Contact with contaminated soil may occur during collection of mud or wet soil for construction of cell partitions by *Osmia* (Kunz et al. 2014; Sgolastra et al. 2019; Fortuin et al. 2021). Estimates for the weight of single partitions and the average weight of mud collected for nest partitions by a nesting *Osmia* are available (Bosch and Vicens 2005; Pinilla-Gallego et al. 2018; Sgolastra et al. 2019). Soil-nesting bees also come in contact with soil throughout their nesting life, and the amount of soil moved by a nesting bee has been estimated (Willis Chan et al. 2019b).

Fortuin et al. (2021) exposed adult *Osmia* to wet soil with different concentrations of the insecticide imidacloprid for 20 mins and found effects on subsequent survival and nesting activity. Although the observed effects were variable and did not follow a dose response curve, the effects appeared to be dependent on the level of soil moisture with higher water content leading to higher effects. Willis Chan et al. (2019) estimated that a female *E. pruinosa* moves 33.5 g of soil during her nesting life, and that the entire compound mass in the soil moved by the bee corresponds to the chronic exposure of the adult bee (assuming a life span of 30 days) or the corresponding acute exposure (from 2.23 g of soil in 48 h). However, no experimental data were available to support this assumption. Contact exposure studies conducted in the laboratory by exposing adult bees to a pesticide via liquid droplets assume that the exposure concentration in the droplet corresponds to contact exposure from soil with the same concentration (Kopit and Pitts-Singer 2018; Lehmann and Camp 2021). However, it is unclear whether the uptake from contact with soil corresponds to uptake from compound dissolved in water.

*M. rotundata* is cavity-nesting like the model *Osmia* species but uses leaf pieces to line each nest cell (Klostermeyer et al. 1973). Sgolastra et al. (2019) suggested a calculation for chronic pesticide exposure ( $\mu\text{g}$  of active ingredient/day) via plant surface for the adults of *M. rotundata*:

$$\text{Plant surface exposure } (\mu\text{g a.i./day/bee}) = \text{AR} * \text{F} * \text{TC} * \text{ET}$$

Where:

AR = pesticide application rate ( $\mu\text{g a.i./cm}^2$ )

F = % fraction of application rate available for transfer to bees (US Environmental Protection Agency 1996)

TC = transfer coefficient ( $\text{cm}^2/\text{unit time}$ )

ET = exposure time to foliage (unit time)

We use this approach to calculate the exposure of nesting females that use plant material to line brood cells. No data are currently available for the transfer coefficient (TC). In the model, the time a (leaf-cutting) bee interacts with leaves (cutting and lining brood cells) is used instead. The exposure time to

foliage (ET) can be estimated from the proportion of time a nesting bee spends collecting leaves and the foraging time per day (Pitts-Singer and Cane 2011).

A similar approach is used in the exposure-effect module for estimating the contact exposure to contaminated soil in soil-nesting bees and cavity-nesting bees that use soil (or mud) in the construction of the brood cells:

$$\text{Soil exposure } (\mu\text{g a.i./day/bee}) = \text{SC} * \text{TC}_s * \text{ET}$$

Where:

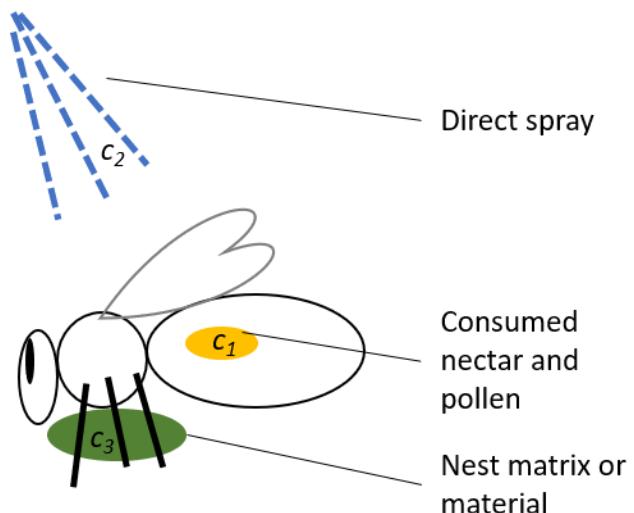
SC = pesticide concentration in the soil ( $\mu\text{g a.i./g soil}$ )

TC<sub>s</sub> = transfer coefficient from soil (g/unit time)

ET = exposure time to soil per day (unit time)

As for plant material, data are not available to parameterize the transfer coefficient from soil. The exposure time per day can be assumed to correspond to the proportion of time a bee spends collecting soil or digging nests in the soil.

The sum of daily contact exposures from direct spray and contact with nest material (or matrix) corresponds to the daily contact exposure of an adult female bee. The daily oral and contact exposures of adult bees are added (Figure 6). The toxicokinetic-toxicodynamic model for survival that was adapted for honey bees (BeeGUTS; (Baas et al. 2022)) and uses the total daily exposure to calculate effects (mortality rate).



*Figure 6. Exposures to post-emergent adult female bees in the model. c<sub>1</sub>: residue concentration in consumed nectar and pollen (including nectar collected for nest provisions) is assumed directly apply as dietary (oral) exposure concentration to the bee; c<sub>2</sub>: residue concentration in direct spray is assumed to directly apply as contact exposure concentration to the bee; c<sub>3</sub>: residue concentration in nest matrix (soil in ground-nesting bees) or nest material in above-ground nesting bees (soil/mud cell partitions or leaves). The sum of the daily exposures c<sub>1</sub>, c<sub>2</sub> and c<sub>3</sub> are used to calculate lethal effects using BeeGUTS.*

### c) Exposures to in-nest life stages

	Question	Yes	No
3	Are lethal effects measures available?	4	7
4	Can the available study data be used to fit / apply a time-variable effects model, e.g. toxicokinetic-toxicodynamic model (TKTD / GUTS)?	Represent effects of time-variable exposures based on all study data; continue with 7	Represent effects as dose-response functions or effects thresholds (e.g., NOEC, LC <sub>x</sub> ); continue with 5
5	Are lethal effects endpoints available from studies with different durations, e.g., acute and chronic studies?	6	7
6	Are exposures occurring / represented exclusively as temporally limited pulses ( $\leq$ duration of acute studies)?	Use data from acute (short-term) toxicity study data for the representation of effects; continue with 7	Use effects from chronic study data, and apply it to time-averaged exposures, or represent acute and chronic effects separately; continue with 7

In most solitary bees (including all model species), nesting females build an individual cell for each offspring. Females provision a cell with pollen and nectar, deposit an egg and close the cell. The larva generally consumes the entire provision before defecating and entering a dormant pre-pupal stage or pupating. During the larval growth and feeding, the larva is in direct contact with the food provision and the brood cell lining. Accordingly, oral and contact exposures are not separated (Figure 7).

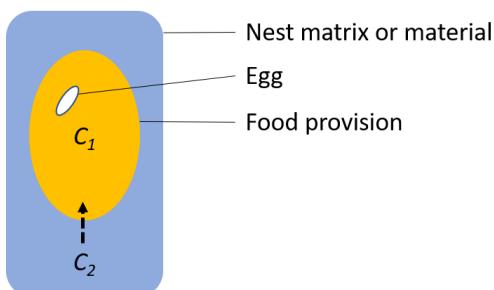


Figure 7. Exposures to in-nest life stages,  $c_1$ : residue concentration in food provision is assumed directly apply as exposure concentration to the developing bee;  $c_2$ : residue concentration in nest matrix (soil in ground-nesting bees) or nest material in above-ground nesting bees (soil/mud cell partitions or leaves);  $c_2$  is only considered if it is larger than  $c_1$  in which case transfer from residue from nest matrix/material to the provisioning/bee is assumed and the exposure concentration experienced by the developing bee is assumed to be  $c_2$ .

In the model, it is assumed that the residue in the provision corresponds to the residue in nectar and pollen collected by the nesting female on the day the egg is laid (even if the cell was started on the previous day). Daily residue concentrations in crop nectar and pollen are inputs to the model. Each female bee collects a percentage of nectar and pollen from crop and non-crop whereby the percentages are identical between nectar and pollen. Accordingly, the residue level in nectar collected for a cell provision is a percentage of the residue in crop nectar. The residue in pollen is calculated accordingly. The composition of brood cell provisions (nectar:pollen) are reported for some species (Klostermeyer et al. 1973; Pitts-Singer and Cane 2011; Ruddle et al. 2018). The residue levels in nectar and pollen inform the residue concentration in the entire cell provision accordingly. The residue levels are assumed to be constant, i.e., no dissipation or degradation of compound occurs in the nest.

As for adult bees, we assume that above-ground cavities used for nesting are not a source of exposure to developing bees. Accordingly, in-nest life stages may be exposed to residues in nesting materials brought in by the nesting female (in above-ground nesting bees) or to the nest matrix (in soil-nesting bees) but not both. The exposure of nest material or matrix is assumed to be constant, i.e., the application occurs prior to the nesting period of the bee and that it does not differ between source sites of nesting material (or within a population of soil-nesting bees).

Transfer of residue from the nesting matrix or nesting material to the developing bee (or the provisioning) is not well understood (Sgolastra et al. 2019). (Willis Chan et al. 2019a) assume no transfer between soil and developing bee/provisioning due to nest lining applied by the mother bee. In contrast, other studies assume that exposure to larvae of erosoil-nesting bees can be simulated in the laboratory via liquid application of a pesticide to the larva whereby the concentration in the liquid corresponds to measured concentrations in soils (Anderson and Harmon-Threatt 2019; Lehmann and Camp 2021). The uptake of pesticides from contaminated soils was studied in earthworms. Most uptake of a toxicant from soil through the earthworm's skin occurred within the first 5 days of exposure, particularly for hydrophile compounds (Jager et al. 2003). If uptake occurs similarly in developing bees, it can be assumed that the internal concentration of the growing larva is in equilibrium with the contaminated nesting material or matrix because combined egg and larval (feeding stage) development times range from 10 to 50 days (Danforth et al. 2019).

In the model, exposure to in-nest life stages from nest material or matrix can be switched on and off separately, allowing to test scenarios with and without these routes of exposure and reflecting the uncertainty about whether toxicants transfer from the nesting material or matrix to the developing bee or its provision. When exposure from the nest material or matrix is switched on, equilibrium toxicant concentration in the developing bee (and its provision) with the nest matrix is assumed in soil-nesting bees. However, nesting materials that line or partition individual brood cells may have less mass than the provision (and consequently, the larva at the end of feeding). In this case, the conservative (worst-case) assumption is applied that the residue (mass, not concentration) corresponds to the exposure of the developing bee. Thereby, it is not distinguished whether the residue transfers to the provision (and is subsequently consumed by the larva) or the developing bee directly. For *M. rotundata*, (Sgolastra et al. 2019) calculate the exposure of a developing bee from the leaf material lining the cell as follows:

$$\text{Exposure } (\mu\text{g a.i./bee}) = \text{AR} * \text{F} * \text{SA}_i$$

Where:

AR = pesticide application rate ( $\mu\text{g a.i./cm}^2$ )

F = % fraction of application rate available for transfer to bees (US Environmental Protection Agency 1996)

SA<sub>i</sub> = internal surface area of nest cell (cm<sup>2</sup>)

Similarly, the residue amount in a single cell partition between brood cells in *Osmia* can be assumed as conservative scenario of exposure from the nesting material:

$$\text{Exposure } (\mu\text{g a.i./bee}) = \text{SC} * \text{SM}$$

Where:

SC = pesticide concentration in the soil ( $\mu\text{g a.i./g soil}$ )

SM = mass of a single soil/mud cell partition (g soil)

Residue in the nesting matrix or material can transfer to the provisioning/bee up to equilibrium concentrations between provisioning/bee and the other matrix, i.e., it is assumed that residues coming from the nest matrix or material do not accumulate in the provisioning/bee and that all mass is preserved in the system (e.g., no water loss the provision or developing bee). In other words, exposure from nest material or matrix is only considered if the exposure concentration in the bee/provision resulting from it is higher than the exposure present in the provision (from nectar and pollen). However, residues in nectar and pollen are assumed to stay in the provision (and are consumed by the larva) and do not transfer to the nest material or matrix.

Consequently, the exposure of the in-nest life stages corresponds to the higher of the two possible exposures: 1) exposure concentration present in the provision at time of egg laying (from nectar and pollen collected by the mother bee) or 2) transferred exposure from the nest material or matrix. The exposure concentration is assumed to correspond to a chronic exposure. Effects on developing bees correspond to the effects on honey bee larvae (from standard larval toxicity studies). Honey bee larvae are exposed through feeding solution (combining oral and contact exposure) throughout their larval stage (~5 days). Note that bee size is not considered because the exposure is based on a concentration (not toxicant mass per bee). Alternatively, larval toxicity data from a model species can be used if available. Effects are represented as logistic concentration-response function:

$$S(c) = I + s \log_{10}(c)$$

where  $S$  give the survival probability,  $c$  is the concentration,  $I$  is the intercept and  $s$  is the slope. Note that a background mortality will be assumed in the model rather than represented in the concentration-response function. Mortality from the exposure of in-nest life stages is applied at the time of emergence from the nest. The assumption of mortality occurring at time of emergence is arbitrary. However, timing of mortality up to emergence does not affect model dynamics.

## Temporal Representation

	<b>Question</b>	<b>Yes</b>	<b>No</b>
1	Are seasonal differences important to the species' life cycle and need to be considered to adequately describe species and chemical co-occurrence?	Temporal resolution should be < 1 year, reflecting temporal scale of seasonal changes	2
2	Are important toxicological processes represented at different resolutions (e.g., TKTD processes)	Time step consistent with temporal resolution of process with shortest time step; or nest functions with shorter time steps within larger time step.	Temporal resolution does not need to be further adapted

Most solitary bee species go through their entire life cycle in one year (univoltine species) or multiple times per year (multivoltine species). Univoltine species or individuals of multivoltine species spend most of their life time within the nest in a dormant stage (as pre-pupa or pre-emergent adult) over the winter or other unfavorable season (Michener 2007).

Adult females are only actively foraging and nest building for a few weeks during their life time. Accordingly, the food provision of a single nest is usually collected within a time period of one to two days and is highly dependent on the floral resource availability on a daily basis. For the future extension of the model with pesticide exposures and effects, the exposure of nesting adults may also vary dependent on application timing and crop flowering. The timing of provision collection governs the exposure of each offspring. Thus, the temporal resolution of the model captures the active season of the bees in daily time steps to reflect the accuracy of data available on female active foraging phases and larval development times.

## 2. MODEL DESCRIPTION

### 2.1. Overview

#### 2.1.1. Purpose

The model is intended as a tool to represent the population dynamics of multiple solitary bee species in agricultural landscapes. Different species can be simulated using species-specific parameterizations which correspond to the ecological traits of the species. Exposures to a pesticide via different routes relevant by species are represented along with effects on adults and developing bees.

#### 2.1.2. Entities, state variables and scales

The entities in the model are individual bees, and the environment is represented non-spatially. The bee agents are characterized by their nesting strategy (*nest.strategy*), sex (sex: female, male) and developmental stage (*life.stage*: egg, larva, cocoon, emerged, nesting). A bee has an stage-specific age (*age.stage*: number of days spent in the current life stage). Bees in in-nest (pre-emergent) life stages have a state variable defining the day of emergence from the nest (*emerge.doy*). Adult females reach maturity within a short time period after emergence and start nesting. During nesting, females have a daily background mortality probability (*mort.prob*). Nesting females are actively building brood cells at a variable rate (*cell.prod*). The probability of producing a female or male offspring is defined by the female sex ratio (*sex.ratio*) which depends on the nesting female's age and resource availability.

The environment of the bees is defined by daily input time series which provide the time available for foraging (derived from weather data) relative to the maximum length of a foraging day, the resource availability form crop and non-crop floral resources and the proportional foraging on crop. Additional daily time series define the exposures to a pesticide as concentration in nectar, pollen, direct spray, soil and leaves. The input times series are described in detail in Appendix B. The environment is also characterized by the day of year (*doy*) and the current simulated year (*year*). The model's state variables along with their descriptions are listed in the file “SolBeePop\_ecotox\_Tables.xlsx.” The exposure to in-nest life stages is driven by the exposures across relevant matrices occurring at time of brood cell production. At time of emergence, simulated bees experience lethal effects from exposures according to a concentration-response function. Post-emergent females experience variable daily exposures from relevant matrices, and lethal effects are implemented using a toxicokinetic-toxicodynamic effect module (BeeGUTS; Baas et al. 2022).

The model proceeds in daily time steps. The simulated total duration of a simulation is defined in years (*Num.repeat.yr*, in increments of 365 time steps). Alternatively, different yearly input files can be defined, and the number of listed years defines the simulation duration (see Appendix B).

#### 2.1.3. Process overview and scheduling

At the beginning of each simulated year (*doy* = 1), a new yearly environmental input defining the proportional foraging day length (0 – 1), the floral resource quality of crop and non-crop (0 – 1) and the proportional foraging on crop (0 – 1) is read in, defining these variables in each time step (day) (see also Appendix B).

The bee agents are conducting daily life-stage specific activities in random order (*life.cycle*; Submodel 2.4.1). In-nest life stages include eggs, larvae and cocoons. The life stage ‘cocoon’ summarizes all developmental stages from 5<sup>th</sup> larval instar (after the larva ceases feeding) through adult prior to emergence from the nest. This applies to all simulated species regardless of whether the species produce a cocoon or not. The in-nest life stages do not experience a chance of mortality on a daily basis. The only activity in-nest life stages engage in is the progression to the next life stage (*life.stage*). For eggs and larvae, this happens when they reach the maximum stage-specific age and transition to the next life stage (larva or cocoon, respectively). Cocoons transition to emerged females on their specified date (day of year) of emergence (*emerge.doy*). Bee agents have a chance of mortality upon emergence that combines the background mortality across the entire in-nest development (*max.survival.e.f* and *max.survival.e.m* for females and males, respectively) with the provision-size dependent mortality (see Submodel 2.4.1).

Post-emergent adult female bees (*life.stage* = “emerged”) spend a defined maturation time before initiation of nesting. At time of maturation, they experience a defined chance of mortality. All males in life stage “emerged” die when they reach the male maximum adult life span. If adult female bees reach the age of maturity in a given time step, they transition to nesting females (*life.stage* = “nesting”). During the nesting life stage, females experience a daily mortality probability. All nesting females die if they reach the maximum adult life span. In each time step, nesting females engage in nest building (*nest.building*; see Submodel 2.4.2). Each brood cell completed in a time step results in the creation of a new bee agent in egg stage. The daily rate of brood cell production (*cell.prod*) of each nesting female is dependent on its age (since emergence) and the daily floral resource quality in the environment. Unfinished brood cells (digits after the point of *cell.prod*) carry over to the next day. If density dependence is included in a simulation, the daily brood cell production rate declines with the number of bee in pre-emergent life stages (see Submodel 2.4.3). All life stages increase their stage-specific age by one at the end of each time step.

The exposure of a developing bee (across in-nest life stages) is determined at time (simulated day) of brood cell completion by the nesting female. The exposure (in ng a.i./bee) of each bee is calculated from the total compound in nectar and pollen making up the provision. If the exposure concentration in the nesting material (soil or leaves) is higher than in the provision (from nectar and pollen), the effective exposure to the developing bee is calculated from the nesting material exposures instead. At time of emergence, the developing bee experiences a probability of mortality calculated from the exposure and a concentration-response function. Post-emergent female bees may be exposed via consumption of nectar and pollen as oral exposure route, and via direct spray (during pesticide application) or contact to exposed nesting material on a daily basis, as defined by the daily input time series. Exposures from the different exposure routes are combined into an “effective exposure” according to BeeGUTS (Baas et al. 2022). On days with effective exposure larger than 0, the bee experiences a probability of death.

## 2.2. Design concepts

### 2.2.1. Basic principles

The model uses a trait-based approach to the simulation of solitary bee populations. While the model only simulates a population of a single bee species at a time, it can represent different species through

specific parameterizations. Bees are simulated individually and the temporal variability in life stages within a population is captured by the model.

The nest building submodel (2.4.2) addresses the main factors, nesting female age and resource availability, identified in the literature affecting the number of daily brood cells built by a nesting female, the sex of the offspring and the provision size.

## 2.2.2. Emergence

Because the model does not include adaptation or learning by the simulated bees, the model outputs emerge based on the interaction between daily floral resource quality (from input), species-specific inputs and model stochasticity. In simulation including density dependence, the reproductive rates are impacted by the number of bees in pre-emergent life stages. The emergent properties include the daily offspring production, offspring and adult survival. Accordingly, the population size over time is emergent from the model.

## 2.2.3. Adaptation

Adaptation of the agents is not included in the model.

## 2.2.4. Objectives

Agent objectives are not implemented in the model.

## 2.2.5. Learning

Learning is not implemented in the model.

## 2.2.6. Prediction

Prediction is not implemented in the model.

## 2.2.7. Sensing

Sensing is not implemented in the model.

## 2.2.8. Interaction

If density dependence is switched on in a simulation, reproductive rates of nesting females decline with increasing numbers of bees in pre-emergent life stages (see Submodel 2.4.3).

## 2.2.9. Stochasticity

Stochasticity is used in multiple ways in the model. In Table 1, the stochastic processes in the model are listed.

Table 1. Stochastic processes in SolBeePop.

Stochastic process	Submodel	Description
Timing of emergence from nest	2.4.1. Life cycle	The day of year of emergence ( <i>emerge.doy</i> ) of each simulated bee is chosen from a normal distribution defined by the inputs <i>day.emerge.f</i> or <i>day.emerge.m</i> (mean emergence day) and <i>var.emerge.f</i> or <i>var.emerge.m</i> (standard deviation of emergence day) for females and males, respectively.
Survival at time of emergence	2.4.1. Life cycle	Survival probability at time of emergence is applied stochastically dependent on maximum survival rate, <i>max.survival.e.f</i> or <i>max.survival.e.m</i> (egg through emergence, model parameter) for females and males, respectively, and the relative provision size, <i>prov.size</i> .
Female survival from emergence to first nesting	2.4.1. Life cycle	Females' probability ( <i>emerged.survival</i> , model parameter) of survival between emergence and onset of nesting applied stochastically at time of transition from emerged to nesting stage. Survival in the model corresponds to successful initiation of nesting within the simulated population. Accordingly, 'mortality' after emergence and prior to nesting summarizes rates of deaths, failure to nest and dispersal.
Daily survival of nesting females	2.4.1. Life cycle	Daily survival probability of nesting females applied stochastically.
Offspring sex determination	2.4.2 Reproduction	The female sex ratio of the offspring produced by a nesting female is used to stochastically determine the sex of each offspring (often only 1 per day): <i>sex.ratio</i> corresponds to the probability of a female offspring.
Foraging decision	2.4.2 Reproduction	If <i>stoch.crop.forag</i> is switched 'on': proportion of daily foraging on crop is chosen randomly by each nesting female (for daily values from input file > 0 and < 1); see also Section 2.4.2 for further details.
Individual GUTS-IT lethal threshold	Exposures and effects of post-emergent females (BeeGUTS)	If effects from exposures on adult bees are simulated using GUTS-IT, each newly 'created' bee in the model (either at time of model initialization or when a new brood cell is completed) randomly chooses a threshold of internal concentration that leads to death. The threshold is chosen from a pre-calculated distribution defined by GUTS-IT parameters.
Mortality due to exposure at time of emergence	Exposures and effects to in-nest life stages	If exposure in the provision or nesting materials occurred, the bee has a probability of death according to the defined concentration-response function.
Daily mortality due to exposures of post-emergent females	Exposures and effects of post-emergent females (BeeGUTS)	If exposure from any relevant exposure route occurs on a given day ( <i>C.effective</i> > 0), the bee has a probability of death according to GUTS-SD or GUTS-IT

## 2.2.10. Collectives

No collectives are used in the model.

## 2.2.11. Observation

The main observations from the model are the population size over time, the offspring production by nesting females, and the sex ratio of the offspring. The population size (number of individuals) is observed as the total number of bees in the population each day (including all life stages), the total number of bees (*bees.emerged.yr*) as well as the number of females (*f.emerged.yr*) and males (*m.emerged.yr*) that have emerged in simulated year (cumulative number reset to 0 on the first day of each year). The number of nesting females is observed each day (*bees.nesting.today*) and as a cumulative number for the simulated year (*bees.nesting*).

The offspring (= brood cell) production is observed at the level of the population. The daily production of total brood cells (*sum.cells.today*), brood cells with female (*sum.f.cells.today*) and male offspring (*sum.m.cells.today*) report the number completed across nesting females on a given day. The cumulative numbers of brood cells completed to date are also used as outputs (*sum.cells*, *sum.f.cells*, *sum.m.cells*). The average daily and cumulative yearly brood cell production to date per nesting female is reported by *mean.cells.today* and *mean.cells*, respectively. The means and cumulative sums across the population are also reported by sex (*mean.f.cells.today*, *mean.m.cells.today*, *mean.f.cells*, *mean.m.cells*, *sum.f.cell.today*, *sum.m.cells.today*, *sum.f.cells*, *sum.m.cells*). Additional outputs of the model are the number of deaths from exposures of in-nest life stages (total number during the simulated year up to the current date, *deaths.exp.in*), and daily and yearly numbers of deaths of post-emergent adults (*deaths.exp.ad.today* and *deaths.exp.ad*, respectively). Note that the absolute numbers of deaths are dependent on the simulate population size: the population-level effects need to be characterized as proportions of observations (excluding death counts) in simulations with and without exposures. See file SolBeePop\_ecotox\_Tables.xlsx for listing and description of model outputs.

## 2.3. Details

### 2.3.1. Initialization

Upon model initialization, the initial number of female and male bee agents (*Initial.num.f* and *Initial.num.m*, respectively) is created. All bees start in the same life stage. The initial life stage of the bees is set on the interface (*Initial.stage*) along with the age (in days) in the life stage (*Initial.age*). The initial age of each individual is assigned stochastically within a range around the input value to avoid an initial population with identical ages. Note that the age applies to the specific life stage, not to the total age of a bee. For eggs and larvae, the age is drawn from a normal distribution, whereby the *Initial.age* is used as average of the distribution and the standard deviation as ¼ of the development time of the respective stage (*dev.egg* or *dev.larva*). All cocoons are directly assigned with *Initial.age* because emergence from cocoons is not dependent on age after the bee is fully developed (*dev.cocoon*). Emerged bees are assigned a randomly chosen age of their stage between 0 days and *Initial.age* + 1. Adult bees' initial ages are also drawn from a normal distribution, with the mean corresponding to *Initial.age* and the standard deviation to the variance in emergence date (*var.emerge.f* or *var.emerge.m*). Ages (*age.stage*) smaller than 0 are set to 0.

To simulate a natural population (i.e., cocoons overwinter and emerge in the field), the simulation should be started prior to the earliest emergence date with all individuals in ‘cocoon’ stage.

The simulation of density dependence can be switched on or off prior to simulation start (selecting ‘On’ or ‘Off’ for *Density.dep*). The function (*DD.funct*) used for the density dependence has to be selected (‘linear’ or ‘log’).

### 2.3.2. Input data

The input file to the model defines a time series of daily foraging and floral resource quality values. An input file must contain 366 rows with the first row stating the column headers and the 365 subsequent rows including the daily data. The input is organized in five columns (in the format “.csv”) as listed below. See Appendix B for a description how input files for SolBeePop can be generated.

1. “doy” – Day of year as a numerical (1 – 365)
2. “Prop\_foraging\_day” – The proportion of a given day available for foraging. This value reflects the daily weather and can take values between 0 (no foraging due to inclement weather) and 1 (bees can forage the maximum daily duration).
3. “Quality\_crop” – Daily floral resource quality of a flowering, bee-attractive crop. The quality summarizes the distance of the flowering crop from the nesting location and the resource availability within the patch (field). Values can range between 0 (no flowering crop within the foraging distance of the bee) and 1 (highly attractive flowering crop within short distance from nest the location).
4. “Quality\_nat” - Daily floral resource quality of wildflower or mixed flower (non crop) resources within the foraging range of the bee. The quality summarizes the distance of the areas with flowers from the nesting location and the resource availability within the (closest and/or most attractive) areas. Values can range between 0 (no wildflowers within the foraging distance of the bee) and 1 (highly attractive flowers within short distance from the nest location).
5. “Prop\_foraging\_crop” – Daily proportion of foraging on crop. The foraging on wildflower (non-crop) resources corresponds to (1 – Prop\_foraging\_crop).
6. “Concentration\_nectar” – Daily concentration of a pesticide in nectar from the (treated) crop resource; concentration in µg a.i. per g nectar.
7. “Concentration\_pollen” – Daily concentration of a pesticide in pollen from the (treated) crop resource; concentration in µg a.i. per g pollen.
8. “Concentration\_spray” – Daily concentration of a pesticide in direct spray (application rate in mg a.i. per L) which the bees are exposed to while foraging in crop.
9. “Concentration.nest.mat” – Daily concentration of a pesticide in soil or mud used as nesting matrix or material (soil concentrations only need to be defined for bees that are soil nesting or use soil/mud as nesting materials, e.g., *Osmia* sp., *N. melanderi*, *E. pruinosa*); concentration in µg a.i. per g soil/mud.
10. “Concentration.leaf” – Daily concentration of a pesticide in leaves used as nesting material (leaf concentrations only need to be defined for above-ground nesting bees that use leaf pieces as nesting materials, e.g., *M. rotundata*); concentration in µg a.i. per cm<sup>2</sup> leaf surface.

Two options are available in the model to provide the input data:

- 1) If “*MultiYearInput*” is switched “Off,” a single input file (*input.floral*) is used by the model and repeated each simulated year (the number of years simulated is defined by *Num.repeat.yr* in this case).
- 2) If “*MultiYearInput*” is switched “On,” a text file (“.txt”) is read in (*List.input.floral*). The first row of the text file states the number of years simulated and needs to correspond to the number of file names listed in the following rows of the file. In each following row, a file name (format “.csv”) is listed which identifies an input file organized as described above. At the beginning of each simulated year, the model reads the next input file from the list. An example of a file used as *List.input.file* is provided in Appendix B.

## 2.4. Submodels

### 2.4.1. Life cycle

Each simulated bee goes through its life cycle from egg through larva and cocoon to emerged bee. Males die at the end of the defined male post-emergent life span (*m.life*). Post-emergent females transition to nesting stage after a defined period (corresponding to maturation, *t.maturity*). The egg stage corresponds to the time period between egg laying by the nesting female and hatching of the larva. The egg stage is characterized solely by its development time (*dev.egg*) which is assumed to be determinate. Correspondingly, the larva stage is defined by its duration (*dev.larva*). The development times of eggs and larvae are assumed to be the same in females and males. In actual bees, the larvae consume the provision and grow to the maximum size during their life span. However, the consumption of the provision and growth are not represented explicitly in the model. The life stage “cocoon” in the model summarizes all developmental stages occurring after the cessation of feeding and growth until emergence from the nest (irrespective of whether the simulated bee species produces a cocoon or not). These include pre-pupa (5<sup>th</sup> larval instar), pupa and pre-emergent adults. Depending on the bee species, developing bees overwinter either as pre-pupae or as pre-emergent adults. The duration of the “cocoon” stage is determined by the emergence date from the nest (*emerge.doy*), rather than a fixed developmental time period, with separate inputs for female and male emergence dates (and ranges): *day.emerge.f* for females (and standard deviation around this date defined by *var.emerge.f*) and *day.emerge.m* for males (SD: *var.emerge.m*). If the model is set to simulate multivoltine (including bivoltine) life cycles (*Voltinism* = “multivoltine”), *emerge.doy* is set on the day the bee completes its development if it occurs prior to the latest emergence date (*latest.emerge*). Otherwise, *emerge.doy* is set in the same way as described for univoltine life cycles.

In-nest life stages (egg, larva, and cocoon) do not experience mortality in the model. Rather, mortality is applied at time of emergence from the nest, summarizing mortality occurring across in-nest life stages in bees. Accordingly, the maximum survival rate to emergence, *max.survival.e.f* (for females) and *max.survival.e.m* (for males), reflects the background mortality due to failure to develop prior to cocoon production and failure to emerge from the cocoon. The background mortality in the model simulates the mortality in bees in the field due to infestations by nest parasites or other unspecified causes of death before or after pupation.

Post-emergent adults (life stage “emerged”) do not experience mortality on a daily basis. Males die at the end of their defined post-emergence life span (*m.life*). Females spend a fixed number of days in the emerged life stage (defined by *t.maturity* and simulating the time between emergence and first nest building activity). Females have a probability of survival (*emerged.survival*) applied at the end of their “emerged” life stage. The daily survival rate of females in “nesting” life stage is derived from the model input defining the maximum adult life span, *max.nesting.life* and the probability, *p.max.nesting.life*, to reach this age. The probability of death on a given day is constant, i.e., it applies to all nesting bees in the simulation and does not change with their age.

## 2.4.2. Reproduction (nest building)

Once the simulated female bees reach the “nesting” life stage, they engage in brood cell production every day until they die. A nesting female can complete between 0 and *max.cells* on a given day. Each completed brood cell in the model contains an egg, i.e., a newly created bee agent in *life.stage* = “egg”. The daily rate of brood cell production is dependent on the nesting female age (*age.stage*) and the floral resource quality of the given day (calculated from the daily input). Note that nests are not represented explicitly in the model, i.e., it is not defined in the model when a nest with multiple brood cells is capped by the bee and a new nest cavity is used (or dug) to house new brood cells.

With the nesting female’s age, she decreases the rate of brood cell building, shifts to increasing male offspring production and decreases the provision sizes for both female and male offspring. In parallel, floral resource availability impacts the same measures: the lower the floral resource availability, the slower a female can produce new brood cells, the more brood cells with male offspring are produced and a smaller provision supplied to each offspring. Note that the shift to male offspring production with increasing nesting female age and decreasing resource availability is likely specific to solitary bee species in which females are larger than males. This is the case in *Osmia* sp., *Megachile rotundata* and *Eucera pruinosa*. Note that in *Nomia melanderi*, males are larger than females, and the shift in sex ratio due to nesting female age and resource availability may not apply; data on these relationships in *N. melanderi* could not be identified.

While these relationships are qualitatively well established in the literature for *Osmia* and *Megachile* (see Section 3.1), the functional relationships are not fully described. For the model, we assumed linear relationships because they correspond to the simplest assumptions. The two factors (nesting female age and floral resource availability) affecting the same measures (rate of nest building, sex ratio and offspring provision size) are assumed to act independently, i.e., their effects are additive.

In the model, the maximum number of brood cells produced by a nesting female is defined by the parameter *max.cells*, including both female and male offspring. The maximum ratio of female offspring in the brood cells produced on a given day is defined by the parameter *max.f.ratio*. The number of brood cells with female and male offspring constructed by each nesting female bee agent on a given day, and the provision size provided is calculated in three steps: 1) calculation of the proportional daily production rate of total brood cells dependent on female age and resource availability; 2) the sex ratio of brood cells dependent on nesting female age and resource availability; and 3) the relative provision size provided to offspring dependent on the same factors. The sex ratio is calculated as ratio of females / (females + males). The provision size is expressed as relative to the maximum provision size for each sex and is assumed to apply to both sexes. Note that the offspring sex ratio is calculated for each nesting

female and day in the model, and effectively corresponds to the probability of any brood cell produced by that female on the given day to be female.

### ***Calculation of daily resource availability from floral resource input***

In the floral resource input file (see Section 2.3.2), daily weather-related foraging opportunities, quality of floral resources available from crops and from natural and semi-natural areas (wildflowers) are defined. These three daily inputs can take values between [0, 1] whereby 0 means no foraging and no resource availability, respectively, on the given day. In addition, the proportion of foraging on crop is also included in the input file. This input can also take values between [0, 1]. A value of 0 means that the bees do not forage on crop but forage exclusively on wildflower resources. Conversely, a proportion of foraging on crop resources of 1 means that no foraging on non-crop resources occurs that day. In Appendix B, a description is provided of the input file and how it can be generated.

For values of proportion of foraging on crop > 0 and < 1, two alternative implementations can be used.

- a) If the interface parameter *stoch.crop.forag* is set to 'On', each nesting bee chooses a proportion of foraging on crop between 0 and 1. This effectively leads to an average of 50% of crop foraging on that day across a large simulated population of nesting females. However, the smaller the population, the higher the fluctuations around this average will be.
- b) If *stoch.crop.forag* is set to 'Off', the value defined in the input file will be used.

The two options are included in the model to capture different levels of information available about foraging of the bees in the landscape. Option a) allows to simulate scenarios without defining the proportion of foraging on crop, reflecting cases in which the preferences of the bees are not well understood when both crop and wildflower resources are available in the landscape at the same time. The uncertainty is captured partially by the implemented stochastic process. Note that this stochastic option always results in an average of 50% foraging on crop across the population. Option b) allows the definition of foraging on crop on a daily basis for scenarios assuming the preference of the bees are known. Note that if the proportion of foraging on crop is set to 0 in the input file, no foraging on crop occurs in both options and if it is set to 1, only foraging on crop occurs. The effective foraging on non-crop resources for each female and day corresponds to (1 - proportion of foraging on crop).

From these generalized definitions of the resource availability in the landscape (surrounding the nest location), the resource-related efficiency of brood cell provisioning, *prov.today*, is calculated in steps as follows:

1. The efficiency is set to the proportion of foraging from the input file. This reflects the proportion of the bees' day with weather conditions suitable for foraging. If the weather is suitable for foraging during the entire activity period of the bee on a given day, this value is 1 (see also Appendix B).
2. The efficiency is then split into foraging in crop (by the proportion from input) and foraging on wildflowers (the remainder).
3. For crop and wildflower resources, the relative efficiency is calculated separately by scaling it to the quality of crop and wildflower resources, respectively. Note that the quality from the input summarizes the distance between resource patch and nest site, the density of suitable flowers in the patch, and the effort needed by the bee to collect pollen and nectar from the flowers. The

input can represent different levels of detail of information available about those aspects (see also Appendix B).

4. The final daily resource-related efficiency of brood cell provisioning, *prov.today*, is the sum of the two efficiencies.

The daily value of *prov.today* is used for the calculation of the resource-related reproductive relationships described in the following paragraphs.

### **Daily number of brood cells (female and male offspring) produced by a nesting female**

The daily maximum number of brood cells produced per day is defined by the model parameter *max.cells*. The effective number of brood cells produced by a nesting female in a simulated day is progressively reduced dependent on the nesting female's age and the resource availability (defined by the floral resource input).

Equation 2.1 gives the relationship between the nesting female's age (*age.stage*) and the relative number of brood cells produced (*cell.age*) whereby *cell.age* can take values between [0, 1]. The parameter *a.cell.age* is derived from literature (see file "SolBeePop\_Tables.xlsx" and Section 3.2.1).

*Equation 2.1*

$$\text{cell.age} = \text{a.cell.age} \times \text{age.stage} + 1$$

Equation 2.2 gives the relationship between the daily resource-related efficiency of brood cell provisioning, *prov.today* (calculated from the floral resource input file, see above), and the relative number of brood cells produced (*cell.res*) whereby *cell.res* can take values between [0, 1]. The parameter *a.cell.resource* is derived from literature (see file "SolBeePop\_Tables.xlsx" and Section 3.2.2).

*Equation 2.2*

$$\text{cell.res} = \text{a.cell.resource} \times \text{prov.today} + (1 - \text{a.cell.resource})$$

The production rate of brood cells (female and male), *cell.prod*, that day is then calculated using Equation 2.3.

*Equation 2.3*

$$\text{cell.prod} = \text{max.cells} \times \text{cell.age} \times \text{cell.res}$$

In the model, the nesting female can only produce whole brood cells, i.e., the number of brood cells produced that day by the female corresponds to the rounded down whole number from *cell.prod*. The decimals from *cell.prod* are carried over to the next day and added to the new day's *cell.prod*.

### **Daily number of female offspring brood cells produced by an adult female**

Equation 2.4 gives the relationship between the nesting female's age (*age.stage*) and the relative ratio of female offspring produced (*sex.age*) whereby *sex.age* can take values between [0, 1]. The input parameter *a.sex.age* is derived from literature (file "SolBeePop\_Tables.xlsx" and Section 3.2.3).

*Equation 2.4*

$$\text{sex.age} = a.\text{sex.age} \times \text{age.stage} + 1$$

Equation 2.5 gives the relationship between the daily resource-related efficiency of brood cell provisioning, *prov.today* (calculated from the floral resource input file, see above), and relative ratio of female offspring produced (*sex.res*) whereby *sex.res* can take values between [0, 1]. The input parameter *a.sex.resource* is derived from literature (file “SolBeePop\_Tables.xlsx” and Section 3.2.4).

*Equation 2.5*

$$\text{sex.res} = a.\text{sex.resource} \times \text{prov.today} + (1 - a.\text{sex.resource})$$

The sex ratio of the brood cell production on the given day is calculated using Equation 2.6.

*Equation 2.6*

$$\text{sex.ratio} = \text{max.f.ratio} \times \text{sex.age} \times \text{sex.res}$$

If *cell.prod*  $\geq 1$ , a new brood cell (with a bee agent) is produced by the nesting female. The sex of the new offspring is determined stochastically whereby the probability of a female egg corresponds to *sex.ratio*. This process is repeated for each whole number in *cell.prod*. The decimal remainder is added to next day’s *cell.prod*.

### **Daily provision size provided to female offspring**

Each brood cell produced on a given day is assigned with a relative size of the provision, *prov.size*, whereby the maximum size is 1. In the solitary bees simulated by the model, provision sizes of offspring are directly related to the adult size of the developing bee (Klostermeyer et al. 1973). Accordingly, the smaller body size of adult male compared to female bees is reflected in their provision sizes. For the model, we assume that the proportional reduction in provisions size occurs irrespective of sex. Bee size at time of emergence has been linked with emergence success (see Section 3.1).

The relative provision size is dependent on the nesting female age, *age.stage* (Equation 2.7) and the daily resource-related efficiency of brood cell provisioning, *prov.today* (calculated from the floral resource input file, see above) (Equation 2.8). The input parameter *a.sex.resource* is derived from literature (file “SolBeePop\_Tables.xlsx” and Section 3.2.5).

*Equation 2.7*

$$\text{size.age} = a.\text{size.age} \times \text{age.stage} + 1$$

*Equation 2.8*

$$\text{size.res} = a.\text{size.resource} \times \text{prov.today} + (1 - a.\text{size.resource})$$

The relative provision size, *prov.size*, is calculated according to Equation 2.9. The input parameter *a.sex.resource* is derived from literature (file “SolBeePop\_Tables.xlsx” and Section 3.2.6).

*Equation 2.9*

$$\text{prov.size} = \text{size.age} \times \text{size.res}$$

The survival rate to emergence,  $e$ , is dependent on proportional to the relative provision size of offspring whereby  $\text{max.survival.e.f}$  and  $\text{max.survival.e.m}$  are inputs that define the maximum survival rates of females and males, respectively (Equation 2.10).

*Equation 2.10*

$$e = \text{max.survival.e} \times \text{prov.size}$$

### 2.4.3. Density dependence of brood cell production

Intra-specific competition for nest sites is considered as the density-dependent process in the model. The density-dependent process can be switched on or off for a given simulation (using *Density.dep* on the interface). The available nesting space is used as proxy for density-dependent resource limitation. With decreasing nesting resources, the brood cell production rates of nesting females are assumed to decline. The occupied brood cells correspond to the number of bees in the model in pre-emergent life stages. Two alternative mathematical formulations of the relationship are implemented and graphed in Figure 8.

The following characterizations of the density-dependence are needed (i.e., parameter values for the model):

- $\text{DD.max.cells.s}$ : maximum number of brood cells that could fit (theoretically) into the nesting site.
- $\text{DD.thresh.s}$ : maximum number of brood cells in the population that do not lead to density-dependent changes in brood cell production rates.

For the linear relationship (Figure 8, Top), no additional parameters are necessary. Note that the brood cell number leading to 50% reduction in brood cell production rate corresponds to Equation 2.11.

*Equation 2.11*

$$(\text{DD.max.cells.s} - \text{DD.thresh.s})/2$$

No reduction in brood cell production rate occurs if the total number of bees in in-nest life stages ( $\text{occ.cells}$ ) is below the threshold ( $\text{DD.thresh}$ ). If the number of bees in in-nest life stages exceeds the threshold, the factor for the brood cell production rate reduction,  $\text{rel.cell.prod}$ , is calculated using Equation 2.12 if the linear relationship is used and Equation 2.13 if the logistic relationship is used (Figure 8, Bottom), the slope of the logistic function is defined by the input parameter  $\text{DD.log.slope}$ .

*Equation 2.12*

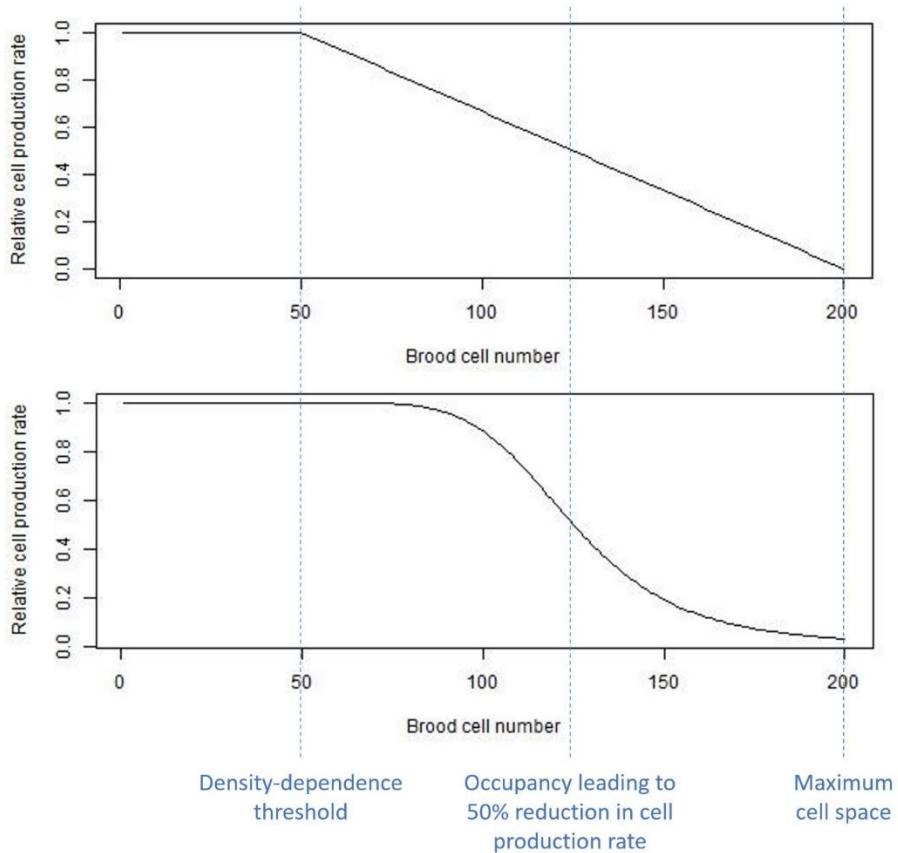
$$\text{rel.cell.prod} = (-1) \frac{\text{occ.cells} - \text{DD.thresh}}{\text{DD.max.cells} - \text{DD.thresh}} + 1$$

*Equation 2.13*

$$\text{rel.cell.prod} = \left( 1 + \exp \left( \ln(\text{occ.cells} - \text{DD.thresh}) - \ln \left( \frac{\text{DD.max.cells} - \text{DD.thresh}}{2} \right)^{\text{DD.log.slope}} \right) \right)^{-1}$$

The parameters for the density dependence function, *DD.max.cells.s*, *DD.thresh.s* and *DD.log.slope* are defined as interface parameters if *MultiYearInput* is 'Off'. In this case, each simulated year (if multiple years are simulated) has the same floral resource input, assuming identical environmental conditions. Accordingly, identical density-dependence parameters are assumed for each simulated year. If *MultiYearInput* is 'On', different floral resource input files are provided for each simulated year. In this case, the density dependence parameters need to be provided for each year in the file *List.input.floral*. This allows for the density dependence parameters to vary between years (see Section 2.3.2 and Appendix B).

Note that the density-dependent process includes the assumption that pre-emergent bees take up a brood cell space. This does not explicitly capture studies in which bees are released in pre-emergent life stages outside of available nesting space. In such studies, cocoons are generally incubated in the laboratory under identical conditions, ensuring that bees emerge from the cocoons within a short time period (e.g., semi-field or field studies with *Osmia* sp. or *M. rotundata*) which can be captured by the model. However, if emergence overlaps considerably with the nesting activity of adult females in simulations of studies with release of pre-emergent bees, the brood cell production rate may falsely be affected by density dependence until all released bees are emerged.

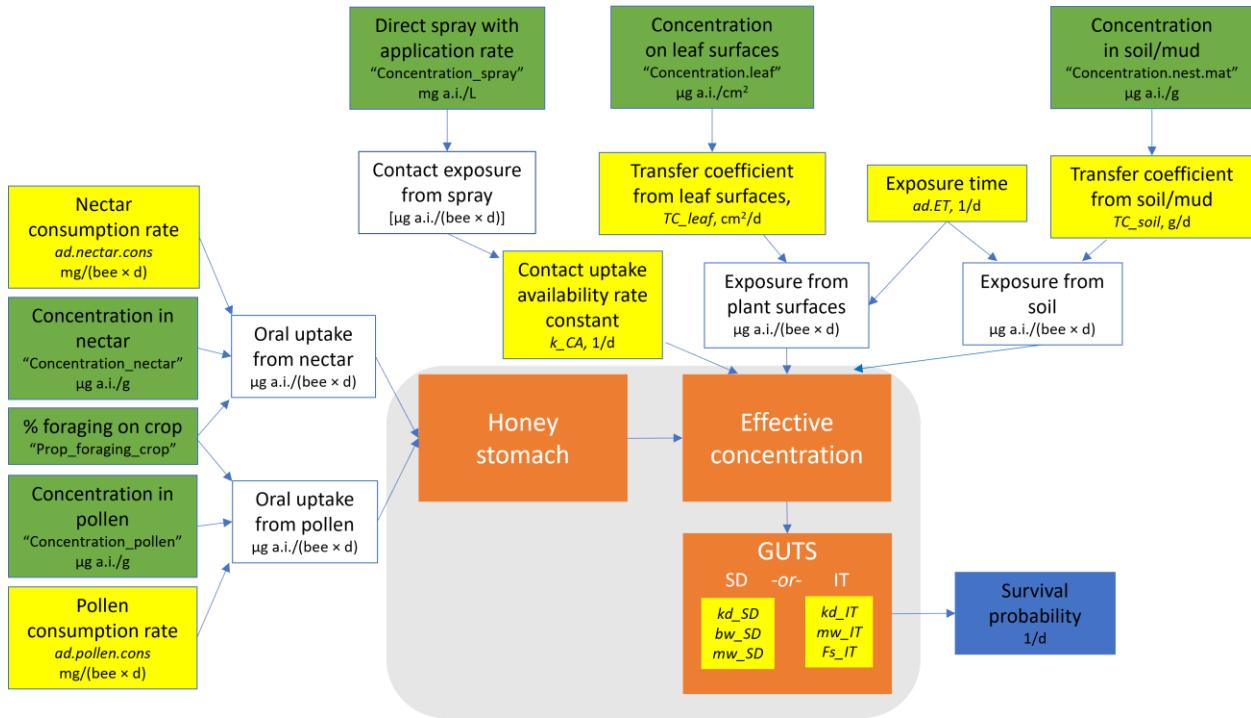


*Figure 8. Function shapes for the relationship between brood cell number (number of bee agents in pre-emergent life stages) and the relative reproductive rate of nesting females. Top: linear relationship. Bottom: logistic relationship.*

#### 2.4.4. Exposures and effects of post-emergent females (BeeGUTS)

##### *Exposures*

Post-emergent females can be exposed to a pesticide via multiple routes which can co-occur on a single simulated day. Thus, exposures are processed in the model to inform a single, daily effective concentration (Figure 9). Exposures and effects on post-emergent males are not simulated by SolBeePop because males are assumed to die within a short time period (*m.life*) after emergence, and they do not contribute to reproduction (i.e., mating is not explicitly represented).



*Figure 9. Overview of exposures (green, read from input time series) and effects on post-emergent females in the model. Boxes in green indicate values defined in the SolBeePop<sub>ecotox</sub> input (daily time series), yellow boxes indicate model parameters (parameter names listed), white boxes are calculations conducted by the submodel, and the blue box indicates the output of the submodel (survival probability). The orange boxes (on the grey background) indicate the exposure and effects in the bee, following the BeeGUTS concept (Baas et al. 2022). Note that the exposure via leaf surfaces and soil/mud are alternatives dependent on the bee's nesting strategy. The concentration of direct spray with application rate is adjusted to bee size (body surface, e.g., by using a body surface factor) in the input.*

The daily exposures from the different exposure routes are read from the input time series and are applicable to all females in post-emergent life stages as well as developing bees (see Section 2.4.5). The daily exposures include the concentration of a pesticide in nectar (from treated floral resources, in  $\mu\text{g a.i./g}$ ), in pollen (from treated floral resources, in  $\mu\text{g a.i./g}$ ), in direct spray (corresponding to the application rate in  $\text{mg a.i./L}$ ), and in soil or mud (in  $\mu\text{g a.i./g}$ ) or pesticide on leaf surfaces (in  $\mu\text{g a.i./cm}^2$  leaf area) (Figure 9).

The consumption of exposed (from treated crop floral resources) and non-exposed (from untreated semi-natural floral resources) is defined in an additional daily input time series, “Prop\_foraging\_crop”. The concentration in consumed nectar and pollen, respectively, is calculated assuming that the exposed food is diluted with unexposed food, unless Prop\_foraging\_crop = 1 in which case all nectar and pollen a bee consumes is assumed to originate from the treated source. The compound mass in nectar and pollen consumed by the bee is assumed to be digested and taken up in full on the same day by the bee, i.e., all compound in consumed nectar and pollen contributes to the effective exposure concentration of

the bee on a simulated day. This means that the stomach uptake rate,  $k_{SR}$ , applied in BeeGUTS to account for digestion of exposed sugar solution in acute oral honey bee toxicity tests (Baas et al. 2022) is not considered in SolBeePop. The daily consumption rate is assumed to be constant throughout a female's post-emergent life and not dependent age. The daily nectar and pollen consumption is scaled according to weather-related foraging: if foraging is limited or not occurring at all, the food consumption is assumed to be reduced accordingly. Daily nectar and pollen consumption excludes nectar and pollen collected by nesting females for brood cell provisioning. This corresponds to the assumption in BeeGUTS that the stomach (of honey bees) is inert and no uptake of compounds occurs prior to digestion (Baas et al. 2022). Pollen collected for brood cell provisioning are transported externally in specialized hair (scopa) by most solitary bees, including model species (Michener 2007; Danforth et al. 2019). Thus, uptake of compound present in pollen by the bee is not considered relevant. The total compound,  $C_{stomach}$  (ng a.i./bee), taken up per bee and day due to food consumption is calculated according to Equation 2.14.

#### *Equation 2.14*

$$C_{stomach} = ((ad.\text{nectar}.\text{cons} * conc.\text{nectar}) + (ad.\text{pollen}.\text{cons} * conc.\text{pollen})) \\ * (prop.\text{forag}.\text{day} * crop.\text{forag})$$

Where  $ad.\text{nectar}.\text{cons}$  and  $ad.\text{pollen}.\text{cons}$  are the daily nectar and pollen consumption rate of post-emergent females, respectively (model parameters),  $conc.\text{nectar}$  and  $conc.\text{pollen}$  are the concentrations of the pesticide in nectar and pollen from treated crop resources (from daily input time series),  $prop.\text{forag}.\text{day}$  is the proportion of the day available for foraging and  $crop.\text{forag}$  is the proportion of foraging on the treated crop resource that day (both read from daily input time series).

If a spray application occurs on a given day ("Concentration\_spray" > 0), a proportion of post-emergent females are assumed to be exposed to the defined amount of compound of direct spray on the application day. The proportion of exposed post-emergent females is defined by the proportion of foraging occurrence on application day. If bees cannot forage on application day ("Prop\_foraging\_day" = 0), no exposure to direct spray occurs. If foraging conditions are optimal ("Prop\_foraging\_day" = 1), all bees are assumed to be foraging during application and can be exposed to direct spray. If "Prop\_foraging\_day" falls between 0 and 1, each simulated post-emergent female has a maximum probability of "Prop\_foraging\_day" to be exposed to direct spray. This means that an individual simulated bee can either receive the entire exposure per bee from direct spray or no exposure at all (no scaling of the amount of exposure from direct spray). The probability of exposure of a bee from direct spray can be further reduced by the proportion of foraging on the treated crop. If bees are assumed not to forage on the treated crop on application day ("Prop\_foraging\_crop" = 0), no exposure to direct spray occurs. Correspondingly, individual post-emergent females have an increasing probability to be exposed to direct spray with their proportion of foraging on the treated crop, whereby "Prop\_foraging\_crop" = 1 means that all post-emergent females are foraging exclusively in the treated crop.

The concentration of the direct spray in the input time series is given as mg a.i./L and corresponds to the application rate. A single encounter with direct spray per day is assumed (i.e., a bee is assumed to fly through direct spray no more than once per day). The compound mass reaching a bee from direct spray is assumed to correspond to the compound mass in 1 µL of the spray. The compound is assumed to stay on the cuticula of the bee and taken up to contribute to the effective exposure following simple kinetics

according to Baas et al. (2022). The kinetics are applied per time step of the GUTS submodel (see details below) (Equation 2.15).

#### *Equation 2.15*

$$C.\text{direct.spray}(t + 1) = C.\text{direct.spray}(t) * e^{-\frac{k_{CA}}{t.guts}}$$

Where  $C.\text{direct.spray}$  is the concentration of direct spray (ng a.i./bee) contributing to the effective concentration,  $k_{CA}$  is the uptake rate (contact availability rate constant; Baas et al. 2022) and  $t.guts$  is the time step of the GUTS model ( $t.guts$  defines the number of GUTS iterations calculated per SolBeePop<sub>ecotox</sub> time step; see below). The uptake rate of  $k_{CA} = 0.4$  from Baas et al. (2022) is used as default in SolBeePop<sub>ecotox</sub> and results in exposures from direct spray contributing to a bee's effective exposure that can extend beyond a single simulated day (i.e., the exposure is carried over to the following day).

Bee may also come into contact with exposed matrices during their nesting activity. Exposure through contact to exposed soil in soil-nesting bees, including *N. melanderi* and *E. pruinosa*, and bees using soil or mud in the construction of above-ground brood cells, including *Osmia sp.* is considered. In leaf-cutting bees, including *M. rotundata*, exposure due to contact to exposed leaves is considered instead. Compound from exposed nesting material ( $\text{conc.mat}$  in µg a.i./g soil or µg a.i./cm<sup>2</sup> leaf) is assumed to be taken up at a constant rate  $TC$  (model parameters  $TC_{soil}$  in g/d or  $TC_{leaf}$  in cm<sup>2</sup>/d, respectively) while the bee is interacting with the material, whereby the contribution to the effective exposure from contact ( $C.\text{contact.mat}$  in ng a.i./bee) with exposed nesting material is calculated in each GUTS time step using Equation 2.16.

#### *Equation 2.16*

$$C.\text{contact.mat} = TC * (\text{conc.mat} * 1000)$$

Contact exposure to nesting material contributes to the effective concentration (GUTS external exposure) for either a defined part of the day (*ad.ET*) during which a nesting bee of the species is reported to interact with nesting material (collection of nesting material and placement in the brood cell or active nest digging) or for the entire day if *Exposure.resting.soil* = TRUE. The latter case can be used if soil-nesting females are assumed to spend most of their day in direct contact with the soil either digging or provisioning brood cells or resting within the nest. Compound transferred from nesting material to the bee matrices is assumed not to stay on the cuticula of the bee, i.e., it does not carry over to the following day.

## **Effects**

The effective concentration is the sum of all three exposure routes ( $C.\text{stomach}$ ,  $C.\text{direct.spray}$ ,  $C.\text{contact.mat}$ ) to post-emergent females and corresponds to the external concentration in the generalized unified threshold model for survival (GUTS) (Jager et al. 2011; Ashauer et al. 2013; Ashauer et al. 2016; EFSA Panel on Plant Protection Products and their Residues (PPR) et al. 2018; Jager and Ashauer 2018). GUTS is a simplified toxicokinetic-toxicodynamic model for the calculation of the survival probability corresponding to the external concentration. Two versions of the GUTS model have been developed and were recommended to be tested as alternatives (EFSA Panel on Plant Protection Products and their Residues (PPR) et al. 2018). GUTS-SD assumes stochastic deaths based on a

distribution of survival thresholds to internal concentrations applicable across individuals in a population. GUTS-IT assumes individual thresholds of mortality based on internal concentrations. In SolBeePop<sub>ecotox</sub>, both GUTS models are implemented as alternatives. In case of GUTS-IT, individual-level thresholds are assigned from a distribution defined by the GUTS-IT parameters to each bee at time of model initialization or ‘creation’ of a new bee in the model (at time of completion of a brood cell by a nesting female). Either GUTS model is applied in sub-daily time steps (number of steps per day defined by *t.guts*) whereby the external (=effective) concentration is recalculated in each time step because *C.direct.spray* changes due to uptake kinetics (Equation 2.15), and *C.contact.mat* is only contributing to the external concentration until the number of guts steps conducted correspond to *ad.ET* (see above). *C.stomach* remains constant during a simulated day. The survival probability from GUTS is applied to individual bees in the model as a probability of survival in addition to assumed background mortality rates that are independent of exposures (see Section 2.4.1). In the model, the survival probability due to exposures is only calculated if the external concentration is larger than 0; otherwise, no reduction in survival due to effects from exposures is assumed.

## 2.4.5. Exposures and effects to in-nest life stages

### *Exposures*

In-nest life stages (egg through pre-emergent adult) can be exposed to a pesticide in their provision (nectar and/or pollen) or from exposed nesting material. Thereby, exposures are not distinguished between oral or contact uptake because the developing bee is assumed to be in constant contact with the provision that they completely consume by the end of their larval development. In addition, the provision is in contact with the nesting material prior to consumption. As the larva grows, it fills the space in the brood cell and thus, comes into contact with the nesting material. Accordingly, transfer of pesticide from nesting material (soil or leaves) to the provision cannot be distinguished from the transfer to the growing larva.

The pesticide concentration in the provision (prior to contact with exposed nesting material) is determined by the concentration in nectar (from treated floral resources, in µg a.i./g) and pollen (from treated floral resources, in µg a.i./g) collected by the nesting female on the day of the completion of the brood cell, and by the composition of the provision, defined by the proportion of nectar in the provision (*nectar\_prop*) (Figure 10). The proportion of exposed (from treated crop floral resources) and non-exposed (from untreated semi-natural floral resources) nectar and pollen is defined by “*Prop\_foraging\_crop*” on the day of brood cell completion, assuming that the exposed food is diluted with unexposed food, unless *Prop\_foraging\_crop* = 1 in which case all nectar and pollen a bee consumes is assumed to originate from the treated source. The concentration of pesticide in the provision (*c.provision*, in µg a.i./g) is calculated according to Equation 2.17.

### *Equation 2.17*

$$c.provision = ((nectar\_prop * conc.nectar) + ((1 - nectar\_prop) * conc.pollen)) * crop.forag$$

Where *conc.nectar* and *conc.pollen* are the concentrations of the pesticide in nectar and pollen from treated crop resources and *crop.forag* is the proportion of foraging on the treated crop resource that

day (both are defined by the daily input time series). The compound mass in the provision is assumed to be taken up completely by the developing bee. No dissipation or degradation of the pesticide is assumed prior to uptake by the bee. The pesticide concentration taken up by the provision prior to consumption by the larva) from soil or mud by soil-nesting bees (including *N. melanderi* and *E. pruinosa*) or above-ground nesting bees that use soil or mud in the construction of the brood cells (including *Osmia* sp.), is calculated from the concentration in soil defined in daily input time series on the day of brood cell completion (Figure 10). For soil-nesting bees, the provision (and subsequently, the developing bee) is assumed to be in contact with the exposed soil for extended time, resulting in an assumed equilibrium of pesticide concentration between the soil and the provision. However, equilibrium is only assumed to occur if the pesticide concentration in the provision (from compound in nectar and pollen) is lower than in the soil. If the concentration in the provision prior to exposure to the soil is higher than in the soil, the exposure concentration calculated from nectar and pollen ( $c_{provision}$ , see Equation 2.17) is assumed to remain as-is. If the concentration in the provision prior to exposure to soil is lower than in the soil (including no exposure from nectar and pollen), the concentration in soil is the assumed concentration in the provision. In bees using soil or mud for capping brood cells in above-ground cavities (including *Osmia* sp.), the concentration in a single partition (calculated using the mass of a single partition,  $SM$ ) is compared to the pesticide concentration in the provision prior to exposure to the partition. If the compound mass in the partition is higher than the compound mass in the provision, the compound mass from the partition is used to calculate the new concentration in the provision. Correspondingly, if a leaf-cutting bee species (including *M. rotundata*) is simulated, the compound mass corresponding the surface area of one brood cell ( $SA_i$ ) is compared to the compound mass in the provision, and used as exposure in case it results in a higher concentration in the provision than present from exposures of nectar and pollen.

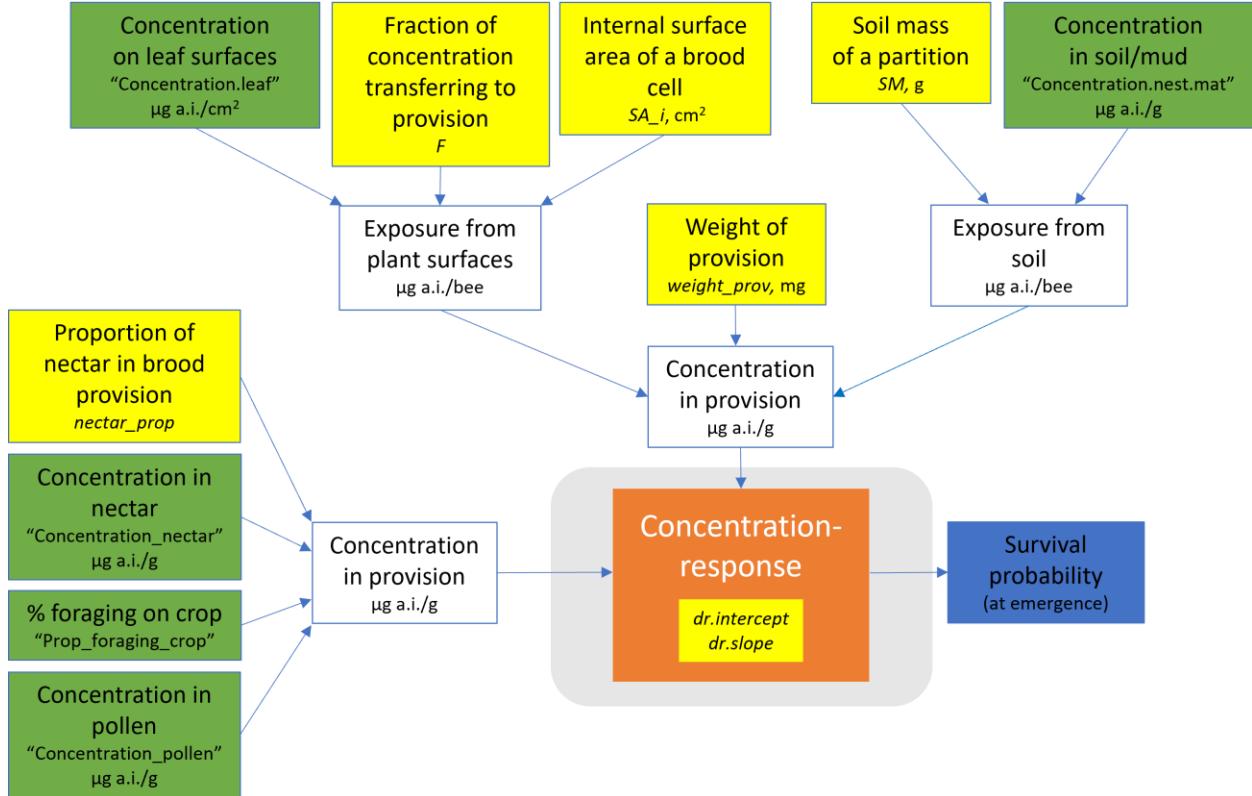


Figure 10. Overview of exposures (green, read from input time series) and effects on in-nest life stages in the model. Boxes in green indicate values defined in the SolBeePop input (daily time series) whereby the concentration on the day of the completion of the brood cell (or 'creation' of a bee in egg stage in the model) determines the concentrations relevant for that bee. Yellow boxes indicate model parameters (parameter names listed), white boxes are calculations conducted by the submodel, and the blue box indicates the output of the submodel (survival probability of the bee at time of emergence), implemented as a concentration-response function.

## Effects

The concentration in the provision is assumed to correspond to a constant, chronic exposure of the developing bees. The survival rate due to the exposure of in-nest life stages is applied at the time of emergence, summarizing pre-emergent deaths. The reduced survival probability ( $P_{survival}$ ) is applied in addition to and independent of the background survival rate in the absence of exposure (see Section 2.4.1). The survival probability due to exposure is calculated as a concentration-response function (Equation 2.1).

*Equation 2.18*

$$P_{survival} = dr.intercept + dr.slope * \log_{10} concentration$$

Where *dr.intercept* is the intercept of the function and *dr.slope* defines the slope (both are model parameters).

# 3. DATA EVALUATION FOR MODEL CONCEPUTALIZATION AND PARAMETERIZATION

## 3.1. Species-specific trait data

Data relevant for the development and parameterization of SolBeePop were compiled in data tables following Pop-GUIDE (Phase 2) (Raimondo et al. 2021). Tables for the model species (*E. pruinosa*, *M. rotundata*, *N. melanderi* and *Osmia* sp.) are presented in Appendix A. The data compilation makes data gaps explicit, and the realism and precision of available data are addressed. Default trait values used for the simulations with the model (and ranges, where applicable) were derived from this data compilation, and are listed for each species in the file “SolBeePop\_Tables.xlsx”.

The trait-specific data compilation facilitates the revision of parameter values used for model simulations if new data becomes available. Additional bee species can be simulated with the model based on corresponding data compilations.

## 3.2. Estimating relationships of reproductive output

In solitary bees, fecundity (total brood cells, containing one egg each, produced per female) is mainly determined by mature adult life span. In addition, the resource availability, particularly the availability of pollen and nectar influences the rate of brood cell provisioning, and accordingly, the life-time eggs produced per female (Goodell 2003). In species that build strings of brood cells in cavities, the first batch of brood cells contain female eggs, and the last batch male eggs, resulting in the earlier emergence of males (Hurd et al. 1974; Bosch et al. 2001; Pitts-Singer and Cane 2011). The ratio of female to male eggs produced may shift with the female bee’s age: early in the season, more female offspring is produced. Towards the end of the season (and the life-time of the female), she produces more male eggs (Torchio and Tepedino 1980; Bosch and Vicens 2005; Giejdasz et al. 2016). The shift in offspring sex ratio with increasing female age occurs in parallel with declining provisioning activity and provisioning sizes provided to each offspring. While resource availability impact provisioning rates and sizes, the shift related to female age has been mainly attributed to reduced foraging capacity (Tepedino and Torchio 1982a; Bosch and Vicens 2005).

In the model, we consider both factors impacting brood cell production by nesting females: the decline in brood cells produced dependent on female age, and the reduction in brood cell production rate with decline in floral resource availability. In response to decreasing habitat quality, females will a) reduce the total daily egg laying rate (Kim 1999; Goodell 2003; Peterson and Roitberg 2006b), b) shift to a higher rate of male egg laying (Bosch and Vicens 2005), i.e., reducing the rate of female offspring production, and c) reduce sizes of provisions, lowering the offspring’s chance of survival to emergence (Tepedino and Torchio 1982b; Bosch and Kemp 2004; Bosch and Vicens 2006; Bosch 2008).

While these relationships are qualitatively well established in the literature, the functional relationships are not fully described. For the model, we will assume linear relationships because they correspond to the simplest assumptions. The two factors (nesting female age and floral resource availability) affecting the same measures (rate of nest building, offspring provision size and sex ratio) are assumed to act independently, i.e., their effects are additive. In this section, we describe the estimation of the parameters of the linear relationships from available literature data. Due to the limited data availability, the relationships are applied across simulated bee species even though relationships are derived from different empirical studies conducted with different species (*Osmia* sp., *Megachile* sp.). Bee species lacking any of the relationships can be captured by setting the corresponding parameter to 0 (*a.cell.age*, *a.sex.age*, *a.size.age*, *a.cell.resource*, *a.sex.resource*, *a.size.resource*).

### 3.2.1. Proportional brood cell production rate dependent on nesting female age

Bosch and Vicens (2005) conducted a 2-year study with *Osmia cornuta* with the goal to identify parental investment into female and male offspring. The authors reported the brood cells produced per female and nesting day for the first half (H1) and second half (H2) of the nesting period at the study site for both study years (Table 2).

The split date between H1 and H2 was identified after the end of the study period as the date when 50% of all brood cells had been produced. In study year 1994, the split date was 24 March and in 1995, 30 March. The first nesting activity was observed on 6 March 1994 and 8 March 1995, respectively. In 1994, 44 females were engaged in nesting activity over 52 days in total, and in 1995, 42 females were nesting over 50 days in total.

For the estimation of the relationship between female age and daily brood cell production rate, we assumed that the two halves of the study periods correspond to two age classes of the females, i.e., females in H2 were assumed to be, on average, 26 and 25 days older than females in H1 in 1994 and 1995, respectively. The slope of the linear relationship between the nesting female's age and the relative number of brood cells produced daily is described by Equation 3.1.

*Equation 3.1*

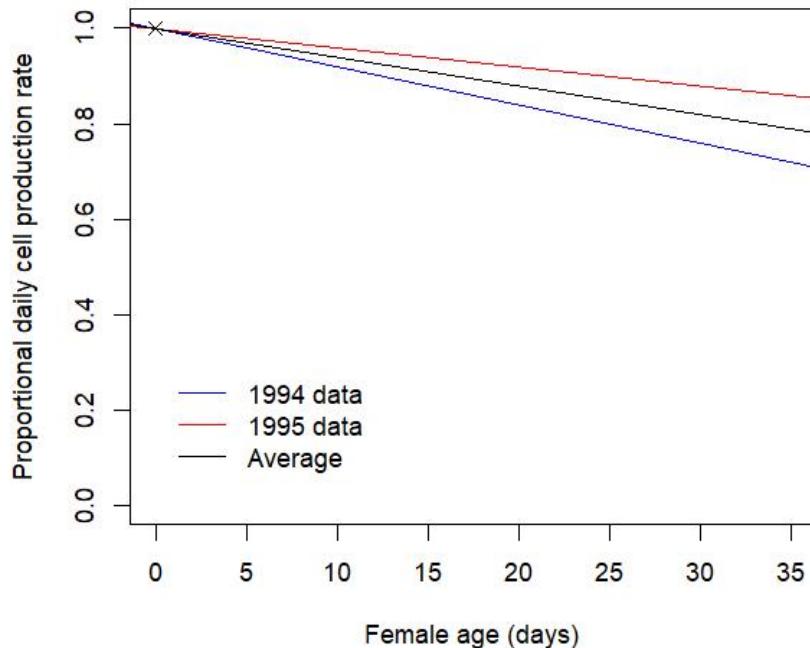
$$a.cell.age = \Delta \text{ cells} / \Delta \text{ age}$$

In Table 2, the estimated relationship, *a.cell.age*, is listed for the data from the two study years. The resulting linear relationships are shown as graphs in Figure 11. The estimates for *a.cell.age* are used as parameter range across simulated bee species in the model because no quantitative data for other species could be found in the literature. The intercept of the linear relationship is set to 1 because it is assumed that the maximum rate of brood cell production occurs at the beginning of a female's nesting activity (*age.stage* = 1).

The quantitative relationship listed in Table 2 should be regarded as highly uncertain because the relationship was derived from study data that was not designed to inform the relationship. Nesting bee ages were not recorded in the study and females building nests across the first half of the nesting season already includes bees with above-average life spans (average life span of post-emergent *Osmia* females: 20-25 days).

*Table 2.* Brood cells/female/day (mean  $\pm$  SE) of *O. cornuta* by study year and half season (data from Bosch and Vicens 2005, Table 1). The proportional difference,  $\Delta$  brood cells, is calculated as (brood cells (H2) – brood cells (H1))/brood cells (H1).

Study year	Brood cells H1	Brood cells H2	$\Delta$ brood cells	$\Delta$ age	$a.cell.age$
1994	0.78 $\pm$ 0.03	0.61 $\pm$ 0.04	-0.218	26	-0.008
1995	0.59 $\pm$ 0.03	0.53 $\pm$ 0.04	-0.102	25	-0.004
				Average:	-0.006



*Figure 11.* Linear relationship between days into *O. cornuta* nesting season (corresponding to nesting female age) and production of brood cells/female/day by study year and half season (data from Bosch and Vicens 2005, Table 1). The relationship is assumed to be proportionally declining from the maximum rate occurring on the first day of nesting.

### 3.2.2. Proportional brood cell production rate dependent on resource availability

Three studies were identified providing quantitative data relevant for the relationship between brood cell production rate and resource availability in solitary bees. (1) Goodell (2003) conducted an experiment with *Osmia pumila* in a greenhouse setting where bees were treated with two levels of floral resource availability (in a cage) and cleptoparasites were either present or absent (all combinations tested). (2) Kim (1999) conducted a similar study with *Megachile apicalis* but did not introduce parasites

into the cages with the nesting female bees. (3) Peterson and Roitberg (2006a) studied *M. rotundata* in a semi-field study with tents set up over flowering alfalfa fields, providing three resource levels. In the following, the three studies and the relevant data are summarized.

In the study by Goodell (2003), it can be assumed that all days provided good conditions for foraging due to the green house setting. From the reported results, we estimated the relationship between the average daily brood cell production per female (presented in Goodell (2003), Figure 4A) and the average floral units per female (presented in Goodell (2003), Figure 3). Data from the figures was extracted using ‘WebPlotDigitizer’ (<https://apps.automeris.io/wpd/>).

On average, the ‘sparse’ treatment provided 0.704 floral units per bee for each floral unit in the ‘rich’ treatment. Females constructed on average 1.16 brood cells per day in the sparse floral treatment and 1.55 brood cells in the rich treatment in the absence of the cleptoparasite. In the cages where the cleptoparasite was introduced, females produced on average 0.85 brood cells per day in the sparse vs. 1.45 in the rich treatment (Table 3). The slope of the linear relationship between the nesting female’s age and the relative number of brood cells produced daily is described by Equation 3.2. For the relative relationship, it is assumed that the daily brood cell production rate is proportional to the maximum daily brood cell production rate occurring if the resource availability is optimal, corresponding to *prov.today* = 1 (see Section 2.4.2). Accordingly, the intercept of the linear relationship is calculated according to Equation 3.3 in the model. Daily brood cell production rates < 0 are set to 0 in the model. This corresponds to the assumption that no brood cell production occurs on days with inclement weather (resulting in low foraging activity) or the lack of suitable floral resources within the bee’s foraging range.

$$\text{Equation 3.2} \quad a.\text{cell.resource} = \Delta \text{ cells} / \Delta \text{ resource}$$

$$\text{Equation 3.3} \quad \text{Intercept} = 1 - a.\text{cell.resource}$$

In the study by Kim (1999), floral resources were provided as bouquets of cut thistles, with low resource availability corresponding to two bouquets of cut thistles spiked with 5 drops of 50% sucrose solution each, and high resource availability to four bouquets of cut thistles spiked with 5 drops of 50% sucrose solution each. For the purpose of estimating the relative impact of resource availability on offspring sex ratio, we assumed that the high resource treatment provided double the resource compared to the low resource treatment. The slope estimate derived from these data are listed in Table 3.

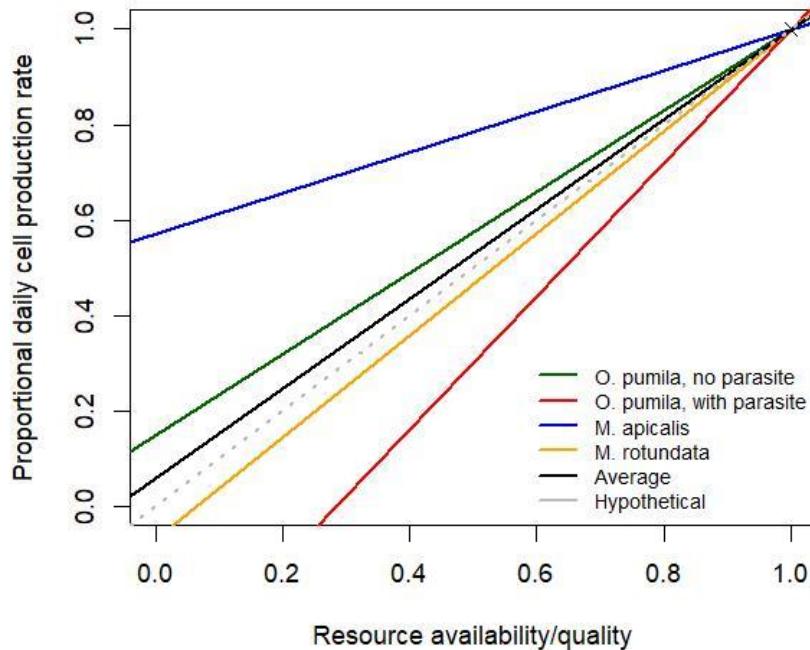
In the study by Peterson and Roitberg (2006a), three resource levels were achieved by covering parts of flowering alfalfa fields with mesh tents whereby in the high resource treatment level, the entire tent area ( $6 \text{ m}^2$ ) was covered with alfalfa plants. In the medium treatment level, half the area was covered with alfalfa plants, and in the low level, three quarters. The total number of brood cells per treatment (25 females per tent) at the end of the nesting season was recorded, i.e., no daily brood cell production data were available. To use the relationship, the data were used as relative to the highest treatment (set to 1) in Table 3.

In Figure 12, the relationships from the three studies are shown graphically. The range of parameters of the relationship derived from the study data (Table 3) show the considerable uncertainty in the quantitative relationship. The uncertainty is introduced due to limitations of quantifying the resource level available to the bees: the optimal resource level that allows bees the highest reproductive rate is not defined, and the count of flower heads or flowering area is an incomplete measure of effective

resource availability. The testing of different bee species (and in case of the study by Goodell (2003), different parasite treatments) introduces additional variability. Lastly, the relationships may not be linear in reality. The data from Peterson and Roitberg (2006a) may be considered the most relevant because the study was conducted under semi-field conditions and had the highest sample size (6-7 repetitions per treatment). It also is directly relevant for one of our model species (*M. rotundata*). For the default parameters used in the model across bee species, the average *a.cell.resource* across data sets (as shown in Table 3) or the data from Peterson and Roitberg (2006a) should be considered. It is assumed that no brood cell production occurs on days with *prov.today* = 0 (see Section 2.4.2), corresponding to days with weather conditions not allowing foraging or the complete absence of floral resources within the foraging range of the nesting bee. In the model, no brood cell production is assumed to occur if the resource availability is 0 (*prov.today* = 0). The relative brood cell production rate cannot drop below 0. Thus, a steepness of the relationship of *a.cell.resource* = 1, shown as "hypothetical" in Figure 12, may be considered as default relationship in the model.

*Table 3. Average brood cells/female/day of *O. pumila* and *M. apicalis* dependent on treatment (data from Goodell 2003, Figures 3 and 4A and Kim 1999, Figure 1A, respectively), and *M. rotundata* average total brood cells per treatment relative to brood cells in highest treatment (data from Peterson and Roitberg 2006, Fig. 2A). The proportional difference,  $\Delta$  brood cells, is calculated as (brood cells (sparse) – brood cells (rich))/brood cells (rich).*

Study	Species	Clepto-parasite	Sparse floral resources	Medium floral resource	Rich floral resources	$\Delta$ brood cells	$\Delta$ resource	<i>a.cell.resource</i>	Intercept
Goodell 2003	<i>O. pumila</i>	Absent	1.16		1.55	0.252	0.296	0.851	0.149
Goodell 2003	<i>O. pumila</i>	Present	0.85		1.45	0.414	0.296	1.399	-0.399
Kim 1999	<i>M. apicalis</i>	--	1.24 ± 0.08 (SE)		1.58 ± 0.08 (SE)	0.215	0.5	0.43	0.57
Peterson and Roitberg 2006	<i>M. rotundata</i>	--	0.20	0.41	1	0.8 (high to low)	0.75 (high to low)	1.07	-0.07
							Average:	0.94	0.063



*Figure 12. Linear relationship between resource availability (or quality) and production of brood cells/female by study (data for *O.pumila* from Goodell 2003; data for *M. apicalis* from Kim 1999; data for *M. rotundata* from Peterson and Roitberg 2006). The average uses the average steepness across data sets without considering sample sizes. The hypothetical relationship is the diagonal with  $a.cell.resource = 1$ . Proportionally highest brood cells production rate is assumed to occur at optimal resource availability of 1.*

### 3.2.3. Offspring sex ratio dependent on nesting female age

We derived an estimation of the relationship between nesting female age and offspring sex ratio from the study by Bosch and Vicens (2005; introduced in Section 3.2.1) and Seidelmann et al. (2010). Note that the authors report the sex ratio of the offspring as  $r_d$  = females/male. In the model, we use the female sex ratio:  $r_m$  = females/(females+males) =  $r_d/(r_d + 1)$ . The sex ratio reported in Table 4 is converted to  $r_m$ . The female nesting age was not reported directly in the study, but the days between the first and second half of the nesting season.

Seidelmann et al. (2010) marked individual nesting females of *O. bicornis* (=rufa) and assessed the impact of multiple factors on offspring sex ratio, including the timing of offspring production. The start of each study year's nesting season was determined as the day with the first nesting activity observed. The sex ratio was assessed per completed nest. Each nest was assigned with the season day, calculated as the intermediate date between start and completion of the nest, with respect to the season start. Linear effects models were applied, and the linear relationship between season day and offspring sex ratio (females per total offspring) was reported (Seidelmann et al. 2010, Table 3).

The slope of the linear relationship between the adult female's age and the relative number of brood cells produced daily is described by Equation 3.4.

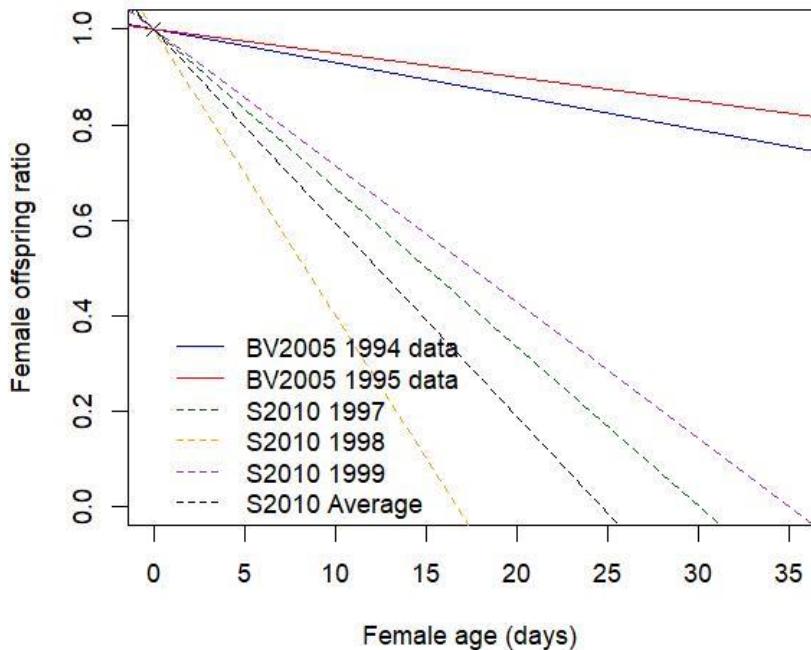
*Equation 3.4*

$$a.sex.age = \Delta \text{ sex ratio} / \Delta \text{ age}$$

In Table 4, the estimated relationship,  $a.sex.age$ , is listed for the data from the two studies. The intercept of the linear relationship is set to 1 because it is assumed that the maximum female sex ratio of brood cells (probability to produce female offspring) occurs at the beginning of a female's nesting activity ( $age.stage = 1$ ). Figure 13 shows the linear relationship as graph. The estimates for  $a.sex.age$  are used as parameter range across simulated bee species in the model because no quantitative data for other species could be found in the literature.

*Table 4. Sex ratio,  $f/(f+m)$ , of *O. cornuta* by study year and half season (BV2005: data from Bosch and Vicens 2005, Table 1). The difference,  $\Delta$  sex ratio, is calculated as (sex ratio (H2) – sex ratio (H1)) and of *O. bicornis* by study year and season day (S2010: data from Seidelmann et al. 2010, Table 3). The relationship from Seidelmann et al. 2010 (S2010) is used as default model parameterization.*

Study	Study year	H1	H2	$\Delta$ sex ratio ( $f/(f+m)$ )	$\Delta$ age	$a.sex.age$
BV2005	1994	0.462	0.281	-0.181	26	-0.007
BV2005	1995	0.415	0.286	-0.129	25	-0.005
BV2005					Average:	-0.006
S2010	1997					-0.0333
S2010	1998					-0.0599
S2010	1999					-0.0286
S2010					Average:	-0.0406



*Figure 13. Linear relationship between days into *O. cornuta* nesting season (corresponding to nesting female age) and ratio of female offspring produced by study year and half season (BV2005, data from Bosch and Vicens 2005, Table 1) and data on *O. bicornis* from Seidelmann et al. (2010), Table 3 (S2010). The relationship is assumed to be proportionally declining from the maximum rate occurring on the first day of nesting.*

A decline in female offspring production with nesting female age was also observed by Giejdasz et al. (2016) in a study with *O. bicornis*. In bees that built brood cells in more than one nest,  $0.7 \pm 0.1$  offspring were female in nests 1, declining to  $0.3 \pm 0.06$  females in nests 3 and 4. Note that females build brood cells in only one nest at a time. Because the dates of starting or completing a nest or nesting female ages were not reported in the article, a quantitative relationship between offspring sex ratio and nesting female age could not be derived from these data.

The two quantitative data sets suggest very different relationships between nesting female age and offspring sex ratio. Note that in Bosch and Vicens (2005), the offspring sex ratio in the first half of the season is already male-biased with a significant increase of this bias in the second half of the season. The relationship derived from this data set would suggest that the sex ratio remains female biased (assuming that the bees start the season with female-biased offspring production). This is contradictive to the data presented.

In contrast, the relationship estimated from Seidelmann et al.'s linear effects models suggest that females will produce males only toward the end of their adult lives which is in line with the literature (Bosch and Vicens 2005; Seidelmann 2006; Seidelmann et al. 2010; Giejdasz et al. 2016). For the model, we use the average relationship from Seidelmann et al. (2010) as default assumption.

### 3.2.4. Offspring sex ratio dependent on resource availability

In an experiment with *Megachile apicalis*, Kim (1999) compared the brood cell completion rate, the brood cell weight, and the female offspring ratio dependent on the floral resource treatment. The female bees were held in a cage and either presented with low resource availability (two bouquets of cut thistles spiked with 5 drops of 50% sucrose solution each) or high resource availability (four bouquets of cut thistles spiked with 5 drops of 50% sucrose solution each). Each female bee in the trial was presented with both resource levels.

For the purpose of estimating the relative impact of resource availability on offspring sex ratio, we assume that the high resource treatment provided double the resource compared to the low resource treatment. The slope of the linear relationship between the resource availability and the relative number of brood cells produced daily is described by Equation 3.5.

*Equation 3.5*

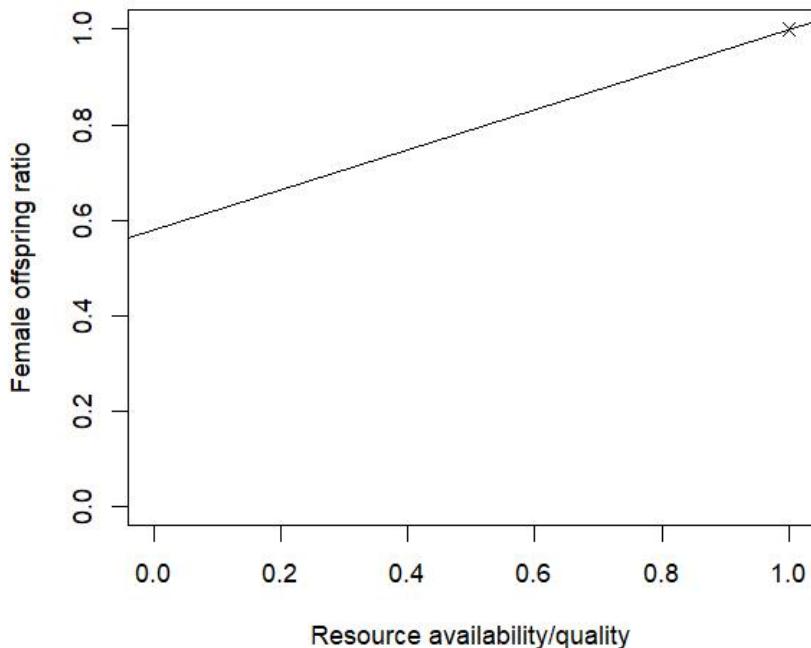
$$a.sex.resource = \Delta \text{ sex ratio} / \Delta \text{ resource}$$

In Table 5, the slope of the estimated linear relationship, *a.sex.resource*, is listed for data from Kim (1999, Figure 2C). Data from the figure was extracted using ‘WebPlotDigitizer’ (<https://apps.automeris.io/wpd/>). Figure 14 shows the linear relationship graphically.

The estimates for *a.sex.resource* are used as parameter range across simulated bee species in the model because no quantitative data for other species could be found in the literature. Note that Peterson and Roitberg (2006a) did not find significant differences in offspring sex ratio due to different resource levels provided to nesting female *M. rotundata* in a semi-field setting. However, the authors assumed that the highest resource level provided may already have been limiting.

*Table 5. Sex ratio, f/(f+m), of M. apicalis by floral resource treatment level (data from Kim 1999, Figure 2C). The difference, Δ sex ratio, is calculated as (sex ratio (high) – sex ratio (low)).*

Low resource treatment	High resource treatment	Δ sex ratio (f/(f+m))	Δ resource	<i>a.sex.resource</i>	Intercept
0.29 ± 0.09	0.5 ± 0.08	0.21 ± 0.09	0.5	0.42	0.58



*Figure 14. Linear relationship between relative resource availability and ratio of female offspring produced by *M. apicalis* (data from Kim 1999). The maximum female offspring ratio is assumed to occur under optimal foraging conditions and floral resource availability.*

### 3.2.5. Proportional female offspring provision size dependent on nesting female age

For the estimation of the relationship between nesting female age and the offspring sex ratio, we rely on the study by Bosch and Vicens (2005; introduced in Section 3.2.1) with *O. cornuta* and Seidelmann et al. (2010; introduced in Section 3.2.3) with *O. bicornis* (=rufa). Bosch and Vicens (2005, Table 1) report the mean weight of female cocoons (pre-wintering). The weight combined the weight of the adult and the cocoon. This weight is assumed to closely correspond to the weight of the provision provided in a brood cell.

The slope of the linear relationship between the adult female's age and the relative provision size is described by Equation 3.6.

*Equation 3.6*

$$a.size.age = \Delta size / \Delta age$$

In Table 6, the estimated relationship, *a.size.age*, is listed for the data from the two study years. The intercept of the linear relationship is set to 1 because it is assumed that the maximum relative provision size is provided to female offspring at the beginning of a female's nesting activity (*age.stage* = 1). Figure 15 shows the linear relationship as graph. The estimates for *a.size.age* are used as parameter range across simulated bee species in the model because no quantitative data for other species could be found in the literature.

Seidelmann et al. (2010) also looked at the weight of female and male offspring dependent on the assigned season day of nest construction (see section 3.2.3). The female offspring weight tended to be lower later in the season, but the relationship was not significant. Seidelmann et al. (2010) fit a linear model to cocoon weights relative to season day when the cocoon was produced. The average female cocoon weight was given as  $108.4 \pm 23.96$  mg. The relationship given in Seidelmann et al., Table 3, was given in mg. For the relative relationship,  $a.size.age$ , this was converted to a regression based on relative weight. The average age of nesting females was assumed to correspond to the reported season length (1997, 42 days; 1998, 31 days; and 1999, 30 days). The average weight of produced female cocoons was assumed to correspond to the reported average female cocoon weight at half of the nesting period (1997, 21 days; 1998, 15.5 days; and 1999, 15 days). The relationships from the individual data sets and the average are plotted in Figure 15.

The average is used as default (baseline) value for the model, the values listed for  $a.size.age$  in Table 6 provides the range of values. Although both data sets used for estimating  $a.size.age$  did not come from studies that were designed to inform this relationship, and the reduction in female cocoon weight was not significant in the study by Seidelmann et al. (2010), the consistency of the relationships between the two studies point to a reasonable assumption, at least for *Osmia* species. The value range is applied across model species.

*Table 6. Cocoon weight (corresponding to provisions size) of *O. cornuta* by study year and half season (BV2005: data from Bosch and Vicens (2005), Table 1). The difference,  $\Delta$  size, is calculated as (size (H2) – size (H1))/size (H1). The relationship between female cocoon weights of *O. bicornis* by study year and season day was given in mg body mass in Seidelmann et al. (2010), Table 3 (S2010). Using the overall reported average female cocoon weight in the study (108.4 mg), the relative reduction was calculated ( $a.size.age$ ). Note that the reduction in body (cocoon) weight of female offspring was not significant in the study. For the body (cocoon) weight of male offspring (data not shown), the reduction was only significant in one of the three study years.*

Study	Study year	H1 (weight in mg; mean $\pm$ SE)	H2 (weight in mg; mean $\pm$ SE)	$\Delta$ size	$\Delta$ age (days)	$a.size.age$
BV2005	1994	$182.9 \pm 2.4$	$158.9 \pm 5.2$	-0.126	26	-0.005
BV2005	1995	$189.4 \pm 4.0$	$180.1 \pm 8.7$	-0.049	25	-0.002
				Average BV2005		-0.0035
S2010	1997			-0.0471 mg	42	-0.001
S2010	1998			-0.2177 mg	31	-0.002
S2010	1999			-0.3666 mg	30	-0.003
				Average S2010		-0.002
				Average across studies		-0.0028

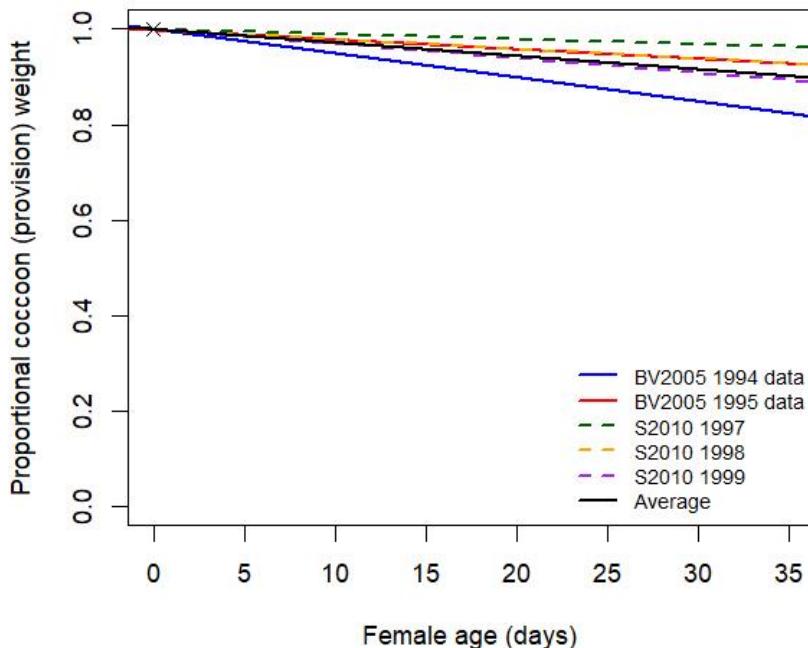


Figure 15. Linear relationship between days into nesting season (assumed to correspond to nesting female age) and female offspring cocoon/provision weight. BV2005: data from the study by Bosch and Vicens (2005) conducted over 2 years with *O. cornuta*. S2010: data from the study by Seidelmann et al. (2010) conducted over 3 years with *O. bicornis*. The relationship is assumed to be proportionally declining from the maximum weight occurring on the first day of nesting.

### 3.2.6. Proportional female offspring provision size dependent on resource availability

In the experiment by Kim (1999), the author also reports the weight of female brood dependent on resource treatment. The data is reported in Kim (1999), Figure 3A, for each female in the trial. Note that 3 of the 10 nesting females in the trial only produced male offspring. The slope of the linear relationship between the resource availability/quality and the female offspring brood cell weight is provided in Equation 3.7.

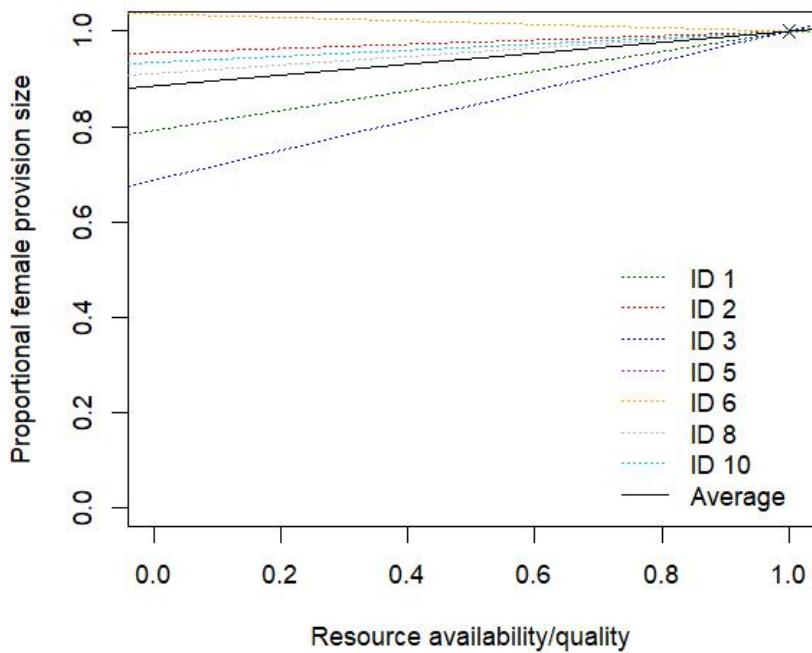
Equation 3.7

$$a.size.resource = \Delta size / \Delta resource$$

The slope estimates,  $a.size.resource$ , derived from these data are listed in Table 7 and are graphed in Figure 16. The estimates for  $a.size.resource$  in Table 7 are used as parameter range across simulated bee species in the model because no quantitative data for other species could be found in the literature. Note that no brood cells are produced if either no foraging occurs during a given day or no floral resources are available at all (within the foraging range).

**Table 7.** Average brood cell weight (mg) of female offspring of *M. apicalis* dependent on treatment (data from Kim (1999), Figure 3A). Floral resource provided in the 'high' treatment was double the resource provided in the 'low' treatment. The relative change in brood cell weight was calculated as  $\Delta$  size = (high – low)/high.

Female code	Low floral resources	High floral resources	$\Delta$ size	$\Delta$ resource	$a.size.resource$	Intercept
1	166.4	185.8	0.104	0.5	0.208	0.792
2	136.7	139.9	0.023	0.5	0.046	0.954
3	133.5	158.1	0.156	0.5	0.312	0.688
5	158.3	168	0.058	0.5	0.116	0.884
6	177.1	173.9	-0.018	0.5	-0.036	1.036
8	186.9	195.4	0.044	0.5	0.088	0.912
10	152.8	158	0.033	0.5	0.066	0.934
				Average	0.114	0.886



**Figure 16.** Linear relationship between relative resource availability and proportional provision size provided to female offspring by *M. apicalis* (data from Kim 1999). The maximum female provision size is assumed to occur under optimal foraging conditions and floral resource availability. The IDs refer to brood cells produced by individual nesting females in the experiment.

# 4. MODEL IMPLEMENTATION VERIFICATION

## 4.1. Review of the model code

Chiara Accolla (Waterborne Environmental) reviewed the model code to assess whether it was implemented according to the model description (provided in Chapter 2). The model implementation review was conducted on an earlier version of the model. Chiara was not involved in the model development, and thus, acted as third-party reviewer of the model implementation.

## 4.2. Verification of model procedures

During the model implementation, procedures were tested for their correct functioning. Single simulations were conducted (using the NetLogo interface), and values of model variables were observed through outputs to the ‘command center’ in NetLogo or by observing individual bees and the values of their state variables.

During implementation of the version of the model presented here, changes to the model code were applied. After each change to model procedures, model outputs were compared to outputs of the previous version to assure that the functionality of the model did not change, but rather, was only expanded according to each change applied.

Model outputs were qualitatively assessed for consistency with expected population dynamics and temporal sequences. For instance, timing of bee emergence is defined by mean dates for females and males along with the variance around those dates. The observed emergence in the model corresponds to the defined dates. Reproductive relationships implemented in the model are reflected in corresponding model outputs, i.e., mean daily brood cell production rate per female and mean daily offspring sex ratio. Offspring with reduced sizes are produced later in the simulated season (corresponding to older nesting females).

### 4.2.1. Verification of input file data handling

More extensive, formalized testing was conducted to assure the correct handling of the time series provided in the input file. The verification confirmed that the input file is read in correctly by the model. If a daily value in ‘Prop\_foraging\_day’ (2<sup>nd</sup> column of the input file) is set to zero on days when nesting females are present, no brood cells are produced in the model according to expectation.

Correspondingly, no brood cells are produced if both ‘Quality\_crop’ and ‘Quality\_nat’ (3<sup>rd</sup> and 4<sup>th</sup> columns of the input file, respectively) are set to zero. Total number of brood cells produced on a given day correctly increases with increasing ‘Prop\_foraging\_day’ and with increasing ‘Quality\_crop’ and ‘Quality\_nat’ (whereby ‘Prop\_foraging\_crop’ was either set to 0 or 1 to achieve bees foraging only on one of the resource types per simulation).

### 4.2.2. Verification of model initialization

The model is implemented to allow a range of initial conditions relevant for simulations of natural (unmanaged) populations as well as specific study conditions. The parameters defining the initial population in each simulation include the initial number of females and males present (*Initial.num.f* and *Initial.num.m*). At the start of a simulation, all bees are in the same life stage, defined by the model parameter *Initial.stage* and the (average) age of the bees specific to the life stage, *Initial.age* (see also Section 2.3.1). The model checks for the consistency of the defined initial settings. For instance, if bees are assigned to be in life stage ‘egg’ at the start of a simulation, their stage-specific age cannot exceed the defined egg development time, *dev.egg*.

The most commonly used first date of simulation is assumed to be 1 January of a simulated year (*Start.day* = 1). This initial date was used for all simulations presented in Chapter 6 (Analysis of parameter uncertainty and Cross-species simulations). All model bees are inactive on 1 January and occur in the life stage ‘cocoon’ (pre-pupa or pre-emergent adult). With this initial setting, bees in the simulations correctly emerge during the specified time window. If *Voltinism* = ‘multivoltine’, a second generation of bees emerges later in the year. All bees that do not complete their development time prior to the date defined by *latest.emerge* do not emerge until the following simulated year. No second generation emerges if *Voltinism* = ‘univoltine’.

The defined date of latest emergence (*latest.emerge*) can be set to fall within the time window of emergence of the first (in case of univoltine life cycles, only) generation of the year. In that case, some simulated bees may remain in cocoon stage in the season after their were laid as eggs. The model code captures this unrealistic case (for our model species) by removing bees that remained in cocoon stage for more than one year (365 days).

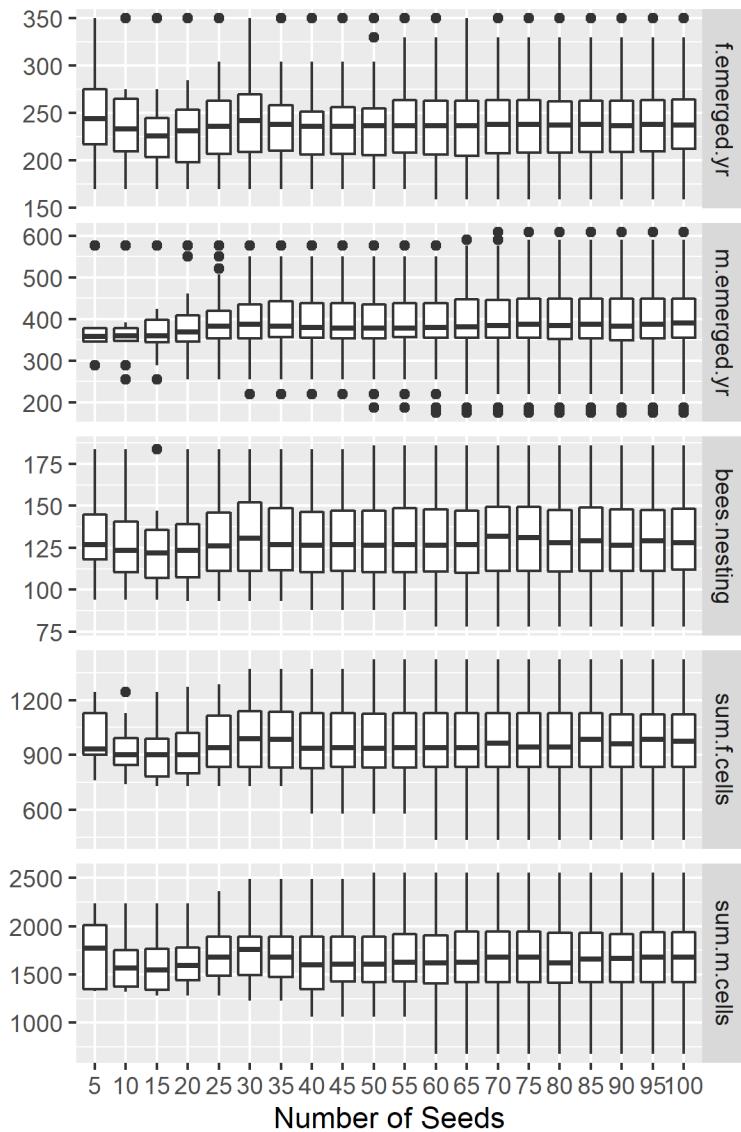
For the simulation of specific studies in which bees are released (usually as cocoons) on a certain date, *Start.day* is set to that date (see also Chapter 7.1). Both uni- and multi-voltine life cycles are correctly captured by the model if the start date is later in the year than 1 January. However, users need to make sure that study-specific emergence dates are also used in such simulations, avoiding start days occurring later than the emergence (in case studies with bees released as cocoons are simulated).

## 4.3. Repeat simulations (model stochasticity)

We conducted repeat simulations with a previous version of the model using identical parameter settings but different random number seeds. This test allows to gain insight about the model behavior due to stochasticity in the model (see Table 1 for a listing of stochastic processes implemented in the model). In addition, it can help identify the number repeat simulations necessary to achieve stable means or medians of model outputs. A total of 100 repeat simulations with identical parameter settings were conducted. In Figure 17, the medians and ranges of five model outputs are shown with increasing the number of repeat simulations (in increments of 5).

This test shows that some median model outputs change considerably from five repetitions to 10. Medians and ranges of model outputs across repeat simulations show only very small changes with fifty or more repetitions. For model analysis, 10 repetitions were chosen because they capture most of the variability in model outputs due to model stochasticity while also limiting the number of total

simulations (see Sections 6.1 and 7.1.2). For the simulations with four model species, 50 repetitions were applied because the test of repeat simulations indicates that no additional information is gained from conducting a higher number of repetitions (see Section 6.2).



*Figure 17. Test of repeat simulations with the SolBeePop model. The number of seeds refers to the number of repetitions conducted with different random number seeds but identical model parameter settings. The median, 25<sup>th</sup> and 75<sup>th</sup> percentile range of model outputs due to stochasticity in the model are shown as boxes, the whiskers indicate 1.5 times the interquartile range.*

## 4.4. Verification of units in SolBeePop<sub>ecotox</sub>

In SolBeePop<sub>ecotox</sub>, different units for the concentrations are used for the characterization of the pesticide exposure concentration in different exposure matrices and within the bee. The correct implementation of units (as defined in the parameter table) and their conversion in the model (where applicable) were verified. The following points and Table 8 list the use of concentrations and their units in the model.

- Concentrations for the calculation of effects (BeeGUTS) in adult (post-emergent) bees are used in ng/bee.
  - Note that in the publication of BeeGUTS (Baas et al. 2022), effective concentrations are given in ng/bee or µg/bee dependent on compound.
- Model parameters defining weights are used in mg in the model, including the daily consumption of nectar and pollen in adults (*ad.nectar.cons* and *ad.pollen.cons*, respectively), provision mass (*weight.prov*) and soil mass used for partitions between brood cells (*SM*; *Osmia* species only).
- Exposure concentrations are defined in the daily input time series (for exposure to direct spray, residues in nectar, pollen, soil and leaves). The units of the input time series are listed in Table 8.
- Exposure from direct spray: exposure to direct spray corresponds to acute contact laboratory tests, ng/bee corresponds to ng a.i. in the applied droplet (reported droplet size 1-2 µL in acute contact tests)

Table 8. Input times series in the input file for SolBeePop<sub>ecotox</sub> defining concentrations of pesticide per exposure route.

Column header in input file	Unit	Description	Remarks
Concentration_nectar	µg/g	µg a.i. per g nectar	
Concentration_pollen	µg/g	µg a.i. per g pollen	
Concentration_spray	mg/L (=ng/µL)	mg a.i. per L formulation sprayed	Corresponds to application rate; assumption that 1 µL spray droplet received per bee (droplet of that volume applied in adult bee acute contact laboratory tests) (OECD 1998a)
Concentration.nest.mat	µg/g	µg a.i. per g soil for soil-nesting bees or mud used for nest partitions ( <i>Osmia</i> sp.)	
Concentration.leaf	µg/cm <sup>2</sup>	µg a.i. per cm <sup>2</sup> surface area of leaf pieces used for nesting lining ( <i>Megachile</i> sp.)	

# 5. MODEL OUTPUT VERIFICATION

The calibration and validation of SolBeePop with *O. bicornis* control semi-field study data is described in Chapter 7.1.

The calibration and validation of SolBeePop<sub>ecotox</sub> with a different set of *O. bicornis* semi-field study data was conducted, including the comparison of model outputs to control and treatment study data (Chapter 7.2).

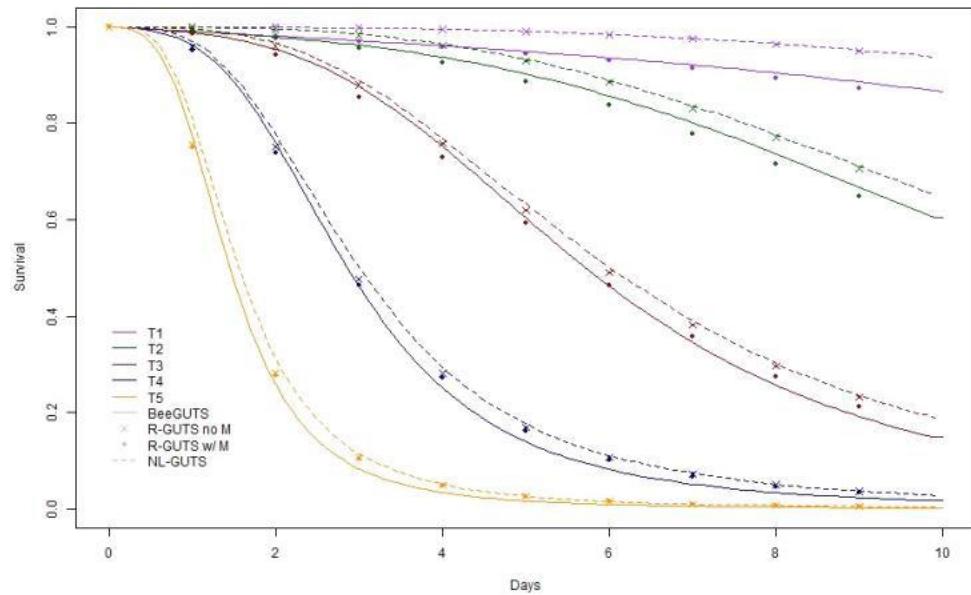
## 5.1. Verification of the effective exposure (adult bees)

The “effective exposure” in BeeGUTS (Baas et al. 2022) corresponds to the “external exposure” in GUTS (Jager and Ashauer 2018). Because adult bees can be exposed via their diet or contact exposure, the two exposure routes need to be reconciled in BeeGUTS, using a defined uptake rate for each ( $k_{SR}$  and  $k_{CA}$ , respectively). The combined exposure present within the bee at each simulated time point is then used as input to the GUTS model. In SolBeePop<sub>ecotox</sub>, the uptake rate from dietary exposure in the simulated bees is assumed to correspond to the full uptake of all residue consumed with diet within a single day ( $k_{SR} = 1$ ). This means that we assume that the bees consume all nectar and pollen the same day they collect it. Note that this refers to the food they collect for their own consumption and does not include nectar and pollen collected for the provisioning of brood. The uptake rate from spray (a droplet applied to the bee’s cuticula) was assumed to correspond to  $k_{CA} = 0.4$  as used in BeeGUTS (Baas et al. 2022).

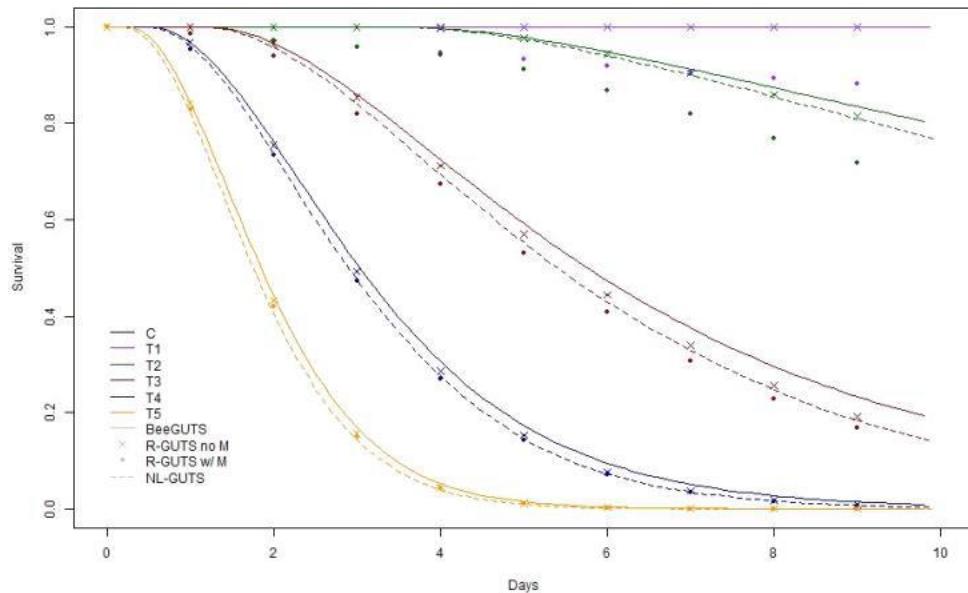
The effective exposure calculated in SolBeePop<sub>ecotox</sub> for each adult female was verified by comparing the model variable *C.effective* over time with the effective concentration calculated independently from the model in R (R Core Team 2022). The effective concentration calculated in SolBeePop<sub>ecotox</sub> and by the external script were identical.

## 5.2. Verification of GUTS implementation

The GUTS implementation was verified by comparing the proportional survival of bees simulated with SolBeePop<sub>ecotox</sub> and the outputs of the dimethoate runs with BeeGUTS, provided by Jan Baas. In addition, GUTS outputs from the implementation in R were also compared. In the R-script, the background mortality in GUTS could be included or not. In the BeeGUTS outputs, background mortality was included, in SolBeePop<sub>ecotox</sub>, no background mortality is included in GUTS because background mortality is captured independent of GUTS in the model. In Figure 18 and Figure 19, the results of the output verifications are shown for GUTS-IT and GUTS-SD, respectively. The expected match between the R-implementation without background mortality (crosses) and the SolBeePop<sub>ecotox</sub> output are fulfilled.



*Figure 18. Survival rates simulated with different GUTS-IT implementations for five diemthoate treatment levels (from the chronic dietary exposure test with honey bee workers. T1 – T5 refer to the treatment levels. Solid lines correspond to BeeGUTS outputs, dashed lines to SolBeePop<sub>ecotox</sub> outputs. Crosses are outputs from the implementation of GUTS in R without background mortality and dots of the same R implementation including background mortality. A perfect match would mean that dashed lines and the crosses are identical, and the dots and the solid lines.*



*Figure 19. Survival rates simulated with different GUTS-SD implementations for five diemthoate treatment levels (from the chronic dietary exposure test with honey bee workers. T1 – T5 refer to the treatment levels. Solid lines correspond to BeeGUTS outputs, dashed lines to SolBeePop<sub>ecotox</sub> outputs. Crosses are outputs from the implementation of GUTS in R without background mortality and dots of the same R implementation including background mortality. A perfect match would mean that dashed lines and the crosses are identical, and the dots and the solid lines.*

### 5.3. Verification of effects in in-nest life stages

For the simulations with SolBeePop<sub>ecotox</sub> presented in this documentation, dimethoate was used as example pesticide. Dimethoate is an insecticide that is often used as positive control in standard laboratory- and field-based bee effects studies. While the compound is highly toxic to adult bees at low concentrations, the bee larvae are comparatively less sensitive to the compound. To characterize the response of in-nest life stages to exposures to dimethoate in simulations with SolBeePop<sub>ecotox</sub>, effects on adult bees have to be excluded because adult bees are always exposed to the same matrices as larvae (although at different levels). For the purpose of testing effects only on in-nest life stages, the model includes the possibility of “NoEffects” in the parameter “GUTS”. Using this setting, exposures in larval provisions corresponding to concentrations resulting in effects in honey bee larval chronic tests can be tested with the model.

For the verification of effects in in-nest life stages from exposures to dimethoate, the concentrations of dimethoate in the feeding solution in the honey bee larval toxicity test was applied as concentration in nectar and pollen in the corresponding SolBeePop<sub>ecotox</sub> input file time series. The concentrations applied (as constant), the percent survival from honey bee laboratory tests (OECD 2016: 239) and from the simulations are shown in Table 9. The simulated survival rates are marginally lower than the ones calculated from the dimethoate laboratory data.

*Table 9. Verification of larval effects using dimethoate as example compound.*

Treatment ID	Concentration (mg a.i./kg diet = µg/g)	Calculated survival % (from OECD 2016)	Simulated average % survival (SolBeePop <sub>ecotox</sub> )
E1	1.75	96.20	95.00
E2	3.5	72.49	72.24
E3	7	48.78	48.75
E4	8	44.22	44.11
E5	14	25.07	25.18
E6	16	20.51	20.38
E7	28	1.37	1.35

# 6. MODEL ANALYSIS

## 6.1. Analysis of parameter uncertainty without exposures and effects

### 6.1.1. Methods

The analysis of parameter uncertainty was conducted to assess the impact of uncertainty in input parameter (trait) values on population-level outputs for the example model species *O. bicornis* and *N. melanderi*. *O. bicornis* was chosen for the model analysis because the most comprehensive data was available from the literature for this species (compared to the other model species addressed by SolBeePop). *N. melanderi* was chosen as second species with traits (and their ranges) differing considerably from *O. bicornis*. The data availability did not only allow an estimate for most species-specific model parameters but also an estimate of the possible range of the parameter values. Ranges of parameter values reported in the literature may stem from a variability of individual trait values within or across populations of the species, a range of environmental conditions interacting with the trait (e.g., time to maturation after emergence may strongly depend on the weather conditions) or a combination of both. The default parameter values applied to *O. bicornis* along with the minimum and maximum values derived for this species from the literature and applied in the model analysis are listed in Table 10, the default parameters and their ranges for *N. melanderi* in Table 11. Literature references are listed for each species-specific parameter. Remarks in the table indicate where no data were available from the literature and how these data gaps were addressed for the purpose of the analysis.

The simulations for the model analysis were conducted representing two years whereby the outputs related to reproductive rates from the first simulation year were analyzed and the emergence rates from the second simulation year (reproductive rates of the second generation were not included in the analysis). The simulations were conducted without density dependence. All model parameters applied are listed Table 10 and Table 11, including parameters that were not species-specific and were not changed across simulations.

The parameters included in the model analysis (parameters with a range of values listed in Table 10 and Table 11) were explored for their impact on model outputs by sampling the parameter space with a Monte Carlo method, latin hypercube (LHC), which results in even sampling of the parameter space (Blower and Dowlatabadi 1994). For the drawing of random parameter values from the parameter space defined by the ranges in Table 10, the method “randomLHS” from the R-package “lhs” was applied (Carnell 2022; R Core Team 2022). The method assumes uniform distributions of all parameters. A Latin Hypercube for 3800 samples<sup>1</sup> from the parameter space was calculated. Simulations with each of these

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<sup>1</sup> (Blower and Dowlatabadi 1994) state that minimum number of samples from the LHC space need to be:  $N > 4/3K$ . In this SA,  $K = 14$ , i.e.,  $N > 18.67$  or the minimum is  $N_{min} = 19$ . The chosen sample number corresponds to  $200 \times N_{min}$ .

parameter combinations were repeated 10 times with different random number seeds<sup>2</sup>. Because the species-specific parameters (traits) were expected to interact differently with different scenarios of temporal floral resource availability, the model analysis was conducted for both example species with three alternative input files (floral resource scenarios):

**Scenario 1:** Optimal foraging conditions (input file name: `Floral_generic_optimal.csv`; the same input file was used for both species given the floral resource availability is constant across the year): floral resource availability is set to the optimal value of 1 throughout the year corresponding to the assumption that the bees have optimal weather conditions for foraging, short flight distances to floral resources and low effort collecting the resources throughout their active flight and nesting phase.

**Scenario 2:** Uniform half of optimal foraging conditions (input file name: `Floral_generic_Sce2.csv`; the same input file was used for both species given the floral resource availability is constant across the year): floral resource availability is set to half the optimal value of 0.5 throughout the year corresponding to the assumption that the bees encounter invariable, suboptimal weather conditions for foraging, longer flight distances to floral resources and/or need a higher effort collecting the resources throughout their active flight and nesting phase than optimal.

**Scenario 3:** Uniform half of optimal with 10-day foraging gap (input file names: `Floral_generic_Sce3_Osmia.csv` and `Floral_generic_Sce3_Nomia.csv`): floral resource availability is set to half of the optimal value of 0.5 throughout the year with a period of 10 days (days of year 113-122 for *Osmia* and 182-191 for *Nomia*) without any forage resource availability (value of 0). This corresponds to the assumption that the bees encounter suboptimal weather conditions for foraging, longer flight distances to floral resources and/or need a higher effort collecting the resources for most of their active flight and nesting phase than optimal. A foraging gap corresponds to a stretch of weather that does not allow foraging at all or a complete absence of foraging resources within the bees' foraging range around the nest site.

Note that all three floral resource availability scenarios are generic and are not intended to assess the interaction between the phenology of the bee and the resources in the landscape. Accordingly, the emergence date (`day.emerge.f` and `day.emerge.m`) of the bees was not included in the model analysis. Although the timing of emergence and subsequent active flying and nesting of the bees is a species-specific trait, it can only influence model outputs if the timing of floral resources availabilities is variable in time and is not synchronized with the bees' shift in phenology. Addressing the impacts of the interaction between flower and bee phenology was not the objective of the model analysis but would require a separate analysis with more realistic and time-variable floral resource input scenarios.

The parameter values defining the reproductive relationships in the model were derived from multiple studies conducted with several different species (see Section 3.1). Data specific for the two example species for all reproductive parameters were not available from the literature. In the model analysis, the six parameters for the reproductive relationships (`a.cell.age`, `a.sex.age`, `a.size.age`, `a.cell.resource`,

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<sup>2</sup> The number of repetitions was chosen from conducting 100 replicate simulations using the default parameter settings and input file “`Floral_generic_optimal.csv`”. Mean values of outputs from 10 repeat simulations were not markedly different from means of 100 repeat simulations.

*a.sex.resource, a.size.resource*) were used with their ranges determined based on the data across species (see also remarks in Table 10).

Model outputs from the LHC were analyzed defining the reproductive output of the population (*sum.f.cells, sum.m.cells*), the total number of female bees nesting (*bees.nesting*) in the simulated first year and the total number of bees emerging in the following season (*f.emerged.yr, m.emerged.yr*). From the LHC simulation outputs with each of the three floral resource input scenarios, the partial rank correlation coefficient (PRCC) was calculated. The PRCC correlates the impact of the applied range of each parameter on outputs across LHC samples (Blower and Dowlatabadi 1994). The analysis was conducted in R using the package “sensitivity” and plots were generated using the package “ggplot2” (Wickham 2016; Iooss et al. 2022; R Core Team 2022).

**Table 10.** Model parameter values applied in the model analysis (without exposures and effects) with example species *Osmia bicornis*.

Parameters not included in the model analysis were used with their default value in all simulations. If no remarks are included for parameters not included in the analysis, these parameters are not species-specific but define initial conditions in the simulations, number of years simulated and the input method of the floral resource input file(s).

Interface parameter name	<i>Osmia bicornis</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
<i>Start.day</i>	1	No	--	--		
<i>Species</i>	O.bicornis	No	--	--		
<i>Voltinism</i>	univoltine	No	--	--		
<i>Initial.num.f</i>	100	No	--	--		
<i>Initial.num.m</i>	200	No	--	--		
<i>Initial.stage</i>	cocoon	No	--	--		
<i>Initial.age</i>	200	No	--	--		
<i>RndSeed</i>		see remarks			Different random numbers used for each of the 10 repeat simulations	
<i>MultiYearInput</i>	FALSE	No	--	--		
<i>List.input.floral</i>	NA	No	--	--		
<i>Num.repeat.yr</i>	2	No	--	--		
<i>input.floral</i>		see remarks			Analysis repeated for 3 scenarios: (1) optimal foraging conditions, (2) half-optimal, (3) half-optimal with 10-day foraging gap during nesting season, see text	
<i>stoch.crop.forag</i>	FALSE	No	--	--		
<i>Density.dep</i>	FALSE	No				
<i>DD.thresh.s</i>	NA	No				

Interface parameter name	<i>Osmia bicornis</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
<i>DD.max.cells.s</i>	NA	No				
<i>DD.funct</i>	NA	No				
<i>DD.log.slope</i>	NA	No				
<i>day.emerge.f</i>	105	No	--	--	Species-specific but not included in the model analysis. See text.	
<i>var.emerge.f</i>	3	Yes	1	7	values need to be integers	No quantitative information available informing the range (time window) of emergence per population and season: generic range applied assuming a short emergence period (up to 1 week)
<i>day.emerge.m</i>	91	No	--	--	Species-specific but not included in the model analysis. See text.	
<i>var.emerge.m</i>	2	No	--	--	Species-specific but not included in the model analysis: no data available (see <i>var.emerge.f</i> ) and male emergence timing does not affect reproductive rates in the model.	
<i>latest.emerge</i>	365	No	--	--	Parameter used for multi-voltine life cycles only; unused if Voltinism = 'univoltine'	
<i>dev.egg</i>	8	No	--	--	Species-specific but not included in the model analysis: in-nest development times do not impact reproductive or emergence rates in the model	
<i>dev.larva</i>	32	No	--	--	Species-specific but not included in the model analysis: in-nest development times do not impact reproductive or emergence rates in the model	

Interface parameter name	<i>Osmia bicornis</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
<i>dev.cocoon</i>	68	No	--	--	Species-specific but not included in the model analysis: in-nest development times do not impact reproductive or emergence rates in the model	
<i>t.maturity</i>	3	Yes	1	10	values need to be integers	(Bosch et al. 2008; Sgolastra et al. 2016)
<i>m.life</i>	21	No	--	--	Species-specific but not included in the model analysis: post-emergent male life span not reported in the literature and not impactful for model outputs	
<i>max.nesting.life</i>	36	Yes	26	36	values need to be integers	(Tepedino and Torchio 1982b; Frohlich and Tepedino 1986; Sugiura and Maeta 1989; Bosch 1994; Bosch et al. 2001; Bosch and Vicens 2005; Bosch and Vicens 2006; Bosch 2008; Sgolastra et al. 2016)
<i>p.max.nesting.life</i>	0.04	Yes	0.01	0.1		Parameter does not correspond to a trait measured in any published study: generic value range applied
<i>max.f.ratio</i>	0.59	Yes	0.38	1		(Bosch and Vicens 2005; Bosch and Vicens 2006; Seidelmann 2006; Seidelmann et al. 2010; Giejdasz et al. 2016; Sgolastra et al. 2016)
<i>max.cells</i>	2	Yes	1	3		(Bosch 1994; Goodell 2003; Bosch and Vicens 2005; Bosch and Vicens 2006; Bosch 2008; Bosch et al. 2008; Palladini and Maron 2014; Giejdasz et al. 2016; Sgolastra et al. 2016)

Interface parameter name	<i>Osmia bicornis</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
<i>max.survival.e.f</i>	0.74	Yes	0.58	0.89		(Bosch 1992; Bosch and Vicens 2005; Sedivy et al. 2011)
<i>max.survival.e.m</i>	0.74	see remarks			No separate data for females and males available for survival to emergence: the same value was applied to <i>max.survival.e.f</i> and <i>max.survival.e.m</i> in the simulations	(Bosch 1992; Bosch and Vicens 2005; Sedivy et al. 2011)
<i>emerged.survival</i>	0.544	Yes	0.5	0.75		(Bosch and Kemp 2002; Bosch et al. 2021)
<i>a.cell.age</i>	-0.006	Yes	-0.004	-0.008	Values derived from study with <i>O. cornuta</i> , see also Section 3.2.1	(Bosch and Vicens 2005)
<i>a.sex.age</i>	-0.0406	Yes	-0.0286	-0.0599	Values derived from study with <i>O. bicornis</i> , see also Section 3.2.3	(Seidelmann et al. 2010)
<i>a.size.age</i>	-0.003	Yes	-0.001	-0.005	Values derived from studies with <i>O. bicornis</i> and <i>O. cornuta</i> , see also Section 3.2.5	(Bosch and Vicens 2005; Seidelmann et al. 2010)
<i>a.cell.resource</i>	0.94	Yes	0.43	1.4	Values derived from study with <i>O. pumila</i> , <i>M. apicalis</i> and <i>M. rotundata</i> , see also Section 3.2.2	(Kim 1999; Goodell 2003; Peterson and Roitberg 2006a)
<i>a.sex.resource</i>	0.42	Yes	0.2	0.6	Default value derived from study with <i>M. apicalis</i> ; study data not suitable for estimation of range, see also Section 3.2.4	(Kim 1999); generic range (min and max)
<i>a.size.resource</i>	0.114	Yes	0	0.312	Values derived from study with <i>M. apicalis</i> , see also Section 3.2.6	(Kim 1999)

*Table 11. Model parameter values applied in the model analysis with example species *Nomia melanderi*. Parameters not included in the model analysis were used with their default value in all simulations. If no remarks are included for parameters not included in the analysis, these parameters are not species-specific but define initial conditions in the simulations, number of years simulated and the input method of the floral resource input file(s).*

Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
<i>Start.day</i>	1	--	--	--		
<i>Species</i>	N.melanderi	--	--	--		
<i>Voltinism</i>	univoltine	--	--	--		
<i>Initial.num.f</i>	100	--	--	--		
<i>Initial.num.m</i>	200	--	--	--		
<i>Initial.stage</i>	cocoon	--	--	--		
<i>Initial.age</i>	200	--	--	--		
<i>RndSeed</i>		see remarks			10 random number seeds per parameter combination	
<i>MultiYearInput</i>	FALSE	--	--	--		
<i>List.input.floral</i>	NA	--	--	--		
<i>Num.repeat.yr</i>	2	--	--	--		
<i>input.floral</i>		see remarks			Analysis repeated for 3 scenarios: (1) optimal foraging conditions, (2) half-optimal, (3) half-optimal with 10-day foraging gap during nesting season, see text	
<i>stoch.crop.forag</i>	FALSE	--	--	--		
<i>Density.dep</i>	FALSE	--	--	--	Density dependence not included in this analysis	
<i>DD.thresh.s</i>	NA	--	--	--		
<i>DD.max.cells.s</i>	NA	--	--	--		

Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
<i>DD.funct</i>	NA	--	--	--		
<i>DD.log.slope</i>	NA	--	--	--		
<i>day.emerge.f</i>	174	--	--	--	only meaningful to test in the context of floral phenology scenarios	
<i>var.emerge.f</i>	6	Yes	3	9	values need to be integers	Mayer and Miliczky 1998; Vinchesi et al. 2013
<i>day.emerge.m</i>	167	--	--	--		
<i>var.emerge.m</i>	8	--	--	--		
<i>latest.emerge</i>	365	--	--	--	only meaningful to test for facultatively bivoltine life cycles	
<i>dev.egg</i>	2	--	--	--	development times not influential to model outputs (in univoltine life cycles)	
<i>dev.larva</i>	6	--	--	--		
<i>dev.cocoon</i>	20	--	--	--		
<i>t.maturation</i>	1	Yes	1	7	values need to be integers	Bohart and Cross 1955; Johansen et al. 1978
<i>m.life</i>	14	--	--	--	not impactful to model dynamics or outputs (other than number of post-emergent males)	
<i>max.nesting.life</i>	26	Yes	22	30	values need to be integers	Bohart and Cross 1955
<i>p.max.nesting.life</i>	0.04	Yes	0.01	0.1		Not available; generic large range included
<i>max.f.ratio</i>	0.51	Yes	0.35	0.51		Mayer and Miliczky 1998
<i>max.cells</i>	1	Yes	0.5	1	generic range applied because no variation in daily brood cell production reported; authors explicitly state that a bee does not start a second brood cell in a given day	Bohart and Cross 1955

Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
<i>max.survival.e.f</i>	0.868	Yes	0.729	0.868	apply the same value to max.survival.e.f and max.survival.e.m	Rust 2006
<i>max.survival.e.m</i>	0.868	see remarks			apply the same value to max.survival.e.f and max.survival.e.m	
<i>emerged.survival</i>	0.544	Yes	0.5	0.75	generic range applied in the absence of data (same range as applied to Osmia)	
<i>a.cell.age</i>	-0.006	Yes	-0.008	-0.004	Reproductive relationships characterized using data from multiple species (see also Table 10)	Bosch and Vicens 2005
<i>a.sex.age</i>	-0.0406	Yes	-0.0599	0		Seidelmann et al. 2010
<i>a.size.age</i>	-0.003	Yes	-0.005	-0.001		Bosch and Vicens 2005; Seidelmann et al. 2010
<i>a.cell.resource</i>	0.94	Yes	0.43	1.4		Kim 1999; Goodell 2003; Peterson and Roitberg 2006
<i>a.sex.resource</i>	0.42	Yes	0	0.6		Kim 1999 (no range; range for testing in SA not supported by data)
<i>a.size.resource</i>	0.114	Yes	0	0.312		Kim 1999

## 6.1.2. Results

From the outputs of the model analysis, the uncertainty range of the species-specific parameters included could be identified as a) highly influential to one or several model outputs analyzed in all three scenarios, b) influential to outputs in at least one of the scenarios, or c) not influential to model outputs irrespective of floral resource availability scenario (Table 12 and Table 13). The PRCC for each parameter included in the model analysis can range between -1 (increase in the parameter value is correlated with a corresponding decrease in the output value irrespective of all other parameter values) and 1 (increase in the parameter value is correlated with a corresponding increase in the output value irrespective of all other parameter values). A PRCC = 0 denotes no impact of the parameter value on outputs. Here, we arbitrarily define parameters as impactful to model outputs if  $|PRCC| \geq 0.25$ . In addition, we identify model parameters as highly impactful if  $|PRCC| \geq 0.5$  for 3 or more of the outputs analyzed. Parameters were classified as not impactful if  $|PRCC| \leq 0.1$ .

*Table 12. Results of the model analysis with O. bicornis by model parameter and floral resource input scenario.* +: PRCC > 0.25 for at least one output and the increase in parameter value corresponds to an increase (or no change) across outputs; -: PRCC < -0.25 for at least one output and the increase in parameter value corresponds to a decrease (or no change) across outputs; +/-:  $|PRCC| > 0.25$  for at least one output and the increase in parameter value corresponds to an increase or decrease (or no change) dependent on the output; ++: PRCC > 0.5 for at least 3 outputs and the increase in parameter value corresponds to an increase (or no change) across outputs; --: PRCC < -0.5 for at least one output and the increase in parameter value corresponds to a decrease (or no change) across outputs; grey cells:  $|PRCC| < 0.1$  across all outputs.

Interface parameter name	Osmia bicornis (default parameter value)	Min value in SA	Max value in SA	Scenario 1: Optimal foraging conditions	Scenario 2: Uniform half of optimal foraging conditions	Scenario 3: Half optimal foraging conditions with 10-day foraging gap
var.emerge.f	3	1	7			+
t.maturity	3	1	10			-
max.nesting.life	36	26	36	+	+	+
p.max.nesting.life	0.04	0.01	0.1	++	++	++
max.f.ratio	0.59	0.38	1	+/-	+/-	+/-
max.cells	2	1	3	++	++	++
max.survival.e.f,	0.74	0.58	0.89	++	++	++
emerged.survival	0.544	0.5	0.75	++	++	++
a.cell.age	-0.006	-0.004	-0.008			
a.sex.age	-0.0406	-0.0599	-0.0286	+/-	+/-	+/-
a.size.age	-0.003	-0.005	-0.001			
a.cell.resource	0.94	0.43	1.4		--	--
a.sex.resource	0.42	0.2	0.6		+/-	-
a.size.resource	0.114	0	0.312		-	-

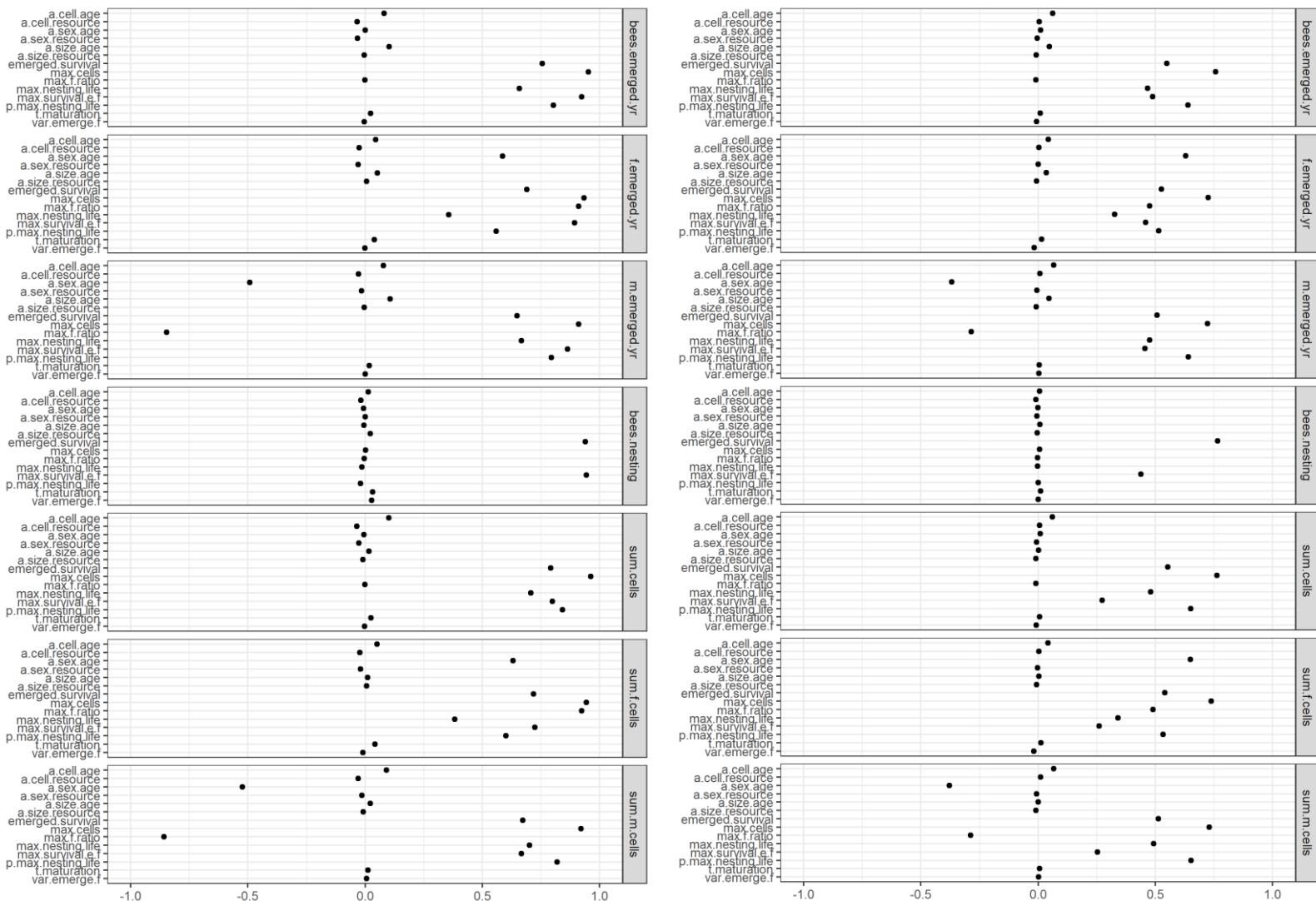
*Table 13. Results of the model analysis with N. melanderi by model parameter and floral resource input scenario.* +: PRCC > 0.25 for at least one output and the increase in parameter value corresponds to an increase (or no change) across outputs; -: PRCC < -0.25 for at least one output and the increase in parameter value corresponds to a decrease (or no change) across outputs; +/-: |PRCC| > 0.25 for at least one output and the increase in parameter value corresponds to an increase or decrease (or no change) dependent on the output; ++: PRCC > 0.5 for at least 3 outputs and the increase in parameter value corresponds to an increase (or no change) across outputs; --: PRCC < -0.5 for at least one output and the increase in parameter value corresponds to a decrease (or no change) across outputs; grey cells: |PRCC| < 0.1 across all outputs.

Interface parameter name	Nomia melanderi (default parameter value)	Min value in SA	Max value in SA	Scenario 1: Optimal foraging conditions	Scenario 2: Uniform half of optimal foraging conditions	Scenario 3: Half optimal foraging conditions with 10-day foraging gap
var.emerge.f	6	3	9			+
t.maturity	1	1	7			-
max.nesting.life	26	22	30	+	+	+
p.max.nesting.life	0.04	0.01	0.1	++	++	++
max.f.ratio	0.51	0.35	0.51	+/-	+/-	+/-
max.cells	1	0.5	1	++	++	++
max.survival.e.f,	0.868	0.729	0.868	+	+	+
emerged.survival	0.544	0.5	0.75	++	+	+
a.cell.age	-0.006	-0.008	-0.004			
a.sex.age	-0.0406	-0.0599	-0.0286	+/-	+/-	+/-
a.size.age	-0.003	-0.001	-0.005			
a.cell.resource	0.94	0.43	1.4		--	--
a.sex.resource	0.42	0	0.6		-	-
a.size.resource	0.114	0	0.312			

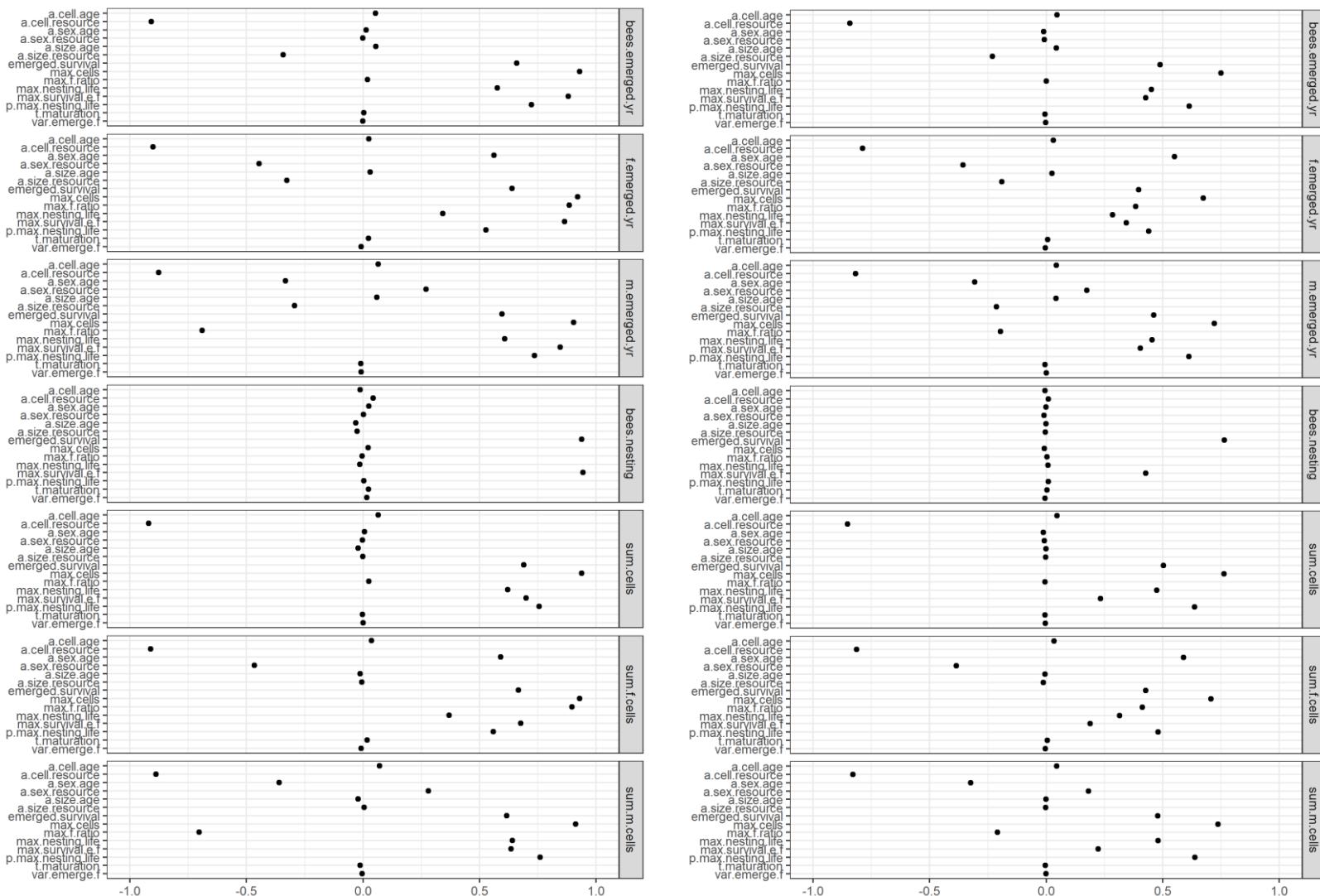
All PRCCs for floral resource availability scenarios 1, 2 and 3 are shown in Figure 20, Figure 21, and Figure 22, respectively, for both example species. The most impactful parameters across scenarios include all parameters characterizing survival of female bees (*p.max.nesting.life*, *max.survival.e.f*, *emerged.survival*) whereby *max.nesting.life* was the least impactful of the survival parameters. In the model, *max.nesting.life* and *p.max.nesting.life* together determine the life span of nesting females. Since a larger range of parameter values for *p.max.nesting.life* was included in the model analysis, reflecting the absence of data informing this parameter, its impact on output variables was expected to be larger than *max.nesting.life*. The parameters characterizing survival impacted outputs for *O. bicornis* as well as *N. melanderi* whereby the parameters *emerged.survival* and *max.survival.e.f* ranked slightly less important for model outputs in *N. melanderi* compared to *O. bicornis* simulations. Apart from the

parameters characterizing survival, three additional parameters were identified as impactful in all scenarios for both species (*max.cells*, *max.f.ratio* and *a.sex.age*). These parameters determine the reproductive rate of nesting females and the sex ratio of the offspring. Accordingly, the six most highly impactful survival and reproductive parameters are important to consider and evaluate in simulations with the model because they are major drivers of the output.

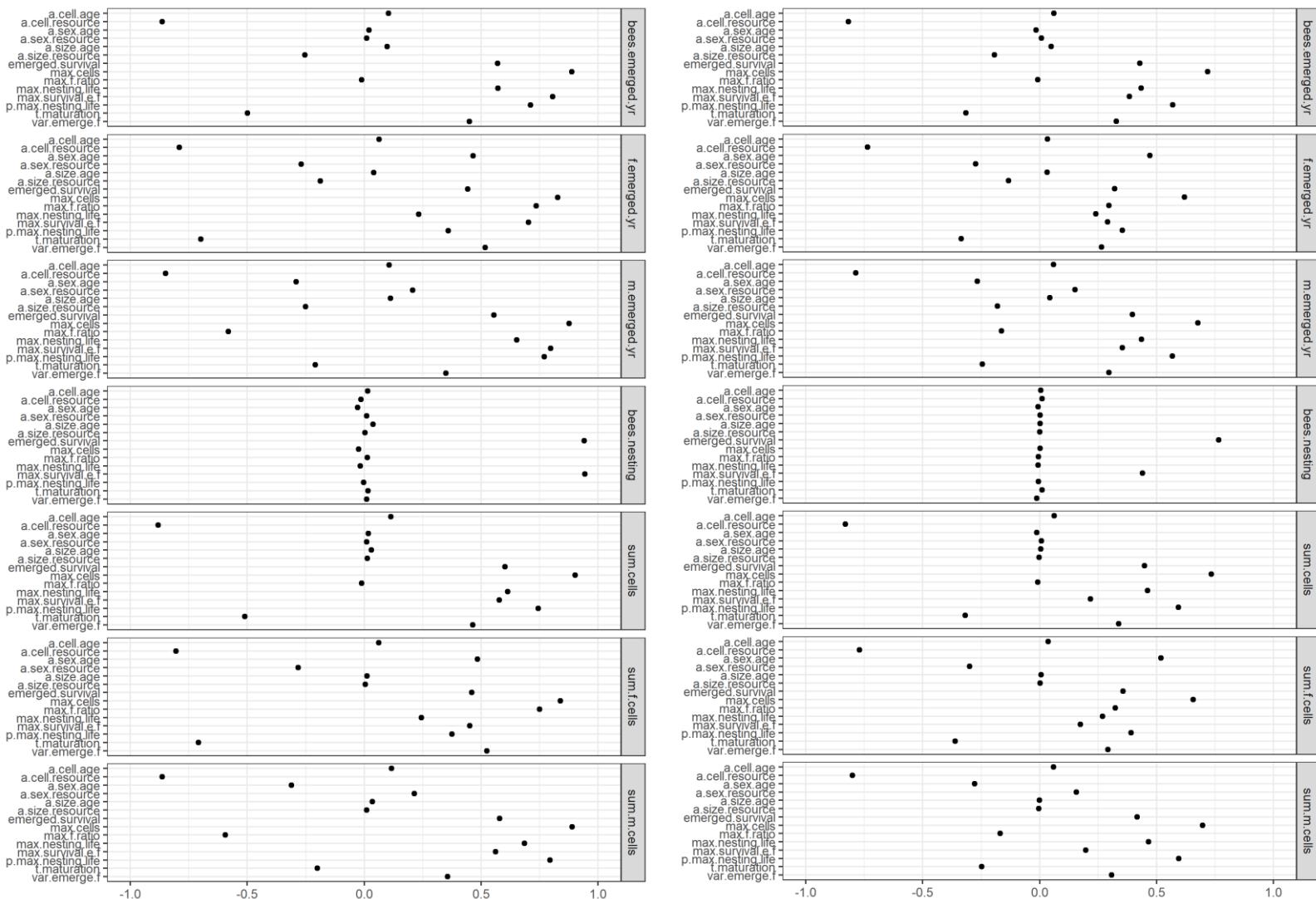
With only half-optimal foraging and floral resource availability (Scenarios 2 and 3), the parameters *a.cell.resource*, *a.sex.resource* were impactful to total emergence numbers (*bees.emerged*) or the sex ratio of the offspring (*f.emerged.yr* vs *m.emerged.yr*) in both species. In *O. bicornis*, *a.size.resource* also ranked as impactful to these model outputs. Because Scenario 3 was the only scenario with a temporal variability in the input, the two parameters related to bee phenology, *t.maturity* and *var.emerge.f*, were also only impactful to the outputs in this scenario (in simulations with both species). Accordingly, the parameters identified as influential to model outputs in Scenarios 2 and 3 are important to address under variable foraging and floral resource availabilities in realistic weather and landscape scenarios. The parameters highly impactful to model outputs may not only drive the quantitative model outputs but may also interact with other stressors, such as exposures and effects, once implemented in the model.



**Figure 20. Scenario 1: optimal foraging and floral resource availability. Left: *O. bicornis*; Right: *N. melanderi*.** Parameters included in the sensitivity analysis and their impact on the model outputs shown as partial rank correlation coefficient (PRCC). Positive PRCCs indicate an increase in the output variable with an increase in the parameter value, negative PRCCs indicate a decrease in the value of the output variable with an increase in the parameter value.



**Figure 21. Scenario 2: uniform half-optimal foraging and floral resource availability. Left: *O. bicornis*; Right: *N. melanderi*.** Parameters included in the sensitivity analysis and their impact on the model outputs shown as partial rank correlation coefficient (PRCC). Positive PRCCs indicate an increase in the output variable with an increase in the parameter value, negative PRCCs indicate a decrease in the value of the output variable with an increase in the parameter value.



**Figure 22. Scenario 3: half-optimal foraging and floral resource availability with a 10-day foraging gap. Left: *O. bicornis*; Right: *N. melanderi*.**  
 Parameters included in the sensitivity analysis and their impact on the model outputs shown as partial rank correlation coefficient (PRCC). Positive PRCCs indicate an increase in the output variable with an increase in the parameter value, negative PRCCs indicate a decrease in the value of the output variable with an increase in the parameter value.

## 6.2. Sensitivity analysis with exposures and effects

### 6.2.1. Exposure scenario applied in the model analyses with exposures and effects

For the analysis of the SolBeePop<sub>ecotox</sub> with exposures and effects, an exposure scenarios was applied using dimethoate as example pesticide. The scenario assumed optimal foraging conditions throughout the simulated bee activity and a spray application date after bee emergence. All resources collected by the bees (pollen, nectar, soil/mud) were assume to be exposed and all post-emergent females present on the day of application were additionally assumed to be exposed to direct spray. The input scenario including the daily exposure characterizations was used for the sensitivity analysis and the uncertainty analysis (Section 6.3).

Note that the input scenarios applied are not meant to represent realistic foraging conditions, floral resource availability or exposure concentrations but had the purpose of assessing the interaction between uncertain parameter values and simulated population-level effects for an example pesticide. The estimation of exposures in the different exposure routes considered by the model were conducted with the goal to obtain exposure concentrations in different matrices with realistic relationships to each other, i.e., assuming all applied exposures could originate from the same hypothetical single application of dimethoate. See also Appendix B how to generate a floral and exposure input file.

For *O. bicornis*, the assumptions used for the generation of the exposure scenario are listed in Table 14. The assumptions used for *N. melanderi* are listed in Table 15. Using the specifications listed for each species, dimethoate concentrations in soil at the relevant depth were estimated using a standard exposure modeling approach and a FOCUS weather scenario for Central Europe. For the estimation of soil exposures (mud collected from the soil surface), a soil exposure model was used, applying a FOCUS weather scenario according to the application date. The application date was chosen to coincide with the time window of emergence of each species.

*Table 14. Exposure scenario for dimethoate applied in the analysis of parameter uncertainty with *O. bicornis*. These exposure assumptions were used to generate the floral and exposure input file (Floral\_Exp1\_Osmia\_Jan2023.csv) for SolBeePop.*

Characteristic	Value	Remarks
Application date (day of year)	22 April (112)	Application date defines the onset of exposure; date corresponds to 1 day prior to median female emergence date used in UA
Application rate	200 a.i. g/ha	High application rate used according to nectar and pollen residue studies (with honey bees) referenced in (European Food Safety Authority 2023) (Annex H)
Kinetics of residues in nectar		Nectar residue data and single first order (SFO) kinetics used from (European Food Safety Authority 2023) (Annex H); see also text for more details

Characteristic	Value	Remarks
Pollen residues		Set identical to nectar (no separate pollen data available)
Concentration in direct spray	2280 mg a.i./l	Corresponds to 2.8 a.i. µg/bee from one drop of 1 µl intercepted by the bee, see text for more explanation
Soil depth	0-9mm	Top soil layer; see text for more details about the soil exposure applied

*Table 15. Exposure scenario applied in the analysis of parameter uncertainty with N. melanderi. These exposure assumptions were used to generate the floral and exposure input file (Floral\_Exp2\_Nomia\_Jan2023.csv) for SolBeePop.*

Characteristic	Value	Remarks
Application date (day of year)	30 June (181)	Application date defines the onset of exposure; date corresponds to 1 day prior to median female emergence date used in UA
Application rate	200 g a.i./ha	High application rate used according to nectar and pollen residue studies (with honey bees) referenced in (European Food Safety Authority 2023) (Annex H)
Kinetics of residues in nectar		Nectar residue data and single first order (SFO) kinetics used from (European Food Safety Authority 2023) (Annex H); see also text for more details
Pollen residues		Set identical to nectar (no separate pollen data available)
Concentration in direct spray	2280 mg a.i./l	Corresponds to 2.8 a.i. µg/bee from one drop of 1 µl intercepted by the bee, see text for more explanation
Soil depth	175mm	Corresponding to reported nest depths of 15-20cm (Batra 1970); see text for more details about the soil exposure applied

Residues in nectar were derived from study data conducted with Phacelia and a dimethoate application rate of 200 g a.i./ha. The study data and the fit to estimate the compound kinetics in nectar are provided in (European Food Safety Authority 2023) (Annex H) and shown in Figure 23. The SFO fit is used as input to SolBeePop for the purpose of the model analysis whereby the application day (0 days after application) corresponds to the application date used for the two model bee species. Because no separate residue data relevant for the estimation of residue kinetics in pollen were identified by (European Food Safety Authority 2023), we applied the residue time series from nectar also to pollen.

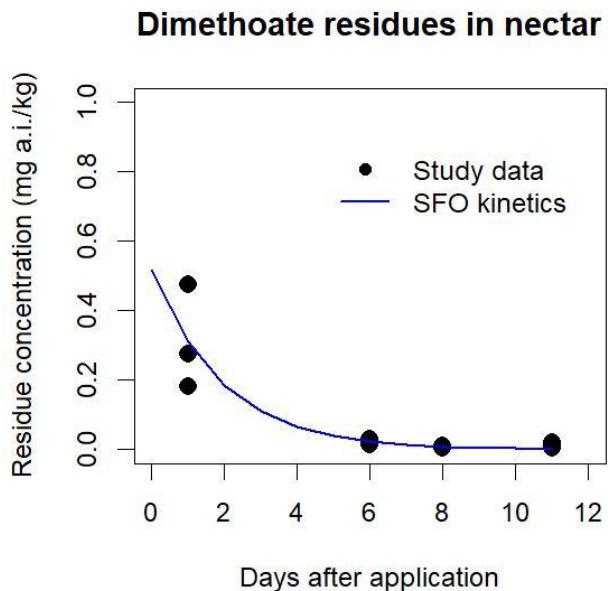


Figure 23. Dimethoate residue concentrations reported in nectar of *Phacelia* flowers at different time points after application (black dots). Data from studies reported by (European Food Safety Authority (EFSA) et al. 2023, Annex H). Single first order (SFO) kinetics fit identified by EFSA (blue) is used as input to SolBeePop for the purpose of the model analysis.

Exposure to direct spray occurs when a bee is foraging within the treated area at time of pesticide application. The amount of compound intercepted by a bee depends on its size with larger bees assumed to intercept more spray than smaller bees. In European Food Safety Authority (EFSA) et al. (2023), a body surface factor (BsF) is provided for honey bees, bumble bees and solitary bees which can be applied to the application rate to estimate the exposure per bee. The BsF is based on bee size. Here, we used the BsF for honey bees ( $0.0114 \text{ dm}^2/\text{bee}$ ) to estimate the dimethoate exposure for *N. melanderi* and *O. bicornis* because females of both species are comparable in size to worker honey bees (see Table 63 and Table 67, respectively). The BsF provided for solitary bees assumes a considerably smaller body surface. SolBeePop requires the concentration (mg/l) as input to define the exposure via direct spray. We assumed that the 2.8 a.i.  $\mu\text{g}/\text{bee}$  are contained in a single droplet of spray with a volume of  $1 \mu\text{l}$ , corresponding to 2280 mg a.i./l.

Generic levels of exposure in soil were estimated using a FOCUS scenario for Central Europe, the application rate of 200 g dimethoate/ha and the application date for each species. The exposure level in the top soil layer was used for *O. bicornis* because the bees collect mud (wet soil) from the soil surface to build partitions between brood cells (in existing, above-ground cavities). *N. melanderi* was reported to build brood cell chambers at soil depths between 15-20 cm (Batra 1970), and thus, exposure levels at a soil depth of 175 mm were used to inform the soil exposure time series for the species. The time series applied are provided in the file *Floral\_Exp2\_Nomia\_Jan2023.csv* for *N. melanderi* and *Floral\_Exp1\_Osmia\_Jan2023.csv* for *O. bicornis*.

## 6.2.2. Methods

The sensitivity analysis was conducted to assess the impact of proportional changes in parameter values population-level effects from exposures with SolBeePop\_ecotox. As an example pesticide, dimethoate was used in the analysis. Dimethoate is an insecticide commonly used as toxic standard (positive control) in bee toxicity studies. Thus, data are available to inform exposures and effects, and the compound is relevant for testing effects in the model.

The analysis used a similar setup applied to the model analysis without exposures and effects (see Section 6.1). The same two example model species were used for the simulations: *O. bicornis* and *N. melanderi*. Parameters potentially influential to model outputs were perturbated in the analysis within a +/-10% range of the identified default value.

For the model parameters no characterizing exposure and effects in the model, the same parameter ranges were applied as in the previous analysis (Section 6.1, Table 10 and Table 11). In addition, parameters defining individual-level exposure (from the input exposure time series) and effects were included in the analysis. In Table 20 (*O. bicornis*) and Table 21 (*N. melanderi*), the default values of the model parameters relevant for the simulations with exposures and effects are listed, their inclusion in the model analysis, default values and ranges. References are provided for reported parameter ranges, or justifications for the ranges applied in case no relevant references could be identified.

Using the same methodology as in the previously described model analyses (Sections 6.1 and 6.2), the parameters included in the model analysis were explored for their impact on simulated effects by sampling the parameter space with a Monte Carlo method, latin hypercube (LHC), which results in even sampling of the parameter space (Blower and Dowlatabadi 1994). For the drawing of random parameter values from the parameter space defined by the ranges in Table 10, the method “randomLHS” from the R-package “lhs” was applied (Carnell 2022; R Core Team 2022). The method assumes uniform distributions of all parameters. Considering the larger number of parameters included in the analysis with exposures and effects, a Latin Hypercube for 7000 samples<sup>3</sup> from the parameter space was calculated. Simulations with each of these parameter combinations were repeated 10 times with different random number seeds.

The sensitivity with exposure and effects was conducted with a single input scenario. The scenario assumes optimal foraging conditions throughout the active seasons of both species (corresponding to Scenario 1 in Section 6.1). For the control simulations, an input file was used that defines no exposure in any matrix (all values in columns in the input file defining daily exposure concentrations in nectar, pollen, direct spray, soil (or mud) and leaves set to 0). For the simulations with exposures, dimethoate concentrations in nectar, pollen, direct spray and soil were estimated, using a worst-case scenario relevant for *O. bicornis* and *N. melanderi*. Residue concentrations on leaves were not estimated because this exposure route is not relevant for the two species. Floral and exposure input files specific for each species were used in the simulations as described in Section 6.2.1.

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<sup>3</sup> (Blower and Dowlatabadi 1994) state that minimum number of samples from the LHC space need to be:  $N > 4/3K$ . In this SA,  $K = 26$ , i.e.,  $N > 34.7$  or the minimum is  $N_{min} = 35$ . The chosen sample number corresponds to  $200 \times N_{min}$ .

Relative effects ( $E_r$ ) were calculated by comparing model outputs from the corresponding control ( $O_c$ ) and exposure simulations ( $O_e$ ) using Equation 6.1. Corresponding control and exposure simulations used identical parameter combinations and random number seeds and differed exclusively in the input file used (without and with exposures, respectively).

*Equation 6.1*

$$E_r = \frac{O_e - O_c}{O_c}$$

The partial rank correlation coefficient (PRCC) was calculated for each relative effect on outputs used in Section 6.1. The PRCC correlates the impact of the applied range of each parameter on outputs across LHC samples (Blower and Dowlatabadi 1994). The analysis was conducted in R using the package “sensitivity” and plots were generated using the package “ggplot2” (Wickham 2016; Iooss et al. 2022; R Core Team 2022).

*Table 16. Model parameter values applied in the sensitivity analysis (SA) with exposures and effects for simulations with O. bicornis. Parameters not included in the model analysis were used with their default value in all simulations. Note that parameters defining the organism-level concentration-response relationship (GUTS for adults, concentration-response function for larvae) are derived from studies with honey bees and are specific to the example pesticide, dimethoate.*

Interface parameter name	Osmia bicornis (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks
Start.day	1	No	--	--	
Species	O.bicornis	No	--	--	
Volitinism	univoltine	No	--	--	
Initial.num.f	100	No	--	--	
Initial.num.m	200	No	--	--	
Initial.stage	cocoon	No	--	--	
Initial.age	200	No	--	--	
RndSeed		see remarks			Different random numbers used for each of the 10 repeat simulations
MultiYearInput	FALSE	No	--	--	
List.input.floral	NA	No	--	--	
Num.repeat.yr	2	No	--	--	
input.floral		see remarks			Control simulations (no exposure): Floral_generic_control_exposure_Jan2023.csv; exposure simulations: Floral_Exp1_Osmia_Jan2023.csv See Section 6.2.1 for description of the exposure scenario applied
stoch.crop.forag	FALSE	No	--	--	
Density.dep	FALSE	No			
DD.thresh.s	NA	No			
DD.max.cells.s	NA	No			
DD.funct	NA	No			
DD.log.slope	NA	No			

Interface parameter name	<i>Osmia bicornis</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks
<i>day.emerge.f</i>	113	No	--	--	Species-specific but not included in the sensitivity analysis. Different date used than in 6.1; in the optimal foraging scenario applied, the emergence date is only relevant relative to the pesticide application date; see also text
<i>var.emerge.f</i>	3	Yes	2	4	values need to be integers; smallest possible perturbation used (>10% because it needs to be an integer)
<i>day.emerge.m</i>	99	No	--	--	Species-specific but not included in the sensitivity analysis. See also <i>day.emerge.f</i>
<i>var.emerge.m</i>	2	No	--	--	Species-specific but not included in the sensitivity analysis: no data available (see <i>var.emerge.f</i> ) and male emergence timing does not affect reproductive rates in the model.
<i>latest.emerge</i>	365	No	--	--	Parameter used for multi-voltine life cycles only; unused if Voltinism = 'univoltine'
<i>dev.egg</i>	8	No	--	--	Species-specific but not included in the sensitivity analysis: in-nest development times do not impact reproductive or emergence rates in the model
<i>dev.larva</i>	32	No	--	--	Species-specific but not included in the sensitivity analysis: in-nest development times do not impact reproductive or emergence rates in the model
<i>dev.cocoon</i>	68	No	--	--	Species-specific but not included in the sensitivity analysis: in-nest development times do not impact reproductive or emergence rates in the model
<i>t.maturity</i>	3	Yes	2	4	values need to be integers; smallest possible perturbation used (>10% because it needs to be an integer)
<i>m.life</i>	21	No	--	--	Species-specific but not included in the sensitivity analysis: post-emergent male life span not reported in the literature and not impactful for model outputs
<i>max.nesting.life</i>	36	Yes	32	40	values need to be integers; rounded up perturbation to meet requirement of integer values
<i>p.max.nesting.life</i>	0.04	Yes	0.036	0.044	

Interface parameter name	<i>Osmia bicornis</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks
<i>max.f.ratio</i>	0.59	Yes	0.531	0.649	
<i>max.cells</i>	2	Yes	1	3	
<i>max.survival.e.f</i>	0.74	Yes	0.666	0.814	
<i>max.survival.e.m</i>	0.74	see remarks			No separate data for females and males available for survival to emergence: the same value was applied to <i>max.survival.e.f</i> and <i>max.survival.e.m</i> in the simulations
<i>emerged.survival</i>	0.544	Yes	0.4896	0.5984	
<i>a.cell.age</i>	-0.006	Yes	-0.0066	-0.0054	Values derived from study with <i>O. cornuta</i> , see also Section 3.2.1
<i>a.sex.age</i>	-0.0406	Yes	-0.04466	-0.03654	Values derived from study with <i>O. bicornis</i> , see also Section 3.2.3
<i>a.size.age</i>	-0.003	Yes	-0.0033	-0.0027	Values derived from studies with <i>O. bicornis</i> and <i>O. cornuta</i> , see also Section 3.2.5
<i>a.cell.resource</i>	0.94	Yes	0.846	1.034	Values derived from study with <i>O. pumila</i> , <i>M. apicalis</i> and <i>M. rotundata</i> , see also Section 3.2.2
<i>a.sex.resource</i>	0.42	Yes	0.378	0.462	Default value derived from study with <i>M. apicalis</i> ; study data not suitable for estimation of range, see also Section 3.2.4
<i>a.size.resource</i>	0.114	Yes	0.1026	0.1254	Values derived from study with <i>M. apicalis</i> , see also Section 3.2.6
<i>Effects</i>	TRUE	--			Aim of the SA is to test the sensitivity to effects
<i>ad.nectar.cons</i>	208.34	Yes	187.506	229.174	

Interface parameter name	<i>Osmia bicornis</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks
<i>ad.pollen.cons</i>	11.6	Yes	10.44	12.76	
<i>k_CA</i>	0.4	--	--	--	Parameter from BeeGUTS (honey bee); it remained unchanged in the BeeGUTS (and interacts with GUTS from contact exposure, and thus, should not be changed independent of the GUTS parameters)
<i>Transfer.mat.adult</i>	TRUE	--	--	--	Testing all aspects of exposure and effects included in the model
<i>ad.ET</i>	0.072	Yes	0.0648	0.0792	Strohm et al. provide time for construction of a single brood cell; range: min = average-sd; max = 2x(average-sd) (if the bee builds two cells per day); range corresponds to data point shown in <a href="#">European Food Safety Authority (EFSA) et al. 2023, Annex B, Fig. 18: ~0.4 h for <i>O. bicornis</i></a> ;
<i>TC_soil</i>	0.5	Yes	0.45	0.55	Parameter only applicable to <i>Osmia</i> (soil/mud brood cell partitions) and soil-nesting bees
<i>TC_leaf</i>	NA	--	--	--	Not applicable to <i>O. bicornis</i> : only applicable to <i>Megachile</i> (leaf-cutter bees)
<i>Exposure.resting.soil</i>	FALSE	--	--	--	Not applicable to <i>O. bicornis</i> : only applicable to soil-nesting bees
<i>GUTS</i>	GUTS-SD, GUTS-IT	--	--	--	Model analysis conducted separately with each GUTS version
<i>t.guts</i>	10	--	--	--	Time step used for GUTS fitting in BeeGUTS
<i>kd_SD</i>	0.39	Yes	0.351	0.429	BeeGUTS parameter estimates and ranges for <b>dimethoate</b> using all data (honey bee); range used for simulations with GUTS-SD
<i>bw_SD</i>	0.014	Yes	0.0126	0.0154	
<i>mw_SD</i>	13	Yes	11.7	14.3	
<i>kd_IT</i>	0.012	Yes	0.0108	0.0132	BeeGUTS parameter estimates and ranges for <b>dimethoate</b> using all data (honey bee); range used for simulations with GUTS-IT
<i>mw_IT</i>	2.4	Yes	2.16	2.64	
<i>Fs_IT</i>	3	Yes	2.7	3.3	
<i>nectar_prop</i>	0.78	Yes	0.702	0.858	Data used from <a href="#">European Food Safety Authority (EFSA) et al. 2023 (Table 14)</a> and assuming 30% sugar content (w/w) of nectar (see section 5.3.6); data specific to <i>O. bicornis</i>
<i>weight.prov</i>	306	Yes	275.4	336.6	
<i>Transfer.mat.dev</i>	TRUE	--	--	--	
<i>SM</i>	187	Yes	168.3	205.7	Wet weight of single brood cell partition; applies only to <i>Osmia</i>

Interface parameter name	<i>Osmia bicornis</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks
<i>F</i>	NA	--	--	--	Not applicable to <i>O. bicornis</i> : only applicable to <i>Megachile</i> (leaf-cutter bees)
<i>SA_i</i>	NA	--	--	--	Not applicable to <i>O. bicornis</i> : only applicable to <i>Megachile</i> (leaf-cutter bees)
<i>dr.intercept</i>	1.1534	Yes	1.03806	1.26874	Dose-response parameters from honey bee larval toxicity studies with dimethoate
<i>dr.slope</i>	-0.7876	Yes	-0.86636	-0.70884	

*Table 17. Model parameter values applied in the sensitivity analysis (SA) with example species Nomia melanderi. Parameters not included in the sensitivity analysis were used with their default value in all simulations. If no remarks are included for parameters not included in the analysis, these parameters are not species-specific but define initial conditions in the simulations, number of years simulated and the input method of the floral resource input file(s).*

Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks
<i>Start.day</i>	1	--	--	--	
<i>Species</i>	N.melanderi	--	--	--	
<i>Voltinism</i>	univoltine	--	--	--	
<i>Initial.num.f</i>	100	--	--	--	
<i>Initial.num.m</i>	200	--	--	--	
<i>Initial.stage</i>	cocoon	--	--	--	
<i>Initial.age</i>	200	--	--	--	
<i>RndSeed</i>		see remarks			10 random number seeds per parameter combination
<i>MultiYearInput</i>	FALSE	--	--	--	
<i>List.input.floral</i>	NA	--	--	--	
<i>Num.repeat.yr</i>	2	--	--	--	
<i>input.floral</i>		see remarks			Analysis repeated for 3 scenarios: (1) optimal foraging conditions, (2) half-optimal, (3) half-optimal with 10-day foraging gap during nesting season, see text
<i>stoch.crop.forag</i>	FALSE	--	--	--	
<i>Density.dep</i>	FALSE	--	--	--	Density dependence not included in this analysis
<i>DD.thresh.s</i>	NA	--	--	--	
<i>DD.max.cells.s</i>	NA	--	--	--	

Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks
<i>DD.funct</i>	NA	--	--	--	
<i>DD.log.slope</i>	NA	--	--	--	
<i>day.emerge.f</i>	182	--	--	--	Species-specific but not included in the sensitivity analysis. Different date used than in 6.1; in the optimal foraging scenario applied, the emergence date is only relevant relative to the pesticide application date; see also text
<i>var.emerge.f</i>	6	Yes	5	7	values need to be integers; smallest possible perturbation used (>10% because it needs to be an integer)
<i>day.emerge.m</i>	167	--	--	--	Species-specific but not included in the sensitivity analysis. See also <i>day.emerge.f</i>
<i>var.emerge.m</i>	8	--	--	--	
<i>latest.emerge</i>	365	--	--	--	only meaningful to test for facultatively bivoltine life cycles
<i>dev.egg</i>	2	--	--	--	development times not influential to model outputs (in univoltine life cycles)
<i>dev.larva</i>	6	--	--	--	
<i>dev.cocoon</i>	20	--	--	--	
<i>t.maturity</i>	1	Yes	1	2	values need to be integers; smallest possible perturbation used (>10% because it needs to be an integer)
<i>m.life</i>	14	--	--	--	not impactful to model dynamics or outputs (other than number of post-emergent males)
<i>max.nesting.life</i>	26	Yes	23	29	values need to be integers; rounded up perturbation to meet requirement of integer values
<i>p.max.nesting.life</i>	0.04	Yes	0.036	0.044	
<i>max.f.ratio</i>	0.51	Yes	0.459	0.561	

Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks
<i>max.cells</i>	1	Yes	0.9	1.1	
<i>max.survival.e.f</i>	0.868	Yes	0.7812	0.9548	apply the same value to <i>max.survival.e.f</i> and <i>max.survival.e.m</i>
<i>max.survival.e.m</i>	0.868	see remarks			apply the same value to <i>max.survival.e.f</i> and <i>max.survival.e.m</i>
<i>emerged.survival</i>	0.544	Yes	0.4896	0.5984	
<i>a.cell.age</i>	-0.006	Yes	-0.0066	-0.0054	Reproductive relationships characterized using data from multiple species (see also Table 10)
<i>a.sex.age</i>	-0.0406	Yes	-0.04466	-0.03654	
<i>a.size.age</i>	-0.003	Yes	-0.0033	-0.0027	
<i>a.cell.resource</i>	0.94	Yes	0.846	1.034	
<i>a.sex.resource</i>	0.42	Yes	0.378	0.462	
<i>a.size.resource</i>	0.114	Yes	0.1026	0.1254	
<i>Effects</i>	TRUE	--			Aim of the SA is to test the sensitivity to effects
<i>ad.nectar.cons</i>	208.34	Yes	187.506	229.174	
<i>ad.pollen.cons</i>	11.6	Yes	10.44	12.76	
<i>k_CA</i>	0.4	--	--	--	Parameter from BeeGUTS (honey bee); it remained unchanged in the BeeGUTS (and interacts with GUTS from contact exposure, and thus, should not be changed independent of the GUTS parameters)
<i>Transfer.mat.adult</i>	TRUE	--	--	--	Testing all aspects of exposure and effects included in the model
<i>ad.ET</i>	0.75	Yes	0.675	0.825	

Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks
TC_soil	0.5	Yes	0.45	0.55	Parameter only applicable to <i>Osmia</i> (soil/mud brood cell partitions) and soil-nesting bees
TC_leaf	NA	--	--	--	Not applicable to <i>N. melanderi</i> : only applicable to <i>Megachile</i> (leaf-cutter bees)
Exposure.resting.soil	FALSE	--	--	--	Not included because setting this parameter to 'TRUE' corresponds to the setting of ad.ET = 1
GUTS	GUTS-SD, GUTS-IT	--	--	--	Model analysis conducted separately with each GUTS version
t.guts	10	--	--	--	Time step used for GUTS fitting in BeeGUTS
kd_SD	0.39	Yes	0.351	0.429	BeeGUTS parameter estimates and ranges for <b>dimethoate</b> using all data (honey bee); range used for simulations with GUTS-SD
bw_SD	0.014	Yes	0.0126	0.0154	
mw_SD	13	Yes	11.7	14.3	
kd_IT	0.012	Yes	0.0108	0.0132	
mw_IT	2.4	Yes	2.16	2.64	BeeGUTS parameter estimates and ranges for <b>dimethoate</b> using all data (honey bee); range used for simulations with GUTS-IT
Fs_IT	3	Yes	2.7	3.3	
nectar_prop	0.67	Yes	0.603	0.737	
weight.prov	270	Yes	243	297	Using reported adult female weight and relation to provision weight reported by Neff 2008
Transfer.mat.dev	TRUE	--	--	--	
SM	NA	--	--	--	Not applicable to <i>N. melanderi</i> : parameter applies only to <i>Osmia</i> (mud/soil brood cell partition)
F	NA	--	--	--	Not applicable to <i>N. melanderi</i> : only applicable to <i>Megachile</i> (leaf-cutter bees)
SA_i	NA	--	--	--	Not applicable to <i>N. melanderi</i> : only applicable to <i>Megachile</i> (leaf-cutter bees)
dr.intercept	1.1534	Yes	1.03806	1.26874	Dose-response parameters from honey bee larval toxicity studies with <b>dimethoate</b>
dr.slope	-0.7876	Yes	-0.86636	-0.70884	

### 6.2.3. Results

From the outputs (relative effects compared to control simulations) of the sensitivity analysis, the perturbation range of the species-specific parameters included could be identified as a) highly influential to one or several model outputs analyzed, b) influential to at least one model output, or c) not influential to model outputs (Table 22 and Table 23). The PRCC for each parameter included in the sensitivity analysis can range between -1 (increase in the parameter value is correlated with a corresponding decrease in the output value irrespective of all other parameter values) and 1 (increase in the parameter value is correlated with a corresponding increase in the output value irrespective of all other parameter values). A PRCC = 0 denotes no impact of the parameter value on outputs. Here, we arbitrarily define parameters as impactful to model outputs if  $|PRCC| \geq 0.25$ . In addition, we identify model parameters as highly impactful if  $|PRCC| \geq 0.5$  for 3 or more of the outputs analyzed. Parameters were classified as not impactful if  $|PRCC| \leq 0.1$ . The results of the PRCC from the sensitivity are shown in Figure 24 and Figure 25.

*Table 18. Results of the sensitivity analysis with O. bicornis by model parameter whereby relative effects were analyzed as outputs. +: PRCC > 0.25 for at least one output and the increase in parameter value corresponds to an increase (or no change) across outputs; -: PRCC < -0.25 for at least one output and the increase in parameter value corresponds to a decrease (or no change) across outputs; +/-: |PRCC| > 0.25 for at least one output and the increase in parameter value corresponds to an increase or decrease (or no change) dependent on the output; ++: PRCC > 0.5 for at least 3 outputs and the increase in parameter value corresponds to an increase (or no change) across outputs; --: PRCC < -0.5 for at least one output and the increase in parameter value corresponds to a decrease (or no change) across outputs; grey cells: |PRCC| < 0.1 across all outputs.*

Interface parameter name	Osmia bicornis (default parameter value)	Min value in SA	Max value in SA	GUTS-IT	GUTS-SD
var.emerge.f	3	1	7	+	+
t.maturity	3	1	10	-	-
max.nesting.life	36	26	36		
p.max.nesting.life	0.04	0.01	0.1		
max.f.ratio	0.59	0.38	1		
max.cells	2	1	3		
max.survival.e.f,	0.74	0.58	0.89		
emerged.survival	0.544	0.5	0.75		
a.cell.age	-0.006	-0.008	-0.004		
a.sex.age	-0.0406	-0.0286	-0.0599		
a.size.age	-0.003	-0.001	-0.005		
a.cell.resource	0.94	0.43	1.4		
a.sex.resource	0.42	0.2	0.6		

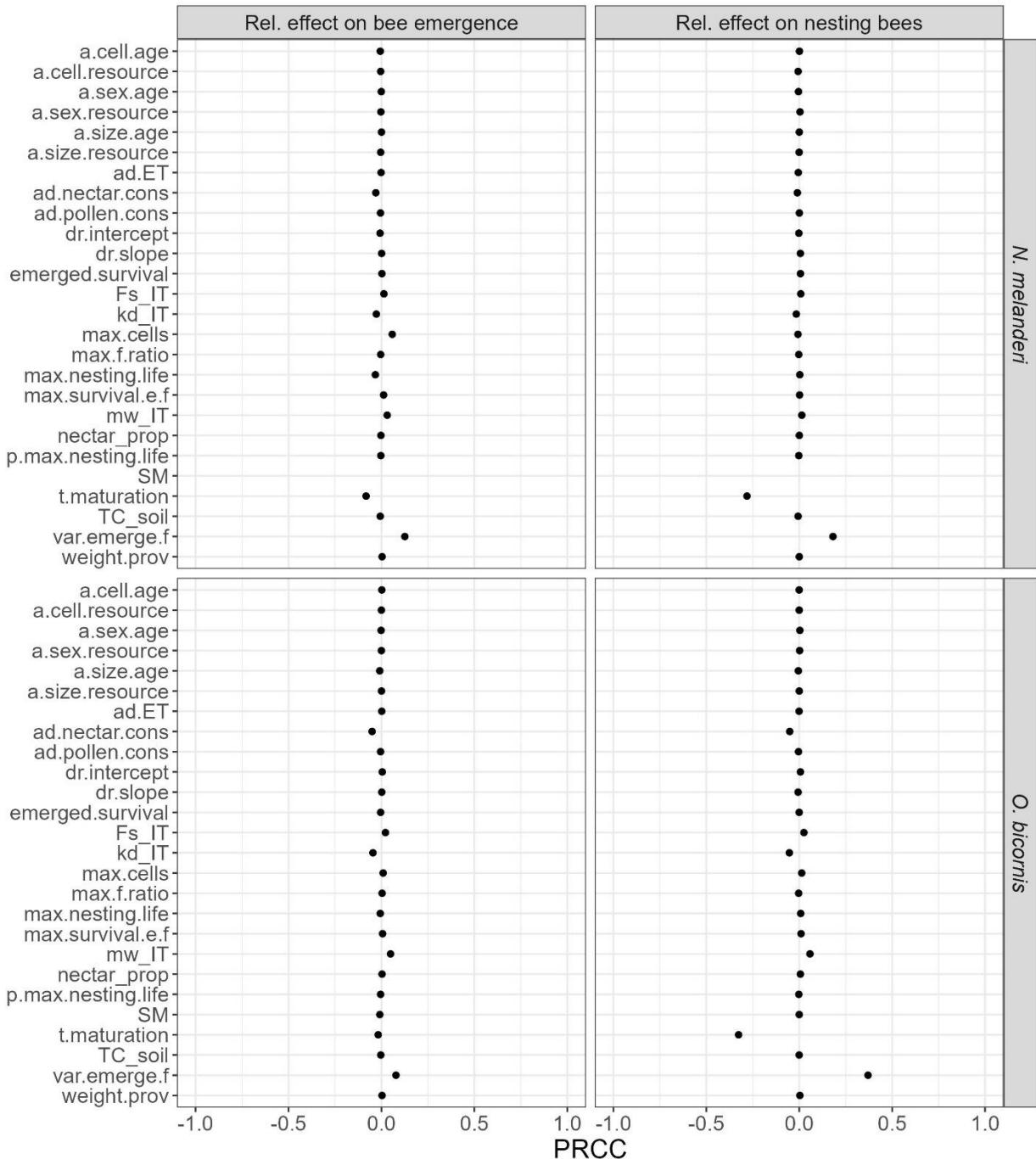
Interface parameter name	Osmia bicornis (default parameter value)	Min value in SA	Max value in SA	GUTS-IT	GUTS-SD
<i>a.size.resource</i>	0.114	0	0.312		
<i>ad.nectar.cons</i>	208.34	140	276.67		
<i>ad.pollen.cons</i>	11.6	0	23.2		
<i>ad.ET</i>	0.072	0.0175	0.157		
<i>TC_soil</i>	0.5	0	1		
<i>kd_SD</i>	0.39	0.3	0.51	NA	
<i>bw_SD</i>	0.014	0.011	0.017	NA	
<i>mw_SD</i>	13	12	15	NA	
<i>kd_IT</i>	0.012	0.0016	0.051		NA
<i>mw_IT</i>	2.4	0.32	9.6		NA
<i>Fs_IT</i>	3	2.7	3.4		NA
<i>nectar_prop</i>	0.78	0.77	0.79		
<i>weight_prov</i>	306	257.1	354.9		
<i>SM</i>	187	135.5	238.5		
<i>dr.intercept</i>	1.1534	0.8419	1.514		
<i>dr.slope</i>	-0.7876	-1.157	-0.507		

Table 19. Results of the sensitivity analysis with *N. melanderi* by model parameter whereby relative effects were analyzed as outputs. +: PRCC > 0.25 for at least one output and the increase in parameter value corresponds to an increase (or no change) across outputs; -: PRCC < -0.25 for at least one output and the increase in parameter value corresponds to a decrease (or no change) across outputs; +/-: |PRCC| > 0.25 for at least one output and the increase in parameter value corresponds to an increase or decrease (or no change) dependent on the output; ++: PRCC > 0.5 for at least 3 outputs and the increase in parameter value corresponds to an increase (or no change) across outputs; --: PRCC < -0.5 for at least one output and the increase in parameter value corresponds to a decrease (or no change) across outputs; grey cells: |PRCC| < 0.1 across all outputs.

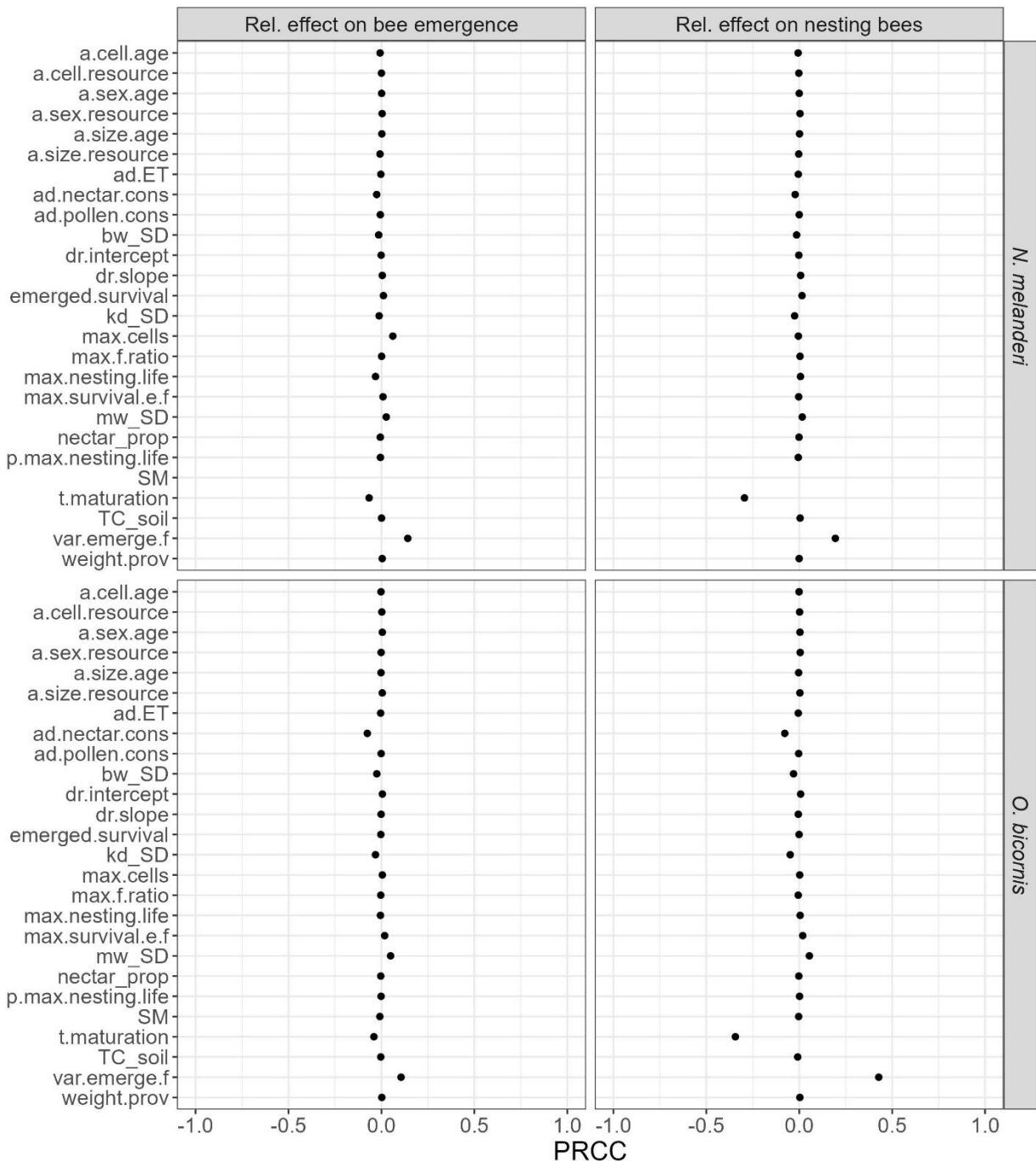
Interface parameter name	Nomia melanderi (default parameter value)	Min value in SA	Max value in SA	GUTS-IT	GUTS-SD
<i>var.emerge.f</i>	3	3	9		
<i>t.maturity</i>	3	1	7	-	-
<i>max.nesting.life</i>	26	22	30		
<i>p.max.nesting.life</i>	0.04	0.01	0.1		
<i>max.f.ratio</i>	0.51	0.35	0.51		

Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Min value in SA	Max value in SA	GUTS-IT	GUTS-SD
<i>max.cells</i>	1	0.5	1		
<i>max.survival.e.f,</i>	0.868	0.729	0.868		
<i>emerged.survival</i>	0.544	0.5	0.75		
<i>a.cell.age</i>	-0.006	-0.008	-0.004		
<i>a.sex.age</i>	-0.0406	-0.0599	0		
<i>a.size.age</i>	-0.003	-0.005	-0.001		
<i>a.cell.resource</i>	0.94	0.43	1.4		
<i>a.sex.resource</i>	0.42	0	0.6		
<i>a.size.resource</i>	0.114	0	0.312		
<i>ad.nectar.cons</i>	208.34	140	276.67		
<i>ad.pollen.cons</i>	11.6	0	23.2		
<i>ad.ET</i>	0.75	0.25	1		
<i>TC_soil</i>	0.5	0	1		
<i>kd_SD</i>	0.39	0.3	0.51	<b>NA</b>	
<i>bw_SD</i>	0.014	0.011	0.017	<b>NA</b>	
<i>mw_SD</i>	13	12	15	<b>NA</b>	
<i>kd_IT</i>	0.012	0.0016	0.051		<b>NA</b>
<i>mw_IT</i>	2.4	0.32	9.6		<b>NA</b>
<i>Fs_IT</i>	3	2.7	3.4		<b>NA</b>
<i>nectar_prop</i>	0.67	0.53	0.81		
<i>weight_prov</i>	270	158	305		
<i>SM</i>	NA	NA	NA	<b>NA</b>	<b>NA</b>
<i>dr.intercept</i>	1.1534	0.8419	1.514		
<i>dr.slope</i>	-0.7876	-1.157	-0.507		

Simulated relative effects in *O. bicornis* were impacted by parameters of bee phenology (*var.emerge.f* and *t.maturity*). In simulations with *N. melanderi*, only perturbations of *t.maturity* resulted in  $|PRCC| > 0.25$ . These parameters influence the timing of bee emergence and onset of nesting relative to the simulated pesticide application date. More variability in female emergence dates (larger range of *var.emerge.f*) results in less overlap with exposures across the population (particularly with the exposure via direct spray which is assumed to occur only on a single day). A longer maturation time (larger values of *t.maturity*) result in less females that emerge prior to exposure (application date) able to initiate nesting. No other parameters were consistently influential to relative effects in the sensitivity analysis.



*Figure 24. Analysis of the impact of parameter perturbations (+/-10% from default value) on simulated relative effect sizes in simulations using GUTS-IT. Parameters included in the model analysis of SolBeePop<sub>ecotox</sub> (with exposure and effects) and their impact on simulated relative effects sizes shown as partial rank correlation coefficient (PRCC). Positive PRCCs indicate an increase in parameter value results in increase in output value (smaller relative effect), negative PRCCs indicate an increase in parameter value results in a decrease in output value (higher relative effect).*



*Figure 25. Analysis of the impact of parameter perturbations (+/-10% from default value) on simulated relative effect sizes in simulations using GUTS-SD. Parameters included in the model analysis of SolBeePop<sub>ecotox</sub> (with exposure and effects) and their impact on simulated relative effects sizes shown as partial rank correlation coefficient (PRCC). Positive PRCCs indicate an increase in parameter value results in increase in output value (smaller relative effect), negative PRCCs indicate an increase in parameter value results in a decrease in output value (higher relative effect).*

## 6.3. Analysis of parameter uncertainty with exposures and effects

### 6.3.1. Methods

The analysis of parameter uncertainty was conducted to gain understanding of the interaction between parameter uncertainty and simulated population-level effects from exposures with SolBeePop\_ecotox. As an example pesticide, dimethoate was used in the analysis. Dimethoate is an insecticide commonly used as toxic standard (positive control) in bee toxicity studies. Thus, data are available to inform exposures and effects, and the compound is relevant for testing effects in the model.

The analysis used the same setup applied to the analysis without exposures and effects (see Section 6.1). The same two example model species were used for the simulations: *O. bicornis* and *N. melanderi*. For the model parameters no characterizing exposure and effects in the model, the same parameter ranges were applied as in the previous analysis (Section 6.1, Table 10 and Table 11). In addition, parameters defining individual-level exposure (from the input exposure time series) and effects were included in the analysis. In Table 20 (*O. bicornis*) and Table 21 (*N. melanderi*), the default values of the model parameters relevant for the simulations with exposures and effects are listed, their inclusion in the model analysis, default values and ranges. References are provided for reported parameter ranges, or justifications for the ranges applied in case no relevant references could be identified.

Using the same methodology as in the previously described model analyses (Sections 6.1 and 6.2), the parameters included in the model analysis were explored for their impact on simulated effects by sampling the parameter space with a Monte Carlo method, latin hypercube (LHC), which results in even sampling of the parameter space (Blower and Dowlatabadi 1994). For the drawing of random parameter values from the parameter space defined by the ranges in Table 10, the method “randomLHS” from the R-package “lhs” was applied (Carnell 2022; R Core Team 2022). The method assumes uniform distributions of all parameters. Considering the larger number of parameters included in the analysis with exposures and effects, a Latin Hypercube for 7000 samples<sup>4</sup> from the parameter space was calculated. Simulations with each of these parameter combinations were repeated 10 times with different random number seeds.

The analysis of parameter uncertainty with exposure and effects was conducted with a single input scenario. The scenario assumes optimal foraging conditions throughout the active seasons of both species (corresponding to Scenario 1 in Section 6.1). For the control simulations, an input file was used that defines no exposure in any matrix (all values in columns in the input file defining daily exposure concentrations in nectar, pollen, direct spray, soil (or mud) and leaves set to 0). For the simulations with exposures, dimethoate concentrations in nectar, pollen, direct spray and soil were estimated, using a worst-case scenario relevant for *O. bicornis* and *N. melanderi*. Residue concentrations on leaves were not estimated because this exposure route is not relevant for the two species. Floral and exposure input files specific for each species were used in the simulations as described in Section 6.2.1.

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<sup>4</sup> (Blower and Dowlatabadi 1994) state that minimum number of samples from the LHC space need to be:  $N > 4/3K$ . In this SA,  $K = 26$ , i.e.,  $N > 34.7$  or the minimum is  $N_{min} = 35$ . The chosen sample number corresponds to  $200 \times N_{min}$ .

Relative effects ( $E_r$ ) were calculated by comparing model outputs from the corresponding control ( $O_c$ ) and exposure simulations ( $O_e$ ) using Equation 6.2. Corresponding control and exposure simulations used identical parameter combinations and random number seeds and differed exclusively in the input file used (without and with exposures, respectively).

*Equation 6.2*

$$E_r = \frac{O_e - O_c}{O_c}$$

The partial rank correlation coefficient (PRCC) was calculated for each relative effect on outputs used in Section 6.1. The PRCC correlates the impact of the applied range of each parameter on outputs across LHC samples (Blower and Dowlatabadi 1994). The analysis was conducted in R using the package “sensitivity” and plots were generated using the package “ggplot2” (Wickham 2016; Iooss et al. 2022; R Core Team 2022).

*Table 20. Model parameter values applied in the analysis of parameter uncertainty (UA) with exposures and effects for simulations O. bicornis. The species-specific values applied to model parameters not specific to simulations with exposures and effects correspond to the values listed in Table 10 (with the exception of the emergence dates, day.emerge.f and day.emerge.m, and the input file, input.floral). Parameters not included in the model analysis were used with their default value in all simulations. Note that parameters defining the organism-level concentration-response relationship (GUTS for adults, concentration-response function for larvae) are derived from studies with honey bees and are specific to the example pesticide, dimethoate.*

Interface parameter name	Osmia bicornis (default parameter value)	Included in UA	Min value in UA	Max value in UA	Remarks	Value ranges based on
Start.day	1	No	--	--		
Species	O.bicornis	No	--	--		
Voltinism	univoltine	No	--	--		
Initial.num.f	100	No	--	--		
Initial.num.m	200	No	--	--		
Initial.stage	cocoon	No	--	--		
Initial.age	200	No	--	--		
RndSeed		see remarks			Different random numbers used for each of the 10 repeat simulations	
MultiYearInput	FALSE	No	--	--		
List.input.floral	NA	No	--	--		
Num.repeat.yr	2	No	--	--		
input.floral		see remarks			Control simulations (no exposure): Floral_generic_control_exposure_Jan2023.csv; exposure simulations: Floral_Exp1_Osmia_Jan2023.csv	See text for description of the exposure scenario applied
stoch.crop.forag	FALSE	No	--	--		
Density.dep	FALSE	No				
DD.thresh.s	NA	No				
DD.max.cells.s	NA	No				

Interface parameter name	<i>Osmia bicornis</i> (default parameter value)	Included in UA	Min value in UA	Max value in UA	Remarks	Value ranges based on
<i>DD.funct</i>	NA	No				
<i>DD.log.slope</i>	NA	No				
<i>day.emerge.f</i>	113	No	--	--	Species-specific but not included in the sensitivity analysis. Different date used than in 6.1; in the optimal foraging scenario applied, the emergence date is only relevant relative to the pesticide application date; see also text	
<i>var.emerge.f</i>	3	Yes	1	7	values need to be integers	No quantitative information available informing the range (time window) of emergence per population and season: generic range applied assuming a short emergence period (up to 1 week)
<i>day.emerge.m</i>	99	No	--	--	Species-specific but not included in the sensitivity analysis. See also <i>day.emerge.f</i>	
<i>var.emerge.m</i>	2	No	--	--	Species-specific but not included in the sensitivity analysis: no data available (see <i>var.emerge.f</i> ) and male emergence timing does not affect reproductive rates in the model.	
<i>latest.emerge</i>	365	No	--	--	Parameter used for multi-voltine life cycles only; unused if Voltinism = 'univoltine'	
<i>dev.egg</i>	8	No	--	--	Species-specific but not included in the sensitivity analysis: in-nest development times do not impact reproductive or emergence rates in the model	
<i>dev.larva</i>	32	No	--	--	Species-specific but not included in the sensitivity analysis: in-nest development times do not impact reproductive or emergence rates in the model	

Interface parameter name	<i>Osmia bicornis</i> (default parameter value)	Included in UA	Min value in UA	Max value in UA	Remarks	Value ranges based on
<i>dev.cocoon</i>	68	No	--	--	Species-specific but not included in the sensitivity analysis: in-nest development times do not impact reproductive or emergence rates in the model	
<i>t.maturity</i>	3	Yes	1	10	values need to be integers	(Bosch et al. 2008; Sgolastra et al. 2016)
<i>m.life</i>	21	No	--	--	Species-specific but not included in the sensitivity analysis: post-emergent male life span not reported in the literature and not impactful for model outputs	
<i>max.nesting.life</i>	36	Yes	26	36	values need to be integers	(Tepedino and Torchio 1982b; Frohlich and Tepedino 1986; Sugiura and Maeta 1989; Bosch 1994; Bosch et al. 2001; Bosch and Vicens 2005; Bosch and Vicens 2006; Bosch 2008; Sgolastra et al. 2016)
<i>p.max.nesting.life</i>	0.04	Yes	0.01	0.1		Parameter does not correspond to a trait measured in any published study: generic value range applied
<i>max.f.ratio</i>	0.59	Yes	0.38	1		(Bosch and Vicens 2005; Bosch and Vicens 2006; Seidelmann 2006; Seidelmann et al. 2010; Giejdasz et al. 2016; Sgolastra et al. 2016)
<i>max.cells</i>	2	Yes	1	3		(Bosch 1994; Goodell 2003; Bosch and Vicens 2005; Bosch and Vicens 2006; Bosch 2008; Bosch et al. 2008; Palladini and Maron 2014; Giejdasz et al. 2016; Sgolastra et al. 2016)

Interface parameter name	<i>Osmia bicornis</i> (default parameter value)	Included in UA	Min value in UA	Max value in UA	Remarks	Value ranges based on
<i>max.survival.e.f</i>	0.74	Yes	0.58	0.89		(Bosch 1992; Bosch and Vicens 2005; Sedivy et al. 2011)
<i>max.survival.e.m</i>	0.74	see remarks			No separate data for females and males available for survival to emergence: the same value was applied to <i>max.survival.e.f</i> and <i>max.survival.e.m</i> in the simulations	(Bosch 1992; Bosch and Vicens 2005; Sedivy et al. 2011)
<i>emerged.survival</i>	0.544	Yes	0.5	0.75		(Bosch and Kemp 2002; Bosch et al. 2021)
<i>a.cell.age</i>	-0.006	Yes	-0.004	-0.008	Values derived from study with <i>O. cornuta</i> , see also Section 3.2.1	(Bosch and Vicens 2005)
<i>a.sex.age</i>	-0.0406	Yes	-0.0286	0.0599	Values derived from study with <i>O. bicornis</i> , see also Section 3.2.3	(Seidelmann et al. 2010)
<i>a.size.age</i>	-0.003	Yes	-0.001	-0.005	Values derived from studies with <i>O. bicornis</i> and <i>O. cornuta</i> , see also Section 3.2.5	(Bosch and Vicens 2005; Seidelmann et al. 2010)
<i>a.cell.resource</i>	0.94	Yes	0.43	1.4	Values derived from study with <i>O. pumila</i> , <i>M. apicalis</i> and <i>M. rotundata</i> , see also Section 3.2.2	(Kim 1999; Goodell 2003; Peterson and Roitberg 2006a)
<i>a.sex.resource</i>	0.42	Yes	0.2	0.6	Default value derived from study with <i>M. apicalis</i> ; study data not suitable for estimation of range, see also Section 3.2.4	(Kim 1999); generic range (min and max)
<i>a.size.resource</i>	0.114	Yes	0	0.312	Values derived from study with <i>M. apicalis</i> , see also Section 3.2.6	(Kim 1999)
<i>Effects</i>	TRUE	--			Aim of the UA is to test the sensitivity to effects	
<i>ad.nectar.cons</i>	208.34	Yes	140	276.67	No quantitative data for <i>O. bicornis</i> ; default: range from honey bee pollen and nectar foragers	(European Food Safety Authority 2023) (Table 15) and assuming 30% sugar content (w/w) of nectar (see section 5.3.6)

Interface parameter name	<i>Osmia bicornis</i> (default parameter value)	Included in UA	Min value in UA	Max value in UA	Remarks	Value ranges based on
<i>ad.pollen.cons</i>	11.6	Yes	0	23.2	No quantitative data for <i>O. bicornis</i> ; default from honey bee nurses used; large range applied	(European Food Safety Authority 2023) (Table 13)
<i>k_CA</i>	0.4	--	--	--	Parameter from BeeGUTS (honey bee); it remained unchanged in the BeeGUTS (and interacts with GUTS from contact exposure, and thus, should not be changed independent of the GUTS parameters)	(Baas et al. 2022)
<i>Transfer.mat.adult</i>	TRUE	--	--	--	Testing all aspects of exposure and effects included in the model	
<i>ad.ET</i>	0.072	Yes	0.0175	0.157	Strohm et al. provide time for construction of a single brood cell; range: min = average-sd; max = 2x(average-sd) (if the bee builds two cells per day); range corresponds to data point shown in EFSA et al. 2023, Annex B, Fig. 18: ~0.4 h for <i>O. bicornis</i> );	(Strohm et al. 2002; European Food Safety Authority 2023)
<i>TC_soil</i>	0.5	Yes	0	1	Parameter only applicable to <i>Osmia</i> (soil/mud brood cell partitions) and soil-nesting bees	Not available; entire possible range of parameter included
<i>TC_leaf</i>	NA	--	--	--	Not applicable to <i>O. bicornis</i> : only applicable to <i>Megachile</i> (leaf-cutter bees)	
<i>Exposure.resting.soil</i>	FALSE	--	--	--	Not applicable to <i>O. bicornis</i> : only applicable to soil-nesting bees	
<i>GUTS</i>	GUTS-SD, GUTS-IT	--	--	--	Model analysis conducted separately with each GUTS version	
<i>t.guts</i>	10	--	--	--	Time step used for GUTS fitting in BeeGUTS	(Baas et al. 2022)
<i>kd_SD</i>	0.39	Yes	0.3	0.51	BeeGUTS parameter estimates and ranges for <b>dimethoate</b> using all data (honey bee); range used for simulations with GUTS-SD	(Baas et al. 2022) (SI, §4.3.1, p. 36)
<i>bw_SD</i>	0.014	Yes	0.011	0.017		
<i>mw_SD</i>	13	Yes	12	15		
<i>kd_IT</i>	0.012	Yes	0.0016	0.051		
<i>mw_IT</i>	2.4	Yes	0.32	9.6		(Baas et al. 2022) (SI, §4.3.2, p. 37)

Interface parameter name	<i>Osmia bicornis</i> (default parameter value)	Included in UA	Min value in UA	Max value in UA	Remarks	Value ranges based on
<i>Fs_IT</i>	3	Yes	2.7	3.4	BeeGUTS parameter estimates and ranges for <b>dimethoate</b> using all data (honey bee); range used for simulations with GUTS-IT	
<i>nectar_prop</i>	0.78	Yes	0.77	0.79	Data used from EFSA et al. 2023 (Table 14) and assuming 30% sugar content (w/w) of nectar (see section 5.3.6); data specific to <i>O. bicornis</i>	(European Food Safety Authority 2023)
<i>weight.prov</i>	306	Yes	257.1	354.9		(Strohm et al. 2002)
<i>Transfer.mat.dev</i>	TRUE	--	--	--		
<i>SM</i>	187	Yes	135.5	238.5	Wet weight of single brood cell partition; applies only to <i>Osmia</i>	(Strohm et al. 2002)
<i>F</i>	NA	--	--	--	Not applicable to <i>O. bicornis</i> : only applicable to <i>Megachile</i> (leaf-cutter bees)	
<i>SA_i</i>	NA	--	--	--	Not applicable to <i>O. bicornis</i> : only applicable to <i>Megachile</i> (leaf-cutter bees)	
<i>dr.intercept</i>	1.1534	Yes	0.8419	1.514	Dose-response parameters from honey bee larval toxicity studies with <b>dimethoate</b>	(OECD 2021) (data provided in Appendix)
<i>dr.slope</i>	-0.7876	Yes	-1.157	-0.507		

*Table 21. Model parameter values applied in the sensitivity analysis with example species Nomia melanderi. Parameters not included in the sensitivity analysis were used with their default value in all simulations. If no remarks are included for parameters not included in the analysis, these parameters are not species-specific but define initial conditions in the simulations, number of years simulated and the input method of the floral resource input file(s).*

Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
<i>Start.day</i>	1	--	--	--		
<i>Species</i>	N.melanderi	--	--	--		
<i>Voltinism</i>	univoltine	--	--	--		
<i>Initial.num.f</i>	100	--	--	--		
<i>Initial.num.m</i>	200	--	--	--		
<i>Initial.stage</i>	cocoon	--	--	--		
<i>Initial.age</i>	200	--	--	--		
<i>RndSeed</i>		see remarks			10 random number seeds per parameter combination	
<i>MultiYearInput</i>	FALSE	--	--	--		
<i>List.input.floral</i>	NA	--	--	--		
<i>Num.repeat.yr</i>	2	--	--	--		
<i>input.floral</i>		see remarks			Analysis repeated for 3 scenarios: (1) optimal foraging conditions, (2) half-optimal, (3) half-optimal with 10-day foraging gap during nesting season, see text	
<i>stoch.crop.forag</i>	FALSE	--	--	--		
<i>Density.dep</i>	FALSE	--	--	--	Density dependence not included in this analysis	
<i>DD.thresh.s</i>	NA	--	--	--		
<i>DD.max.cells.s</i>	NA	--	--	--		

Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
<i>DD.funct</i>	NA	--	--	--		
<i>DD.log.slope</i>	NA	--	--	--		
<i>day.emerge.f</i>	182	--	--	--	Species-specific but not included in the sensitivity analysis. Different date used than in 6.1; in the optimal foraging scenario applied, the emergence date is only relevant relative to the pesticide application date; see also text	
<i>var.emerge.f</i>	6	Yes	3	9	values need to be integers	(Mayer and Miliczky 1998; Vinchesi et al. 2013)
<i>day.emerge.m</i>	167	--	--	--	Species-specific but not included in the sensitivity analysis. See also <i>day.emerge.f</i>	
<i>var.emerge.m</i>	8	--	--	--		
<i>latest.emerge</i>	365	--	--	--	only meaningful to test for facultatively bivoltine life cycles	
<i>dev.egg</i>	2	--	--	--	development times not influential to model outputs (in univoltine life cycles)	
<i>dev.larva</i>	6	--	--	--		
<i>dev.cocoon</i>	20	--	--	--		
<i>t.maturity</i>	1	Yes	1	7	values need to be integers	(Bohart and Cross 1955; Johansen et al. 1978)
<i>m.life</i>	14	--	--	--	not impactful to model dynamics or outputs (other than number of post-emergent males)	
<i>max.nesting.life</i>	26	Yes	22	30	values need to be integers	(Bohart and Cross 1955)

Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
<i>p.max.nesting.life</i>	0.04	Yes	0.01	0.1		Not available; generic large range included
<i>max.f.ratio</i>	0.51	Yes	0.35	0.51		(Mayer and Miliczky 1998)
<i>max.cells</i>	1	Yes	0.5	1	generic range applied because no variation in daily brood cell production reported; authors explicitly state that a bee does not start a second brood cell in a given day	(Bohart and Cross 1955)
<i>max.survival.e.f</i>	0.868	Yes	0.729	0.868	apply the same value to <i>max.survival.e.f</i> and <i>max.survival.e.m</i>	(Rust 2006)
<i>max.survival.e.m</i>	0.868	see remarks			apply the same value to <i>max.survival.e.f</i> and <i>max.survival.e.m</i>	
<i>emerged.survival</i>	0.544	Yes	0.5	0.75	generic range applied in the absence of data (same range as applied to <i>Osmia</i> )	
<i>a.cell.age</i>	-0.006	Yes	-0.008	-0.004	Reproductive relationships characterized using data from multiple species (see also Table 10)	Bosch and Vicens 2005
<i>a.sex.age</i>	-0.0406	Yes	-0.0599	0		Seidelmann et al. 2010
<i>a.size.age</i>	-0.003	Yes	-0.005	-0.001		Bosch and Vicens 2005; Seidelmann et al. 2010
<i>a.cell.resource</i>	0.94	Yes	0.43	1.4		Kim 1999; Goodell 2003; Peterson and Roitberg 2006
<i>a.sex.resource</i>	0.42	Yes	0	0.6		Kim 1999 (no range; range for testing in SA not supported by data)
<i>a.size.resource</i>	0.114	Yes	0	0.312		Kim 1999
<i>Effects</i>	TRUE	--			Aim of the UA is to test the sensitivity to effects	

Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
<i>ad.nectar.cons</i>	208.34	Yes	140	276.67	No quantitative data for <i>N. melanderi</i> ; default: range from honey bee pollen and nectar foragers	(European Food Safety Authority 2023) (Table 15) and assuming 30% sugar content (w/w) of nectar (see section 5.3.6)
<i>ad.pollen.cons</i>	11.6	Yes	0	23.2	No quantitative data for <i>N. melanderi</i> ; default from honey bee nurses used; large range applied	(European Food Safety Authority 2023) (Table 13)
<i>k_CA</i>	0.4	--	--	--	Parameter from BeeGUTS (honey bee); it remained unchanged in the BeeGUTS (and interacts with GUTS from contact exposure, and thus, should not be changed independent of the GUTS parameters)	(Baas et al. 2022)
<i>Transfer.mat.adult</i>	TRUE	--	--	--	Testing all aspects of exposure and effects included in the model	
<i>ad.ET</i>	0.75	Yes	0.25	1	Large range based on observational account and indication that bees might engage in brood cell digging and preparation at night; min corresponds to 6h	(Bohart and Cross 1955)
<i>TC_soil</i>	0.5	Yes	0	1	Parameter only applicable to <i>Osmia</i> (soil/mud brood cell partitions) and soil-nesting bees	Not available; entire possible range of parameter included
<i>TC_leaf</i>	NA	--	--	--	Not applicable to <i>N. melanderi</i> : only applicable to <i>Megachile</i> (leaf-cutter bees)	
<i>Exposure.resting.soil</i>	FALSE	--	--	--	Not included because setting this parameter to 'TRUE' corresponds to the setting of <i>ad.ET</i> = 1	
<i>GUTS</i>	GUTS-SD, GUTS-IT	--	--	--	Model analysis conducted separately with each GUTS version	

Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
<i>t.guts</i>	10	--	--	--	Time step used for GUTS fitting in BeeGUTS	(Baas et al. 2022)
<i>kd_SD</i>	0.39	Yes	0.3	0.51	BeeGUTS parameter estimates and ranges for <b>dimethoate</b> using all data (honey bee); range used for simulations with GUTS-SD	(Baas et al. 2022) (SI, §4.3.1, p. 36)
<i>bw_SD</i>	0.014	Yes	0.011	0.017		
<i>mw_SD</i>	13	Yes	12	15		
<i>kd_IT</i>	0.012	Yes	0.0016	0.051	BeeGUTS parameter estimates and ranges for <b>dimethoate</b> using all data (honey bee); range used for simulations with GUTS-IT	(Baas et al. 2022) (SI, §4.3.2, p. 37)
<i>mw_IT</i>	2.4	Yes	0.32	9.6		
<i>Fs_IT</i>	3	Yes	2.7	3.4		
<i>nectar_prop</i>	0.67	Yes	0.53	0.81	No data for <i>N. melanderi</i> ; (European Food Safety Authority 2023) assuming 30% sugar content (w/w) of nectar (see section 5.3.6); composition of provision from <i>M. rotundata</i> from Cane et al. 2011, using sugar + water as nectar in provision	(Cane et al. 2011; European Food Safety Authority 2023)
<i>weight.prov</i>	270	Yes	158	305	Using reported adult female weight and relation to provision weight reported by Neff 2008	(Neff 2008; Cane et al. 2011; Cane et al. 2017)
<i>Transfer.mat.dev</i>	TRUE	--	--	--		
<i>SM</i>	NA	--	--	--	Not applicable to <i>N. melanderi</i> : parameter applies only to <i>Osmia</i> (mud/soil brood cell partition)	
<i>F</i>	NA	--	--	--	Not applicable to <i>N. melanderi</i> : only applicable to <i>Megachile</i> (leaf-cutter bees)	
<i>SA_i</i>	NA	--	--	--	Not applicable to <i>N. melanderi</i> : only applicable to <i>Megachile</i> (leaf-cutter bees)	
<i>dr.intercept</i>	1.1534	Yes	0.8419	1.514		

Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
<i>dr.slope</i>	-0.7876	Yes	-1.157	-0.507	Dose-response parameters from honey bee larval toxicity studies with dimethoate	(OECD 2021) (data provided in Appendix)

### 6.3.2. Results

From the outputs (relative effects compared to control simulations) of the model analysis, the uncertainty range of the species-specific parameters included could be identified as a) highly influential to one or several model outputs analyzed, b) influential to at least one model output, or c) not influential to model outputs (Table 22 and Table 23). The PRCC for each parameter included in the sensitivity analysis can range between -1 (increase in the parameter value is correlated with a corresponding decrease in the output value irrespective of all other parameter values) and 1 (increase in the parameter value is correlated with a corresponding increase in the output value irrespective of all other parameter values). A PRCC = 0 denotes no impact of the parameter value on outputs. Here, we arbitrarily define parameters as impactful to model outputs if  $|PRCC| \geq 0.25$ . In addition, we identify model parameters as highly impactful if  $|PRCC| \geq 0.5$  for 3 or more of the outputs analyzed. Parameters were classified as not impactful if  $|PRCC| \leq 0.1$ .

*Table 22. Results of the analysis of parameter uncertainty with O. bicornis by model parameter whereby relative effects were analyzed as outputs. +: PRCC > 0.25 for at least one output and the increase in parameter value corresponds to an increase (or no change) across outputs; -: PRCC < -0.25 for at least one output and the increase in parameter value corresponds to a decrease (or no change) across outputs; +/-: |PRCC| > 0.25 for at least one output and the increase in parameter value corresponds to an increase or decrease (or no change) dependent on the output; ++: PRCC > 0.5 for at least 3 outputs and the increase in parameter value corresponds to an increase (or no change) across outputs; --: PRCC < -0.5 for at least one output and the increase in parameter value corresponds to a decrease (or no change) across outputs; grey cells: |PRCC| < 0.1 across all outputs.*

Interface parameter name	Osmia bicornis (default parameter value)	Min value in SA	Max value in SA	GUTS-IT	GUTS-SD
var.emerge.f	3	1	7	+	+
t.maturation	3	1	10	-	-
max.nesting.life	36	26	36		
p.max.nesting.life	0.04	0.01	0.1		
max.f.ratio	0.59	0.38	1		
max.cells	2	1	3		
max.survival.e.f,	0.74	0.58	0.89		
emerged.survival	0.544	0.5	0.75		
a.cell.age	-0.006	-0.008	-0.004		
a.sex.age	-0.0406	-0.0286	-0.0599		
a.size.age	-0.003	-0.001	-0.005		
a.cell.resource	0.94	0.43	1.4		
a.sex.resource	0.42	0.2	0.6		
a.size.resource	0.114	0	0.312		
ad.nectar.cons	208.34	140	276.67		
ad.pollen.cons	11.6	0	23.2		
ad.ET	0.072	0.0175	0.157		
TC_soil	0.5	0	1		

Interface parameter name	<i>Osmia bicornis</i> (default parameter value)	Min value in SA	Max value in SA	GUTS-IT	GUTS-SD
kd_SD	0.39	0.3	0.51	NA	
bw_SD	0.014	0.011	0.017	NA	
mw_SD	13	12	15	NA	
kd_IT	0.012	0.0016	0.051	-	NA
mw_IT	2.4	0.32	9.6	+	NA
Fs_IT	3	2.7	3.4		NA
nectar_prop	0.78	0.77	0.79		
weight_prov	306	257.1	354.9		
SM	187	135.5	238.5		
dr.intercept	1.1534	0.8419	1.514		
dr.slope	-0.7876	-1.157	-0.507		

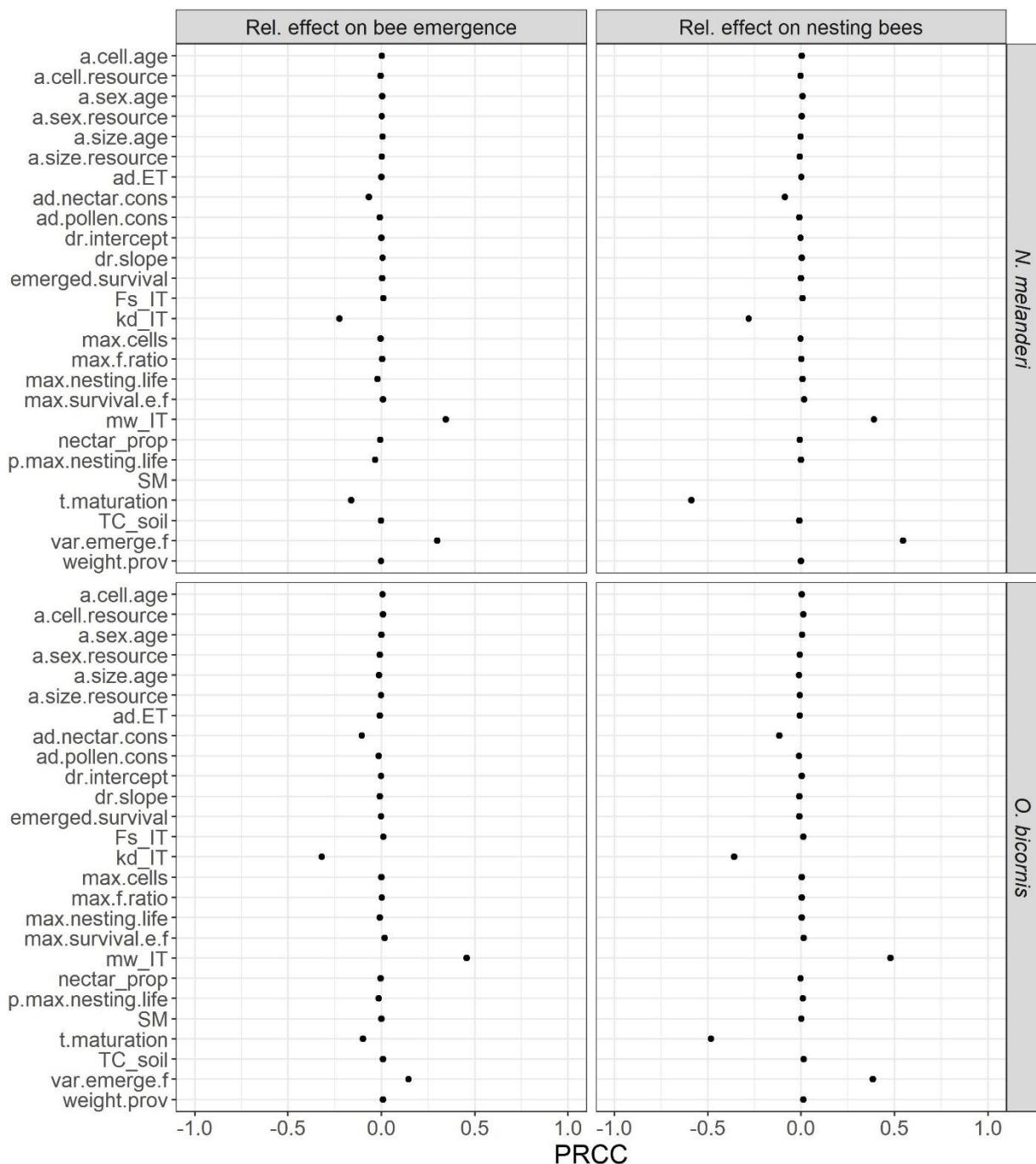
Table 23. Results of the analysis of parameter uncertainty with *N. melanderi* by model parameter whereby relative effects were analyzed as outputs. +: PRCC > 0.25 for at least one output and the increase in parameter value corresponds to an increase (or no change) across outputs; -: PRCC < -0.25 for at least one output and the increase in parameter value corresponds to a decrease (or no change) across outputs; +/-: |PRCC| > 0.25 for at least one output and the increase in parameter value corresponds to an increase or decrease (or no change) dependent on the output; ++: PRCC > 0.5 for at least 3 outputs and the increase in parameter value corresponds to an increase (or no change) across outputs; --: PRCC < -0.5 for at least one output and the increase in parameter value corresponds to a decrease (or no change) across outputs; grey cells: |PRCC| < 0.1 across all outputs.

Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Min value in SA	Max value in SA	GUTS-IT	GUTS-SD
var.emerge.f	3	3	9	+	+
t.maturity	3	1	7	-	-
max.nesting.life	26	22	30		
p.max.nesting.life	0.04	0.01	0.1		
max.f.ratio	0.51	0.35	0.51		
max.cells	1	0.5	1		
max.survival.e.f,	0.868	0.729	0.868		
emerged.survival	0.544	0.5	0.75		
a.cell.age	-0.006	-0.008	-0.004		
a.sex.age	-0.0406	-0.0599	0		
a.size.age	-0.003	-0.005	-0.001		
a.cell.resource	0.94	0.43	1.4		
a.sex.resource	0.42	0	0.6		
a.size.resource	0.114	0	0.312		

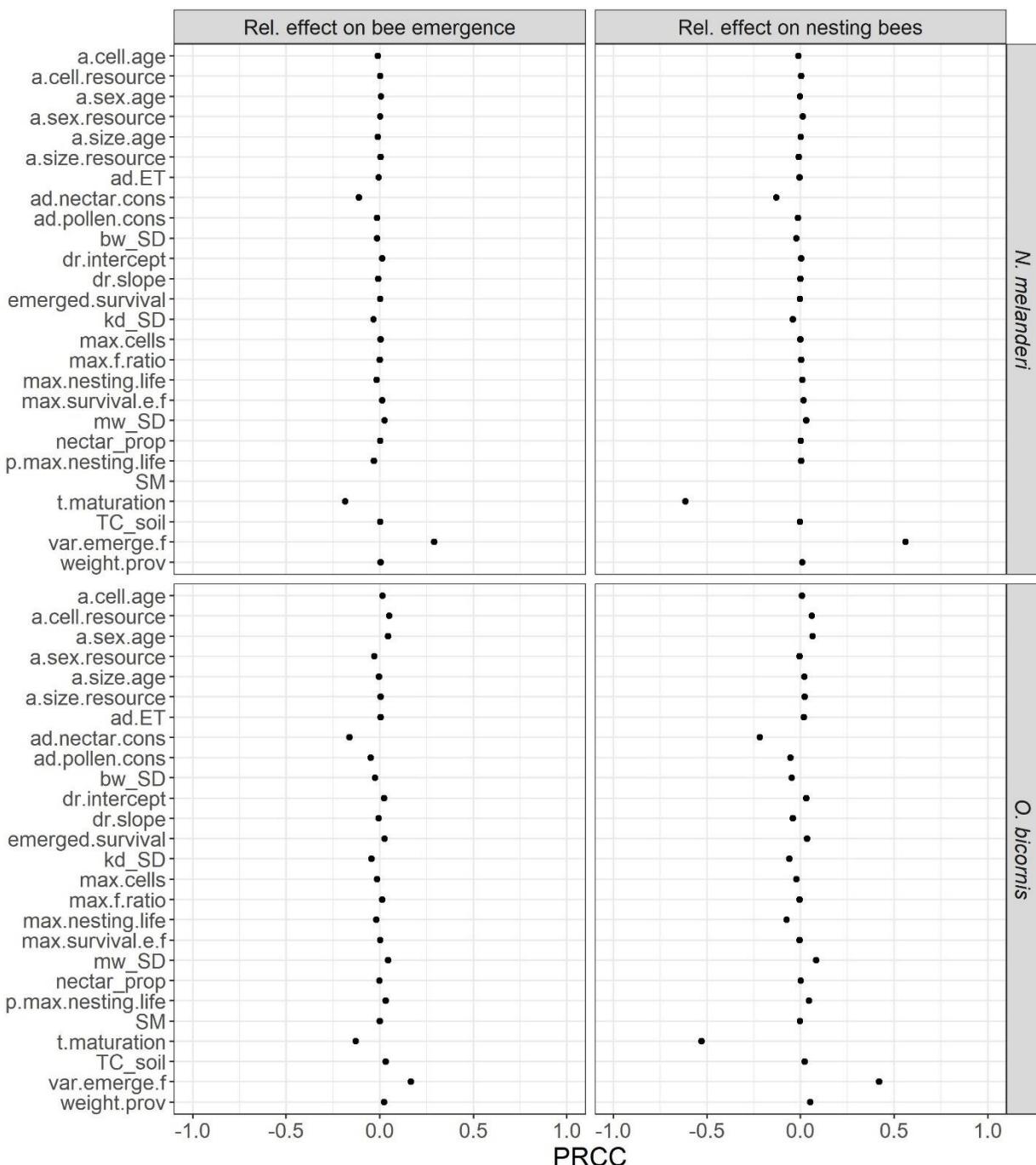
Interface parameter name	<i>Nomia melanderi</i> (default parameter value)	Min value in SA	Max value in SA	GUTS-IT	GUTS-SD
<i>ad.nectar.cons</i>	208.34	140	276.67		
<i>ad.pollen.cons</i>	11.6	0	23.2		
<i>ad.ET</i>	0.75	0.25	1		
<i>TC_soil</i>	0.5	0	1		
<i>kd_SD</i>	0.39	0.3	0.51	<b>NA</b>	
<i>bw_SD</i>	0.014	0.011	0.017	<b>NA</b>	
<i>mw_SD</i>	13	12	15	<b>NA</b>	
<i>kd_IT</i>	0.012	0.0016	0.051	-	<b>NA</b>
<i>mw_IT</i>	2.4	0.32	9.6	+	<b>NA</b>
<i>Fs_IT</i>	3	2.7	3.4		<b>NA</b>
<i>nectar_prop</i>	0.67	0.53	0.81		
<i>weight_prov</i>	270	158	305		
<i>SM</i>	NA	NA	NA	<b>NA</b>	<b>NA</b>
<i>dr.intercept</i>	1.1534	0.8419	1.514		
<i>dr.slope</i>	-0.7876	-1.157	-0.507		

Simulated relative effects were impacted by parameters of bee phenology (*var.emerge.f* and *t.maturity*) for both species. These parameters influence the timing of bee emergence and onset of nesting relative to the simulated pesticide application date. More variability in female emergence dates (larger range of *var.emerge.f*) results in less overlap with exposures across the population (particularly with the exposure via direct spray which is assumed to occur only on a single day). A longer maturation time (larger values of *t.maturity*) result in less females that emerge prior to exposure (application date) able to initiate nesting.

For simulations with GUTS-IT, two GUTS parameters were influential to simulated relative effects. The parameters are important for the determination of individual-level effects to post-emergent females, and thus, are expected to interact with population-level effects. However, corresponding parameters in GUTS-SD were not influential to relative effects in SolBeePop. Ranges of the GUTS parameters were used according to the confidence ranges in the GUTS fits to dimethoate honey bee toxicity data (Baas et al. 2022). Although both GUTS versions provided good fits when using all available data sets (adult honey bee toxicity studies with dimethoate) for fitting (GUTS-SD:  $R^2 = 0.8$ ; GUTS-IT:  $R^2 = 0.829$ ), the confidence ranges of the GUTS-IT parameters were considerably larger for GUTS-IT than GUTS-SD (see Table 22 and Table 23). The adult nectar consumption had a small but consistent impact on relative effect sizes. No other parameters were influential to relative effect sizes for the compound and exposure scenario tested. For both species, PRCCs for relative effects on numbers of bees emerging (in the year after simulated exposure) and nesting females are shown in Figure 26 for GUTS-IT and Figure 27 for GUTS-SD.



*Figure 26. Analysis of the impact of parameter uncertainty on simulated relative effect sizes in simulations using GUTS-IT. Parameters included in the model analysis of SolBeePop<sub>ecotox</sub> (with exposure and effects) and their impact on simulated relative effects sizes shown as partial rank correlation coefficient (PRCC). Positive PRCCs indicate an increase in parameter value results in increase in output value (smaller relative effect), negative PRCCs indicate an increase in parameter value results in a decrease in output value (higher relative effect).*



*Figure 27. Analysis of the impact of parameter uncertainty on simulated relative effect sizes in simulations using GUTS-SD. Parameters included in the model analysis of SolBeePop<sub>ecotox</sub> (with exposures and effects) and their impact on simulated relative effects sizes shown as partial rank correlation coefficient (PRCC). Positive PRCCs indicate an increase in parameter value results in increase in output value (smaller relative effect), negative PRCCs indicate an increase in parameter value results in a decrease in output value (higher relative effect).*

### 6.3.3. Comparison of sensitivity and parameter uncertainty analysis

The model analyses conducted with SolBeePop<sub>ecotox</sub> (with exposures and effects) differed in the ranges of parameter values tested. The sensitivity analysis was conducted using permutations of the default parameter values by +/-10%. While the default parameter values are derived from literature-

reported trait and exposure or effect values, the range tested is generic. A sensitivity analysis gives insight into model behavior without the explicit consideration of uncertainties in parameter values derived from empirical data or the possible (biologically plausible) range of values each parameter could assume. In contrast, the analysis of parameter uncertainty explicitly considers reported parameter ranges. For parameters for which data from the literature are lacking, large ranges of the parameter values are assumed within possible or plausible limits. Thus, the analysis of parameter uncertainty directly links the uncertainty in empirical data to uncertainties in model outputs.

We presented both types of model analyses in this section, using the same parameters included in the global analyses and the same approach to the analysis of the simulation results. The analyses exclusively differed in the parameter value ranges used. Thus, we can directly compare the two analyses and their results.

### **Parameter ranges applied in the model analyses**

A total of 29 (*O. bicornis*) or 28 (*N. melanderi*) parameters relevant for population-level model outcomes and effects were included in the analyses. The parameter ranges used were larger in the analysis of parameter uncertainty (to various extents) with few exceptions. The following parameters included equal, different, or smaller ranges in the analysis of parameter uncertainty compared to the sensitivity analysis (see Table 16, Table 17, Table 20 and Table 21):

- *max.nesting.life*: in the analysis of parameter uncertainty, the default value was used as the maximum of the value range. Accordingly, the sensitivity analysis a parameter range that included larger values. However, the total range of parameter values was larder in the analysis of parameter uncertainty.
- *max.cells*: the same range of parameter values was included in both analyses.
- *nectar\_prop*: parameter range tested in the sensitivity analysis was slightly larger than in the analysis of parameter uncertainty.
- *mw\_SD*: parameter range tested in the sensitivity analysis was slightly larger than in the analysis of parameter uncertainty.
- *Fs\_IT*: the parameter ranges used in both analyses were only marginally different.

### **Impacts on relative effect sizes**

The pattern of impacts on relative effect sizes corresponded in the two analyses. Impacts of parameters on effect sizes were generally lower in the sensitivity analysis compared to the analysis of parameter uncertainty. The impact of the GUTS-IT parameters on relative effect sizes was mostly absent in the sensitivity analysis due to considerably smaller ranges of parameter values tested compared to the analysis of parameter uncertainty.

### **Conclusions**

A sensitivity analysis with parameter ranges uninformed by specific uncertainties in parameter values can provide an initial insight into model behavior and indicate which parameters might be most influential to model outputs. However, applying a fixed range (e.g., +/-10% of the default value) may not be very informative in the context of model applications in realistic contexts. Model parameters in ecological models generally represent very different measures and have very different possible or plausible ranges. For instance, in the SolBeePop model, several parameters define survival rates of bees. Survival parameters are, by definition, limited to values between 0 (certain death) and 1 (certain survival). Survival of in-nest life stages is summarized into a single parameter (*max.survival.e.f* for females and *max.survival.e.m* for males). The default value identified for *O. bicornis* is 0.74. A perturbation of this value by 10% results in 7.4% more or less bees emerging per

simulated season (one season per year in the univoltine *O. bicornis*). Similarly, the parameters *max.nesting.life* and *p.max.nesting.life* are used by the model to determine the daily survival probability of nesting females. A slight change ( $\leq 10\%$ ) in number of reproductive females was not expected to interact with the relative effect of pesticide exposures.

## 6.4. Comparing model outputs across bee species

The SolBeePop model is a representation of solitary bee populations and can be applied to various species using species-specific input parameter values whereby the input parameters correspond to species' traits. Density dependence can be simulated in the model acting on the brood cell production rate by nesting females. The species' traits interact with the assumed density dependent processes over time.

In the cross-species simulations, the model was applied using the trait values of four species, *Osmia bicornis*, *Megachile rotundata*, *Nomia melanderi* and *Eucera pruinosa*. The goal of the simulations was to demonstrate the functionality of the model in simulating species with different traits and density-dependent population dynamics. The interaction between the species' traits and the density dependence was analyzed.

For all four species, the same number of initial bees was used as well as the same density-dependence parameters. The density-dependence parameters were chosen arbitrarily and do not represent a specific population in the field but rather, were intended to make the simulations comparable. In addition, ideal foraging conditions in the landscape were assumed on all days of the year. The initial population size was also set to the same value for the four species and was well below the ultimate carrying capacity (governed by the density dependence parameters). Accordingly, all populations were expected to increase over the simulated period of 30 years. All simulated populations were expected to reach their carrying capacity within this simulated time period. After reaching the carrying capacity, populations may still vary in abundance between simulated years but not show a sustained increase. Differences between species were expected to result in different numbers of years until the carrying capacity is reached, the population size range at carrying capacity, and the variability between yearly population sizes after the carrying capacity is reached.

### 6.4.1. Simulations

Cross-species simulations were conducted using species-specific parameter values as listed in Table 24. Note that emergence timings were set for *M. rotundata* and *N. melanderi* to achieve univoltine life cycles, simulating populations in the Northern parts of each species ranges. Identical values were applied across species to parameters in the model characterizing the density dependent nesting and initial population conditions (Table 24). For all simulations, the same input file was used to define the foraging in the landscape (file name: *Floral\_generic\_optimal.csv*). The input file defines optimal foraging availability on all days of the year. Simulations were run for 30 years. For each of the four species, 50 simulations were conducted with 50 random number seeds to capture the stochasticity in the model (see also Section 4.3).

*Table 24. Parameter values applied in the cross-species simulations with density dependence.*  
*Identical initial conditions were applied in all simulations and species as well as density-dependence parameters.*

Interface parameter name	<i>Osmia bicornis</i>	<i>Megachile rotundata</i>	<i>Nomia melanderi</i>	<i>Eucera pruinosa</i>
<i>Start.day</i>	1	1	1	1
<i>Species</i>	O.bicornis	M.rotundata	N.melanderi	E.pruinosa
<i>Voltinism</i>	univoltine	univoltine	univoltine	univoltine
<i>Initial.num.f</i>	50	50	50	50
<i>Initial.num.m</i>	75	75	75	75
<i>Initial.stage</i>	cocoon	cocoon	cocoon	cocoon
<i>Initial.age</i>	200	200	200	200
<i>RndSeed</i>	50 different numbers applied (for each repeat simulation)			
<i>MultiYearInput</i>	FALSE	FALSE	FALSE	FALSE
<i>List.input.floral</i>	NA	NA	NA	NA
<i>Num.repeat.yr</i>	30	30	30	30
<i>input.floral</i>	Floral_generic_optimal.csv			
<i>stoch.crop.forag</i>	FALSE	FALSE	FALSE	FALSE
<i>Density.dep</i>	TRUE	TRUE	TRUE	TRUE
<i>DD.thresh.s</i>	250	250	250	250
<i>DD.max.cells.s</i>	2500	2500	2500	2500
<i>DD.funct</i>	linear	linear	linear	linear
<i>DD.log.slope</i> <sup>(a)</sup>	2	2	2	2
<i>day.emerge.f</i>	105	166	174	212
<i>var.emerge.f</i>	3	3 <sup>(b)</sup>	6	30
<i>day.emerge.m</i>	91	164	167	202
<i>var.emerge.m</i>	2	2 <sup>(b)</sup>	8	15
<i>latest.emerge</i>	365	365	365	365
<i>dev.egg</i>	8	3	2	8 <sup>(b)</sup>
<i>dev.larva</i>	32	9	6	15
<i>dev.cocoon</i>	68	8	20	68 <sup>(b)</sup>
<i>t.maturity</i>	3	7	1	4
<i>m.life</i>	21	7	14	14
<i>max.nesting.life</i>	36	52	26	36 <sup>(b)</sup>
<i>p.max.nesting.life</i>	0.04	0.04	0.04	0.04
<i>max.f.ratio</i>	0.59	0.83	0.51	0.7
<i>max.cells</i>	2	2	1	1.65
<i>max.survival.e.f</i>	0.74	0.65	0.868	0.74
<i>max.survival.e.m</i>	0.74	0.65	0.868	0.74
<i>emerged.survival</i>	0.544	0.69	0.544	0.544
<i>a.cell.age</i>	-0.006	-0.006	-0.006	-0.006
<i>a.sex.age</i>	-0.0406	-0.0406	-0.0406	-0.0406
<i>a.size.age</i>	-0.003	-0.003	-0.003	-0.003
<i>a.cell.resource</i>	0.94	0.94	0.94	0.94
<i>a.sex.resource</i>	0.42	0.42	0.42	0.42

Interface parameter name	<i>Osmia bicornis</i>	<i>Megachile rotundata</i>	<i>Nomia melanderi</i>	<i>Eucera pruinosa</i>
<i>a.size.resource</i>	0.114	0.114	0.114	0.114

<sup>(a)</sup> Unused parameter: only applies if *DD.funct* = 'log' is chosen

<sup>(b)</sup> No data found for this trait and species; value from *O. bicornis* used

## 6.4.2. Output analysis

For the cross-species simulations, we were interested in the dynamics of population growth and reaching of stable population sizes due to the density dependence in the model over multiple years. Thus, we analyzed the total number of brood cells produced (*sum.cells*) in a population at the end of each simulated year and the yearly reproductive output per female (which corresponds to the lifetime reproductive output).

The carrying capacity was also defined based on total numbers of brood cells (*sum.cells*). This corresponds to the total number of brood cells produced during the year's nesting season. We defined the carrying capacity as the average number of brood cells (corresponding to the population size) at the end of simulated years 21-30 across simulations with one species, i.e., each species had a carrying capacity defined post-hoc from the simulations.

The years until the carrying capacity was reached by each species was determined as the first simulation year in which the average total number of brood cells (across the 50 repetitions) was equal to or larger than the carrying capacity. To characterize the variability in population sizes in stable populations (after reaching carrying capacity), the smallest and largest population number at the end of the simulation years 21-30 and across all repetitions was identified for each species.

The change in reproductive rates was analyzed from populations not impacted by density dependence (simulated year 1) and populations regulated by density dependence (simulated year 30). The sex ratio of the offspring at the end of years 1 and 30 was calculated as the number of brood cells with female offspring (*sum.f.cells*) produced across all females divided by the total number of brood cells (*sum.cells*). The average sex ratio across the 50 repetitions was calculated. In addition, the reproductive rate per nesting female was compared between simulation years 1 and 30 using the mean number of brood cells (*mean.cells*) produced per female during the previous nesting season. Data analysis were conducted using R and plots were generated using the package "ggplot2" (Wickham 2016; R Core Team 2022).

## 6.4.3. Results

The dynamics of population growth from the initial conditions as well as the population size at carrying capacity differed between species in the simulations. *N. melanderi* had the lowest carrying capacity and it took the longest to reach it. (Table 25; Figure 28). *N. melanderi* also displayed the most variability in total brood cell numbers across simulation years 21-30. *M. rotundata* had the highest carrying capacity and needed the shortest time to reach it. In all simulated species, the average number of brood cells a nesting female produced declined between simulated year 1 and year 30 as expected (Figure 30). This decline was most pronounced in *M. rotundata* whereby numbers were reduced by nearly a factor of 10. *N. melanderi* displayed the smallest difference. In *M. rotundata*, the female sex ratio in the offspring increased considerably while the ratio remained nearly unchanged in *N. melanderi* and even declined slightly in *E. pruinosa* (Table 25; Figure 29).

Table 25. Total number of brood cells produced per year, carrying capacity (average total brood cells numbers in years 11-20), sex ratio and reproductive rate per female by simulated species.

	<i>Osmia bicornis</i>	<i>Megachile rotundata</i>	<i>Nomia melanderi</i>	<i>Eucera pruinosa</i>
Carrying capacity	2464.9	2499.9	1082.6	2048.1
Range of population sizes in years 11-20	2426 - 2494	2497 – 2500	758 – 1402	1865 - 2181
Average years until reaching carrying capacity	6.6	4.2	18.5	5.7
Average offspring sex ratio in year 1	0.389	0.474	0.377	0.457
Average offspring sex ratio in year 20	0.501	0.743	0.372	0.441
Average number of brood cells per female in year 1	20.2	26.9	6.7	16.8
Average number of brood cells per female in year 20	5.0	3.0	5.7	5.8

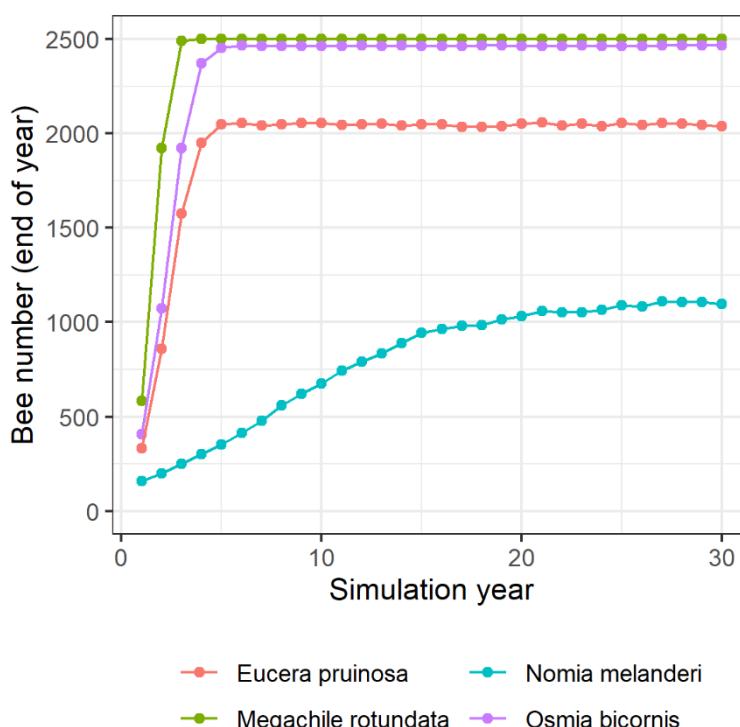


Figure 28. Average total number of bees (brood cells) at the end of each simulated year for the four species. The average of the numbers from years 21-30 are used to calculate the “carrying capacity.”

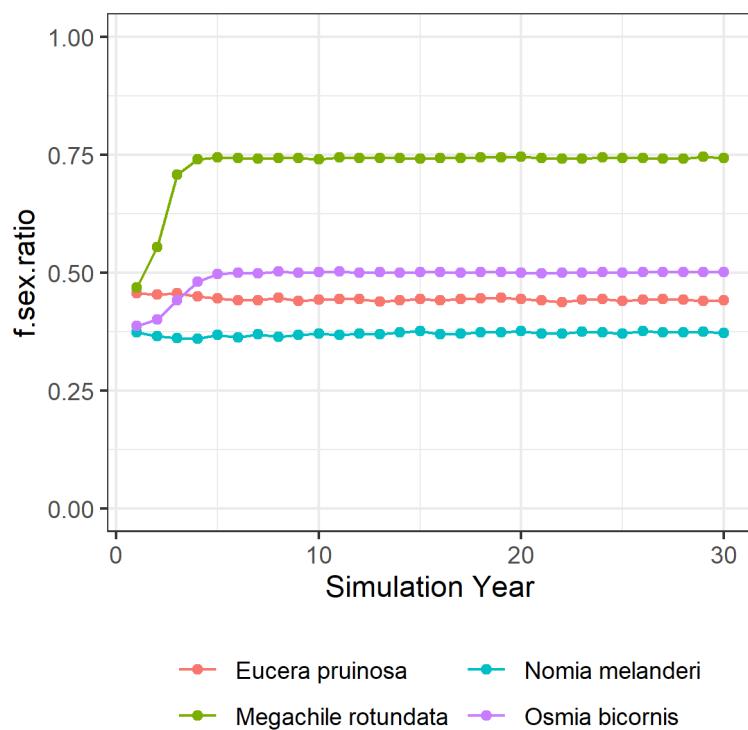


Figure 29. Average female sex ratio (*f.sex.ratio*) of each year's offspring by species.

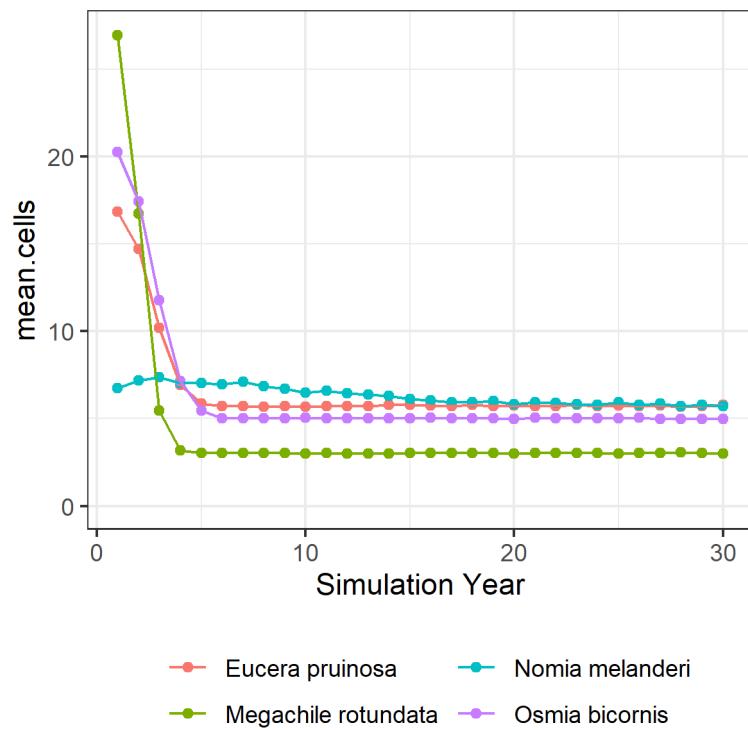


Figure 30. Average number (*mean.cells*) of offspring (brood cells) produced per nesting female in each simulated year.

The differences between species result from species-specific trait values interacting with the density dependence. In *M. rotundata*, a high maximum daily brood cell production rate of 2 is combined with a relatively high survival of females from emergence to maturation and a long lifespan. Due to this high reproductive output, *M. rotundata* reached a carrying capacity in the simulations that corresponds to the maximum number of brood cells that can be used (defined by the model parameter *DD.max.cells.s*). In contrast, *N. melanderi* produces only one brood cell per day and is assumed to have the shortest life span of post-emergent females. As a result, the reduction in reproductive output due to density dependence in the model lead to a much lower carrying capacity than in *M. rotundata*.

The model includes multiple stochastic processes (see Table 1) which result in variability across repeat simulations. The variability in model outputs between repeat simulations decreases when the population reach carrying capacity because most brood is produced early during female nesting, reducing the importance of daily mortality (a stochastic process). However, density dependence is less influential to brood cells production rates in *N. melanderi*, reflected in a minor change in brood cells produced per female and year over the simulated years (Figure 30). Accordingly, the variability in population sizes in the last 10 simulated years is relatively larger for *N. melanderi* compared to the other simulated species (Table 25).

Note that the reproductive relationships linking reproductive outputs to resource availability in the landscape are not relevant in the cross-species simulations because the resource availability was set to be optimal throughout the year. The reproductive rates related to female age apply equally to all simulated species because data specific to the four species were lacking. The relationship results in a high female sex ratio in the offspring produced by young nesting females which subsequently shifts to a male-biased sex ratio. Populations with high density-dependent regulation as occurs in *M. rotundata* are progressively limited in their reproductive rate with the progress of the nesting season. Accordingly, male production is affected more by density dependence than female offspring production.

## 6.5. Case study simulations: hypothetical semi-field studies with *N. melanderi* and *E. pruinosa*

### 6.5.1. Species-specific parameters

The calibration and validation of SolBeePop<sub>ecotox</sub> with semi-field study data indicates the usefulness of the model to estimate effects of *O. bicornis* tested in these study designs. Corresponding semi-field studies are not routinely conducted with other solitary bee species, particularly soil-nesting bees. *Osmia* readily nests in artificial above-ground cavities, easing the collection of cocoons, incubation under controlled conditions and release tailored to the study design. In contrast, soil-nesting species are harder to test because developing bees cannot be easily collected and released in a chosen study environment. However, the model can be applied to gain insights of potential effects from exposures in other solitary bee species in hypothetical semi-field settings.

In the case study application using dimethoate as example pesticide, we simulated two soil-nesting solitary bee species, *N. melanderi* and *E. pruinosa* in hypothetical semi-field studies. Bee trait values that had been identified as each species' default were used in the simulations. In Table 26, the model parameters used in the simulations are listed. Emergence dates (*day.emerge.f* and *day.emerge.m*) were chosen within the range of reported emergence dates for each species. Both species are active mainly in the summer. The alkali bee *N. melanderi* is partially managed for alfalfa pollination, and its active season co-occurs with the crop's flowering period. The hoary squash bee is a specialist for cucurbit pollen (squash and pumpkin) and its activity season is tied to the flowering of the crop. The hypothetical dimethoate application date in the simulations was assumed to occur 10 days after the assumed peak emergence date of each species, matching this temporal relationship with the *O. bicornis* semi-field studies. Study time windows, weather conditions and dimethoate fate in the soil were considered using conditions relevant for each species.

*Table 26. Model parameters used in the simulations of hypothetical dimethoate semi-field studies with *N. melanderi* and *E. pruinosa*. Descriptions of the parameters and references for each species are provided in SolBeePop\_ecotox\_Tables.xlsx.*

Interface parameter name	<i>Nomia melanderi</i>	<i>Eucera pruinosa</i>	Remarks
<i>Start.day</i>	146	168	Day of year; Corresponds to the hypothetical first day in the semi-field study (tunnel phase)
<i>Species</i>	N.melanderi	E.pruinosa	
<i>Voltinism</i>	univoltine	univoltine	
<i>Initial.num.f</i>	90	90	
<i>Initial.num.m</i>	110	110	
<i>Initial.stage</i>	cocoon	cocoon	
<i>Initial.age</i>	300	300	Days
<i>RndSeed</i>			Set of 50 different random number seeds used
<i>MultiYearInput</i>	FALSE	FALSE	
<i>List.input.floral</i>	NA	NA	
<i>Num.repeat.yr</i>	2	2	
<i>input.floral</i>	Floral_semidfield_Nomia	Floral_semidfield_Eucera	Different input files used for each scenario defining exposure to direct spray

Interface parameter name	<i>Nomia melanderi</i>	<i>Eucera pruinosa</i>	Remarks
	DIMexp75_med_resid.csv	DIMexp75_med_resid.csv	
<i>stoch.crop.forag</i>	FALSE	FALSE	
<i>Density.dep</i>	FALSE	FALSE	
<i>DD.thresh.s</i>	1	1	Unused
<i>DD.max.cells.s</i>	1	1	Unused
<i>DD.funct</i>	1	1	Unused
<i>DD.log.slope</i>	1	1	Unused
<i>day.emerge.f</i>	158 (151, 165)	198 (191, 205)	Day of year; adjusted to application date; in brackets: dates for shifted peak emergences simulations
<i>var.emerge.f</i>	6	15	Days
<i>day.emerge.m</i>	158	198	Day of year; adjusted to application date
<i>var.emerge.m</i>	6	8	Days
<i>latest.emerge</i>	195	235	Corresponds to the hypothetical last day in the semi-field study (tunnel phase)
<i>dev.egg</i>	2	8*	Days
<i>dev.larva</i>	6	15	Days
<i>dev.cocoon</i>	20	68*	Days
<i>t.maturity</i>	1	4	Days
<i>m.life</i>	14	21*	Days
<i>max.nesting.life</i>	26	36	Days
<i>p.max.nesting.life</i>	0.04	0.04	
<i>max.f.ratio</i>	0.51	0.7	
<i>max.cells</i>	1	1.65	
<i>max.survival.e.f</i>	0.868	0.74*	
<i>max.survival.e.m</i>	0.868	0.74*	
<i>emerged.survival</i>	0.82	0.82	<i>M. rotundata</i> : rate reported from semi-field study (Pitts-Singer and Bosch 2010); <i>N. melanderi</i> and <i>E. pruinosa</i> : value from <i>O. bicornis</i> calibrated to 2021 Eurofins semi-field study used
<i>a.cell.age</i>	-0.006	-0.006	
<i>a.sex.age</i>	-0.0406	-0.0406	
<i>a.size.age</i>	-0.003	-0.003	
<i>a.cell.resource</i>	0.94	0.94	
<i>a.sex.resource</i>	0.42	0.42	
<i>a.size.resource</i>	0.114	0.114	
<i>Effects</i>	TRUE	TRUE	
<i>ad.nectar.cons</i>	208.34	210.00	mg/d; Nectar consumption of adults derived from European Food Safety Authority (EFSA) et al. (2023) (Table 15); see text for further explanation
<i>ad.pollen.cons</i>	11.6	11.7	mg/d; see text for further explanation
<i>k_CA</i>	0.4	0.4	
<i>Transfer.mat.adult</i>	TRUE	TRUE	

Interface parameter name	<i>Nomia melanderi</i>	<i>Eucera pruinosa</i>	Remarks
<i>ad.ET</i>	0.790	0.790	Species-specific; see text for further explanation
<i>TC_soil</i>	0.50	0.50	g/d; see text for further explanation
<i>TC_leaf</i>	0.00	0.00	cm <sup>2</sup> /d; see text for further explanation
<i>Exposure.resting.soil</i>	FALSE	FALSE	
<i>GUTS</i>	GUTS-SD, GUTS-IT	GUTS-SD, GUTS-IT	All GUTS parameters derived from honey bee standard toxicity studies with dimethoate (Baas et al. 2022)
<i>t.guts</i>	10	10	
<i>kd_SD</i>	0.39	0.39	
<i>bw_SD</i>	0.014	0.014	
<i>mw_SD</i>	13.00	13.00	
<i>kd_IT</i>	0.012	0.012	
<i>mw_IT</i>	2.40	2.40	
<i>Fs_IT</i>	3.00	3.00	
<i>nectar_prop</i>	0.78	0.78	Species-specific
<i>weight.prov</i>	270.00	316.00	mg; Species-specific
<i>Transfer.mat.dev</i>	TRUE	TRUE	
<i>SM</i>	0.00	0.00	Only relevant for bees collecting soil for above-ground nests (e.g., <i>Osmia</i> )
<i>F</i>	0.00	0.00	Only relevant for leafcutter bees; see text for further explanation
<i>SA_i</i>	0.00	0.00	cm <sup>2</sup> ; only relevant for leafcutter bees; see text for further explanation
<i>dr.intercept</i>	1.1534	1.1534	Derived from honey bee larval toxicity studies (OECD 2016, No 239)
<i>dr.slope</i>	-0.7876	-0.7876	Derived from honey bee larval toxicity studies (OECD 2016, No 239)

\*No data found for the species: value from *O. bicornis* used.

For the estimation of individual-level exposures from the dimethoate spray application, bee size (body surface area) as well as consumption rates of pollen and nectar are needed as model parameters. However, literature data are not available for the estimation of these values for the two species. Instead, we used simplifying assumptions suggested in [European Food Safety Authority \(EFSA\) et al. \(2023\)](#). For the body surface factor of bees (addressed in Section 6.2.1), three size categories were listed: honey bees, bumble bees and solitary bees whereby bumble bees are assumed to be slightly larger (heavier) than honey bees and solitary bees considerably smaller. For the simulation of *N. melanderi* and *E. pruinosa*, we chose the surrogate bee category by their reported female sizes rather than assuming the small size of the solitary bee category. Females of *N. melanderi* are similar in size to honey bees (and *O. bicornis* females), and the values for honey bees were used (*ad.nectar.cons* = 208.34 mg/d, *ad.pollen.cons* = 11.6). *E. pruinosa* females are slightly larger than honey bee workers, resulting in the use of the proxy values for bumble bees (*ad.nectar.cons* = 210 mg/d, *ad.pollen.cons* = 11.7).

No data were found for the proportion of nectar in brood provisions of *N. melanderi* and *E. pruinosa*. Thus, the value listed by in [European Food Safety Authority \(EFSA\) et al. \(2023: Table 16\)](#) for *O. bicornis* was used due to lack of species-specific data. In addition, the weights of provisions for

female offspring were also not reported. However, it has been shown that the weight of post-emergent adult bees shows a close relationship with the provision weight. We used the average conversion factor of 2.87 from adult female wet weight to female provision wet weight (Neff 2008). Adult wet weights were reported for *N. melanderi* (Rust 2006; Cane et al. 2017; Table 63) and *E. pruinosa* (Willis Chan 2020; Table 55).

The exposure time per day (*ad.ET*) is an estimate of the time a nesting female bee is in contact with potentially exposed nesting material (mud or soil brood cell partitions in *Osmia* and soil in soil-nesting bees). Soil nesting bees are potentially in contact with the matrix while digging the nest, preparing brood cells, provisioning them as well as while resting in the nest when not foraging. Accordingly, soil-nesting bees have potentially the most contact with the nesting material per day, where time without contact is limited to the time foraging outside the nest. A foraging time of about 5 h per day was reported for *E. pruinosa* (Willis Chan 2020). The adult exposure time is used as a fraction of the day (24 h), i.e., *ad.ET* = 0.79. Because no species-specific data on foraging per day was found for *N. melanderi*, the same value was used (Table 26).

The daily rate of transfer of residues in nesting material to nesting adults has not been measured for either of the simulated species or nesting materials. Effects have been shown to occur in a study with *O. lignaria* brought in contact with imidacloprid-spiked wet soil (Fortuin et al. 2021) but the transfer rate to the bee was not quantified. Thus, a generic factor, *TC\_soil* = 0.5 g/d, was applied in the simulations of the Eurofins semi-field studies with *O. bicornis*. The same generic assumption was applied to the soil-nesting bee species (note that the transfer is assumed to occur only during the exposure time, defined by *ad.ET*).

For the characterization of the exposure of bees developing in the nest, assumptions also had to be applied to estimate residue transfer from potentially exposed nesting materials to the provision or larva. Because the contact with the nesting material occurs throughout the bee's pre-emergent stages, it is assumed that the exposure corresponds to the residue level in soil in soil-nesting bees (see also Section 2.4.5).

## 6.5.2. Exposures and species-specific input files

For the estimated exposures via relevant routes, assumptions corresponding to the exposure estimation for the Eurofins semi-field studies with *O. bicornis* were applied (see Section 7.2.4): for each case, a PEARL scenario was created based on the FOCUS scenarios and adapted to the according local conditions. For the information on soil composition, weather and timing freely available databases were searched to construct the scenarios based on literature information. Compound information was taken from European Food Safety Authority et al. (2018) with DT50 (20°C, 100%FC) 2.8 days, Koc of 28 L/kg, and 1/n of 1.02. Specifications of the soil exposure model scenarios are listed in Table 27.

For simulations of *N. melanderi*, a theoretical scenario for Walla Walla, Washington, USA was constructed. The region is known for its alfalfa production, and *N. melanderi* nesting beds are managed for pollination (Cane 2008). The modeled crop was alfalfa (BBCH 65) treated once at 75 g a.i./ha dimethoate spray with an interception of 90%. The same soil composition was used as for the simulation of the Eurofins 2019 and 2021 semi-field studies with *O. bicornis* as the texture fitted for the purpose of the hypothetical study. The weather conditions were based on data derived from freely available data bases for Walla Walla for the year 2003.

For the simulations of a hypothetical study with *E. pruinosa*, Winchester, Virginia USA, was chosen as location, corresponding a published study with the species (Julier and Roulston 2009). Tomato (BBCH 65) was used as model crop for pumpkin and squash, and a single spray treatment was assumed with 75 g a.i./ha of dimethoate and an interception of 80%. The same soil composition was applied as used for the simulations with *O. bicornis* and *N. melanderi*. The weather conditions were based on data derived from freely available data bases for Winchester for the year 2003.

In Table 27, the assumptions and specifications are listed for the daily exposure time series in the SolBeePop<sub>ecotox</sub> input files. Input files for control simulations (without exposures) and treatment simulations (single dimethoate spray application to the flowering crop during the daylight hours when bees are generally active) were generated using species- and location-relevant data. *N. melanderi* is partially managed for pollination of alfalfa in the Western US. For the simulation of the hypothetical semi-field study, we assumed the pesticide (dimethoate) application date (18 June) after their emergence at the end of spring. As example case, the weather conditions from 2003 in Walla Walla, Washington, USA were used. This corresponds to the nearest weather station to Touchet Valley, Washington, USA where multiple studies with *N. melanderi* were conducted (Johansen et al. 1978; Mayer and Miliczky 1998; Cane 2008; Vinchesi et al. 2013; Cane et al. 2017). From the weather station, daily air temperature and precipitation data were available but not relative humidity or wind speed. Accordingly, whether a bee could forage during a given day dependent on weather conditions was determined based on temperature and precipitation only. For *N. melanderi*, it was assumed that bees only forage (and provision nests) on days with maximum daily temperature at or above 21 °C (Table 28). Because data was not found for temperature suitable for foraging in the species, ranges of suitable temperatures were used as reported for *M. rotundata*, with 21 °C representing the middle of the range reported across studies (Tasei 1975; Stubbs et al. 1994; Pitts-Singer and Cane 2011). Both species are active in the late spring or summer and are managed for alfalfa pollination in similar climates, indicating *M. rotundata* could have similar preferences for weather conditions. No data was available to inform quantitative relationships between precipitation and foraging activity. We applied the generic assumption that *N. melanderi* avoids foraging in rain with a threshold for a rainy day set to 2.5 mm precipitation. *N. melanderi* occurs in arid regions with low rainfall in the summer when the bee is active. Daily precipitation of 2.5 mm corresponds to 10% of the rain level preventing bee foraging across species in study in blueberry fields (Drummond 2016; Drummond et al. 2017), with 25.4 mm of rain resulting in no observed bee activity.

*E. pruinosa* is a specialist for cucurbit crops in North America. For the hypothetical semi-field study simulations, we assumed an application date in summer (28 July) during peak flowering of pumpkin or squash fields at a location around Winchester, Virginia, USA. The weather conditions from the example year 2003 were retrieved, providing air temperature and precipitation data. We assumed a day reaching a maximum temperature of 16 °C or more is suitable for *E. pruinosa* foraging (Hurd et al. 1974) (Table 28). No data on foraging activity of the species relative to precipitation was available, and we applied the generic assumption of no foraging occurring on days with 25.4 mm of rain or more (Drummond 2016; Drummond et al. 2017).

The same application rate of dimethoate (75 g a.i./ha) was used as in the Eurofins semi-field studies with *O. bicornis*. The initial residues in nectar and pollen on the day of application were estimated using the residue unit doses (RUDs) provided by European Food Safety Authority (EFSA) et al. (2023: Table 19). The residues were assumed to decline in both matrices following a simple first-order kinetics (SFO) function with a constant of  $k = 0.5145$  (European Food Safety Authority (EFSA) et al. 2023, Annex H, dimethoate).

The exposure from direct spray was calculated from the application rate and the body surface factor (BSF; European Food Safety Authority (EFSA) et al. 2023), whereby BSFs for honey bees and bumble bees, respectively, were applied according to bee size: BSF = 0.0114 dm<sup>2</sup>/bee (*N. melanderi*), and BSF = 0.0146 dm<sup>2</sup>/bee (*E. pruinosa*) (Table 28).

For the estimation of daily exposures from soil, total soil concentrations of dimethoate were derived from the application rate and weather conditions (see previous paragraph) using a standard soil exposure model. For *N. melanderi*, the average nest depth of 17.5 cm was assumed (Batra 1970), corresponding to the soil depth for the exposure. The nests of *E. pruinosa* were reported to be 12-38 cm or 16-18 cm deep, respectively (Mathewson 1968; Hurd et al. 1974). We used a soil depth of 18.5 cm for the species' exposure from soil.

*Table 27. Definitions of study and environmental conditions for the estimation of exposures from soil over time for the hypothetical semi-field study simulations with *N. melanderi* and *E. pruinosa*.*

Exposure scenario characteristic	<i>N. melanderi</i>	<i>E. pruinosa</i>																																								
1) Application date	18 June DOY: 169 BBCH: 65	28 July DOY: 209 BBCH: 65																																								
2) Application rate	1 x 75 g/ha spray	1 x 75 g/ha spray																																								
3) Crop (in-field)	Alfalfa	Squash or pumpkin (represented by tomato)																																								
4) Off-field	Bare soil	Bare soil																																								
5) Drift rate	0.92%	0.92%																																								
6) Weather scenario	Walla Walla, Washington, US	Winchester, Virginia, US (see Julier and Roulston 2009)																																								
7) Soil type	Soil type for both studies (from a location between the two sites):  <table border="1"> <thead> <tr> <th colspan="2">Soil parameters</th> </tr> </thead> <tbody> <tr> <td>Sand [%]</td><td>7.0</td></tr> <tr> <td>Clay [%]</td><td>6.9</td></tr> <tr> <td>Silt [%]</td><td>86.2</td></tr> <tr> <td>pH (CaCl<sub>2</sub>)</td><td>7.4</td></tr> <tr> <td>pH (H<sub>2</sub>O)</td><td>7.7</td></tr> <tr> <td>Total organic carbon [%]</td><td>1.7</td></tr> <tr> <td>Total carbon [%]</td><td>3.96</td></tr> <tr> <td>Organic matter (calculated TOC x 1.72)</td><td>2.87</td></tr> <tr> <td>Rho [g/cm<sup>3</sup>]</td><td>1.34</td></tr> </tbody> </table>	Soil parameters		Sand [%]	7.0	Clay [%]	6.9	Silt [%]	86.2	pH (CaCl <sub>2</sub> )	7.4	pH (H <sub>2</sub> O)	7.7	Total organic carbon [%]	1.7	Total carbon [%]	3.96	Organic matter (calculated TOC x 1.72)	2.87	Rho [g/cm <sup>3</sup> ]	1.34	Soil type for both studies (from a location between the two sites):  <table border="1"> <thead> <tr> <th colspan="2">Soil parameters</th> </tr> </thead> <tbody> <tr> <td>Sand [%]</td><td>7.0</td></tr> <tr> <td>Clay [%]</td><td>6.9</td></tr> <tr> <td>Silt [%]</td><td>86.2</td></tr> <tr> <td>pH (CaCl<sub>2</sub>)</td><td>7.4</td></tr> <tr> <td>pH (H<sub>2</sub>O)</td><td>7.7</td></tr> <tr> <td>Total organic carbon [%]</td><td>1.7</td></tr> <tr> <td>Total carbon [%]</td><td>3.96</td></tr> <tr> <td>Organic matter (calculated TOC x 1.72)</td><td>2.87</td></tr> <tr> <td>Rho [g/cm<sup>3</sup>]</td><td>1.34</td></tr> </tbody> </table>	Soil parameters		Sand [%]	7.0	Clay [%]	6.9	Silt [%]	86.2	pH (CaCl <sub>2</sub> )	7.4	pH (H <sub>2</sub> O)	7.7	Total organic carbon [%]	1.7	Total carbon [%]	3.96	Organic matter (calculated TOC x 1.72)	2.87	Rho [g/cm <sup>3</sup> ]	1.34
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Total organic carbon [%]	1.7																																									
Total carbon [%]	3.96																																									
Organic matter (calculated TOC x 1.72)	2.87																																									
Rho [g/cm <sup>3</sup> ]	1.34																																									

Exposure scenario characteristic	<i>N. melanderi</i>	<i>E. pruinosa</i>
8) Relevant Soil depth for exposure (output needed)	17.5 cm (average nest depth)	18.5 cm (average nest depth)
9) Relevant concentration	Total + pore water	Total + pore water
10) Residues on leaves	n.a.	n.a.

### 6.5.3. Case study simulations

Capturing the study design of the Eurofins semi-field studies with *O. bicornis*, we simulated a dimethoate application rate of 75 g a.i./ha 10 days after the average emergence of females in *N. melanderi* and *E. pruinosa*.

Different timings of application (relative to the bees' average emergence date) can have impacts on population-level effects. Thus, three temporal scenarios were tested: 1) average female emergence occurring 10 days prior to application which corresponds roughly to the Eurofins semi-field studies with *O. bicornis*, 2) average female emergence 17 days prior to application, and 3) 3 days prior to application. The temporal scenarios were chosen to illustrate the interaction between application timing and population-level effects. The temporal scenarios were tested with *N. melanderi*, *E. pruinosa* and *O. bicornis*. Here, we included *O. bicornis* because the species was reported to differ in synchronization of emergence from the other two species. *O. bicornis* females in a single population tend to emerge within a few days (Bosch et al. 2008). In contrast, *E. pruinosa* was reported to emerge over the duration of a month (Hurd et al. 1974). The range of temporal emergence of females is reflected in the model parameter *var.emerge.f*.

With the baseline study design, we also tested different proportions of bees actively foraging, and thus, exposed to direct spray on application day. In the baseline scenario, we assumed all post-emergent females were exposed to direct spray. Additional scenarios assumed 0, 25, 50, 75% of bees exposed to direct spray (see also Section 7.2.5). Each simulation scenario was repeated 50 times, i.e., identical parameters and input files were used in simulations with different random number seeds to capture the stochasticity in the model.

From the outputs of the simulations, the number of post-emergent females were plotted (using ggplot; Wickham 2016), showing control simulation outputs and treatment scenarios in one plot. Outputs were plotted by calculating the averages across the 50 repeat simulations and the minimum and maximum values generated by the model for each day. Correspondingly, the cumulative number of brood cells produced were plotted as well as the numbers of female and male bees emerged in the following year from the brood produced during the (hypothetical) semi-field phase. In addition, relative effects ( $E_r$ ) were calculated by comparing model outputs from the corresponding control ( $O_c$ ) and exposure simulations ( $O_e$ ) using Equation 6.3. Corresponding control and exposure simulations used identical parameter combinations and random number seeds and differed exclusively in the input file used (without and with exposures, respectively).

*Equation 6.3*

$$E_r = \frac{O_e - O_c}{O_c}$$



Table 28. Specifications for the daily foraging and exposure definitions in the SolBeePop<sub>ecotox</sub> input files.

Specification	<i>N. melanderi</i>	<i>E. pruinosa</i>	Description	Remarks
<b>Foraging specifications (apply to control and treatment simulations)</b>				
Temperature data	WallaWalla\ Wal_Wal_Air.met	Eucera\ Winchester\ Win_7_SE.met	File containing temperature data (maximum daily temperature in °C)	Wal_Wal = Walla Walla, Washington, USA; Win = Winchester, Virginia, USA
Precipitation data	WallaWalla\ Wal_Wal_Air.met	Eucera\ Winchester\ Win_7_SE.met	File containing daily precipitation data (mm)	Wal_Wal = Walla Walla, Washington, USA; Win = Winchester, Virginia, USA
Humidity data	none	none	File containing humidity data (minimum %)	
Wind data	none	none	File containing wind speed data (m/s)	
Sunshine hours	none	none	File containing hours of sunshine per day	
Start date (doy)	19 May 2003 (139)	17 June 2003 (168)	First date with possible foraging (corresponds to start date of study)	Year corresponds to simulated soil exposure
End date (doy)	14 July 2003 (195)	23 August 2003 (235)	Last date with possible foraging (corresponds to end date of study)	
Minimum temperature (min.temp)	21 °C	16 °C	Assumed minimum temperature when foraging of the species occurs; compared to maximum daily temperature	
Maximum wind speed (max.wind)	NA	NA	Assumed maximum wind speed with foraging of the species	
Maximum precipitation (max.precip)	2.5 mm	25.4 mm	Assumed amount of rain per day that still allows foraging (compared to total mm precipitation)	<i>N. melanderi</i> : 10% of limit for other species; description for summer-active species <i>M. rotundata</i> that it does not forage in rain (Stubbs et al. 1994)
Maximum relative humidity (max.humid)	NA	NA	Assumed maximum humidity with foraging of the species (compared to minimum daily humidity because highest humidity generally occurs at night)	

Specification	<i>N. melanderi</i>	<i>E. pruinosa</i>	Description	Remarks
Control input file name (no exposure)	Nomia\ Floral_semifield_Nomia_noexp.csv	Eucera\ Floral_semifield_Eucera_noexp.csv	Input time series generated using the specifications above	No spaces in actual file names
<b>Exposure specifications (treatments only)</b>				
Compound (PPP)	dimethoate	dimethoate		
Application date (doy)	18 June 2003 (169)	28 July 2003 (209)		The year 2003 corresponds to the weather data used
Application rate (AR)	75 g/ha	75 g/ha		Two different application rates simulated in hypothetical semi-field studies
RUD in nectar	0.87 mg/kg x kg/ha	0.87 mg/kg x kg/ha	Defines residue in nectar on application day	residue value calculated from RUD and AR; values for 'med' nectar & pollen residues (see notes from 24 October 2023)
RUD in pollen	67.7 mg/kg x kg/ha	67.7 mg/kg x kg/ha	Defines residue in pollen on application day	see nectar
Soil concentration data	Nomia\ WallaWalla\ off_field_75_total\ ssBARE.out	Eucera\ Winchester\ in_field_75_total\ ssTOMPia.out	Modeled concentrations in soil	
Soil layer	18 (175mm)	19 (185mm)	Soil layer of interest (corresponds to average nest depth)	Nest depth reported for <i>N. melanderi</i> (Batra 1970); <i>E. pruinosa</i> (Mathewson 1968; Hurd et al. 1974)
Soil horizon density	1340 kg/m <sup>3</sup>	1340 kg/m <sup>3</sup>		
Kinetics function for residue dissipation in nectar and pollen	SFO	SFO	see <a href="#">European Food Safety Authority (EFSA) et al. (2023)</a> , Annex H, dimethoate	
Constant of SFO kinetics for nectar and pollen	0.5145	0.5145	see <a href="#">European Food Safety Authority (EFSA) et al. (2023)</a> , Annex H, dimethoate	
Exposure factor from direct spray (EF_co)	1	1	<a href="#">European Food Safety Authority (EFSA) et al. (2023)</a>	

Specification	<i>N. melanderi</i>	<i>E. pruinosa</i>	Description	Remarks
Body surface factor (BSF)	0.0114 dm <sup>2</sup> /bee	0.0146 dm <sup>2</sup> /bee	European Food Safety Authority (EFSA) et al. (2023), Table 9; using honey bee for <i>Osmia</i> and <i>N. melanderi</i> ; bumble bee for <i>E. pruinosa</i>	See text for further explanation
Kinetics function for residue dissipation in and on plant surfaces (leaves)	NA	NA		Note that the initial concentration corresponds to the application rate
Constant of SFO kinetics for leaves	NA	NA		Derived from reported RL50 = 4.6 days for dimethoate <sup>5</sup>
Input file name (with exposure specifications)	Nomia\ Floral_semifield_Nomia_DIMexp75_med_resid.csv	Eucera\ Floral_semifield_Eucera_DIMexp75_med_resid.csv	Input time series generated using the specifications above	No spaces in actual file names

<sup>5</sup> <http://sitem.herts.ac.uk/aeru/ppdb/en/Reports/244.htm>

## 6.5.4. Results

In the hypothetical semi-field studies with *N. melanderi* and *E. pruinosa*, simulated exposures resulted in mortality of nearly all post-emergent females present in the population on application day. This applies to the scenario in which all post-emergent females were assumed to be exposed to direct spray. Because the same individual-level response to exposures was assumed to occur in both simulated species, this result was expected because it corresponds to the response in the simulated semi-field studies with *O. bicornis* (Section 7.2.7) and the individual-level response was simulated using BeeGUTS derived from standard laboratory toxicity studies with the honey bee. Note that effects on in-nest life stages from simulated dimethoate exposure levels did not occur: the pesticide is highly toxic to adults but not to larvae.

Although the effect from the exposures was qualitatively comparable between simulated species, differences were observed in population-level effect sizes (Figure 31). In *N. melanderi*, a comparatively short maximum life span of post-emergent females was assumed (26 days), with most brood cell production occurring prior to exposure to dimethoate. *E. pruinosa* females were assumed to be least synchronized in their emergence, with females emerging in the same population across more than two weeks. Thus, emergence of new females occurred after application even though the application date was set to occur 10 days after peak emergence. Thus, the number of post-emergent females was observed to increase again after the dimethoate application in the species (Figure 31C). These simulated females produced brood, reducing the overall effect on reproductive output. For reference, simulations of the Eurofins 2021 semi-field study with *O. bicornis* are also shown in Figure 31. *O. bicornis* emerge from cocoons within a few days, particularly in the semi-field study setting in which cocoons were incubated at identical temperatures.

In additional simulation sets, we tested the interaction between the proportion of females foraging on the day of application and simulated effects. Females not foraging on the day of application do not experience exposure from direct spray in the model. This had been tested in the simulation of the Eurofins 2019 and 2021 semi-field studies with *O. bicornis* as well (Section 7.2.7). In the case of *O. bicornis*, these scenarios demonstrated that the exposure to direct spray was the main driver of the observed effects, with only very slight effects observed in case no foraging was assumed to occur on application day. This qualitative observation also applied to the simulations of *N. melanderi* and *E. pruinosa*: a lower proportion (50%) of females exposed to direct spray resulted in a reduction in the simulated effect (Figure 32). Without direct exposure to spray, only slight effects occurred in the simulations of the two species (Figure 33). In this case, the bees in the model were still exposed to dimethoate through consumption of residues in nectar and pollen and contact to exposed soil. Accordingly, the exposure routes via pollen, nectar and soil were of lesser importance for spray application of dimethoate. For the compound's mode of action and the application type, *O. bicornis* provides a conservative surrogate for effects for soil-nesting solitary bee species.

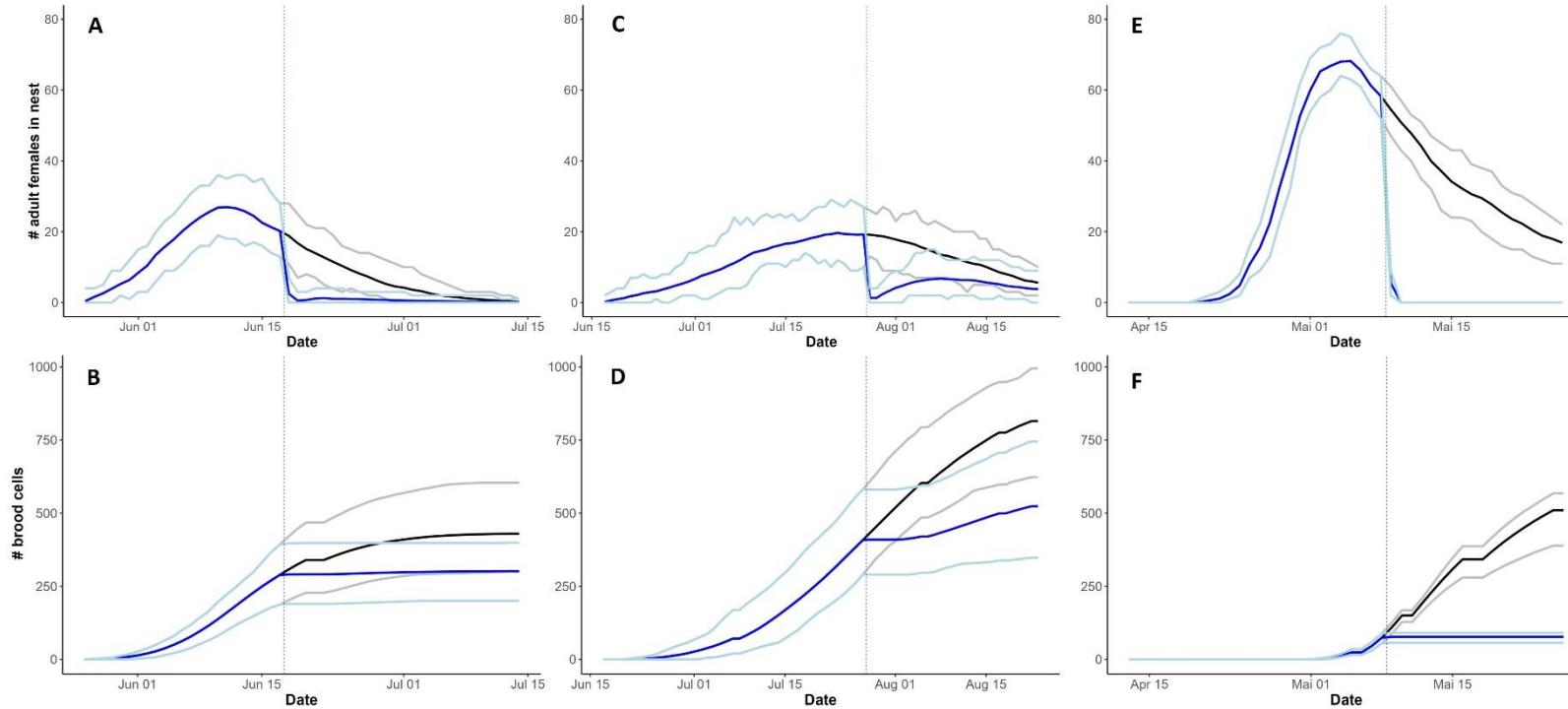


Figure 31. Simulations of hypothetical semi-field studies with *N. melanderi* (A, B), *E. pruinosa* (C, D) and *O. bicornis* (E, F). Controls are shown by their averages (black lines) and ranges (grey lines); treatment averages are shown as blue lines and ranges as light blue lines. Plots in the top row show the number of post-emergent female bees in the nests, bottom the cumulative number of brood cells. In the treatment simulations, **100% exposure of post-emergent females to direct spray** was assumed, and the application data was simulated 10 days after peak emergence of the bees. Simulations with *O. bicornis* correspond to the simulations of the 2021 Eurofins semi-field study.

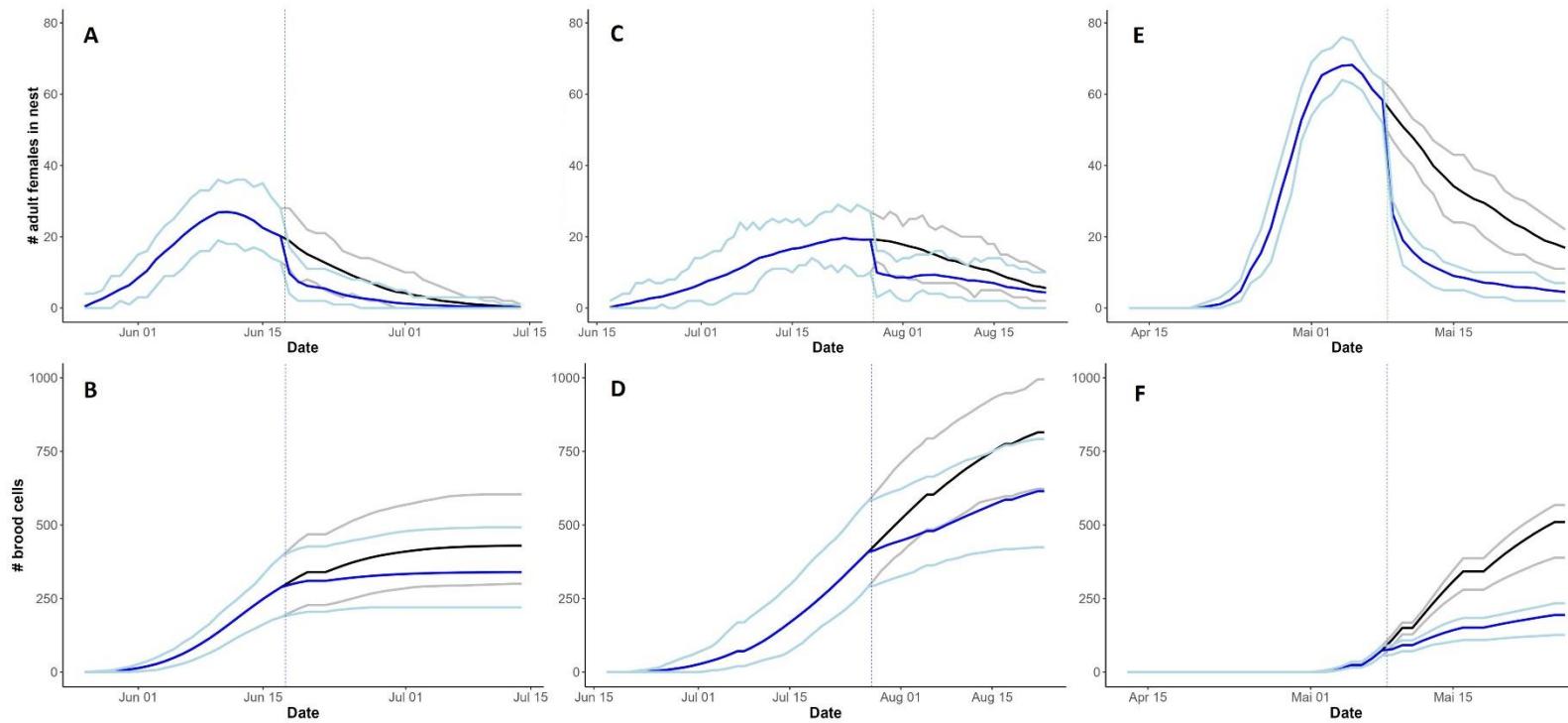


Figure 32. Simulations of hypothetical semi-field studies with *N. melanderi* (A, B), *E. pruinosa* (C, D) and *O. bicornis* (E, F). In the treatment simulations, **50% exposure of post-emergent females to direct spray** was assumed. Controls are shown by their averages (black lines) and ranges (grey lines); treatment averages are shown as blue lines and ranges as light blue lines. Plots in the top row show the number of post-emergent female bees in the nests, bottom the cumulative number of brood cells. The application data was simulated 10 days after peak emergence of the bees. Simulations with *O. bicornis* correspond to the simulations of the 2021 Eurofins semi-field study.

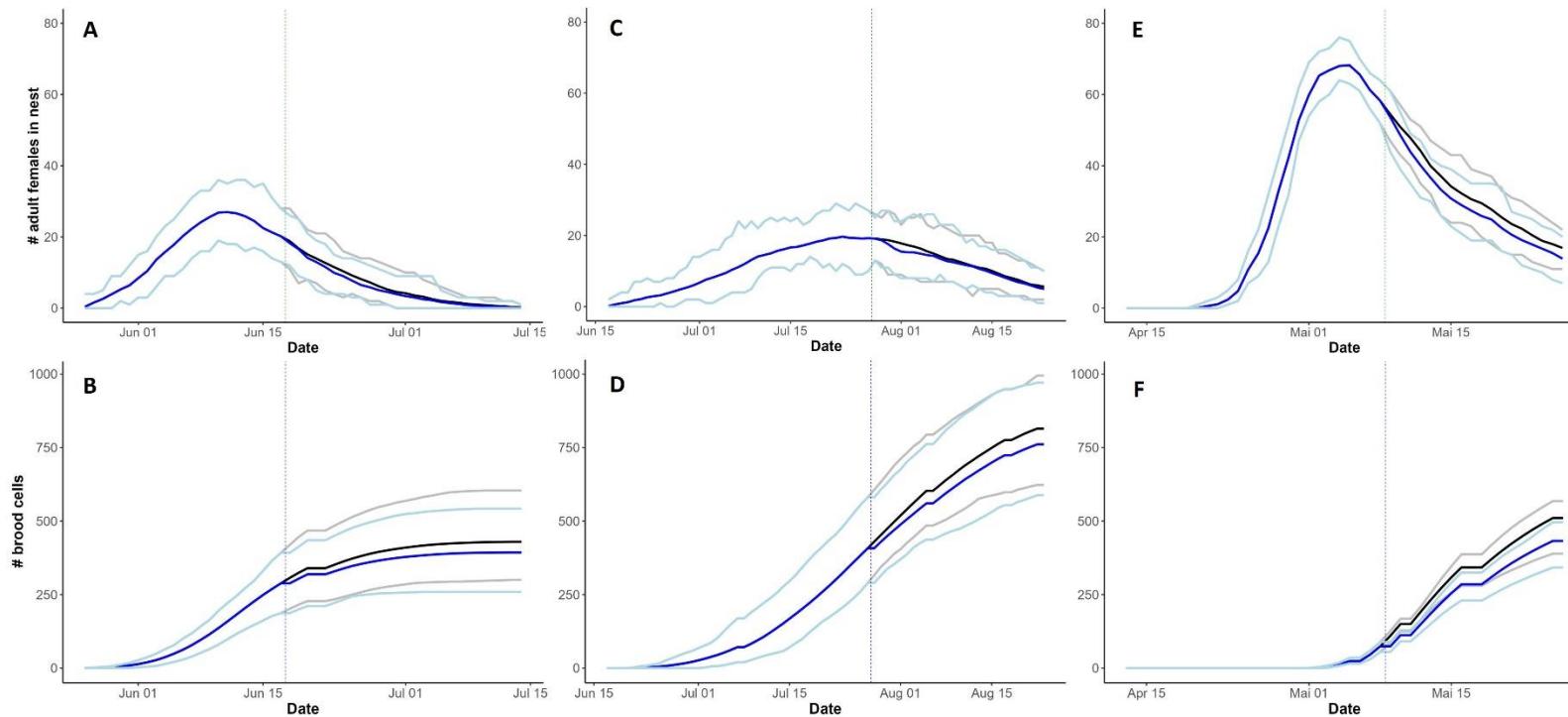
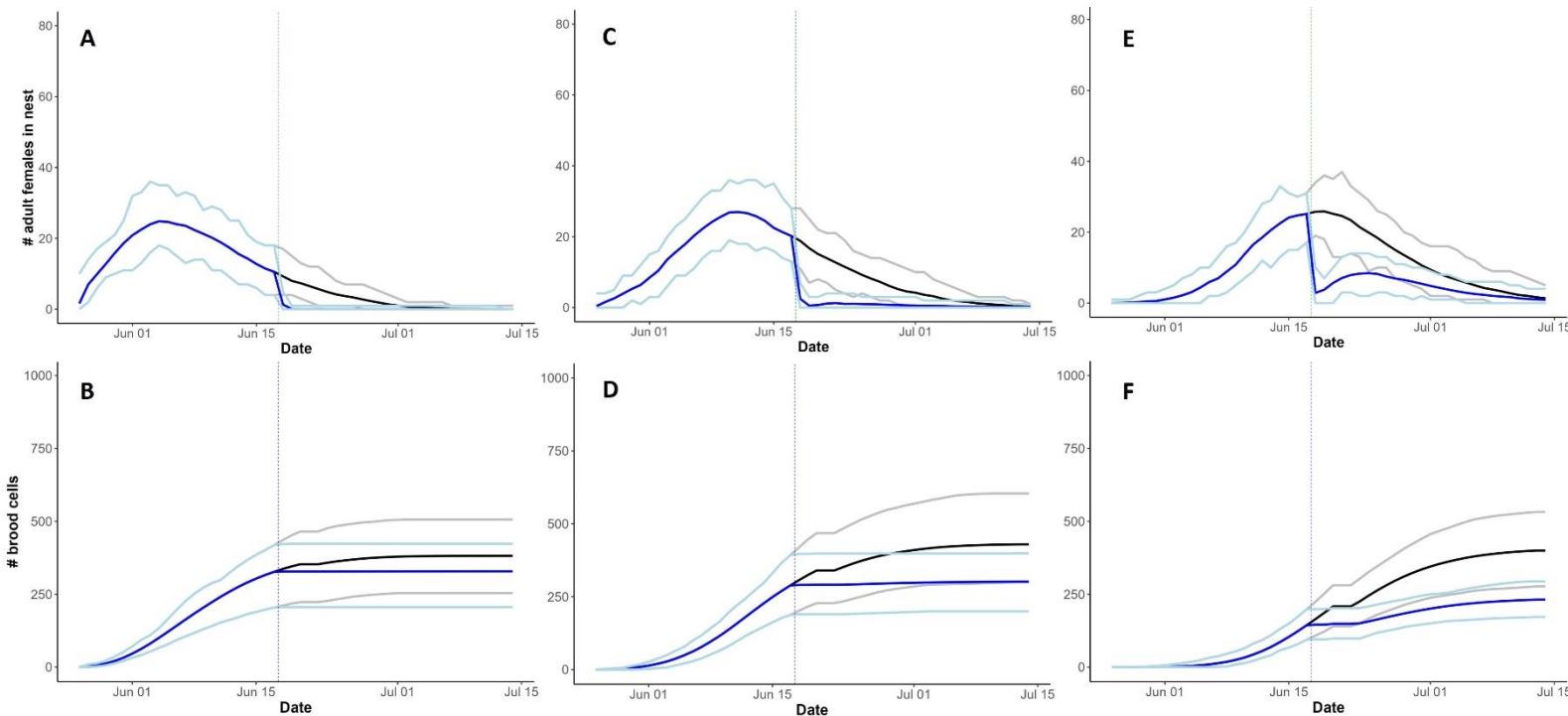


Figure 33. Simulations of hypothetical semi-field studies with *N. melanderi* (A, B), *E. pruinosa* (C, D) and *O. bicornis* (E, F). In the treatment simulations, **0% exposure of post-emergent females to direct spray** was assumed. Controls are shown by their averages (black lines) and ranges (grey lines); treatment averages are shown as blue lines and ranges as light blue lines. Plots in the top row show the number of post-emergent female bees in the nests, bottom the cumulative number of brood cells. The application data was simulated 10 days after peak emergence of the bees. Simulations with *O. bicornis* correspond to the simulations of the 2021 Eurofins semi-field study.

The temporal shift of bees' peak emergence date relative to the application date resulted in different outcomes dependent on simulated species. In *O. bicornis*, the impact of the temporal shift was most pronounced (Figure 36). The shorter the time interval between peak emergence and application, the lower cumulative brood cell production was observed. The application resulted in 100% nesting female mortality, effectively cutting the reproductive season short. In *N. melanderi* (Figure 34) and *E. pruinosa* (Figure 35), this effect could also be observed but was less pronounced than in *O. bicornis*. In those two species, some emergence occurred after the application in case peak emergence occurred only three days before application, compensating for some of the mortality of females.

Relative effect sizes indicate the effect relative to control numbers. Because relative effects are independent of the absolute numbers of individuals, they can be more informative when generalizing beyond a specific study. In Table 29, we list the average and range (minimum and maximum) relative effect sizes in the simulations of the hypothetical semi-field studies. For *N. melanderi* and *E. pruinosa*, relative effects are listed for scenarios with 100%, 50% and 0% of post-emergent females exposed to direct spray. In addition, relative effects in scenarios with temporal shifts, i.e., females' peak emergence date 17 and 3 days prior to exposure, are also listed in Table 29. The scenarios with the temporal shifts between peak emergence and application were also applied to *O. bicornis*, using the settings from the simulations of the 2021 Eurofins semi-field study. Relative effects on numbers of post-emergent females are listed on day 2 after exposure, the relative effects on cumulative brood numbers on the last day of the simulated tunnel phase. Relative effect sizes are listed for simulations using GUTS-SD and GUTS-IT models.



**Figure 34.** Simulations of hypothetical semi-field studies with *N. melanderi* using three different temporal scenarios. A, B: Peak female emergence 17 days prior to dimethoate application; C, D: peak emergence 10 days, and E, F: peak emergence 3 days prior to application. Controls are shown by their averages (black lines) and ranges (grey lines) treatment averages are shown as blue lines and ranges as light blue lines. Plots in the top row show the number of post-emergent female bees in the nests, bottom plots the cumulative number of brood cells.

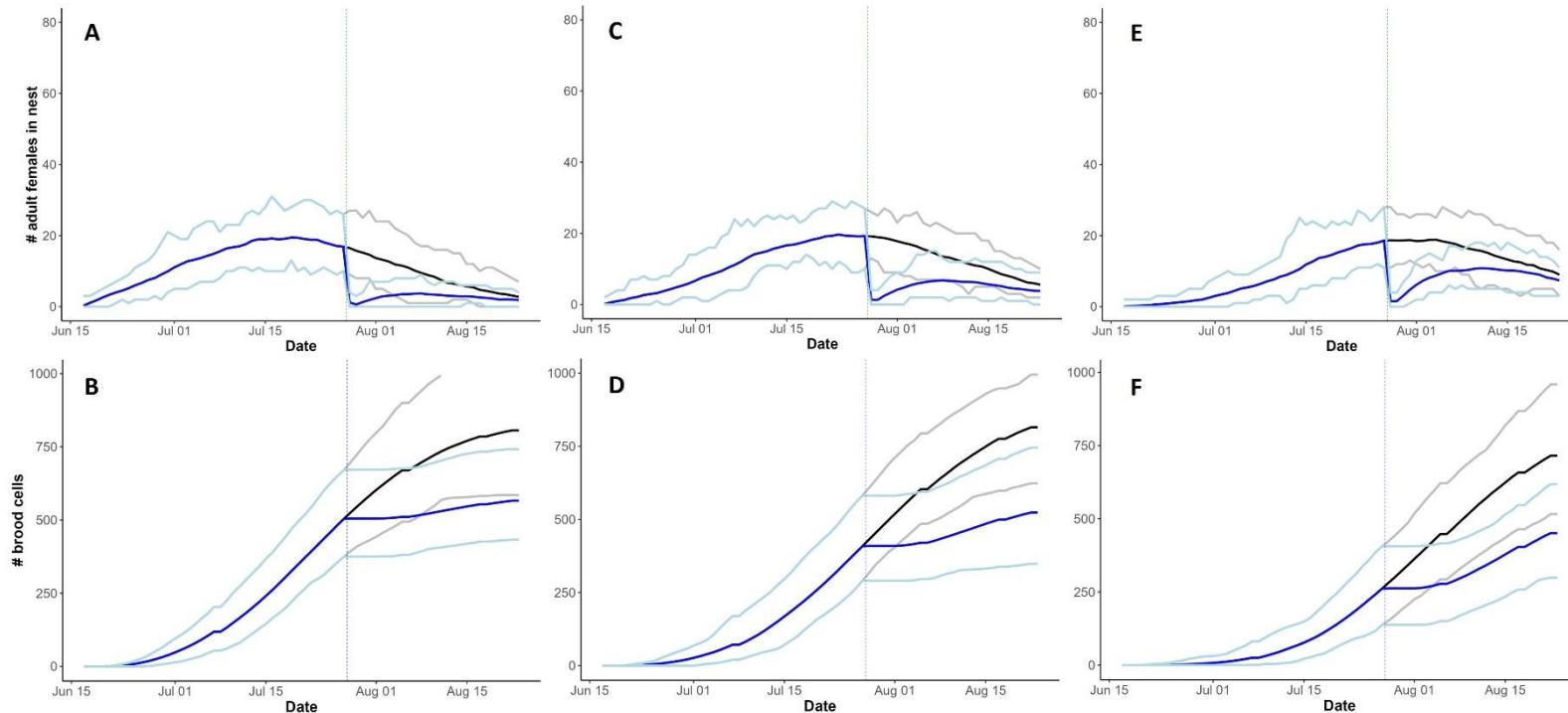
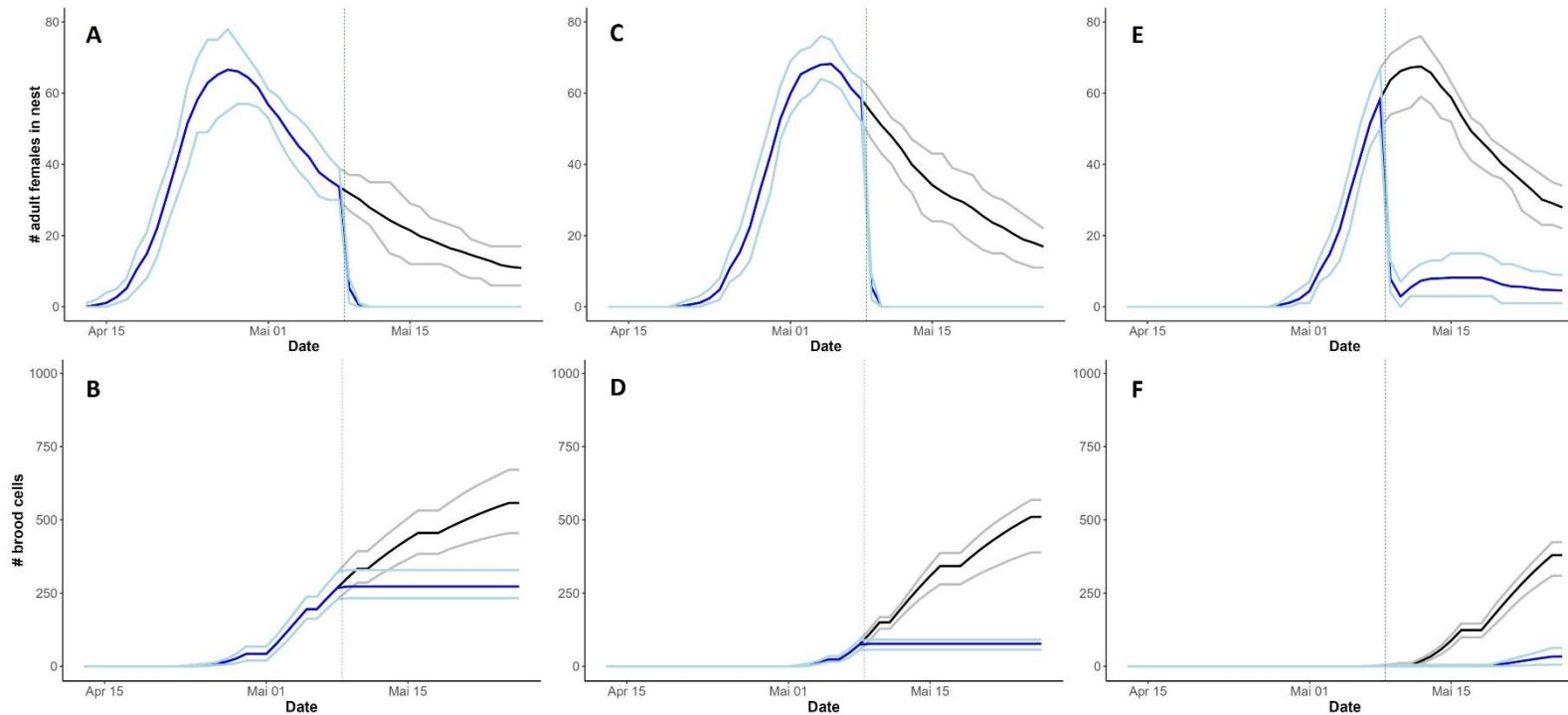


Figure 35. Simulations of hypothetical semi-field studies with *E. pruinosa* using three different temporal scenarios. A, B: Peak female emergence 17 days prior to dimethoate application; C, D: peak emergence 10 days, and E, F: peak emergence 3 days prior to application. Controls are shown by their averages (black lines) and ranges (grey lines) treatment averages are shown as blue lines and ranges as light blue lines. Plots in the top row show the number of post-emergent female bees in the nests, bottom plots the cumulative number of brood cells.



**Figure 36.** Simulations of hypothetical semi-field studies with *O. bicornis* using three different temporal scenarios. A, B: Peak female emergence 17 days prior to dimethoate application; C, D: peak emergence 10 days (corresponding to the 2021 Eurofins semi-field study), and E, F: peak emergence 3 days prior to application. Controls are shown by their averages (black lines) and ranges (grey lines) treatment averages are shown as blue lines and ranges as light blue lines. Plots in the top row show the number of post-emergent female bees in the nests, bottom plots the cumulative number of brood cells.

Table 29. Relative effect sizes (proportion of controls) in the simulations of hypothetical semi-field studies. Relative effects on number of post-emergent females are listed two days after the application; for total brood cell numbers, the relative effects on the last day of the tunnel phase.

Simulated species	Peak emergence prior to simulated application	Assumed % of females exposed to direct spray	GUTS model	Nesting female number (day after application)	Brood cell number (end of tunnel phase)
<i>N. melanderi</i>	10 days	100%	GUTS-SD	-0.949 (-1; -0.813)	-0.296 (-0.421; -0.140)
<i>N. melanderi</i>	10 days	100%	GUTS-IT	-0.940 (-1; -0.800)	-0.300 (-0.426; -0.143)
<i>N. melanderi</i>	10 days	50%	GUTS-SD	-0.582 (-0.824; -0.273)	-0.208 (-0.354; -0.067)
<i>N. melanderi</i>	10 days	50%	GUTS-IT	-0.572 (-0.882; -0.273)	-0.194 (-0.347; -0.022)
<i>N. melanderi</i>	10 days	0%	GUTS-SD	-0.034 (-0.400; 0.625)	-0.082 (-0.211; 0.092)
<i>N. melanderi</i>	10 days	0%	GUTS-IT	0.001 (-0.471; 0.625)	-0.077 (-0.256; 0.074)
<i>N. melanderi</i>	17 days	100%	GUTS-SD	-0.995 (-1; -0.833)	-0.138 (-0.231; -0.052)
<i>N. melanderi</i>	17 days	100%	GUTS-IT	-0.995 (-1; -0.833)	-0.141 (-0.236; -0.052)
<i>N. melanderi</i>	3 days	100%	GUTS-SD	-0.777 (-1; -0.636)	-0.413 (-0.571; -0.242)
<i>N. melanderi</i>	3 days	100%	GUTS-IT	-0.792 (-0.962; -0.609)	-0.418 (-0.575; -0.136)
<i>E. pruinosa</i>	10 days	100%	GUTS-SD	-0.869 (-1; -0.647)	-0.354 (-0.528; -0.103)
<i>E. pruinosa</i>	10 days	100%	GUTS-IT	-0.860 (-1; -0.647)	-0.343 (-0.456; -0.151)
<i>E. pruinosa</i>	10 days	50%	GUTS-SD	-0.503 (-0.706; 0.111)	-0.241 (-0.425; -0.005)
<i>E. pruinosa</i>	10 days	50%	GUTS-IT	-0.505 (-0.750; 0.111)	-0.231 (-0.466; -0.151)
<i>E. pruinosa</i>	10 days	0%	GUTS-SD	-0.045 (-0.389; 0.778)	-0.061 (-0.272; 0.228)
<i>E. pruinosa</i>	10 days	0%	GUTS-IT	-0.039 (-0.381; 0.778)	-0.088 (-0.374; 0.114)
<i>E. pruinosa</i>	17 days	100%	GUTS-SD	-0.911 (-1; -0.625)	-0.293 (-0.456; -0.079)
<i>E. pruinosa</i>	17 days	100%	GUTS-IT	-0.903 (-1; -0.625)	-0.289 (-0.481; -0.079)
<i>E. pruinosa</i>	3 days	100%	GUTS-SD	-0.830 (-1; -0.667)	-0.361 (-0.600; -0.149)
<i>E. pruinosa</i>	3 days	100%	GUTS-IT	-0.833 (-1; -0.667)	-0.379 (-0.600; -0.067)
<i>O. bicornis</i>	10 days	100%	GUTS-SD	-1.000 (-1; -1)	-0.848 (-0.894; -0.823)
<i>O. bicornis</i>	10 days	100%	GUTS-IT	-0.992 (-1; -0.957)	-0.850 (-0.887; -0.823)
<i>O. bicornis</i>	17 days	100%	GUTS-SD	-1.000 (-1; -1)	-0.508 (-0.576; -0.439)
<i>O. bicornis</i>	17 days	100%	GUTS-IT	-0.996 (-1; -0.957)	-0.515 (-0.578; -0.447)
<i>O. bicornis</i>	3 days	100%	GUTS-SD	-0.919 (-0.958; -0.851)	-0.910 (-0.985; -0.830)
<i>O. bicornis</i>	3 days	100%	GUTS-IT	-0.916 (-0.960; -0.881)	-0.913 (-0.954; -0.825)

# 7. MODEL OUTPUT CORROBORATION

## 7.1. Model corroboration with *Osmia bicornis* semi-field study data

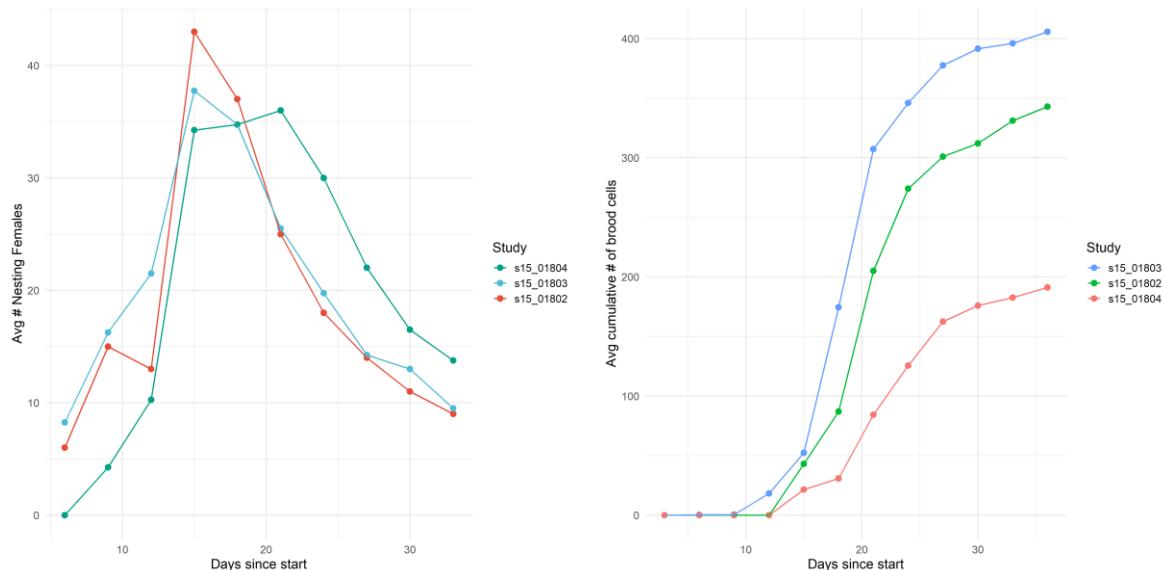
The simulations were conducted using the model version SolBeePop.nlogo (Schmolke et al. 2023a; Schmolke et al. 2023b).

### 7.1.1. Semi-field study data

Data from a semi-field studies conducted with *O. bicornis* (Ruddle et al. 2018) were available for comparison to model outputs. The semi-field studies were conducted by setting up mesh tunnels over portions of oilseed rape fields. Inside each tunnel, nest boxes were set up. Cocoons (60 females and 90 males in each tunnel) were placed in the nesting units at the onset of crop flowering. All cocoons were obtained from the same commercial supplier and stored under the same conditions prior to release. The mesh tunnels prevented released bees from nesting or foraging beyond the tunnel and excluded other bees and predators from reaching the released bees. Three semi-field studies were conducted in 2015 in three separate locations (Table 30). During the tunnel phase of the studies, newly produced brood cells were assessed every three days (a total of 12 assessments). The first assessment was conducted on the first day of the tunnel phase (day of cocoon release) and the last assessment on the last day in the tunnel. Number of adult bees present in the nest boxes were also assessed in three-day intervals with a total of 10 assessments. The first assessment of bees in the nest boxes was conducted three days after the start of the tunnel phase and the last three days before the end of the tunnel phase. At the end of the tunnel phase, nest boxes were closed and stored outside until the fall. Then, cocoons were removed from the nest boxes, cleaned and stored in the laboratory for hibernation under controlled conditions. After hibernation for about four months, a subset of cocoons was incubated at stepwise increasing temperatures to trigger emergence of the adult bees. Emergence success by sex was recorded. Figure 37 shows the average nesting females and cumulative brood cells produced during the tunnel phases of the three studies. The data are plotted relative to the study start date (date of release of cocoons into the tunnels) for better comparison. The plots indicate that the onset of nesting occurred later in the Celle study (S15\_01804) compared to the other two studies. In addition, bees in study S15\_01804 produced clearly less brood cells.

*Table 30. Specifications of semi-field studies conducted with *O. bicornis* from Ruddle et al. (2018). Tunnels were set up over portions flowering oilseed rape fields. In each tunnel, 60 female and 90 male cocoons were released.*

Study ID	Location	Date of cocoon release	End of tunnel phase	Untreated control tunnels
S15-01802	Niefern (Baden-Württemberg, Germany)	21 Apr 2015	27 May 2015	1
S15-01803	Tübingen (Baden-Württemberg, Germany)	23 April 2015	29 May 2015	4
S15-01804	Celle (Niedersachsen, Germany)	29 April 2015	4 June 2015	4



*Figure 37. Data from the three semi-field studies from Ruddle et al. (2018) reported for the tunnel phase. The x-axis shows the days since the release of cocoons into the tunnels for better comparison. **Left:** average number of nesting females observed in the nest blocks. **Right:** average cumulative number of brood cells in the nest blocks.*

### 7.1.2. Model calibration to semi-field study data

For the simulation of the semi-field studies, density dependence was switched off, assuming that the nesting space in the boxes provided in the tunnels was not limiting for the released females. An input file defining the daily floral resource availability was generated for each study location, using available weather data. We assumed that the bees forage 100% on the oilseed rape flowering in the tunnels and that the crop provided excess nectar and pollen throughout the tunnel phase for all nesting females. Thus, the daily forage availability was assumed to vary exclusively due to weather conditions in the simulations. The foraging preferences and crop and weather data used for the generation of the floral resource input file are summarized in Table 31.

In addition to the floral resource input file, the dates of the tunnel phase were study specific, informing the corresponding model parameters listed in Table 32. The onset of nesting (presence of females in the nesting blocks and production of first brood cells) was observed later after study initiation (release of cocoons into the tunnels) in the Celle study (S15-01804) compared to the other studies. The timing of emergence from the released cocoons was not reported in the studies. The reason for the later emergence cannot be derived from reported study data. To account for this difference across studies, two temporal scenarios were applied in the calibration simulations:

- A) Early emergence: emergence 4 and 3 days after introduction into the tunnel by females and males, respectively
- B) Late emergence: emergence 7 and 6 days after introduction into the tunnel by females and males, respectively

Seven SolBeePop parameters were selected for calibration to the semi-field studies because they were identified as uncertain and influential to model outputs in the analysis of parameter uncertainty (Section 6). For these parameters, the same value ranges were used in the calibration as in the model analysis with the exception of the parameter defining the survival of developing bees from egg stage through emergence, *max.survival.e.f* and *max.survival.e.m*. In the semi-field studies, only viable cocoons were released into the tunnels (F0 generation) and incubated over winter after the end of the tunnel phase (F1 generation), resulting in higher emergence rates because deaths prior to emergence are excluded. Thus, we included 100% emergence rates as possible highest parameter value. Note that the two parameters are assigned identical values in the calibration because no separate survival data for females and males through emergence were available (see also Section 6). The parameter *emerged.survival* was not included in the calibration because emergence rates from the cocoons released into the tunnels (F0 generation) were not reported in the studies. Thus, the survival rate of females to maturation (onset of nesting) cannot be separated from the survival rate through emergence. The latter parameter, *max.survival.e.f*, was included in the calibration. The parameter values applied in the calibration simulations are listed in Table 33.

*Table 31. Assumptions and data used for the generation of site-specific floral resource input files for the simulation of the semi-field studies. For the generation of the input file using these assumptions, see Appendix B.*

Specification	Description	Value	Remarks
wind.data	Availability of data on wind speed included in weather data	--	If unavailable: daily foraging not dependent on wind
use.sunshine	Availability (or use) of sunshine hours per data in weather data	--	If unavailable: daily foraging not dependent on sunshine hours per day
min.temp	Minimum temperature (°C) for <i>O. bicornis</i> foraging	10	Foraging assumed to occur if the maximum daily temperature exceeds this threshold
max.wind	Maximum wind speed at which foraging occurs	7.2	Not applied for semi-field simulations because wind speed was not available from the weather data
max.precip	Maximum daily precipitation (mm) at which foraging occurs	25.4	In the semi-field studies, no daily precipitation above this threshold was reported
max.humid	Maximum relative humidity (%) at which foraging occurs	78	
max.forag.hrs	Maximum number of hours of foraging by a bee	10	
crop.start	Start date (Julian day) of crop flowering	Study-specific	Corresponds to the start of the tunnel phase (date of cocoon release) in the studies (see Table 30)
crop.end	End date (Julian day) of crop flowering	Study-specific	Corresponds to the end of the tunnel phase in the studies (see Table 30)
crop.peak	Date (Julian) of peak crop flowering; if no temporal dynamic of flowering is assumed, set to 0	0	Assumes excess availability from oilseed rape throughout the tunnel phase
crop.Q	Relative quality of forage on crop; 1 = maximum quality (low foraging effort and distance); 0 = no forage available from crop within flight range of the bee	1	Assumption that the forage quality from crop is maximal throughout the tunnel phase (oilseed rape corresponding to <i>O. bicornis</i> foraging preferences, ease of pollen collection and very low foraging distance between nest and resource)
min.crop.Q	Minimum relative quality of forage on crop (during crop flowering)	n/a	Not applicable to semi-field simulations because crop.Q was set to 1 throughout the tunnel phase
nat.Q	Relative quality of forage on non-crop resources	0	Assumption that no pollen or nectar resources were available in the tunnels apart from oilseed rape
prop.crop	Proportion of foraging on crop (proportion of foraging on non-crop resources is assumed to be 1 – prop.crop)	1	Assumption that bees forage exclusively on oilseed rape within the tunnels

*Table 32. Model parameters and inputs used in model calibration and validation to the semi-field study data (Ruddle et al. 2018) reflecting study-specific conditions.*

Study-specific model parameter / input	Niefern <b>S15-01802</b>	Tübingen <b>S15-01803</b>	Celle <b>S15-01804</b>	Remarks
<i>Start.day</i>	111	113	119	Day of year of cocoon release into the tunnels; see Table 30
<i>input.floral</i>	Floral_S15_01802_Sce3_Jan2022.csv	Floral_S15_01803_Sce3_Jan2022.csv	Floral_S15_01804_Sce3_Jan2022.csv	For the assumption applied to generate the study-specific input, see text and Table 31
<i>day.emerge.f</i>	115, 118	117, 120	123, 126	Early and late emergence scenarios, see text
<i>day.emerge.m</i>	114, 117	116, 119	122, 125	Early and late emergence scenarios, see text
<i>latest.emerge</i>	147	149	155	Day of year of last day in tunnels; see Table 30

Table 33. SolBeePop model parameter value combinations applied in the semi-field calibration simulations. Parameters included in the calibration are listed with the value range used.

Parameter name	Default value ( <i>O. bicornis</i> )	Included in calibration	Min value in calibration	Max value in calibration	Remarks
<i>Start.day</i>	See remarks	--	--	--	Differs between studies (see Table 32)
<i>Species</i>	<i>O.bicornis</i>	--	--	--	
<i>Voltinism</i>	univoltine	--	--	--	
<i>Initial.num.f</i>	60	--	--	--	Number released in all studies
<i>Initial.num.m</i>	90	--	--	--	Number released in all studies
<i>Initial.stage</i>	cocoon	--	--	--	Life stage released in all studies
<i>Initial.age</i>	300	--	--	--	
<i>RndSeed</i>	See remarks	--	--	--	Different random numbers used for each of the 10 repeat simulations
<i>MultiYearInput</i>	FALSE	--	--	--	
<i>List.input.floral</i>	NA	--	--	--	
<i>Num.repeat.yr</i>	2	--	--	--	2 years to capture emergence of F1
<i>input.floral</i>	See remarks	--	--	--	Differs between studies (see Table 32)
<i>Density.dep</i>	FALSE	--	--	--	
<i>DD.thresh.s</i>	1	--	--	--	unused
<i>DD.max.cells.s</i>	1	--	--	--	unused
<i>DD.funct</i>	linear	--	--	--	unused
<i>DD.log.slope</i>	1	--	--	--	unused
<i>stoch.crop.forag</i>	FALSE	--	--	--	
<i>day.emerge.f</i>	See remarks	--	--	--	Differs between studies; two scenarios included in calibration (see Table 32 and text for further explanation)
<i>var.emerge.f</i>	3	Yes	1	7	Standard deviation around the mean emergence date (day of year) of female bees ( <i>day.emerge.f</i> ); parameter range from model analysis applied (Section 6.1)
<i>day.emerge.m</i>	See remarks	--	--	--	Differs between studies; two scenarios included in calibration (see Table 32 and text for further explanation)
<i>var.emerge.m</i>	2	--	--	--	
<i>latest.emerge</i>	See remarks	--	--	--	Differs between studies (see Table 32)
<i>dev.egg</i>	8	--	--	--	

Parameter name	Default value ( <i>O. bicornis</i> )	Included in calibration	Min value in calibration	Max value in calibration	Remarks
<i>dev.larva</i>	32	--	--	--	
<i>dev.cocoon</i>	68	--	--	--	
<i>t.maturity</i>	3	Yes	1	10	Female maturation time (days between emergence and initiation of nesting); specific to semi-field study because timing of emergence from cocoon after release not reported; parameter range from model analysis applied (Section 6.1)
<i>m.life</i>	21	--	--	--	
<i>max.nesting.life</i>	36	--	--	--	Excluded from calibration because the tunnel phase was shorter than the maximum life span
<i>p.max.nesting.life</i>	0.04	Yes	0.01	0.1	Likelihood of survival to maximum life span; influential in model analysis, parameter range from model analysis applied (Section 6.1)
<i>max.f.ratio</i>	0.59	Yes	0.38	1	Maximum probability of a new brood cell containing female offspring; influential in model analysis, parameter range from model analysis applied (Section 6.1)
<i>max.cells</i>	2	Yes	1	3	Maximum number of brood cells a female can produce in a single day; influential in model analysis, parameter range from model analysis applied (Section 6.1)
<i>max.survival.e.f</i>	0.74	Yes	0.58	1	Maximum survival of females from egg through emergence; higher max value applied than in the model analysis (Section 6.1) because only viable cocoons were released (F0) and incubated (F1)
<i>max.survival.e.m</i>	0.74	see remarks			No separate data for females and males available for survival to emergence: the same value was applied to <i>max.survival.e.f</i> and <i>max.survival.e.m</i> in the simulations
<i>emerged.survival</i>	1	--	--	--	Based on study data, this parameter is not separable from <i>max.survival.e.f</i>
<i>a.cell.age</i>	-0.006	--	--	--	Excluded because it was not impactful in the model analysis (Section 6.1)
<i>a.sex.age</i>	-0.0406	Yes	-0.0286	-0.0599	Defines the relationship between nesting female age and her brood cell production rate; influential in model analysis, parameter range from model analysis applied (Section 6.1)
<i>a.size.age</i>	-0.003	--	--	--	Excluded because it was not impactful in the model analysis (Section 6.1)
<i>a.cell.resource</i>	0.94	--	--	--	Excluded because it was only impactful in the model analysis (Section 6.1) for sub-optimal foraging scenarios
<i>a.sex.resource</i>	0.42	--	--	--	Excluded because it was only impactful in the model analysis (Section 6.1) for sub-optimal foraging scenarios
<i>a.size.resource</i>	0.114	--	--	--	Excluded because it was only impactful in the model analysis (Section 6.1) for sub-optimal foraging scenarios

For the calibration of SolBeePop, the parameter space defined by the value ranges of seven model parameters included in the calibration were explored using the latin hypercube (LHC) simulations (see Section 6.1.1). Thereby, 2000 samples of the parameter space were used, i.e., simulations with different parameter combinations. Each parameter combination was repeated 10 times using different random number seeds to address the stochasticity in SolBeePop. The LHC was set up using the R package “lhs”, model output analysis was conducted in R, and plots were generated using the package “ggplot2” (Wickham 2016; Carnell 2022; R Core Team 2022).

The goal of the calibration was to identify the parameter combinations that result in the best fit of model outputs to study data. Two studies, S15-01803 (Tübingen) and S15-01804 (Celle), were considered equally suitable for model calibration and validation because both studies included repeat tunnels while study S15-0182 (Niefern) consisted of a single trial (see Table 30). We conducted the calibration using S15-01803, and the validation using study data sets S15-01802 and S15-01804 (see Section 7.1.3). In an additional cross-validation, we used S15-01804 for calibration, S15-01802 and S15-01803 for validation.

The best fit to data was determined based on the comparison between means of the measured data (means across the four tunnels) and the means of the repeat simulations (10 repetitions, i.e., simulations with different random number seeds per parameter combination). To assess the goodness-of-fit of the simulations to the observations in the study, we applied the three quantitative indicators, NRMSE, NMAE and RSR, listed in Table 34 following the approach by (Schmolke et al. 2020). The three goodness-of-fit indicators all indicate a better fit between observations and predictions the lower their value. Observed number of female bees in the nest boxes on assessment days were compared to the daily number of simulated actively nesting females. The reported cumulative number of brood cells produced until (and including) the assessment date was compared to the cumulative number of simulated brood cells until the same date. The goodness-of-fit indicators were calculated separately for nesting females and cumulative brood cells.

The number of females and males emerging from the brood cells in the following year were also simulated. In the semi-field studies, only a subset of cocoons was incubated for emergence after overwintering. Accordingly, the number of emerged bees in the second study year (F1 generation) do not reflect the survival through emergence of all offspring produced during the tunnel phase. We assume that a random subset of cocoons was selected for incubation and subsequent assessment of offspring emergence in the studies. Although the reported absolute number of emerged females and males in the studies cannot be compared to model outputs, the sex ratio of the emerged bees should reflect the sex ratio of the total viable offspring produced during the tunnel phase. The sex ratio of the emerged offspring (F1 generation) was compared to the sex ratio of the emerged F1 bees in the simulations using the NMAE and the NRMSE. The RSR cannot be calculated based on a single measurement. Average goodness-of-fit indicators presented in this section are the averages of the indicators calculated for nesting female and cumulative brood cell numbers, respectively. We based the selection of the parameter combination resulting in the best model fit on the average NRMSE across the three comparisons: number of nesting females per sample date, cumulative brood cells numbers per study date, and sex ratio of emerged offspring.

*Table 34. Goodness-of-fit indicators applied to compare predictions from SolBeePop simulations with observations from semi-field study data. In the equations, O are the observations, P the predictions and  $\bar{O}$  the mean of the n observations.*

Goodness-of-fit indicator	Equation	Remarks	References
Normalized mean absolute error (NMAE)	$\text{MAE} = \frac{1}{n} \sum_{i=1}^n  O_i - P_i $ $\text{NMAE} = \frac{\text{MAE}}{\bar{O}}$	Other names used for the same indicator: relative MAE, MARE	(Bennett et al. 2013; Harmel et al. 2014; EFSA Panel on Plant Protection Products and their Residues (PPR) et al. 2018)
Normalized mean square error (NRMSE)	$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (O_i - P_i)^2}$ $\text{NRMSE} = \frac{\text{RMSE}}{\bar{O}}$	Indicator is very sensitive to outliers; NRMSE ≤ 0.5 suggested acceptable performance for TKTD models <sup>1</sup> in EFSA (2018)	(Bennett et al. 2013; Harmel et al. 2014; EFSA Panel on Plant Protection Products and their Residues (PPR) et al. 2018)
RMSE-standard deviation ratio (RSR)	$RSR = \frac{RMSE}{STDEV_{obs}} = \frac{\sqrt{\sum_{i=1}^n (O_i - P_i)^2}}{\sqrt{\sum_{i=1}^n (O_i - \bar{O})^2}}$	Indicator of how well the model explains the variance in the observations; indicator is sensitive to outliers	(Moriasi et al. 2007; Bennett et al. 2013)

<sup>1</sup> Toxicokinetic toxicodynamic models

## Calibration results

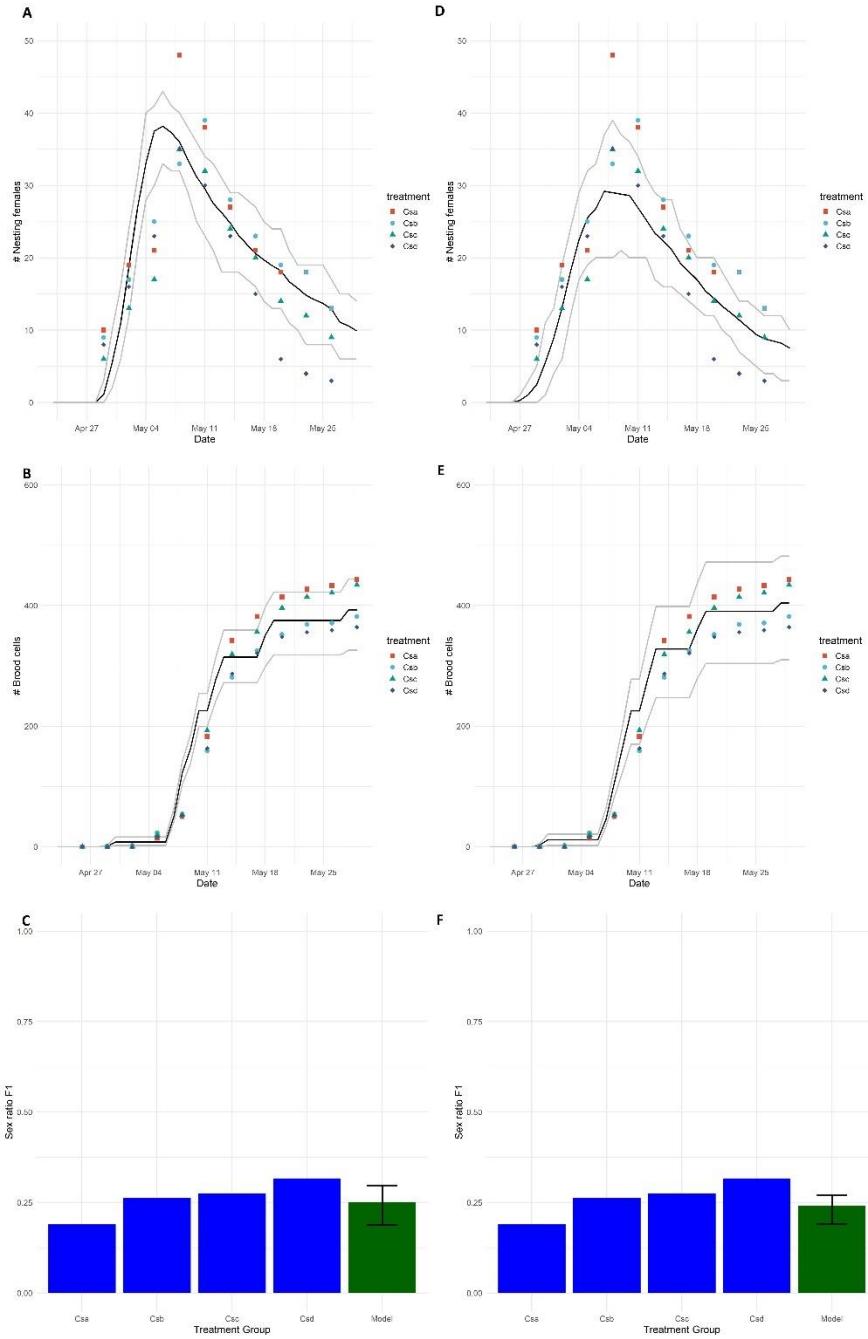
The parameter combinations resulting in the best fit with the study data were identified. The best fit to data were very similar based on NRMSE and NMAE. However, the goodness of fit based on RSR indicated a different parameter combination as the best fit to the data. Because with the RSR, it was not possible to consider the sex ratio of the offspring, we based the selection of the best fit on the NRMSE only.

### Study S15-01803 (Tübingen) as calibration data set

For study S15-01803, the best fits to data are listed based on the early and late emergence scenario (Table 35). In Figure 38, the simulated number of nesting female bees and the cumulative brood cells produced over time are shown along with the emerged bees in the following year for the best fits to study S15-01803. The plots show the range of the simulations (from 10 repetitions) compared to the study data (from 4 repeat tunnels).

*Table 35. Parameter combinations resulting in the best fits (lowest average NRMSE) with to data from study S15-01803 for the early and late emergence scenarios. The average NRMSE and NMAE were calculated from NRMSEs and NMAEs for nesting female numbers, cumulative brood cells, and offspring sex ratio after emergence. The average RSR is based only on the first two.*

Study	Temporal emergence scenario	var.emerge.f	t.maturity	p.max.nesting.life	max.f.ratio	max.cells	max.survival.e.f	a.sex.age	Average NRMSE	Average NMAE	Average RSR
S15-01803	(A) Early	2	6	0.094	0.428	1.664	0.846	-0.0477	0.153	0.108	0.964
S15-01803	(B) Late	3	4	0.091	0.408	1.965	0.750	-0.0597	0.132	0.103	0.681



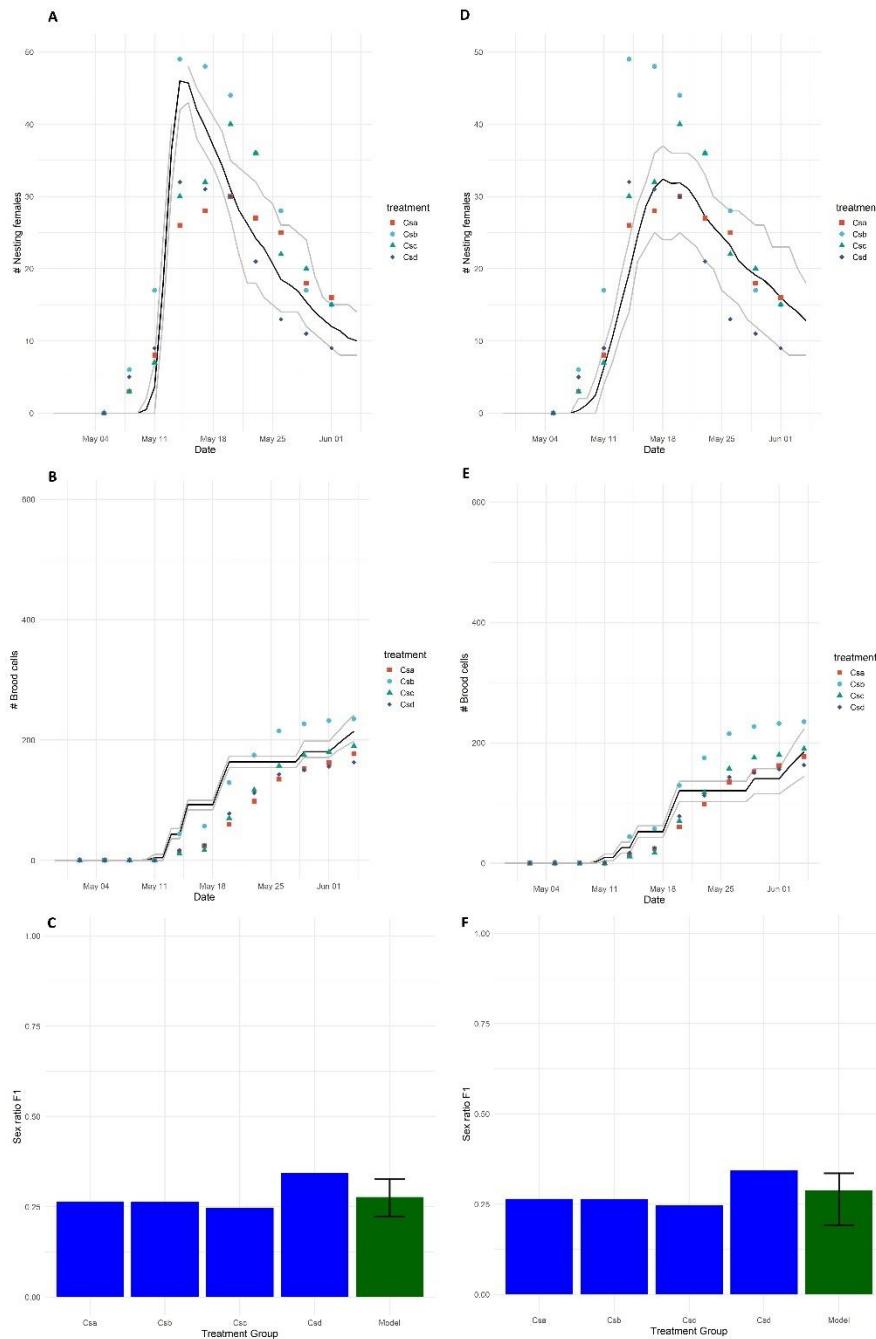
**Figure 38. Best simulations of study S15-01803 based on the comparison between average simulation outputs (predictions) and average of the four tunnels in the study (observations). Comparison of observed and simulated number of nesting females per day (A, D) and cumulative brood cells produced (B, E) during the tunnel phase of the semi-field study S15-01803. The black lines show the average of 10 simulations and the grey lines depict the range. The dots show the data from the four repeat tunnels in the study. The sex ratio of emerged female and male bees after overwintering (F1 generation) are shown in plots C and F. Plots in the **left column** (A, B, C) show the simulations with the best fit using the early emergence scenario; the plots in the **right column** (D, E, F) with the late emergence scenario.**

### Study S15-01804 (Celle) as calibration data set

For an additional cross-validation, we used S15-01804 for calibration, S15-01802 and S15-01803 for validation (see Section 7.1.3). Accordingly, we applied the calibration methodology using the data from study S15-01804, as well as study-specific model parameters (Table 32). For study S15-01804, the best fits to data are listed based on the early and late emergence scenario (Table 36). In Figure 39, the simulated number of nesting female bees and the cumulative brood cells produced over time are shown along with the emerged bees in the following year for the best fits to study S15-01804. The plots show the range of the simulations (from 10 repetitions) compared to the study data (from 4 repeat tunnels).

*Table 36. Parameter combinations resulting in the best fits (lowest average NRMSE) to data from study S15-01804 for the early and late emergence scenarios. The average NRMSE and NMAE were calculated from NRMSEs and NMAEs for nesting female numbers, cumulative brood cells, and offspring sex ratio after emergence. The average RSR is based only on the first two.*

Study	Temporal emergence scenario	var.emerge.f	t.maturity	p.max.nesting.life	max.f.ratio	max.cells	max.survival.e.f	a.sex.age	Average NRMSE	Average NMAE	Average RSR
S15-01804	(A) Early	1	10	0.062	0.419	1.087	0.958	-0.0519	0.224	0.155	1.473
S15-01804	(B) Late	3	9	0.089	0.505	1.121	0.852	-0.0564	0.198	0.144	0.788



**Figure 39. Best simulations of study S15-01804 based on the comparison between average simulation outputs (predictions) and average of the four tunnels in the study (observations). Comparison of observed and simulated number of nesting females per day (A, D) and cumulative brood cells produced (B, E) during the tunnel phase of the semi-field study S15-01804. The black lines show the average of 10 simulations and the grey lines depict the range. The dots show the data from the four repeat tunnels in the study. The sex ratio of emerged female and male bees after overwintering (F1 generation) are shown in plots C and F. Plots in the **left column** (A, B, C) show the simulations with the best fit using the early emergence scenario; the plots in the **right column** (D, E, F) with the late emergence scenario.**

### 7.1.3. Model validation with semi-field study data

#### Study S15-01803 (Tübingen) as calibration data set

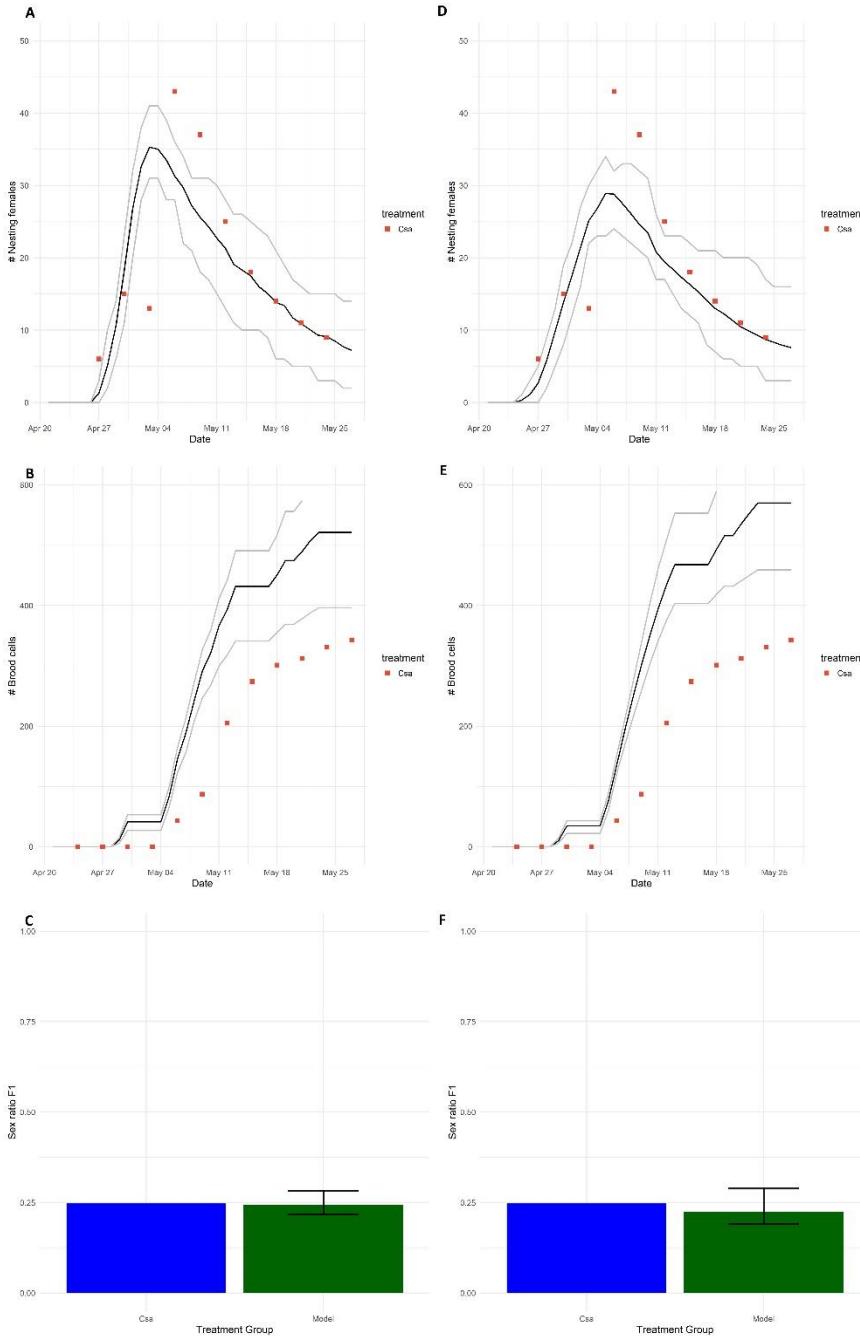
The parameter combinations identified to provide the best fit to the S15-01803 semi-field study data (Table 35) were applied in simulations of the other two studies (S15-01802 and S15-01804). The goodness-of-fit indicators were calculated from these simulations and the corresponding study data. Note that the average predictions from the simulations (across 10 repetitions) were compared with individual data points from the single tunnel used in S15-01802. The goodness-of-fit indicator values for the validation simulations are shown in Table 37.

Simulating study S15-01802 results in overestimation of brood cell production in all scenarios. The goodness-of-fit indicators suggest a better fit when using the early emergence scenario. Simulations using the early emergence scenario result in nesting female numbers in study S15-01802 captured well ( $\text{NRMSE} < 0.5$ ). In Figure 40, the validation simulations of study S15-01802 are shown along with the study data. The figure depicts the simulations of the temporal emergence scenarios using the corresponding best fits to study S15-01803 with the early emergence shown on the left and the late emergence shown on the right.

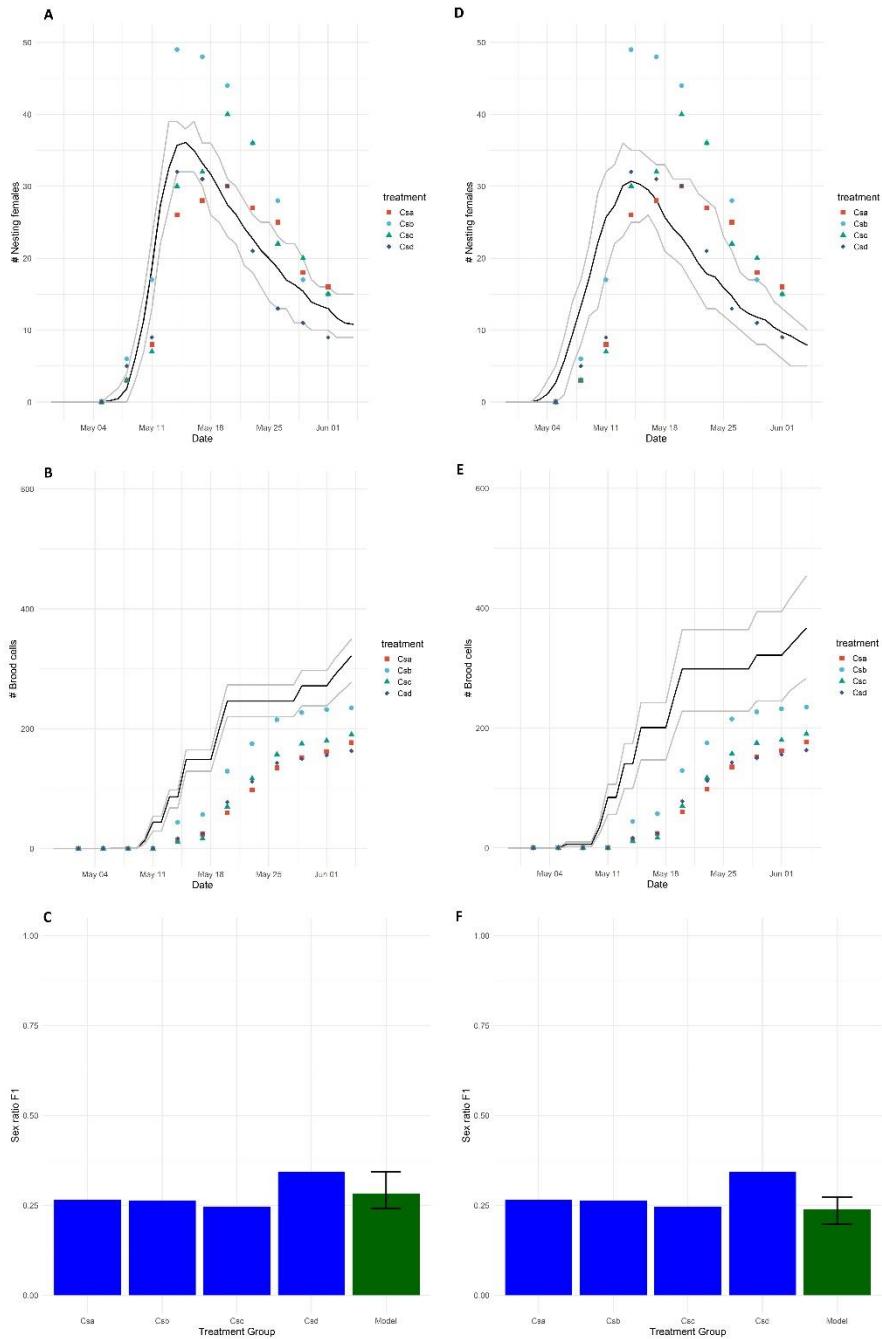
Validation simulations with study S15-01804 indicate that bee emergence and/or onset of nesting occurred later after release of the cocoons into the tunnels compared to the other two studies. The simulations using the late emergence scenario (B) with study S15-01804 using the best fits to study S15-01803 result in lower values of NRMSE compared to simulations with the early emergence scenario (A) (see Table 37). The simulation using the best fit to S15-01803 with early emergence (A) applied to the late emergence scenario (B) results in the best correspondence between simulated and observed data in study S15-01804 with an acceptable NRMSE ( $< 0.5$ ). The simulations of the late emergence scenario (B) of study S15-01804 using the best fits to study S15-01803 with both, early (A) and late (B) emergence scenarios, are shown in Figure 41. Validation simulations indicate an overestimation of brood cell production compared to observed brood cell production in study S15-01804.

**Table 37.** Goodness-of-fit indicator values for the simulations of study **S15-01802** and **S15-01804** using the parameter combinations that resulted in the best fit to study S15-01803. Validation simulations were conducted using the early and late emergence scenarios. The average NRMSE and NMAE were calculated from NRMSEs and NMAEs for nesting female numbers, cumulative brood cells, and offspring sex ratio after emergence. The average RSR is based only on the first two. Acceptable NRMSE < 0.5 are highlighted in green.

Study	Temporal emergence scenario	Best fit to	var.emerge.f	t.maturity	p.max.nesting.life	max.f.ratio	max.cells	max.survival.e.f	a.sex.age	Average NRMSE	Average NMAE	Average RSR
S15-01802	(A) Early	S15-01803(A)	2	6	0.094	0.428	1.664	0.846	-0.0477	0.462	0.360	0.934
S15-01802	(A) Early	S15-01803(B)	3	4	0.091	0.408	1.965	0.75	-0.0597	0.647	0.555	1.298
S15-01802	(B) Late	S15-01803(A)	2	6	0.094	0.428	1.664	0.846	-0.0477	0.505	0.416	1.271
S15-01802	(B) Late	S15-01803(B)	3	4	0.091	0.408	1.965	0.75	-0.0597	0.519	0.420	1.005
S15-01804	(A) Early	S15-01803(A)	2	6	0.094	0.428	1.664	0.846	-0.0477	0.767	0.640	4.214
S15-01804	(A) Early	S15-01803(B)	3	4	0.091	0.408	1.965	0.75	-0.0597	0.876	0.781	4.499
S15-01804	(B) Late	S15-01803(A)	2	6	0.094	0.428	1.664	0.846	-0.0477	0.464	0.377	2.891
S15-01804	(B) Late	S15-01803(B)	3	4	0.091	0.408	1.965	0.75	-0.0597	0.743	0.642	4.152



**Figure 40. Validation simulations of study S15-01802 using the best fits to study S15-01803.**  
 Comparison of observed and simulated number of nesting females per day (A, D) and cumulative brood cells produced (B, E) during the tunnel phase of the semi-field study S15-01802. The black lines show the average of 10 simulations and the grey lines depict the range. The dots show the data from the single tunnel in the study. The sex ratio of emerged female and male bees after overwintering (F1 generation) are shown in plots C and F. Plots in the **left column** (A, B, C) show the simulations with the early emergence scenario (A) and the parameters the were the best fit to the early emergence scenario with study S15-01803 (A); the plots in the **right column** (D, E, F) with the late emergence scenario (B) and the parameters the were the best fit to the late emergence scenario with study S15-01803 (B).



**Figure 41. Validation simulations of study S15-01804 using the best fits to study S15-01803.** Comparison of observed and simulated number of nesting females per day (A, D) and cumulative brood cells produced (B, E) during the tunnel phase of the semi-field study S15-01804. The black lines show the average of 10 simulations and the grey lines depict the range. The dots show the data from the four repeat tunnels in the study. The sex ratio of emerged female and male bees after overwintering (F1 generation) are shown in plots C and F. Plots in the **left column** (A, B, C) show the simulations with the late emergence scenario (B) and the parameters the were the best fit to the early emergence scenario with study S15-01803 (A); the plots in the **right column** (D, E, F) with the late emergence scenario (B) and the parameters the were the best fit to the late emergence scenario with study S15-01803 (B).

### Study S15-01804 (Celle) as calibration data set

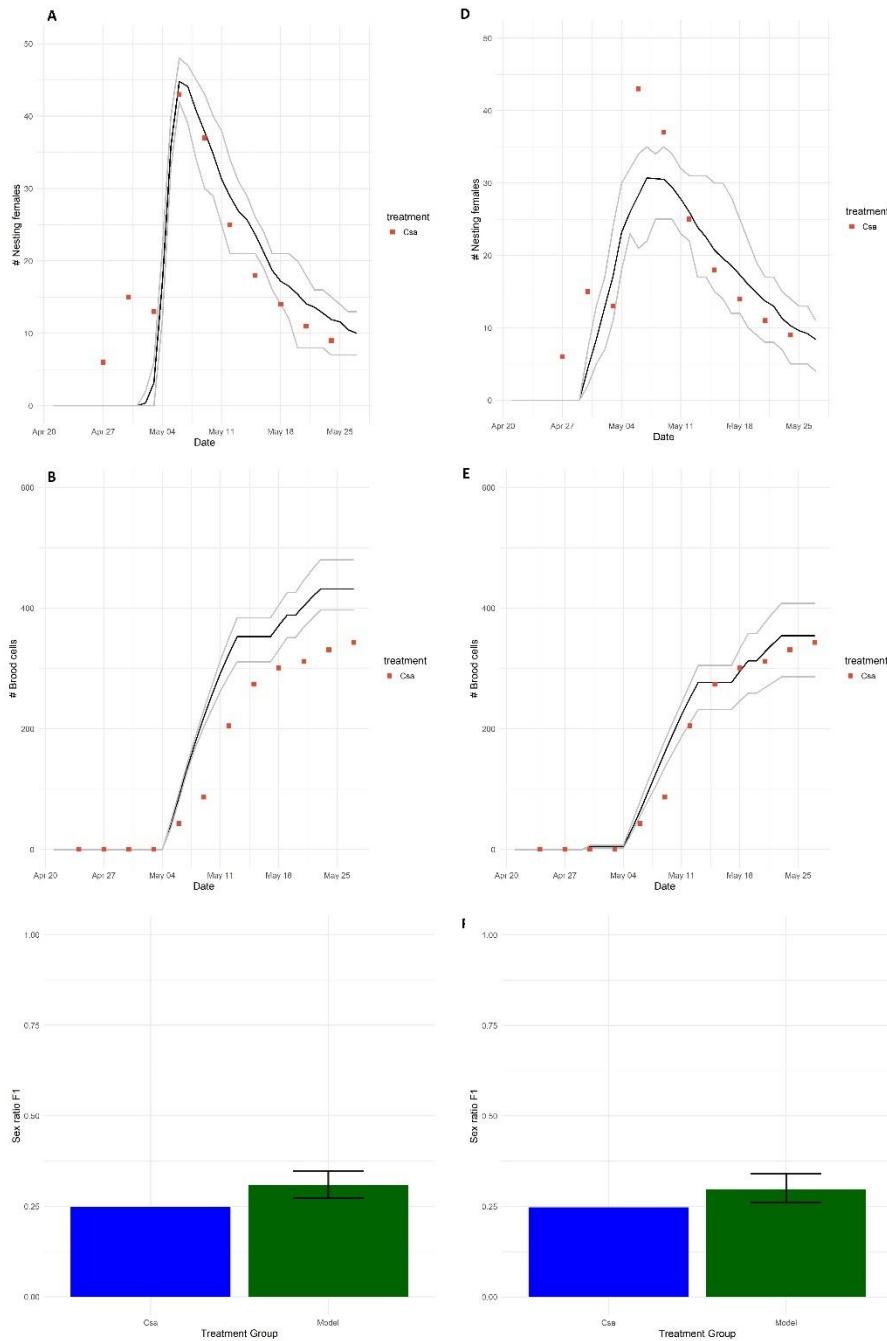
As a cross-validation exercise, the parameter combinations identified to provide the best fit to the S15-01804 semi-field study data (Table 36) were applied in simulations of the other two studies (S15-01802 and S15-01803). The goodness-of-fit indicators were calculated from these simulations and the corresponding study data. Note that the average predictions from the simulations (across 10 repetitions) were compared with individual data points from the single tunnel used in S15-01802. The goodness-of-fit indicator values for the validation simulations are listed in Table 38.

Simulating study S15-01802 with the best fits to S15-01804 results in good representations of the S15-01802 study data in all scenarios ( $\text{NRMSE} < 0.5$ ). The goodness-of-fit indicators suggest a better fit when using the early emergence scenario compared to the late emergence scenario. Because bee emergence and/or onset of nesting occurred later after release of the cocoons into the tunnels in study S15-01804 compared to the other two studies, validation simulations with the early emergence scenario (A) of S15-01802 using the best fit to the late emergence scenario (B) to S15-01804 resulted in the lowest goodness-of-fit indicators. In Figure 42, two sets of validation simulations of study S15-01802 are shown: using the best fit to S15-01804 with the early emergence scenario (A; left column) and the with the late emergence scenario (B; right column).

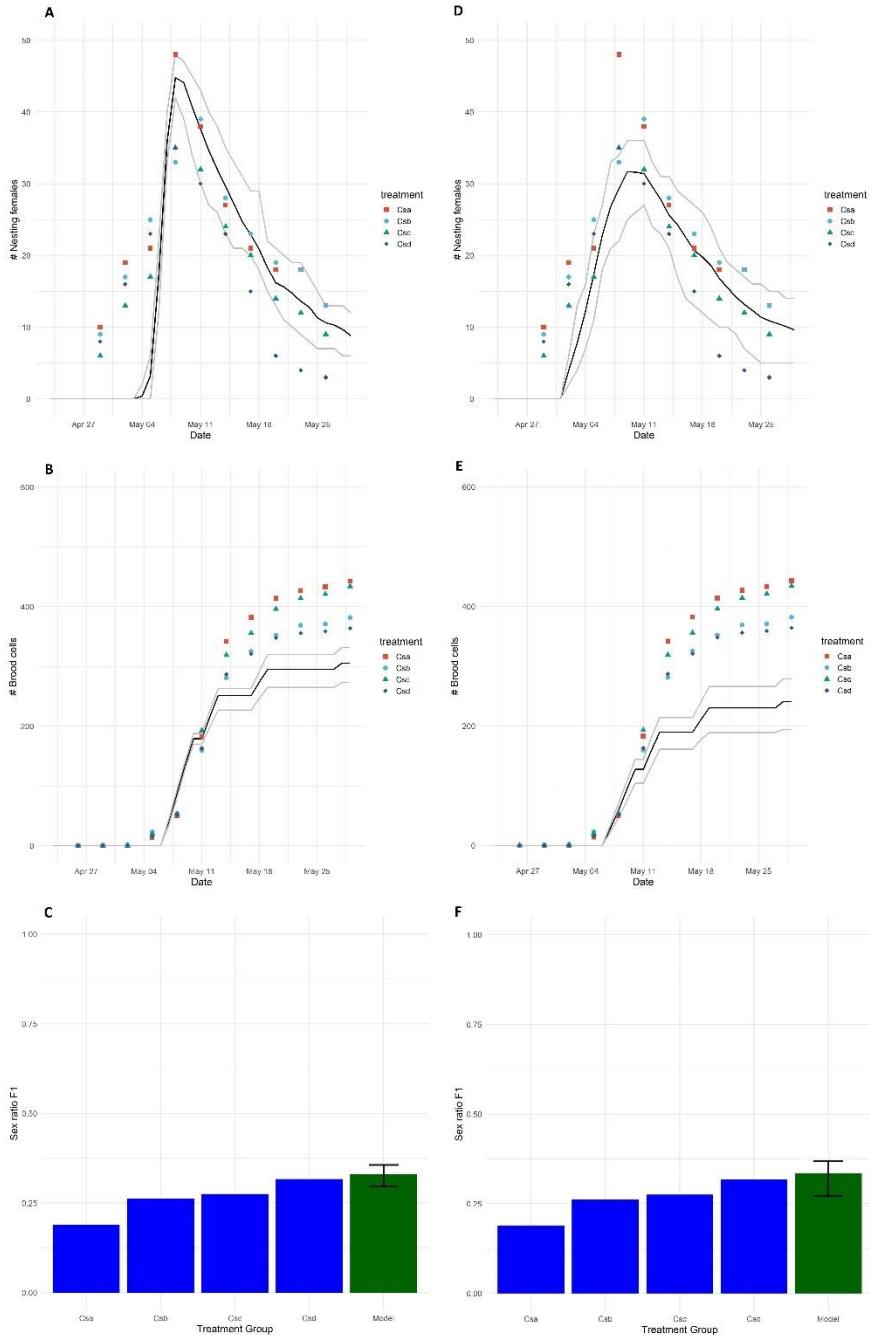
Corresponding to the simulations of study S15-01802, validation simulations with study S15-01803 also showed the best correspondence with data if the early emergence scenario (A) was used, resulting in  $\text{NRMSE} < 0.5$  (see Table 38). The parameter combinations provided in the best fit to study S15-01804 did not result in good correspondence to data if used to simulate S15-01803 in the late emergence scenario. Across validation simulations with S15-01803 (all temporal emergence scenarios), the brood cells production in the study was underestimated by the simulations. In Figure 43, the validation simulations with study S15-01803 are shown, whereby the early emergence scenario was used. In the figure, the left column depicts the simulations with the parameter combination that provided the best fit to S15-01804, early emergence scenario (A), and the right column with the parameter combination that provided the best fit to S15-01804, late emergence scenario (B).

*Table 38. Goodness-of-fit indicator values for the simulations of study S15-01802 and S15-01803 using the parameter combinations that resulted in the best fit to study S15-01804. Validation simulations were conducted using the early and late emergence scenarios. The average NRMSE and NMAE were calculated from NRMSEs and NMAEs for nesting female numbers, cumulative brood cells, and offspring sex ratio after emergence. The average RSR is based only on the first two.*

Study	Temporal emergence scenario	Best fit to	var.emerge.f	t.maturity	p.max.nesting.life	max.f.ratio	max.cells	max.survival.e.f	a.sex.age	Average NRMSE	Average NMAE	Average RSR
S15-01802	(A) Early	S15-01804(A)	1	10	0.062	0.419	1.087	0.958	-0.0519	0.359	0.300	0.962
S15-01802	(A) Early	S15-01804(B)	3	9	0.089	0.505	1.121	0.852	-0.0564	0.244	0.197	0.531
S15-01802	(B) Late	S15-01804(A)	1	10	0.062	0.419	1.087	0.958	-0.0519	0.429	0.360	1.444
S15-01802	(B) Late	S15-01804(B)	3	9	0.089	0.505	1.121	0.852	-0.0564	0.370	0.335	1.038
S15-01803	(A) Early	S15-01804(A)	1	10	0.062	0.419	1.087	0.958	-0.0519	0.348	0.284	1.654
S15-01803	(A) Early	S15-01804(B)	3	9	0.089	0.505	1.121	0.852	-0.0564	0.378	0.308	0.868
S15-01803	(B) Late	S15-01804(A)	1	10	0.062	0.419	1.087	0.958	-0.0519	0.566	0.484	3.518
S15-01803	(B) Late	S15-01804(B)	3	9	0.089	0.505	1.121	0.852	-0.0564	0.537	0.464	2.536



**Figure 42. Validation simulations of study S15-01802 using the best fits to study S15-01804.**  
 Comparison of observed and simulated number of nesting females per day (A, D) and cumulative brood cells produced (B, E) during the tunnel phase of the semi-field study S15-01802. The black lines show the average of 10 simulations and the grey lines depict the range. The dots show the data from the single tunnel in the study. The sex ratio of emerged female and male bees after overwintering (F1 generation) are shown in plots C and F. Plots in the left column (A, B, C) show the simulations with the early emergence scenario (A) and the parameters the were the best fit to the early emergence scenario with study S15-01804 (A); the plots in the right column (D, E, F) with the early emergence scenario (A) and the parameters the were the best fit to the late emergence scenario with study S15-01804 (B).



**Figure 43. Validation simulations of study S15-01803 using the best fits to study S15-01804.**  
 Comparison of observed and simulated number of nesting females per day (A, D) and cumulative brood cells produced (B, E) during the tunnel phase of the semi-field study S15-01803. The black lines show the average of 10 simulations and the grey lines depict the range. The dots show the data from the four repeat tunnels in the study. The sex ratio of emerged female and male bees after overwintering (F1 generation) are shown in plots C and F. Plots in the left column (A, B, C) show the simulations with the early emergence scenario (A) and the parameters the were the best fit to the early emergence scenario with study S15-01804 (A); the plots in the right column (D, E, F) with the early emergence scenario (A) and the parameters the were the best fit to the late emergence scenario with study S15-01804 (B).

## Conclusions

With the calibration and validation of the model to the available semi-field study data, we could demonstrate that the model can capture the dynamics observed in these studies. Two of the three study data sets were conducted with four repetitions each (the Niefern study S15-01802 was conducted with only a single repetition). Both studies, S15-01803 (Tübingen) and S15-01804 (Celle), were used separately to calibrate the model, using ranges of a subset of SolBeePop parameters. Because the data from the three studies indicated that emergence from the released cocoons or the onset of nesting by the released females started at different times (relative to the released date), two temporal emergence scenarios were used in the calibrations.

For validation, the parameter combinations providing the best fit to one study were then applied to the other studies. The parameter set providing the best fit to S15-01803 (assuming early emergence) resulted in acceptable fits to the other two data sets. For the validation simulations with S15-01802, the acceptable fit was observed in case early emergence was used in the simulations, for S15-01804, the late emergence scenario provided an acceptable fit. In the validation simulations of both studies, the brood cell production was overestimated. When conducting the cross-validation, using study S15-01804 for calibration, the best parameter fits to both scenarios resulted in acceptable fits when simulating study S15-01802 (both scenarios) and the early emergence scenario with study S15-01803. In the cross-validation, the validation simulations tended to underestimate the brood cell production.

In addition to the NRMSE, two more goodness-of-fit indicators were calculated. In the comparisons conducted for the calibration and validation of SolBeePop with semi-field data, NMAE indicated similar goodness-of-fit as the NRMSE. Because no recommendations for a threshold of acceptable fit based on NMAE have been proposed in the literature (Schmolke et al. 2020), NMAE was not used for the selection of the best fit or the determination of validation success. The RSR indicates parameter combinations as best fit that differ from the NRMSE. Because no RSR could be calculated for the offspring sex ratio and the studies had only four repetitions (or only one, in case of study S15-01802), the NRMSE was identified as more reliable indicator in our case.

The difference in validation success, dependent on which study was used for calibration and validation, indicates that the choice of study data influences validation outcomes. Existing differences between study results are not fully explained by the model. The studies were conducted in the same year in different locations in Germany. All cocoons released into the tunnels came from the same commercial supplier and were treated identically before transport to each study site. The three studies were initiated (cocoons released into the tunnels) within 9 days. Nevertheless, emergence timing and brood cell production differed considerably between studies. The cause for these differences in the studies was not identified, and they cannot be resolved by the model. The differences captured by SolBeePop were mainly driven by different weather conditions between the study locations. It was assumed that the foraging availability was identical between all oilseed rape fields where the study tunnels were installed. Potential differences between the locations were not reported in the study, but could have occurred. High variabilities between bees within a single population has been reported and may also influence the results.

The calibration and validation of the model shows that it can be applied to this study type and that it captures the dynamics of the bees' life cycle. However, the calibrations are specific to the specific study

and cannot be transferred to studies in which the cocoons may have been treated differently, bees are released at a considerably different time period or to a different crop. For an improved comparability between the simulations and data, the reporting of the timing of emergence of released cocoons in semi-field (or field) studies would be beneficial.

## 7.2. SolBeePop<sub>ecotox</sub>: Model corroboration with *O. bicornis* semi-field study data including exposures to dimethoate

### 7.2.1. Semi-field study data

Data from two semi-field studies conducted with *O. bicornis* were available for comparison to model outputs. The studies were conducted by Eurofins in 2019 and 2021. The semi-field studies were conducted by setting up mesh tunnels over portions of oilseed rape fields. Inside each tunnel, nest boxes were set up. All cocoons were obtained from the same commercial supplier and stored under the same conditions prior to release. The mesh tunnels prevented released bees from nesting or foraging beyond the tunnel and excluded other bees and predators from reaching the released bees.

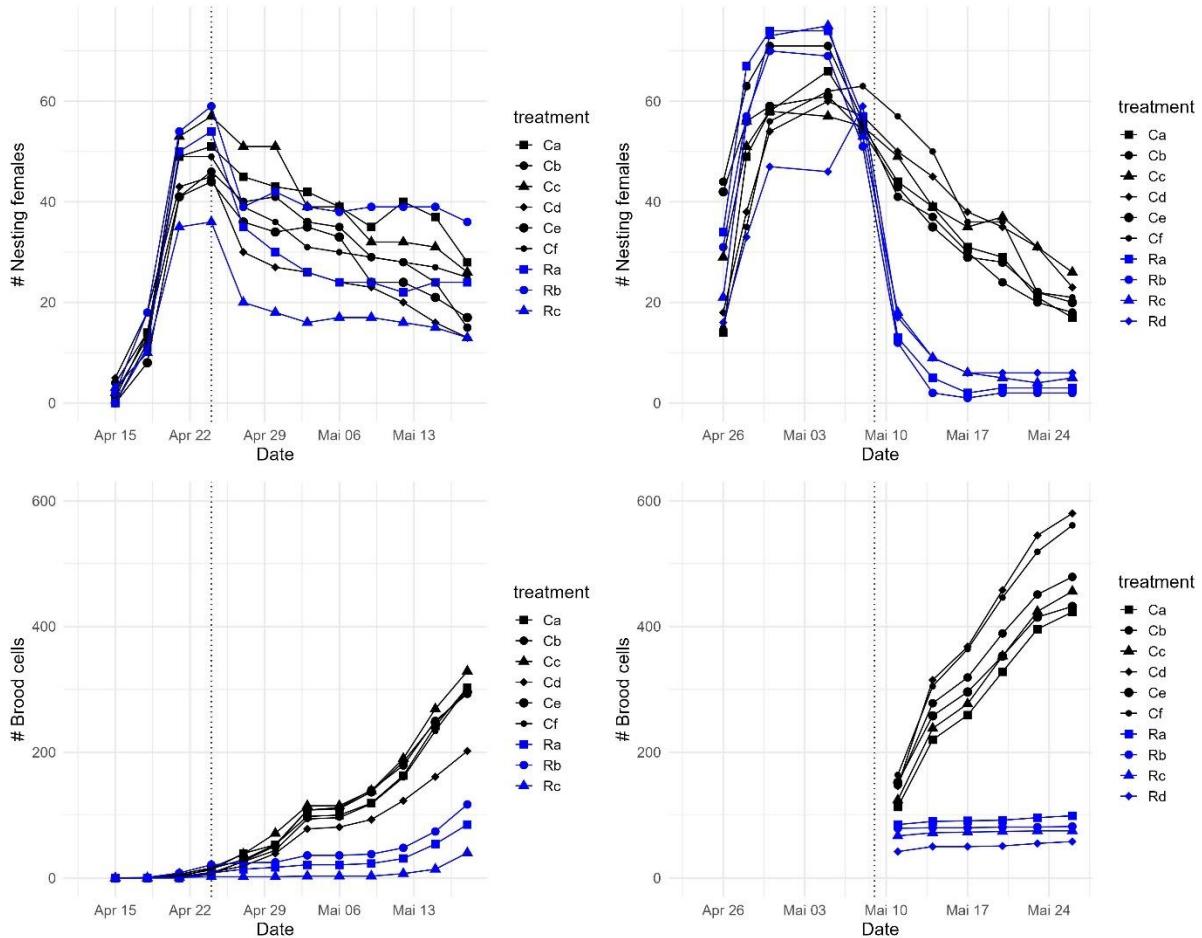
The study conducted in 2019 included 6 untreated control tunnels and 3 tunnels with dimethoate treatment (75 g/ha). Cocoons of *O. bicornis* (60 females and 90 males in each tunnel) were placed in the nesting units at the onset of crop flowering (12 April 2019). Dimethoate treatments occurred on 24 April 2019. The flowering oilseed rape was treated with the insecticide by a spray application during the day when bees can be assumed to be active. Bare soil/mud is used by *O. bicornis* for the construction of partitions between brood cells. Sources of soil/mud within the study tunnels were assumed to be exposed during the dimethoate spray. Nest boxes were closed at the end of the oilseed rape flowering (18 May 2019), ending the tunnel phase of the study. Number of nesting females in the nest boxes as well as completed brood cells were counted starting 15 April 2019 in 3-day intervals until the end of tunnel phase. Cocoon cohorts were marked by their completion date (3-day intervals), live cocoons were taken to the laboratory for overwintering, and brought to emergence the following spring. Emergence rate and sex were reported by cohort.

The study conducted in 2021 included 6 untreated control tunnels and 4 tunnels with dimethoate treatment (75 g a.i./ha). Cocoons of *O. bicornis* (90 females and 110 males in each tunnel) were placed in the nesting units at the onset of crop flowering (23 April 2021). Dimethoate treatments occurred on 9 May 2021. The flowering oilseed rape was treated with the insecticide by a spray application during the day when bees can be assumed to be active. Sources of soil/mud within the study tunnels were assumed to be exposed during the dimethoate spray. Nest boxes were closed at the end of the oilseed rape flowering (26 May 2021), ending the tunnel phase of the study. Number of nesting females in the nest boxes were counted starting on 26 April 2021, and in 3-day intervals until the end of tunnel phase. Counts of completed brood cells started on 11 May 2021. Cocoon cohorts were marked by their completion date (cocoons completed until the first sampling date; thereafter in 3-day intervals), live cocoons were taken to the laboratory for overwintering, and brought to emergence the following spring. Emergence rate and sex were reported by cohort.

Specifications of the 2019 and 2021 semi-field studies by Eurofins are listed in Table 39. Figure 44 shows the number of females observed in the nest boxes as well as the cumulative number of brood cells over the tunnel phase of the studies.

*Table 39. Specifications of semi-field studies conducted with *O. bicornis* by Eurofins in 2019 and 2021. Tunnels were set up over portions flowering oilseed rape fields. Treatments consisted of a spray application of dimethoate (75 g a.i./ha) during daylight (when bees are potentially active).*

Study ID	Location	Date of cocoon introduction	End of tunnel phase	Treatment date	No. control tunnels	No. treatment tunnels	Female cocoons introduced	Male cocoons introduced
Eurofins 2019 study	Niefern (near Pforzheim), Germany	12 April 2019	18 May 2019	24 April 2019	6	3	60	90
Eurofins 2021 study	Niefern (near Pforzheim), Germany	23 April 2021	26 May 2021	9 May 2021	6	4	90	110



*Figure 44. Data from the semi-field studies reported for the tunnel phase. Left: Eurofins 2019 study. Right: Eurofins 2021 study. Top: number of post-emergent females observed in the nest blocks. Bottom: cumulative number of brood cells in the nest blocks. Untreated controls are shown in black (treatment Ca – Cf) and data from treated tunnels (with 75 g a.i./ha dimethoate) are shown in blue (treatment Ra – Rc or Rd). The dotted vertical line indicates the date of the dimethoate application.*

## 7.2.2. Model calibration to control data

Using the data available from 2019 and 2021 semi-field studies, we conducted a calibration to the untreated controls to account for potential differences among the studies, particularly with respect to phenology and survival rates of the bees introduced as cocoons. Simulations including dimethoate exposures and effects according to the study treatment tunnels was conducted in a second step whereby no further calibrations were conducted (Section 7.2.5). The calibration and validation to controls only has the following benefits: a) increased confidence in the ability of the model capture bee population dynamics in the absence of stressors, b) separation of exposure and effect parameters informs usefulness of the toxicity submodel (BeeGUTS) which has been parameterized for the honey bee, c) correspondence with the previously conducted calibration and validation with SolBeePop using control data sets from different semi-field studies (Schmolke et al. 2023b).

The calibration to controls was conducted following the same approach as presented in Section 7.1. However, based on the experience with the previous calibration of SolBeePop to control semi-field study data, we added two parameters to the calibration. Instead of testing different scenarios of emergence timing of the cocoons introduced into the tunnels (early / late emergence scenarios), we included the corresponding parameter, *day.emerge.f*, in the calibration with a relevant range. The parameter *emerged.survival* was also added with a range in the calibration because the study data indicated high emergence rates from the introduced cocoons. The parameters and their ranges in the calibration are listed in Table 40.

*Table 40. SolBeePop<sub>ecotox</sub> parameters varied for the calibration of the model to Eurofins semi-field study data. The parameters included and their ranges are compared to the previous model calibration (see Section 7.1).*

Parameters calibrated	Value range applied in calibration to Ruddle et al. data, see Section 7.1.2	Value range applied in calibration to Eurofins data	Changes for calibration to Eurofins data
<i>day.emerge.f</i>	Not included	2-6 days after Start.day	Added: replaces early/late scenario
<i>var.emerge.f</i>	1 - 7	1 - 3	Reduced value range
<i>t.maturity</i>	1 - 10	5 - 10	Reduced value range
<i>p.max.nesting.life</i>	0.01 - 0.1	0.01 - 0.1	--
<i>max.f.ratio</i>	0.38 - 1	0.38 - 1	--
<i>max.cells</i>	1 – 3	1 – 2	Reduced value range
<i>max.survival.e.f</i>	0.58 – 1	0.75 – 1	Reduced value range
<i>emerged.survival</i>	Not included	0.75 – 1	Added
<i>a.sex.age</i>	-0.0286 - -0.0599	-0.04 - -0.07	Changed value range

The input files for the simulations of the 2019 and 2021 Eurofins studies were generated using similar assumptions as for the simulation of the semi-field studies by Ruddle et al. (2018) (Section 7.1.2). The assumptions and data used are listed in Table 41.

*Table 41. Assumptions and data used for the generation of site-specific floral resource input files for the simulation of the semi-field studies. For the generation of the input file using these assumptions, see Appendix B.*

Specification	Description	Value	Remarks
wind.data	Availability of data on wind speed included in weather data	--	If unavailable: daily foraging not dependent on wind
use.sunshine	Availability (or use) of sunshine hours per data in weather data	--	If unavailable: daily foraging not dependent on sunshine hours per day
min.temp	Minimum temperature (°C) for <i>O. bicornis</i> foraging	10	Foraging assumed to occur if the maximum daily temperature exceeds this threshold
max.wind	Maximum wind speed at which foraging occurs	--	Not applied for semi-field simulations because wind speed was not available from the weather data
max.precip	Maximum daily precipitation (mm) at which foraging occurs	25.4	In the semi-field studies, no daily precipitation above this threshold was reported
max.humid	Maximum relative humidity (%) at which foraging occurs	60	
max.forag.hrs	Maximum number of hours of foraging by a bee	--	Only needs to be specified if sunshine hours are available
crop.start	Start date (Julian day) of crop flowering	Study-specific	Corresponds to the start of the tunnel phase (date of cocoon release) in the studies (see Section 7.2.1)
crop.end	End date (Julian day) of crop flowering	Study-specific	Corresponds to the end of the tunnel phase in the studies (see Section 7.2.1)
crop.peak	Date (Julian) of peak crop flowering; if no temporal dynamic of flowering is assumed, set to 0	0	Assumes excess availability of pollen and nectar from oilseed rape throughout the tunnel phase
crop.Q	Relative quality of forage on crop; 1 = maximum quality (low foraging effort and distance); 0 = no forage available from crop within flight range of the bee	1	Assumption that the forage quality from crop is optimal throughout the tunnel phase (oilseed rape corresponding to <i>O. bicornis</i> foraging preferences, ease of pollen collection and very low foraging distance between nest and resource)
min.crop.Q	Minimum relative quality of forage on crop (during crop flowering)	--	Not applicable to semi-field simulations because crop.Q was set to 1 throughout the tunnel phase
nat.Q	Relative quality of forage on non-crop resources	0	Assumption that no pollen or nectar resources were available in the tunnels apart from oilseed rape
prop.crop	Proportion of foraging on crop (proportion of foraging on non-crop resources is assumed to be 1 – prop.crop)	1	Assumption that bees forage exclusively on oilseed rape within the tunnels

In Table 42, the study-specific inputs are listed that were used for the calibration and validation simulations of the 2019 and 2021 Eurofins semi-field studies.

*Table 42. Model parameters and inputs used in model calibration and validation to the control semi-field study data of the Eurofins semi-field studies reflecting study-specific conditions.*

Study-specific model parameter / input	Eurofins 2019 Study	Eurofins 2021 Study	Remarks
<i>Start.day</i>	102	113	Day of year of cocoon release into the tunnels; compare to Table 39
<i>input.floral</i>	Floral_Eurofins2019_26Apr2023_control.csv	Floral_Eurofins2021_27Apr2023_control.csv	For the assumption applied to generate the study-specific input, see text and Table 41
<i>day.emerge.f</i>	107 (104-108)	118 (115 – 119)	Default: set to five days after cocoon placement in the tunnels, range used for calibration (see also Table 40)
<i>day.emerge.m</i>	107	118	Assumption that females and males emerge on the same day due to incubation of cocoons in the laboratory, male emergence not impactful to other model variables
<i>latest.emerge</i>	138	146	Day of year of last day in tunnels; see Table 39

For each study, 2400 parameter combinations were simulated, each with 10 repetitions using 10 different random number seeds. The number of parameter combinations, or samples from the latin hypercube, were increased compared to the previous calibration (Section 7.1.2) because more parameters (9 instead of 7) were included in the calibration.

The goodness-of-fit of the outputs from the simulations was calculated using the indicators listed in Table 34 (Section 7.1.2). Note that nesting females in the study (females present in the nest boxes at night) were compared to the total number of post-emergent females, i.e., females in the life stages ‘emerged’ and ‘nesting’ in the model.

## ***Calibration results***

The parameter combinations resulting in the best fit with the control study data were identified. The best fit to data were very similar based on NRMSE and NMAE. However, the goodness of fit based on RSR indicated a different parameter combination as the best fit to the data. Because with the RSR, it was not possible to consider the sex ratio of the offspring, we based the selection of the best fit on the NRMSE only.

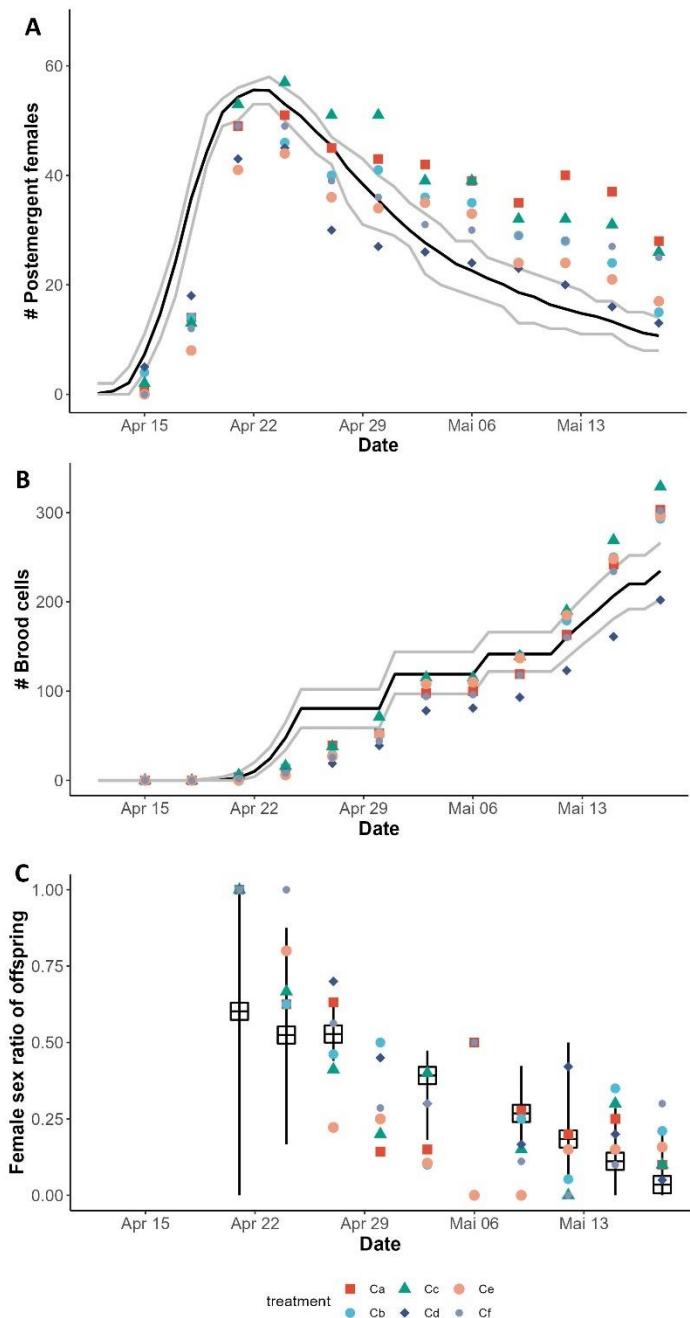
### **Eurofins 2019 study as calibration data set**

For the Eurofins 2019 study, the parameter combination resulting in the best fit to control data is listed in Table 43. In Figure 45, the simulated number of post-emergent female bees and the cumulative brood cells produced over time are shown along with the sex ratio of the emerged bees in the following year for the best fits to the controls in the Eurofins 2019 study. The plots show the range of the simulations (from 10 repetitions) compared to the control study data (from 6 repeat tunnels).

*Table 43. Parameter combinations resulting in the best fits (lowest average NRMSE) to the control data of the Eurofins 2019 study. The average NRMSE and NMAE were calculated from NRMSEs and NMAEs for post-emergent female numbers, cumulative brood cells, and offspring sex ratio after emergence. The average RSR is based only on the first two.*

Study	day.emerge.f	var.emerge.f	t.maturity	p.max.nesting.life	max.f.ratio	max.cells	max.survival.e.f	emerged.survival	a.sex.age	Average NRMSE	Average NMAE	Average RSE
2019	108*	2	7	0.0818	0.553	1.223	0.946	0.996	-0.0424	0.490	0.395	1.312

\* 6 days after introduction of cocoons into tunnels



*Figure 45. Best simulations of the control data of the Eurofins 2019 study based on the comparison between average simulation outputs (predictions) and average of the four tunnels in the study (observations).* **A:** Comparison of observed and simulated number of post-emergent females per day, and **B:** cumulative brood cells produced during the tunnel phase of the semi-field study. The black lines show the average of 10 simulations and the grey lines depict the range. The dots show the data from the four repeat tunnels in the study. **C:** The female sex ratio of offspring (F1 generation). Offspring was reported in 3-day intervals in the study. Average and range of simulated female sex ratios are shown in black; two of the 3-day resulted in no offspring (brood cell) production in the simulation.

## Eurofins 2021 study as calibration data set

For the Eurofins 2021 semi-field study, the parameter combination resulting in the best fit to control data is listed in Table 44. In Figure 46, the simulated number of post-emergent female bees and the cumulative brood cells produced over time are shown along with the sex ratio of the emerged bees in the following year for the best fits to the controls in the Eurofins 2021 study. The plots show the range of the simulations (from 10 repetitions) compared to the control study data (from 6 repeat tunnels).

*Table 44. Parameter combinations resulting in the best fits (lowest average NRMSE) to the control data of the Eurofins 2021 study. The average NRMSE and NMAE were calculated from NRMSEs and NMAEs for post-emergent female numbers, cumulative brood cells, and offspring sex ratio after emergence. The average RSE is based only on the first two.*

Study	day.emerge.f	var.emerge.f	t.maturity	p.max.nesting.life	max.f.ratio	max.cells	max.survival.e.f	emerged.survival	a.sex.age	Average NRMSE	Average NMAE	Average RSE
2021	119*	3	9	0.0836	0.548	1.121	0.812	0.819	-0.0424	0.186	0.157	5.870

\* 6 days after introduction of cocoons into tunnels

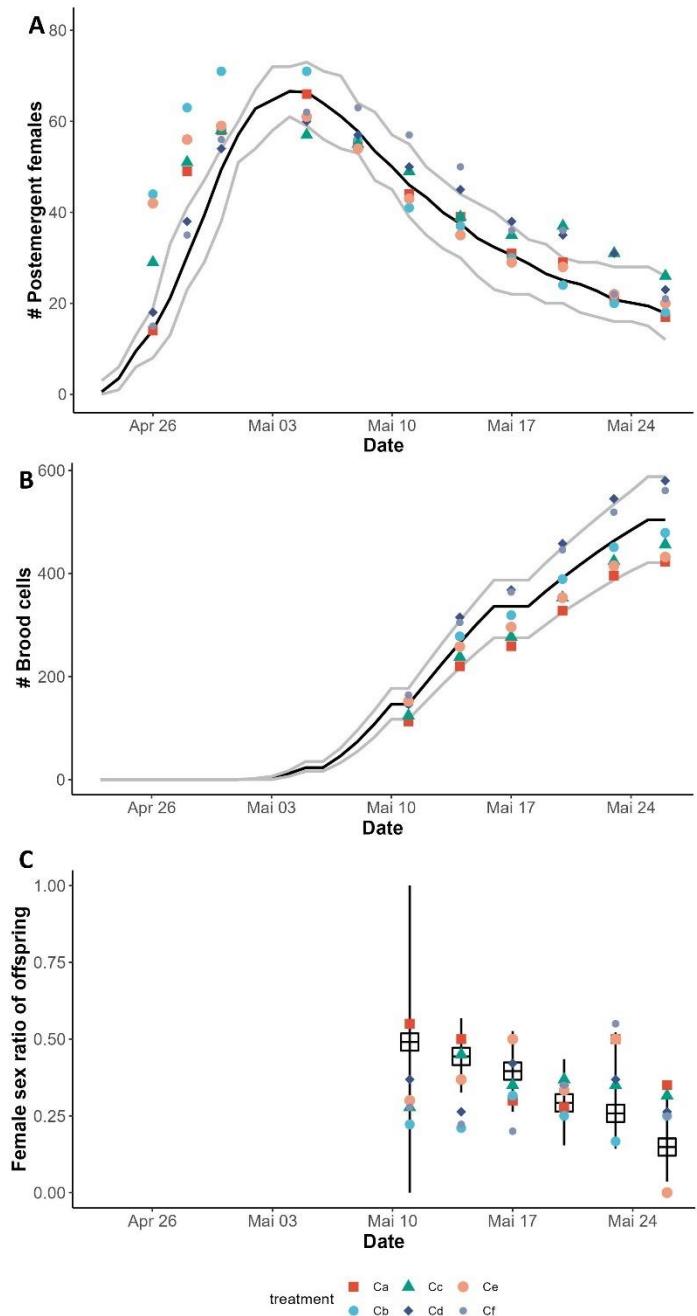


Figure 46. Best simulations of the control data of the Eurofins 2021 study based on the comparison between average simulation outputs (predictions) and average of the four tunnels in the study (observations). **A:** Comparison of observed and simulated number of post-emergent females per day, and **B:** cumulative brood cells produced during the tunnel phase of the semi-field study. The black lines show the average of 10 simulations and the grey lines depict the range. The dots show the data from the four repeat tunnels in the study. **C:** The female sex ratio of offspring (F1 generation). Offspring was reported in 3-day intervals in the study. Average and range of simulated female sex ratios are shown in black.

### 7.2.3. Model validation with control data

The parameter combinations identified to provide the best fit to control data of the Eurofins 2019 study were applied in the simulation of the Eurofins 2021 study. The goodness-of-fit indicators were calculated from these simulations and the corresponding study data. The goodness-of-fit indicator values for the validation simulations are shown in Table 45.

Simulating the Eurofins 2019 study using the best fit to the 2021 study resulted in an underestimation of brood cell production (Figure 47B). The number of post-emergent females in the simulation were also slightly underestimated in the simulation (Figure 47A). The female sex ratio of the offspring (F1 generation) declined in the study with progressing tunnel phase. This trend was captured in the simulations (Figure 47C).

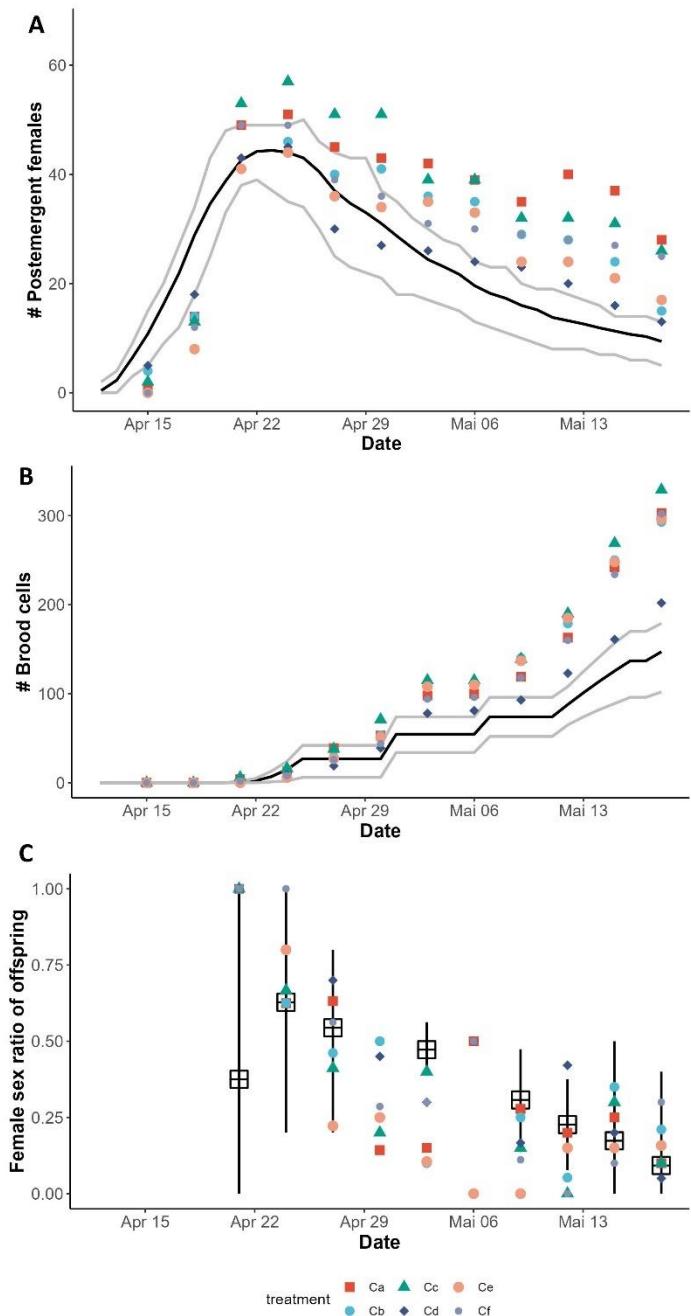
Simulating the Eurofins 2021 study using the best fit to the 2019 study results in the opposite pattern: number of post-emergent females were overestimated by the simulations (Figure 48A). A more pronounced overestimation was seen in the brood cell production (Figure 48B). The offspring sex ratio followed as similar pattern as in the 2019 study and its simulations (Figure 48C).

Due to the discrepancies in validation simulations to the respective study data, the goodness-of-fit was not within the acceptable range defined for other models: in the EFSA opinion addressing TKTD models, NRMSE < 0.5 were suggested to be considered ‘acceptable’ (EFSA Panel on Plant Protection Products and their Residues (PPR) et al. 2018). Average NRMSE of the validation simulations of the Eurofins studies were > 0.5. However, the data from the two studies showed very different dynamics (see Figure 44). Aspects of the study conditions that are not fully described or captured by the model may have differed between the two studies, e.g., incubation of the cocoons introduced into the tunnels, resulting in potentially different emergence times and nesting rates, as well as temporally variable resource availability from the oilseed rape in the tunnels. In addition, assumptions about weather-related foraging in *O. bicornis* are based on limited data, resulting in uncertainties about the foraging activity (and resulting brood cell production). This uncertainty is particularly impactful for study periods with a tendency for inclement weather because it can be assumed that warm and dry weather conditions always allow foraging. The 2019 study had extended stretches of weather with high humidity and precipitation while during the 2021 study, good weather was reported.

*Table 45. Goodness-of-fit indicator values for the simulations of the control data of Eurofins 2019 and 2021 studies using the parameter combinations that resulted in the best fit to the other study, respectively. The average NRMSE and NMAE were calculated from NRMSEs and NMAEs for post-emergent female numbers, cumulative brood cells, and offspring sex ratio after emergence. The average RSR was based only on the first two.*

Study simulated	Parameter combination with best fit to study										Average NRMSE	Average NMAE	Average RSE
2019	2021	108*	3	9	0.0836	0.548	1.121	0.812	0.819	-0.0424	0.575	0.418	1.413
2021	2019	119*	2	7	0.0818	0.553	1.223	0.946	0.996	-0.0424	0.516	0.476	7.698

\* 6 days after introduction of cocoons into tunnels



*Figure 47. Validation simulations of the control data of the Eurofins 2019 study using the best fit to Eurofins 2021 study. A: Comparison of observed and simulated number of post-emergent females per day, and B: cumulative brood cells produced during the tunnel phase of the semi-field study. The black lines show the average of 10 simulations and the grey lines depict the range. The dots show the data from the four repeat tunnels in the study. C: The female sex ratio of offspring (F1 generation). Offspring was reported in 3-day intervals in the study. Average and range of simulated female sex ratios are shown in black; two of the 3-day resulted in no offspring (brood cell) production in the simulation.*

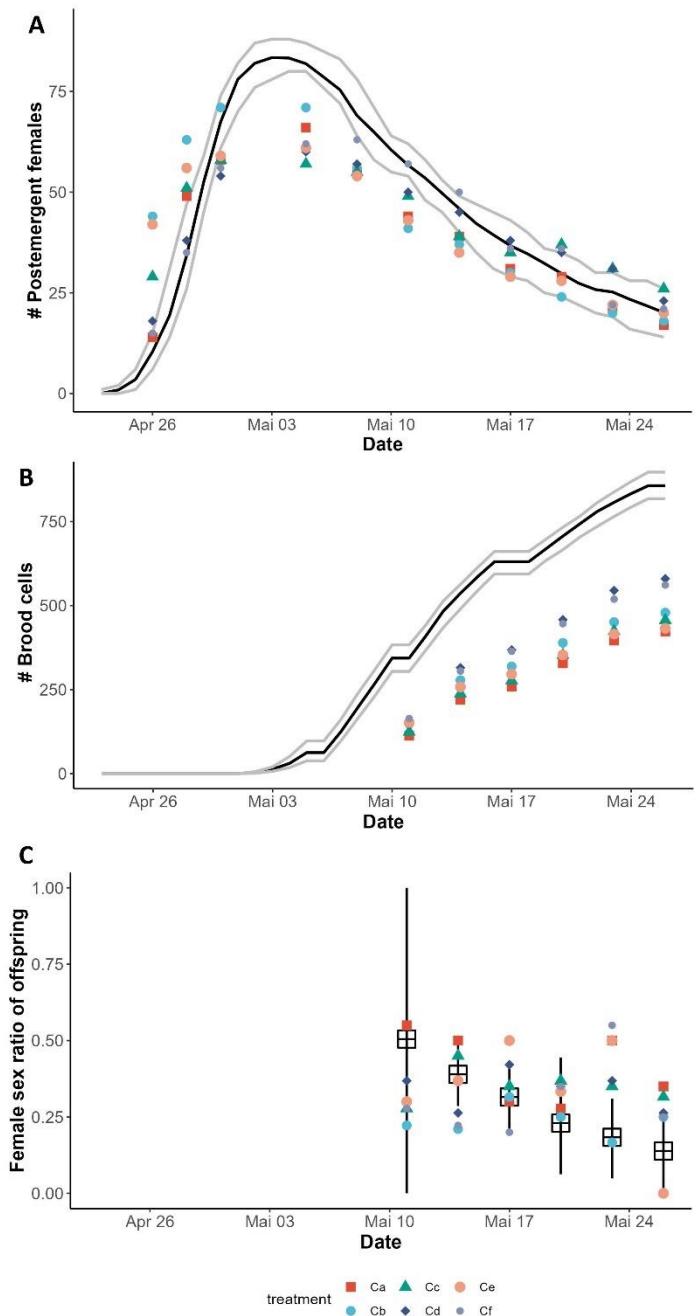


Figure 48. Validation simulations of the control data of the Eurofins 2021 study using the best fit to Eurofins 2019 study. **A:** Comparison of observed and simulated number of post-emergent females per day, and **B:** cumulative brood cells produced during the tunnel phase of the semi-field study. The black lines show the average of 10 simulations and the grey lines depict the range. The dots show the data from the four repeat tunnels in the study. **C:** The female sex ratio of offspring (F1 generation). Offspring was reported in 3-day intervals in the study. Average and range of simulated female sex ratios are shown in black.

## 7.2.4. Dimethoate exposure scenario

In the SolBeePop<sub>ecotox</sub> input, five possible routes of exposures to a pesticide are distinguished: residues in nectar, residues in pollen, exposure from direct spray, residues in soil and residues on leaves used to line brood cells. The latter is only applicable to leafcutter bees, including *M. rotundata*, and does not apply to simulations of *O. bicornis*. The exposure from the other matrices needed to be estimated based on the treatment applied in the semi-field studies (see Section 7.2.1).

### *Residues in nectar and pollen*

Residues in oilseed rape nectar and pollen were not assessed in the Eurofins 2019 and 2021 semi-field studies. The residue per unit dose (RUD) was used to estimate initial residue levels in nectar and pollen occurring shortly after the application (corresponding to the day of application in the model). The residue unit dose (RUD) is an estimate of the residue concentration of a pesticide in pollen and in nectar, standardized to an application rate of 1 kg/ha. In the EFSA bee guidance ([European Food Safety Authority \(EFSA\) et al. \(2023\)](#), Table 19), shortcut RUD values are provided for downward spray pesticide applications. RUDs in pollen were reported significantly higher than RUDs in nectar (Kyriakopoulou et al. 2017; European Food Safety Authority 2023). The initial residue concentrations ( $c_0$ ) in nectar and pollen for the exposure scenarios in the model are listed in Table 46.

*Table 46. RUDs in nectar and pollen used for the residue scenarios in the simulations of the Eurofins semi-field studies. RUD gives the residue concentration in mg/kg matrix, standardized to an application rate of 1 kg/ha. The listed RUDs are applicable to the initial residue concentration on the day of a spray application. Applying the RUDs, the calculated initial concentrations ( $c_0$  in nectar and pollen) are listed for the application rate of dimethoate (75 g a.i./ha).*

Scenario	RUD in nectar	RUD in pollen	Reference	$c_0$ in nectar (µg a.i./g)	$c_0$ in pollen (µg a.i./g)
Median	0.87	67.7	<a href="#">European Food Safety Authority (EFSA) et al. (2023)</a> , Table 19	0.065	5.078

Residue concentrations in nectar and pollen decline over time due to dissipation of the compound. The kinetics of the decline are dependent on the pesticide. In ([European Food Safety Authority 2023](#)) (Annex H), kinetics of dimethoate are provided, fit to available data for nectar. The SFO (single first-order kinetics) fit provided in the EFSA guidance was used to estimate the residue levels over time,  $c_t$  (µg a.i./g), in oilseed rape nectar and pollen in the Eurofins semi-field studies (Equation 7.1).

*Equation 7.1*

$$c_t = c_0 \exp(-k t)$$

The constant  $k$  was determined with a value of  $k = 0.5145 \text{ d}^{-1}$  ([European Food Safety Authority \(EFSA\) et al. \(2023\)](#), Annex H). Because no separate residue data relevant for the estimation of residue kinetics in

pollen were available for dimethoate, we applied the residue kinetics to both, nectar and pollen using the initial residue concentrations,  $c_0$ , listed in Table 46.

### ***Exposure from direct spray***

Exposure from direct spray defines the external exposure a bee receives while present in the field during the spray application. It is assumed that a bee is exposed by a single droplet on the body. The acute contact exposure from direct spray is estimated using Equation 7.2 (from [European Food Safety Authority \(EFSA\) et al. \(2023\)](#), Section 5.1.1.).

*Equation 7.2*

$$PEQ_{co} = AR \cdot EF_{co} \cdot BSF$$

Where

$PEQ_{co}$ : Predicted Exposure Quantity ( $\mu\text{g}/\text{bee}$ )

$AR$ : application rate (g a.i./ha)

$EF_{co}$ : exposure factor for contact exposure (unitless)

$BSF$ : body surface factor ( $\text{dm}^2/\text{bee}$ )

For the exposure from direct spray in the Eurofins semi-field studies,  $AR = 75 \text{ g a.i./ha}$ . The application of dimethoate was conducted via spray during crop flowering. For this case, it is assumed that the bee is not shielded from exposure, i.e.,  $EF_{co} = 1$  ([European Food Safety Authority \(EFSA\) et al. \(2023\)](#), Appendix B). The body surface factor is estimated according to bee size. [European Food Safety Authority \(EFSA\) et al. \(2023\)](#), Table 13 provides BSF for honey bees, bumble bees and solitary bees. We think that given the average size of female *O. bicornis* bees corresponding closely to honey bee workers,  $BSF = 0.0114 \text{ dm}^2/\text{bee}$  estimated for a honey bee worker is most appropriate (rather than the much smaller body surface estimated for a generic solitary bee).

The exposure from direct spray only occurs on the application day in the simulations of the Eurofins semi-field studies. The calculated is  $PEQ_{co} = 75 \text{ g/ha} \times 1 \times 0.0114 \text{ dm}^2/\text{bee} = 0.855 \mu\text{g}/\text{bee} = 855 \text{ ng}/\text{bee}$  (with the latter showing the value in the units of the model input).

### ***Exposure from residues in soil***

Exposures from soil were defined for the simulations of the Eurofins semi-field studies with *O. bicornis* to capture potential transfer of residues in the soil/mud the bees use to cap each brood cell. Exposures due to contact with soil can occur in nesting females as well as developing bees. For the simulations, we assumed that the bees collect soil within the treated field (underneath the oilseed rape plants). The residues in the top layer of the soil are relevant for the species.

The PEARL model (Pesticide Emission Assessment at Regional and Local scales) was used to calculate exposure concentrations in the soil (van den Berg et al. 2016; Tiktak et al.). For each study, a PEARL scenario was created based on the FOCUS scenarios and adapted to the local conditions, including soil composition, weather and timing of application was used (Table 47). Compound information was taken from EFSA peer review with DT50 (20°C, 100%FC) 2.8 days, Koc of 28 L/kg, and 1/n of 1.02 (European Food Safety Authority et al. 2018).

For study 1 and 2, the environmental information from the Eurofins study site were used to construct a PEARL scenario, as location, time, and soil type were measured. The subsoil organic carbon was based on FOCUS Hamburg and soil texture class was characterized as Silt (Rosetta). The modeled crop was winter oilseed rape (BBCH 65) sprayed once with 75 g a.i./ha dimethoate with an interception of 80%. In Table 47, the conditions for the estimation of the soil exposure are summarized.

*Table 47. Definitions of study and environmental conditions for the estimation of exposures from soil over time for the simulations of the Eurofins semi-field studies from 2019 and 2021 with O. bicornis.*

Exposure scenario characteristic	STUDY 1 (2019)	STUDY 2 (2021)																																				
Application date	24 April 2019 DOY: 114 BBCH: 65	9 May 2021 DOY: 129 BBCH 65																																				
Application rate	1 x 75 g/ha spray	1 x 75 g/ha spray																																				
Crop (in-field)	Winter oilseed rape	Winter oilseed rape																																				
Off-field	n.a.	n.a.																																				
Drift rate	n.a.	n.a.																																				
Weather scenario	Location: Katharinentaler Hof near Pforzheim (near Neulingen) ZIP code: 75177 Region: Baden-Württemberg Country: Germany GPS coordinates: N: 48.926242°; E: 8.713765° Alternative: MARS Daten	Location: Katharinentaler Hof near Pforzheim (near Neulingen) ZIP code: 75177 Region: Baden-Württemberg Country: Germany GPS coordinates: N: 48.932076°; E: 8.708179° Alternative: MARS Daten																																				
Soil type	Soil type for both studies (from a location between the two sites):  <table border="1"> <thead> <tr> <th colspan="2">Soil parameters</th> </tr> </thead> <tbody> <tr> <td>Sand [%]</td> <td>7.0</td> </tr> <tr> <td>Clay [%]</td> <td>6.9</td> </tr> <tr> <td>Silt [%]</td> <td>86.2</td> </tr> <tr> <td>pH (CaCl<sub>2</sub>)</td> <td>7.4</td> </tr> <tr> <td>pH (H<sub>2</sub>O)</td> <td>7.7</td> </tr> <tr> <td>Total organic carbon [%]</td> <td>1.7</td> </tr> <tr> <td>Total carbon [%]</td> <td>3.96</td> </tr> <tr> <td>Organic matter (calculated TOC x 1.72)</td> <td>2.87</td> </tr> </tbody> </table>	Soil parameters		Sand [%]	7.0	Clay [%]	6.9	Silt [%]	86.2	pH (CaCl <sub>2</sub> )	7.4	pH (H <sub>2</sub> O)	7.7	Total organic carbon [%]	1.7	Total carbon [%]	3.96	Organic matter (calculated TOC x 1.72)	2.87	Soil type for both studies (from a location between the two sites):  <table border="1"> <thead> <tr> <th colspan="2">Soil parameters</th> </tr> </thead> <tbody> <tr> <td>Sand [%]</td> <td>7.0</td> </tr> <tr> <td>Clay [%]</td> <td>6.9</td> </tr> <tr> <td>Silt [%]</td> <td>86.2</td> </tr> <tr> <td>pH (CaCl<sub>2</sub>)</td> <td>7.4</td> </tr> <tr> <td>pH (H<sub>2</sub>O)</td> <td>7.7</td> </tr> <tr> <td>Total organic carbon [%]</td> <td>1.7</td> </tr> <tr> <td>Total carbon [%]</td> <td>3.96</td> </tr> <tr> <td>Organic matter (calculated TOC x 1.72)</td> <td>2.87</td> </tr> </tbody> </table>	Soil parameters		Sand [%]	7.0	Clay [%]	6.9	Silt [%]	86.2	pH (CaCl <sub>2</sub> )	7.4	pH (H <sub>2</sub> O)	7.7	Total organic carbon [%]	1.7	Total carbon [%]	3.96	Organic matter (calculated TOC x 1.72)	2.87
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Exposure scenario characteristic	STUDY 1 (2019)		STUDY 2 (2021)	
	Rho [g/cm <sup>3</sup> ]	1.34	Rho [g/cm <sup>3</sup> ]	1.34
Relevant Soil depth for exposure (output needed)	Surface layer (0-1 cm)		Surface layer (0-1 cm)	
Relevant concentration	Total + pore water		Total + pore water	
Residues on leaves	n.a.		n.a.	

Table 48. Specifications for the daily foraging and exposure definitions in the SolBeePop input files for the simulations of the Eurofins semi-field studies from 2019 and 2021 with *O. bicornis*.

Specification	<i>O. bicornis</i> (Study 1, 2019)	<i>O. bicornis</i> (Study 2, 2021)
<b>Foraging specifications (applied to control and treatment simulations)</b>		
Temperature data	Weather_data_Air_T_RH_Osmia_2019.csv	Weather_data_Osmia_2021_Air_T_RH.csv
Precipitation data	Weather_data_Rain_Osmia_2019.csv	Weather_data_Osmia_2021_precip.csv
Humidity data	Weather_data_Air_T_RH_Osmia_2019.csv	Weather_data_Osmia_2021_Air_T_RH.csv
Wind data	none	none
Sunshine hours	none	none
Start date (doy)	12 April 2019 (102)	23 April 2021 (113)
End date (doy)	18 May 2019 (138)	26 May 2021 (146)
Minimum temperature (min.temp)	10 °C	10 °C
Maximum wind speed (max.wind)	NA	NA
Maximum precipitation (max.precip)	25.4 mm	25.4 mm
Maximum relative humidity (max.humid)	60%	60%
Control input file name (no exposure)	Floral_Eurofins2019_26Apr2023_control.csv	Floral_Eurofins2021_27Apr2023_control.csv
<b>Exposure specifications (treatments only)</b>		
Compound (PPP)	dimethoate	dimethoate
Application date (doy)	24 April 2019 (114)	9 May 2021 (129)

Specification	<i>O. bicornis</i> (Study 1, 2019)	<i>O. bicornis</i> (Study 2, 2021)
Application rate (AR)	75 g/ha	75 g/ha
RUD in nectar	0.87 mg/kg x kg/ha	0.87 mg/kg x kg/ha
RUD in pollen	67.7 mg/kg x kg/ha	67.7 mg/kg x kg/ha
Soil concentration data	Pforzheim\ 1_in_field_75_total\ ssWOSRpi.out	Pforzheim\ 2_in_field_75_total\ ssWOSRpi.out
Soil layer	1 (0-10mm depth)	1 (0-10mm depth)
Soil horizon density	1340 kg/m <sup>3</sup>	1340 kg/m <sup>3</sup>
Kinetics function for residue dissipation in nectar and pollen	SFO	SFO
Constant of SFO kinetics for nectar and pollen	0.5145	0.5145
Exposure factor from direct spray (EF_co)	1	1
Body surface factor (BSF)	0.0114 dm <sup>2</sup> /bee	0.0114 dm <sup>2</sup> /bee
Kinetics function for residue dissipation in and on plant surfaces (leaves)	NA	NA
Constant of SFO kinetics for leaves	NA	NA
Input file name (with exposure specifications)	Floral_Eurofins2019_25Oct2023_DIMexp_med_resid.csv	Floral_Eurofins2021_25Oct2023_DIMexp_med_resid.csv

## 7.2.5. Simulations with dimethoate exposures and effects

For the simulations of the treatments in the Eurofins semi-field studies, the parameter combinations that resulted in the best fits to the control data were applied (see Section 7.2.2). Default parameters defining the effective exposure of each bee were used (Table 49). For the characterization of the organism-level effects, default (average) parameter values for dimethoate were applied for the BeeGUTS model (Baas et al. 2022) as well as the concentration-response function for the developing bees. The parameters of both toxic responses were derived from honey bee laboratory toxicity study data (Table 49). Separate simulations with GUTS-SD and GUTS-IT were conducted. Each simulation was repeated 10 times (using different random number seeds).

A considerable difference in effect sizes of dimethoate treatments is apparent between Eurofins 2019 and 2021 studies, particularly with effects observed in nesting females (see Section 7.2.1 and Figure 44).

It is possible that the discrepancy in observed effects was related to the flight activity of the bees during application. Only bees foraging within the crop during application can be assumed to be exposed to direct spray. For instance, weather conditions resulting in no or fewer bees foraging on application day in 2019 compared to 2021 could have resulted in different observed effect sizes. To test this hypothesis, we conducted additional simulations, assuming different proportions of the bee foraging occurring on application day. For both studies, the application day was considered available for foraging based on the weather data. However, it is possible that weather conditions were different enough between those days in the two studies. In addition to the assumption that all bees were actively foraging at time of dimethoate spray application (applied in the simulations described above, “Prop\_foraging\_day” = 1 on application day), we tested the assumptions that only 75, 50, 25 or 0% of females were actively foraging (“Prop\_foraging\_day” = 0.75, 0.5, 0.25, 0) on application day (doy = 114 in 2019; doy = 129 in 2021). The proportion foraging per day corresponds to the probability of an individual bee to be directly exposed to the spray application.

*Table 49. Model parameters used in the simulations with dimethoate exposures and effects of Eurofins 2019 and 2021 semi-field studies with *O. bicornis*. Descriptions of the parameters and references for *O. bicornis* are given in SolBeePop\_ecotox\_Tables.xlsx.*

Interface parameter name	Eurofins 2019 Study	Eurofins 2021 Study	Remarks
<i>Start.day</i>	102	113	Day of year; corresponds to date the cocoons were introduced into the tunnels in the study
<i>Species</i>	<i>O.bicornis</i>	<i>O.bicornis</i>	
<i>Voltinism</i>	univoltine	univoltine	
<i>Initial.num.f</i>	60	90	
<i>Initial.num.m</i>	90	110	
<i>Initial.stage</i>	cocoon	cocoon	
<i>Initial.age</i>	300	300	Days
<i>RndSeed</i>			Set of 10 different random number seeds used
<i>MultiYearInput</i>	FALSE	FALSE	
<i>List.input.floral</i>	NA	NA	
<i>Num.repeat.yr</i>	2	2	
<i>input.floral</i>	Floral_Eurofins2019_25Oct2023_DIMexp_med_resid.csv	Floral_Eurofins2021_25Oct2023_DIMexp_med_resid.csv	Actual file names do not contain spaces
<i>stoch.crop.forag</i>	FALSE	FALSE	
<i>Density.dep</i>	FALSE	FALSE	
<i>DD.thresh.s</i>	1	1	Unused
<i>DD.max.cells.s</i>	1	1	Unused

Interface parameter name	Eurofins 2019 Study	Eurofins 2021 Study	Remarks
<i>DD.funct</i>	1	1	Unused
<i>DD.log.slope</i>	1	1	Unused
<i>day.emerge.f</i>	108	119	Day of year; calibrated to controls
<i>var.emerge.f</i>	2	3	Days; calibrated to controls
<i>day.emerge.m</i>	107	118	Day of year
<i>var.emerge.m</i>	1	1	Days
<i>latest.emerge</i>	138	146	Corresponds to the last day in the semi-field study (tunnel phase)
<i>dev.egg</i>	8	8	Days
<i>dev.larva</i>	32	32	Days
<i>dev.cocoon</i>	68	68	Days
<i>t.maturity</i>	9	9	Days; calibrated to controls
<i>m.life</i>	21	21	Days
<i>max.nesting.life</i>	36	36	Days
<i>p.max.nesting.life</i>	0.0818	0.0836	Calibrated to controls
<i>max.f.ratio</i>	0.553	0.548	Calibrated to controls
<i>max.cells</i>	1.223	1.121	Calibrated to controls
<i>max.survival.e.f</i>	0.946	0.812	Calibrated to controls
<i>max.survival.e.m</i>	0.946	0.812	Value for females used
<i>emerged.survival</i>	0.996	0.819	Calibrated to controls
<i>a.cell.age</i>	-0.006	-0.006	
<i>a.sex.age</i>	-0.0424	-0.0424	Calibrated to controls
<i>a.size.age</i>	-0.003	-0.003	
<i>a.cell.resource</i>	0.94	0.94	
<i>a.sex.resource</i>	0.42	0.42	
<i>a.size.resource</i>	0.114	0.114	
<i>Effects</i>	TRUE	TRUE	
<i>ad.nectar.cons</i>	208.34	208.34	mg/d; nectar consumption of adults derived from <a href="#">European Food Safety Authority (EFSA) et al. (2023, Table 15)</a> using honey bee consumption values
<i>ad.pollen.cons</i>	11.6	11.6	mg/d; pollen consumption of adults derived from <a href="#">European Food Safety Authority (EFSA) et al. (2023, Table 15)</a> using honey bee consumption values
<i>k_CA</i>	0.4	0.4	From BeeGUTS for honey bees (Baas et al. 2022)
<i>Transfer.mat.adult</i>	TRUE	TRUE	
<i>ad.ET</i>	0.072	0.072	1/d; time reported for mud collection and partition building per day (scaled to 24 h) (Strohm et al. 2002; European Food Safety Authority 2023)
<i>TC_soil</i>	0.5	0.5	g/d; see text for further explanation

Interface parameter name	Eurofins 2019 Study	Eurofins 2021 Study	Remarks
<i>TC_leaf</i>	0	0	cm <sup>2</sup> /d; unused in <i>Osmia</i>
<i>Exposure.resting.soil</i>	FALSE	FALSE	
<i>GUTS</i>	GUTS-SD, GUTS-IT	GUTS-SD, GUTS-IT	All GUTS parameters derived from honey bee standard toxicity studies with dimethoate (Baas et al. 2022)
<i>t.guts</i>	10	10	From BeeGUTS for honey bees (Baas et al. 2022)
<i>kd_SD</i>	0.39	0.39	From BeeGUTS for honey bees (Baas et al. 2022)
<i>bw_SD</i>	0.014	0.014	From BeeGUTS for honey bees (Baas et al. 2022)
<i>mw_SD</i>	13.00	13.00	From BeeGUTS for honey bees (Baas et al. 2022)
<i>kd_IT</i>	0.012	0.012	From BeeGUTS for honey bees (Baas et al. 2022)
<i>mw_IT</i>	2.40	2.40	From BeeGUTS for honey bees (Baas et al. 2022)
<i>Fs_IT</i>	3.00	3.00	From BeeGUTS for honey bees (Baas et al. 2022)
<i>nectar_prop</i>	0.78	0.78	From European Food Safety Authority (EFSA) et al. (2023), Table 16, assuming 30% sugar in nectar
<i>weight.prov</i>	306	306	mg; Strohm et al. 2002
<i>Transfer.mat.dev</i>	TRUE	TRUE	
<i>SM</i>	187	187	mg; Strohm et al. 2002
<i>F</i>	0	0.00	unused in <i>Osmia</i>
<i>SA_i</i>	0	0.00	cm <sup>2</sup> ; unused in <i>Osmia</i>
<i>dr.intercept</i>	1.1534	1.1534	Derived from honey bee larval toxicity studies (OECD 2016, No 239)
<i>dr.slope</i>	-0.7876	-0.7876	Derived from honey bee larval toxicity studies (OECD 2016, No 239)

## 7.2.6. Analysis of simulations with dimethoate exposures and effects

The simulations of dimethoate treatments in the Eurofins 2019 and 2021 studies were analyzed in two ways: 1) comparing the outputs from the treatment simulations with the treatment data from each study directly, and 2) calculating the relative effect size in the simulations and comparing it to the relative effect sizes observed in the studies. Note that the goodness-of-fit using the direct comparison is expected to be dependent on the fit of the model outputs to the control, i.e., the model performance representing the treatments is not expected to exceed the model performance representing the controls in each study. The comparison of relative effects is expected to be less dependent on the model performance representing control dynamics. For the characterization of goodness-of-fit (NRMSE), the

female sex ratio of the offspring was not considered because few or no new brood cells were produced after dimethoate application.

Relative effects ( $E_r$ ) were calculated by comparing model outputs from the corresponding control ( $O_c$ ) and exposure simulations ( $O_e$ ) using Equation 7.3. Corresponding control and exposure simulations used identical parameter combinations and random number seeds and differed exclusively in the input file used (without and with exposures, respectively).

#### *Equation 7.3*

$$E_r = \frac{O_e - O_c}{O_c}$$

The relative effects were calculated in the same way for the study data. The relative effects were then compared between simulations and study data by calculating the RMSE. Because relative effects are expressed relative to control data or simulations, the RMSE does not need to be normalized to be comparable between different measurement endpoints, i.e., number of females in nests and brood cells.

### 7.2.7. Results

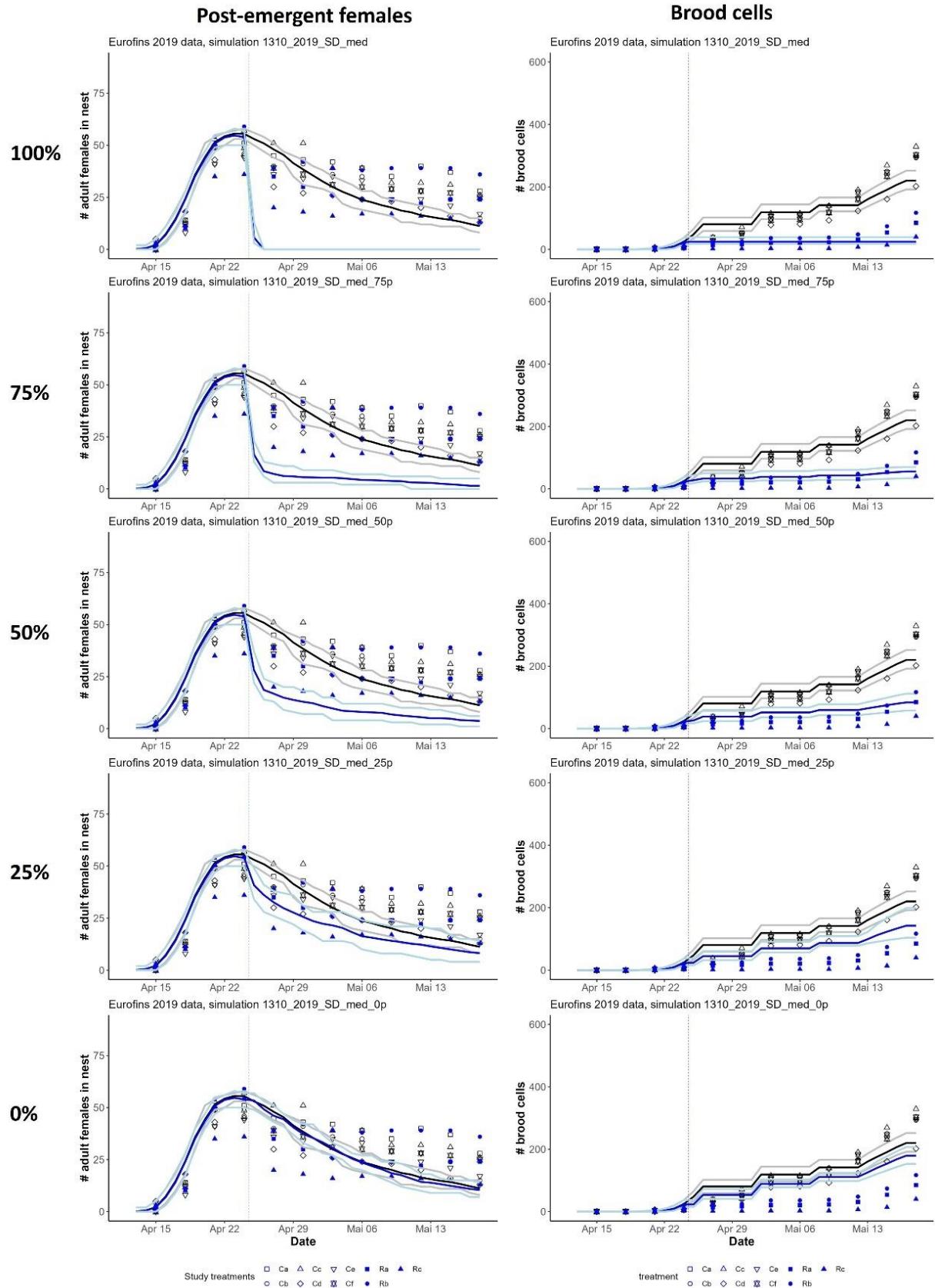
In the simulations of the Eurofins semi-field studies with dimethoate treatments, the application of the pesticide resulted in 100% mortality of the post-emergent females in case all females were assumed to be exposed to direct spray (Figure 49, Figure 50). In contrast, the effects observed in the two Eurofins studies differed considerably, with higher effects observed in 2021 compared to 2019. It could not fully be determined why the differences in effects occurred in the studies. With the model, we tested the hypothesis that different proportions of post-emergent females were actively foraging at time of application, resulting in different proportions of females exposed directly to the spray application. While simulations with the model cannot resolve what caused the differences between the two Eurofins semi-field studies, this approach corresponds to testing a hypothesis: could different levels of effects be caused by differences in female foraging activity? Such differences in foraging activity could occur due to various reasons, e.g., different weather conditions on application day, different timing of application on application day or other unknown reasons. While the weather data from the application days in 2019 and 2021 both indicate favorable conditions for *O. bicornis* foraging, inclement weather started less than two days after application in 2019 while weather conditions in 2021 remained mostly favorable in 2021 for the remainder of the tunnel phase.

In Figure 49, control and effect simulations are plotted along with the Eurofins 2019 study data for assumptions of 0, 25, 50, 75, and 100% of post-emergent females foraging during spray application. If no foraging on application day is assumed (Figure 49A,B), only slight effects occur in the simulations, indicating that the simulated effects in the 100% spray exposure scenario are driven by the direct exposure to spray. The best fit (lowest NRMSE) of the 2019 treatment data (number of nesting females and cumulative brood cells produced) was achieved with the simulations assuming 75% of females exposed to direct spray; the best fit to the relative effect sizes observed in 2019 was reached with the

assumption of 25% exposure to direct spray. The average NRMSE values for simulations of treatment data and the RMSE for relative effects are listed in Table 50 and Table 51, respectively.

We applied the same hypothesis about different proportions of females exposed to direct spray in the simulations of the Eurofins 2021 semi-field study. In this study, observed effects were more pronounced than in the 2019 study, with females observed in the nest boxes dropping to very low numbers after application day. The best fit with the treatment data were simulations assuming 100% of females exposed to direct spray. Relative effects were best captured if 75% females exposed were assumed. The NRMSE values for the simulations of the 2021 study treatment data are listed in Table 52. RMSEs for relative effects are listed in Table 53.

Relative effect sizes indicate the effect relative to control numbers. Because relative effects are independent of the absolute numbers of individuals, they can be more informative when generalizing beyond a specific study. Relative effects on number of post-emergent females were most pronounced shortly after dimethoate application (Table 54). The effects on total number of brood cells produced was cumulative, and thus, most pronounced at the end of the tunnel phase. In Table 54, we list the average and range (minimum and maximum) relative effect sizes on post-emergent female numbers on the first sampling day after application (3 days after application in the 2019 study and 2 days after application in the 2021 study) and relative effect sizes on total brood cells produced (at the end of the tunnel phase). Relative effect sizes are listed for the study data, the simulations using GUTS-SD and GUTS-IT models for effects on adults, and the scenarios defining the proportion of females exposed to direct spray.



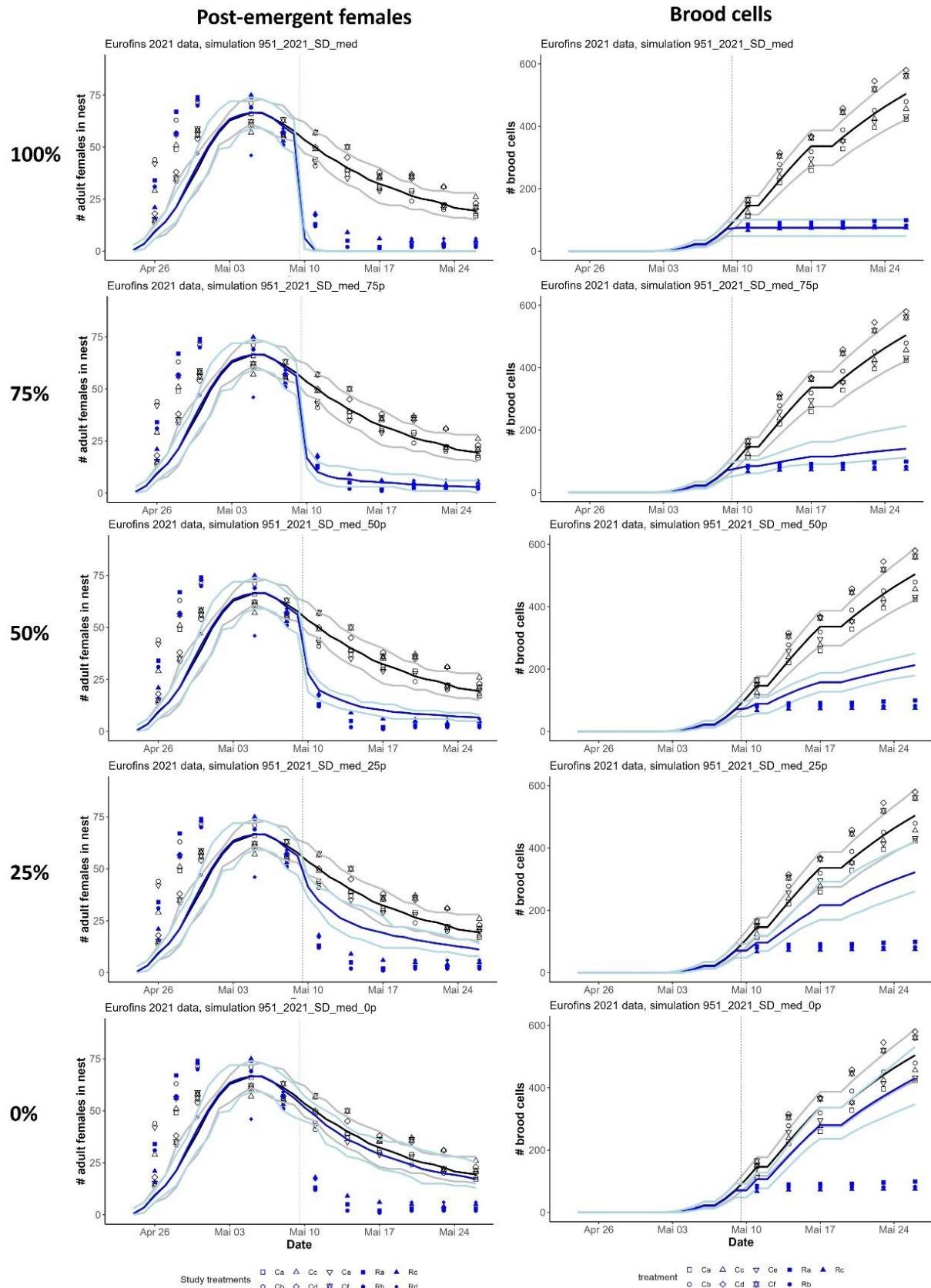
*Figure 49 (previous page). Data and simulations of the Eurofins 2019 semi-field study. Black dots indicate data from repeat control tunnels, blue dots from repeat treatment tunnels. Simulated controls are shown by their averages (black lines) and ranges (grey lines), treatment averages are shown as blue lines and ranges as light blue lines. Plots in the left column show the number of post-emergent female bees in the nests, right plots the cumulative number of brood cells in the nest blocks. In the rows, decreasing proportions of post-emergent females were assumed to be foraging on application day, corresponding the indicated percentages of females exposed to direct spray in the simulations. Treatment simulation outputs using GUTS-SD are shown.*

*Table 50. Goodness of fit (NRMSE) of simulation outputs to dimethoate treatment data from the Eurofins 2019 semi-field study. Simulations used the parameter combination providing the best fit to 2019 control study data (run # 1310). Smaller NRMSE values indicate better fits to the data. Fits to the number of females observed in the nests and the number of brood cells are listed separately, along with the averages of the two values. Simulations using GUTS-SD and GUTS-IT were qualitatively similar with slight differences in outputs. Best fits are highlighted in green.*

Foraging / direct spray exposure	NRMSE female number		NRMSE brood cell number		Average NRMSE	
	GUTS-SD	GUTS-IT	GUTS-SD	GUTS-IT	GUTS-SD	GUTS-IT
100%	0.825	0.822	0.856	0.859	0.841	0.840
75%	0.702	0.671	0.721	0.706	0.711	0.689
50%	0.576	0.518	1.082	1.331	0.829	0.925
25%	0.360	0.386	2.081	2.079	1.221	1.233
0%	0.338	0.314	2.947	3.319	1.643	1.816

*Table 51. Goodness of fit (RMSE) of simulated relative effects to relative effects in the Eurofins 2019 semi-field study. Simulations used the parameter combination providing the best fit to 2019 control study data (run # 1310). Smaller RMSE values indicate better fits to the data. Fits to the number of females observed in the nests and the number of brood cells are listed separately, along with the averages of the two values. Simulations using GUTS-SD and GUTS-IT were qualitatively similar with slight differences in outputs. Best fits are highlighted in green.*

Foraging / direct spray exposure	RMSE relative effect on female number		RMSE relative effect on brood cell number		Average RMSE of relative effects	
	GUTS-SD	GUTS-IT	GUTS-SD	GUTS-IT	GUTS-SD	GUTS-IT
100%	0.737	0.734	0.507	0.507	0.622	0.621
75%	0.602	0.575	0.510	0.510	0.556	0.542
50%	0.465	0.402	0.532	0.548	0.498	0.475
25%	0.179	0.244	0.604	0.604	0.391	0.424
0%	0.153	0.205	0.688	0.720	0.420	0.462



*Figure 50 (previous page). Data and simulations of the Eurofins 2021 semi-field study. Black dots indicate data from repeat control tunnels, blue dots from repeat treatment tunnels. Simulated controls are shown by their averages (black lines) and ranges (grey lines), treatment averages are shown as blue lines and ranges as light blue lines. Plots in the left column show the number of post-emergent female bees in the nests, right plots the cumulative number of brood cells in the nest blocks. In the rows, decreasing proportions of post-emergent females were assumed to be foraging on application day, corresponding the indicated percentages of females exposed to direct spray in the simulations. Treatment simulation outputs using GUTS-SD are shown.*

*Table 52. Goodness of fit (NRMSE) of simulation outputs to dimethoate treatment data from the Eurofins 2021 semi-field study. Simulations used the parameter combination providing the best fit to 2021 control study data (run # 951). Smaller NRMSE values indicate better fits to the data. Fits to the number of females observed in the nests and the number of brood cells are listed separately, along with the averages of the two values. Simulations using GUTS-SD and GUTS-IT were qualitatively similar with slight differences in outputs. Best fits are highlighted in green.*

Foraging / direct spray exposure	NRMSE female number		NRMSE brood cell number		Average NRMSE	
	GUTS-SD	GUTS-IT	GUTS-SD	GUTS-IT	GUTS-SD	GUTS-IT
100%	0.520	0.519	0.044	0.051	0.282	0.285
75%	0.485	0.485	0.583	0.585	0.534	0.535
50%	0.501	0.499	1.222	1.191	0.862	0.845
25%	0.615	0.648	2.174	2.416	1.395	1.532
0%	0.803	0.807	3.121	3.150	1.962	1.978

*Table 53. Goodness of fit (RMSE) of simulated relative effects to relative effects in the Eurofins 2021 semi-field study. Simulations used the parameter combination providing the best fit to 2021 control study data (run # 951). Smaller RMSE values indicate better fits to the data. Fits to the number of females observed in the nests and the number of brood cells are listed separately, along with the averages of the two values. Simulations using GUTS-SD and GUTS-IT were qualitatively similar with slight differences in outputs. Best fits are highlighted in green.*

Foraging / direct spray exposure	RMSE relative effect on female number		RMSE relative effect on brood cell number		Average RMSE of relative effects	
	GUTS-SD	GUTS-IT	GUTS-SD	GUTS-IT	GUTS-SD	GUTS-IT
100%	0.143	0.142	0.067	0.065	0.105	0.103
75%	0.053	0.054	0.141	0.141	0.097	0.098
50%	0.136	0.130	0.252	0.243	0.194	0.186
25%	0.332	0.375	0.418	0.459	0.375	0.417
0%	0.557	0.554	0.596	0.599	0.577	0.577

*Table 54. Relative effect sizes (proportion of controls) in the Eurofins semi-field study data and the SolBeePop<sub>ecotox</sub> simulations. For the simulations of the 2019 and 2021 studies, the respective best fits from the calibration were used. Relative effects on number of post-emergent females are listed on the first sampling day after application; for total brood cell numbers, the relative effects on the last day of the tunnel phase. n/a: not applicable.*

Data set	Assumed % of females exposed to direct spray	GUTS model	Nesting female number (day after application)	Brood cell number (end of tunnel phase)
2019 study data	n/a	n/a	-0.220 (-0.502; -0.029)	-0.719 (-0.861; -0.593)
2019 simulation	100%	GUTS-SD	-1 (-1; -1)	-0.888 (-0.917; -0.813)
2019 simulation	100%	GUTS-IT	-0.996 (-1; -0.979)	-0.890 (-0.922; -0.823)
2019 simulation	75%	GUTS-SD	-0.848 (-0.940; -0.727)	-0.747 (-0.823; -0.665)
2019 simulation	75%	GUTS-IT	-0.785 (-0.860; -0.682)	-0.736 (-0.847; -0.599)
2019 simulation	50%	GUTS-SD	-0.651 (-0.729; -0.551)	-0.618 (-0.754; -0.515)
2019 simulation	50%	GUTS-IT	-0.585 (-0.660; -0.521)	-0.557 (-0.659; -0.485)
2019 simulation	25%	GUTS-SD	-0.320 (-0.449; -0.182)	-0.345 (-0.587; -0.020)
2019 simulation	25%	GUTS-IT	-0.312 (-0.420; -0.208)	-0.378 (-0.544; -0.310)
2019 simulation	0%	GUTS-SD	-0.039 (-0.140; 0)	-0.180 (-0.285; -0.034)
2019 simulation	0%	GUTS-IT	0.007 (-0.140; 0.146)	-0.069 (-0.210; 0.131)
2021 study data	n/a	n/a	-0.683 (-0.746; -0.620)	-0.839 (-0.881; -0.797)
2021 simulation	100%	GUTS-SD	-0.996 (-1; -0.978)	-0.851 (-0.895; -0.779)
2021 simulation	100%	GUTS-IT	-0.994 (-1; -0.979)	-0.856 (-0.889; -0.796)
2021 simulation	75%	GUTS-SD	-0.796 (-0.880; -0.667)	-0.720 (-0.785; -0.575)
2021 simulation	75%	GUTS-IT	-0.803 (-0.872; -0.694)	-0.719 (-0.788; -0.608)
2021 simulation	50%	GUTS-SD	-0.598 (-0.722; -0.500)	-0.573 (-0.696; -0.475)
2021 simulation	50%	GUTS-IT	-0.631 (-0.735; -0.540)	-0.582 (-0.684; -0.399)
2021 simulation	25%	GUTS-SD	-0.305 (-0.421; -0.089)	-0.355 (-0.483; -0.166)
2021 simulation	25%	GUTS-IT	-0.291 (-0.404; -0.149)	-0.307 (-0.445; -0.138)
2021 simulation	0%	GUTS-SD	-0.041 (-0.204; 0.133)	-0.136 (-0.408; 0.162)
2021 simulation	0%	GUTS-IT	-0.047 (-0.222; 0.133)	-0.133 (-0.300; 0.076)

## 7.2.8. Discussion

The simulations of the semi-field studies with exposures and effects of a dimethoate spray treatment show that the model can capture effects without further calibration of model parameters defining individual-level exposures and effects. While the application rate of the pesticide was reported from the studies, the detailed information on the exposure levels reaching individual bees were not characterized, including the residues in pollen and nectar of the treated oilseed rape and the residues in soil collected by the nesting females for the construction of brood cell partitions. The consumption rates of post-emergent *O. bicornis* and the uptake of residues from exposed soil remain uncertain, and the amount of spray received by a single bee present in a crop at time of application are based on simplifying assumptions. For these parameters, we applied conservative assumptions, following recommendations by European Food Safety Authority (EFSA) et al. (2023) for lower-tier risk assessments where available (see Section 7.2.4). For the effects, we used parameters of BeeGUTS for post-emergent bees derived from honey bee standard toxicity studies with dimethoate (adult acute contact, acute oral and chronic oral tests) (OECD 1998a; OECD 1998b; OECD 2017). Honey bee toxicity was used as surrogate because data specific for *O. bicornis* were not available. While laboratory toxicity tests have been conducted with *O. bicornis* for a small number of pesticides (Arena and Sgolastra 2014; Heard et al. 2017; Sgolastra et al. 2017; Spurgeon et al. 2017; Roessink et al. 2018; Anderson and Harmon-Threatt 2019; Azpiazu et al. 2019; Carnesecchi et al. 2019; Eeraerts et al. 2019; Mokkapati et al. 2021; Mokkapati et al. 2022), it cannot be expected that such data will be readily available across compounds and for multiple solitary bee species. Thus, the use of honey bee toxicity parameters served as a test whether these data are relevant for characterizing the effects in another bee species, *O. bicornis*. The application of SolBeePop<sub>ecotox</sub> suggests that the honey bee can serve as an individual-level toxicity (intrinsic sensitivity) surrogate for *O. bicornis*. Using this assumption, the model overpredicts effects experienced by post-emergent bees observed in the semi-field studies, and thus, can be seen as conservative in modeling such studies. Although the reproductive output in the semi-field studies was affected due to the mortality of nesting females, effects on offspring that were produced after application were not observed in the studies and also not predicted by the model. Dimethoate has considerably higher toxicity to adults compared to bee larvae, and thus, this result aligns with the expectations (OECD 2016). Semi-field studies are conducted in the context of higher-tier bee risk assessments. In semi-field studies with honey bees, dimethoate may also be used as reference pesticide (positive control). An application rate of 200 g/ha has been used in the honey bee studies because this rate reliably results in clear effects to honey bee colonies (European Food Safety Authority 2023). The lower rate used in the *O. bicornis* semi-field studies does not necessarily indicate a higher sensitivity of the species to the pesticide but can be explained by the proportion of bees exposed and the measurement endpoints, both differing considerably from studies with honey bee colonies.

We tested the hypothesis that different proportions of post-emergent females foraging in the semi-field studies at time of application could explain the differences in effects observed in the 2019 compared to the 2021 study. Less than 100% of post-emergent females directly exposed to spray improved the goodness of fit of the simulations to the 2019 study treatment data. A lower proportion of females exposed in 2019 compared to 2021 captured the difference between the two studies with the simulations. We cannot conclude that the foraging activity of bees on application day did influence the observed effects in the Eurofins semi-field studies. However, the testing of this hypothesis with the model indicates how the model can be applied to support empirical data. The most important exposure

route (direct spray) comes with an uncertainty related to the proportion of bees exposed. In semi-field trials, the exclusion of bees from exposure to direct spray (e.g., through application at night when bees are not active) could be used to determine effects resulting from other exposure routes (dietary and contact to soil).

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# APPENDIX A

In Table 55 through Table 70, data compiled for the model bee species following Pop-GUIDE (Phase 2) (Raimondo et al. 2021) are presented. Data for the model *Osmia* species (*O. lignaria*, *O. cornuta*, *O. bicornis* and *O. cornifrons*) are summarized in combined tables because the species are similar in life history and size. Citations listed in the tables are included in the Reference list.

## Data summary for *Eucera pruinosa*

Table 55. Organism-level characteristics of *E. pruinosa*, and how the data compilation relates to the bee traits used in Schmolke et al. (2021). Complexity level of data is listed (general-realistic-precise). NA = Not applicable.

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Life span	Nesting period		No data could be found		
Reproductive/breeding season	Combination of emergence time and nesting period	General	Late Jun/July-Sep (aligned with cucurbit flowering); peak observed on July 31; 19-20 June: bees had emerged, but no nest construction; emergence in Ontario: mid to late July; males emerge earlier than females (Ullmann et al. 2016)	Study from Hurd et al. in Sacramento Valley, CA in 1971; dependent on region/climate	(Mathewson 1968; Hurd et al. 1974; Ullmann et al. 2016; Willis Chan 2020)
Reproductive frequency	Voltinism	General	Univoltine		(Hurd et al. 1974)
Reproductive output/clutch size	Fecundity	Realistic	~1 cell/day; up to 1.65 cells/day based on foraging trips		(Willis Chan 2020)

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Egg development time	NA			<i>No data could be found</i>	
Larval development time	Larval feeding period	General	15 days	Reported in supplementary information	(Willis Chan et al. 2019a)
Onset of maturation	NA	General	2-3 weeks (Mathewson); 4 days (Willis Chan)	Time between emergence and start of nesting in females; 4 days more realistic because female emergence was observed (vs. emergence of any bee)	(Mathewson 1968; Hurd et al. 1974; Willis Chan 2020)
Hatching (eggs)/germination (seeds) rate	NA			<i>No data could be found</i>	
Immature transition rate (including metamorphosis) <sup>1</sup>	NA			<i>No data could be found</i>	
Sex ratio	NA	Realistic	2.1 males per female (=0.32 females/total; Willis Chan 2020); ~0.7 female/total sex ratio (Ullmann et al. 2016)		(Ullmann et al. 2016; Willis Chan 2020)
Recruitment rate	NA	NA	NA	Covered by previous characteristics	
Survival rate	NA			<i>No data could be found</i>	

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Growth rate	NA	NA	NA	Growth assumed to be directly determined by provisioning size	
Body size - females	Body size	General	12.5-14 mm length (discoverlife.org); 0.11 +/- 0.002 g (Willis Chan)		(Willis Chan 2020; Discover Life 2021)
Body size - males	NA	General	11-13 mm length (discoverlife.org); 0.07 +/- 0.0008 g (Willis Chan)		(Willis Chan 2020)
Seedling emergence; emergence after hibernation; emergence of new generation	Emergence time of females	General	Late May-Aug (dependent on region/ cucurbit flowering); emergence occurs over extended period (~1 month)		(Hurd et al. 1974; Willis and Kevan 1995; Willis Chan 2020)
Protandrous emergence	NA	General	Males emerge at least 3 days before females		(Willis Chan 2020)
Dormancy duration (inactive life stages, e.g., hibernation, soil seed bank)	NA	General	Overwinter in nest prior to emergence (univoltine)		(Hurd et al. 1974)

Table 56. Population and spatial characteristics. Data for *E. pruinosa* compiled. NA = Not applicable.

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Density dependence	NA	NA	NA		
Population size	NA	NA	NA		
Spatial Metapopulation structure	NA	NA	NA		
Dispersal/migration	NA			Quantitative data on dispersal not available; hard to distinguish from mortality and failure of nest establishment	
Foraging range	Foraging range	General	<260 m		(Willis Chan et al. 2019a)
Habitat features	NA	General	Dependent on cucurbit crops in most of its range		(Hurd et al. 1974; López- Uribe et al. 2016)
Geographical range	NA	General	Most of North America where cucurbit crops are grown Soil nesting, close to or within pumpkin fields; preference for wet soils, under vegetation (e.g., wet leaves); soil clay content negatively correlated with <i>E. pruinosa</i> abundance		(López-Uribe et al. 2016)
Habitat classification/suitability	Nesting substrate	General			(Hurd et al. 1974; Julier and Roulston 2009)

Table 57. External factors. Data for *E. pruinosa* compiled. NA = Not applicable.

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Predation/herbivory	NA				
Competition	NA	General	Rapid pollen depletion in squash flowers observed	Points to competition of this resource across species visiting squash flowers	(Willis Chan 2020)
Environmental conditions	NA				
Stressors - pathogens	NA				
Stressors – abiotic, other	NA				
Existing management	NA	General	No management reported		
Indirect effects (obligatory relationships)	NA				

Table 58. Additional characteristics identified as important for solitary bees and their interactions with their environment. Data for *E. pruinosa* compiled. NA = Not applicable.

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Nesting substrate / strategy	Nesting substrate	General	Soil nesting (below ground)		(Hurd et al. 1974)
Nesting material	Nesting material	General	Burrows in soil; most brood cells at 12-38 cm depth (Hurd et al.); 16-18 cm depth (Mathewson)		(Mathewson 1968; Hurd et al. 1974)
Nesting material weight/size	NA	NA	NA	No additional nesting material collected	
Pollen transport	Pollen transport	General	Legs and abdomen		(Hurd et al. 1974; Michener 2007)
Flower preference	Flower preference	General	Oligolectic for pollen (cucurbits: squash, pumpkin and gourds), polylectic for nectar		(Hurd et al. 1974)
Composition of food provision	NA	Realistic	The mean ( $\pm$ SE) number of [squash] pollen grains in a fully provisioned hoary squash bee nest cell is $62,719.23 \pm 7,900.49$ ( $n = 13$ ; Figure 3.8)	Nectar not reported; total provision mass not reported	(Willis Chan 2020)
Composition of adult food	NA	NA	NA	<i>No data could be found</i>	

## Data summary for *Megachile rotundata*

Table 59. Organism-level characteristics of *M. rotundata*, and how the data compilation relates to the bee traits used in Schmolke et al. (2021). Complexity level of data is listed (general-realistic-precise). NA = Not applicable.

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Life span	Nesting period	General-realistic	7-8 weeks	Post-emergent females	(Tasei 1975; Pitts-Singer and Cane 2011)
Reproductive/breeding season	Combination of emergence time and nesting period	General-realistic	Emergence in summer (June), earlier/later dependent on temperature/ region); activity for 11 weeks after first emergence (including 2 <sup>nd</sup> generation bees) Uni- or bivoltine, dependent on region/climate Plus unknown factors; up to 50% of the early summer brood completes development to yield a second generation	Temperature dependent; varies by species; can be bivoltine in warmer climates	(Tasei and Masure 1978; Pitts-Singer and Cane 2011; Blattschneiderbienen: <i>Megachile rotundata</i> ) <sup>1</sup>
Reproductive frequency	Voltinism	General-realistic	Up to 57 eggs/female under ideal conditions; max. 2 eggs/day (Pitts-Singer and Cane); 25-30 eggs/female (Tasei)		(Pitts-Singer and Cane 2011)
Reproductive output/clutch size	Fecundity	General-realistic		Under ideal conditions; far fewer if floral resources are limited	(Tasei 1975; Pitts-Singer and Cane 2011)
Egg development time	NA	General-precise	3 days (42-120 h)	Reared at 22-26C; see Table 1	(Tasei 1975; Trostle and Torchio 1994)
Larval development time	Larval feeding period	General-precise	8.7 days (5.4-16 days) to cocoon (end of feeding); non-diapausing bees (second generation): 5 days to pupate (after cessation of larval movement); adults remain in the cocoon 2-3 days before emergence (Trostle and Torchio 1994); 3 weeks from hatching to cocoon (Tasei 1975)	Reared at 22-26C; see Table 2	(Tasei 1975; Trostle and Torchio 1994)

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Onset of maturation	NA	General	Within a week after emergence		(Pitts-Singer and Cane 2011)
Hatching (eggs)/germination (seeds) rate	NA	Realistic	4-42% of cells are pollen balls (cells without developing bees)	Can be due to no egg or death early in the development	(Pitts-Singer and James 2008)
Immature transition rate (including metamorphosis)	NA	Realistic	0-65% of cells produce adults (survival through emergence) (Pitts-Singer and Bosch 2010); emergence rate from cells: 70-74% (Peterson and Roitberg 2006) Proportion of female offspring produced: 0.2 – 0.45; average: 0.35 (Peterson and Roitberg 2006); 0.33-0.83 overall; 0.38-0.77 of overwintering brood (Pitts-Singer and Bosch 2010); 0.25-.33 (Tasei 1975)	Includes pollen balls (provisions without developing bee); from semi-field trials (stored in incubator) in both studies; Peterson and Roitberg 2006 do not specifically report pollen balls	(Peterson and Roitberg 2006a; Pitts-Singer and Bosch 2010)
Sex ratio	NA	Realistic	0.33-0.83 overall; 0.38-0.77 of overwintering brood (Pitts-Singer and Bosch 2010); 0.25-.33 (Tasei 1975)	Sex ratio may be dependent on resource availability, but not observed by Peterson and Roitberg 2006b	(Tasei 1975; Peterson and Roitberg 2006a; Pitts-Singer and Bosch 2010)
Recruitment rate	NA	NA	NA	Covered by previous characteristics	
Survival rate	NA	General-realistic	50-88% nesting of released females under semi-field conditions with high floral resource (post-emergent survival to maturity)	See Pitts-Singer and Bosch 2010, Table 1	(Pitts-Singer and Bosch 2010)
Growth rate	NA	NA	NA	Growth assumed to be directly determined by provision size	(Kim 1999)(applicable across model solitary bee species, see also Osmia data table)

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Provision weight – females	NA	Realistic	Average 105 mg (wet weight); average 90 +/- 26 mg (wet weight) (median: 88 mg; not separated by sex)	Klostermeyer et al. (1973), Table 4 (data from 3 nests); Cane et al. 2011 (not separated by sex)	(Klostermeyer et al. 1973; Cane et al. 2011)
Provision weight – males	NA	Realistic	Average: 85 mg (wet weight)	Klostermeyer et al. (1973), Table 4 (data from 3 nests); see Cane et al. 2011 for provision weight not separated by sex	(Klostermeyer et al. 1973; Cane et al. 2011)
Body size - females	Body size	General-realistic	8-10 mm length; ~5-16mg (adult dry weight); 10.9-12.3 mg (adult dry weight); prepupal: 42.6-49.8 mg (wet weight)	Note that the low weight observed on exclusive buckwheat diet; second generation tend to be smaller than diapausing	(Peterson and Roitberg 2006a; Pitts-Singer and Bosch 2010; Frewin et al. 2019; Blattschneiderbienen: <i>Megachile rotundata</i> ; discoverlife.org)
Body size – males	NA	General-realistic	6-8mm length; 9.1-9.3 mg (adult dry weight); prepupal: 39-43.3 mg (wet weight)		(Peterson and Roitberg 2006a; Pitts-Singer and Bosch 2010); discoverlife.org
Seedling emergence; emergence after hibernation; emergence of new generation	Emergence time of females	General		See reproductive/breeding season	
Protandrous emergence	NA	General	First males emerge 1-3 days before females		(Pitts-Singer and Cane 2011)
Dormancy duration (inactive life stages, e.g., hibernation, soil seed bank)	NA	General	<i>M. rotundata</i> overwinters as prepupa (after 1-2 generations); no diapause in first generation if bivoltine		(Pitts-Singer and Cane 2011)

<sup>1</sup> Tasei and Masure 1978: *Megachile pacifica* = *Megachile rotundata*

Table 60. Population and spatial characteristics. Data for *M. rotundata*. compiled. NA = Not applicable.

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Density dependence	NA	General	Nesting cavities and floral resources may be limiting	see Osmia data table	(Pitts-Singer and James 2008)
Population size	NA			Data for unmanaged populations not available	
Spatial Metapopulation structure	NA			No data available for use in model	
Dispersal/migration	NA			Quantitative data on dispersal not available; hard to distinguish from mortality and failure of nest establishment	
Foraging range	Foraging range	General-realistic	0.1 – 1.8 km (Greenleaf); usually 10-40m, but up to 1.5 km (Tasei)	Mostly within 100m from nest	(Tasei 1975; Peterson and Roitberg 2006b; Greenleaf et al. 2007; Pitts-Singer and Cane 2011)
Habitat features	NA	General-realistic	Sand and clay, dry slopes, forest edges, parks, agricultural landscapes		(Blattschneiderbienen: <i>Megachile rotundata</i> )
Geographical range	NA	General-realistic	South and central Europe; introduced to the US for alfalfa pollination		(Blattschneiderbienen: <i>Megachile rotundata</i> )
Habitat classification/suitability	Nesting substrate	General-realistic	Nest above-ground in pre-existing cavities		(Sgolastra et al. 2019)

Table 61. External factors. Data for *M. rotundata* compiled. NA = Not applicable.

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Predation/herbivory	NA	General	Cleptoparasites	Can affect significant proportion of brood	(Pitts-Singer and Cane 2011)
Competition	NA	General	Intra-specific competition for floral resources suggested in semi-field study (not quantified)		(Peterson and Roitberg 2006a)
Environmental conditions	NA	General-realistic	Weather-dependent reproductive success	Regional differences in empty cells linked to weather	(Pitts-Singer and James 2008)
Stressors - pathogens	NA	General	Chalkbrood	Can affect significant proportion of brood	(Pitts-Singer and Cane 2011)
Stressors – abiotic, other	NA				
Existing management	NA	General	Managed for alfalfa pollination in the US		(Pitts-Singer and Cane 2011)
Indirect effects (obligatory relationships)	NA				

*Table 62. Additional characteristics identified as important for solitary bees and their interactions with their environment. Data for M. rotundata compiled. NA = Not applicable.*

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Nesting substrate / strategy	Nesting substrate	General	Above-ground nests in existing cavities		(Pitts-Singer and Cane 2011)
Nesting material	Nesting material	General	Leaf pieces used as brood cell lining and capping		(Pitts-Singer and Cane 2011)
Nesting material weight/size	NA	General	Each brood cell requires 14-15 leaf pieces		(Pitts-Singer and Cane 2011)
Pollen transport	Pollen transport	General	Abdomen: Megachilidae have hairs (scopa) on the underside of their abdomen for pollen transport, rather than on their legs (like many other bee species)  Polylectic; provisions mainly composed of alfalfa pollen in bees managed for alfalfa pollination		(Michener 2007)
Flower preference	Flower preference	General			(Tasei 1975; Cane et al. 2011; Pitts-Singer and Cane 2011)
Factors impacting provision size for female offspring	NA	Realistic	Lower resource availability leads to lower female provision and female offspring size	Resource limitation also results in lower overall offspring production	(Peterson and Roitberg 2006a; Peterson and Roitberg 2006b)
Composition of food provision	NA	Realistic	64-67% nectar, 33-36% pollen by weight; provision contains 1.3 million pollen grains and is 47% sugar by weight		(Klostermeyer et al. 1973; Cane et al. 2011; Pitts-Singer and Cane 2011)

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Composition of adult food	NA			<i>No data could be found</i>	

## Data summary for *Nomia melanderi*

Table 63. Organism-level characteristics of *N. melanderi*, and how the data compilation relates to the bee traits used in Schmolke et al. (2021). Complexity level of data is listed (general-realistic-precise). NA = Not applicable.

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Life span	Nesting period	General-realistic	15-26 days	Nesting female, corresponds to age after emergence	(Bohart and Cross 1955)
Reproductive/breeding season	Combination of emergence time and nesting period	General-realistic	6-8 weeks (in WA, univoltine); longer in bivoltine populations (Utah); early/mid June- mid July (WA); late June – late August (UT); starting late May in 2018 in WA	August probably due to second generation; season may be shorter in WA (univoltine)	(Bohart and Cross 1955; Cross and Bohart 1960; Johansen et al. 1978; Vinchesi et al. 2013; Smith et al. 2019)
Reproductive frequency	Voltinism	General-realistic	Univoltine (in WA); partially bivoltine in UT		(Bohart and Cross 1955; Cane 2008)
Reproductive output/clutch size	Fecundity	Realistic	15-20 cells/nest; 1 nest/female; 1 cell/day	Pattern of provisioning on one day and egg laying by the following observed; slower rate reported for nests older than 20 days	(Bohart and Cross 1955)
Egg development time	NA	Realistic-precise	2 days; 7 days	Cache Valley, UT, 1952; Touchet Valley, WA, 1973-75 (Johansen et al., Table 1)	(Bohart and Cross 1955; Johansen et al. 1978)
Larval development time	Larval feeding period	Realistic-precise	6 days (larval growth); plus 2-3 days to transform to prepupa (overwintering stage); 10 days until prepupa	Cache Valley, UT, 1952; Touchet Valley, WA, 1973-75 (Johansen et al., Table 1)	(Bohart and Cross 1955; Johansen et al. 1978)
Onset of maturation	NA	Realistic-precise	Pupation in June; pupal stage takes ~2 weeks; adults remain in nest for 3-4 days before taking flight; females mate and start nesting on the day of emergence	Cache Valley, UT, 1952; partial bivoltinism suggested in some locations (not investigated); pupation time corresponds in WA (Johansen et al., Table 1)	(Bohart and Cross 1955; Johansen et al. 1978; Mayer and Miliczky 1998)

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Hatching (eggs)/germination (seeds) rate	NA	NA		<i>No data could be found</i>	
Immature transition rate (including metamorphosis)	NA	General- precise	Mortality rates larvae – emergence (lab reared): 13.2 – 27.1% (higher deaths in populations from lower latitudes)	Larvae overwintered and incubated in lab under step-wise temperature regimens; larvae collected from 24 populations across NA	(Rust 2006)
Sex ratio	NA	Realistic- precise	Average: 45% females (of total emergence); range: 35-51%	Touchet Valley, WA; data from 2 study years; 5 emergence cages total	(Mayer and Miliczky 1998)
Recruitment rate	NA	NA	NA	Covered by previous characteristics	
Survival rate	NA	NA		<i>No data could be found</i>	
Growth rate	NA	General	NA	Growth assumed to be directly determined by provisioning size	
Body size - females	Body size	General- precise	Average adult ITD: 2.44-2.49mm (small: 2.3 +/- 0.09 mm; large: 2.58 +/- 0.08 mm) from Smith et al. 2019; adult weight: 83.0 +/- 14.4 mg from Rust 2006		(Rust 2006; Smith et al. 2019)

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Body size - males	NA	General-precise	Adult weight: 96.8 +/- 15.8 mg		(Rust 2006)
Seedling emergence; emergence after hibernation; emergence of new generation	Emergence time of females	General-realistic	June (reported dates of first emergence: <28 May in 2018; 10 June; 11 June; 23 June in earlier studies in WA); peak emergence in late June; temperature- dependent; emergence of females can continue for up to a month (emergence observed after 29 Jun in WA)	Emergence of (partial) second generation observed in August in Utah	(Bohart and Cross 1955; Johansen et al. 1978; Cane 2008; Vinchesi et al. 2013; Cane et al. 2017; Smith et al. 2019)
Protandrous emergence	NA	General	Males start emerging up to a week before females		(Cane 2008)
Dormancy duration (inactive life stages, e.g., hibernation, soil seed bank)	NA	General-realistic	Until emergence in the following season; overwintering as prepupa	No data on bivoltine populations (univoltine in WA; partially bivoltine UT)	(Bohart and Cross 1955; Cane 2008)

Table 64. Population and spatial characteristics. Data for *N. melanderi* compiled. NA = Not applicable.

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Density dependence	NA	General	Nest sites limiting: increase in population with increase in area of managed nest beds in WA		(Cane 2008)
Population size	NA	General-precise	Up to 5.3 million in a single managed nesting bed; 16.7 million in Touchet Valley, WA	Populations were increasing due to management between 1999 and 2006	(Cane 2008)
Spatial Metapopulation structure	NA	General	Location and size of nest aggregations in Touchet Valley, WA	Exchange between nesting beds unclear (may collectively be a well-connected, single population) Quantitative data on dispersal not available; hard to distinguish from mortality and failure of nest establishment WA sites suggest shorter flight distances due to proximity to alfalfa fields	(Cane 2008)
Dispersal/migration	NA	NA	NA		
Foraging range	Foraging range	General	1.6 - 11.3 km		(Greenleaf et al. 2007)
Habitat features	NA	NA			
Geographical range	NA	General	Arid desert basins of Western North America		(Cane 2008)
Habitat classification/suitability	Nesting substrate	General	Soil-nesting in alkali/salty and moist soils		(Johansen et al. 1978; Cane 2008)

Table 65. External factors. Data for *N. melanderi* compiled. NA = Not applicable.

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Predation/herbivory	NA	NA	Parasite of female ovaries reported		(Bohart and Cross 1955)
Competition	NA	NA	NA		
Environmental conditions	NA	Realistic-precise	Optimum temperature for larval growth: 29.4 °C (85 °F); for prepupal development (post-diapause): optimum at 29 °C, range: 17-35 °C		(Cross and Bohart 1960; Stephen 1965; Vinchesi et al. 2013)
Stressors - pathogens	NA	NA	NA		
Stressors – abiotic, other	NA	NA	NA		
Existing management	NA	General	Populations (nest sites) managed for alfalfa populations		(Johansen et al. 1978; Cane 2008)
Indirect effects (obligatory relationships)	NA	NA	NA		

Table 66. Additional characteristics identified as important for solitary bees and their interactions with their environment. Data for *N. melanderi* compiled. NA = Not applicable.

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Nesting substrate / strategy	Nesting substrate	General	Soil nesting (below ground)		(Cane 2008)
Nesting material	Nesting material	General	Burrows in soil; brood cells at 15-20 cm depth (Batra)		(Batra 1970; Cane 2008)
Nesting material weight/size	NA	NA		No additional nesting material collected	
Pollen transport	Pollen transport	General	Legs and abdomen		(Cane et al. 2017)
Flower preference	Flower preference	General	Polylectic; in population managed for alfalfa pollination (WA), bees forage on alfalfa only		(Cross and Bohart 1960; Cane 2008; Cane et al. 2017)
Composition of food provision	NA	Realistic (incomplete)	4,068,000±184,000 alfalfa pollen grains per completed provision	Nectar not reported; total provision mass not reported	(Cane et al. 2017)
Composition of adult food	Adult food	Realistic-precise (incomplete)	Includes pollen irrespective of female bee age; 33,953±2440 alfalfa pollen grains in a full crop (volume = 34 mm <sup>3</sup> )	Nectar not reported	(Cane et al. 2017)

## Data summary for *Osmia*

Table 67. Organism-level characteristics of *O. lignaria*, *O. cornuta*, *O. bicornis* and *O. cornifrons*, and how the data compilation relates to the bee traits used in Schmolke et al. (2021). Complexity level of data is listed (general-realistic-precise). Remarks include notes about the four species in grey, as applicable. NA = Not applicable.

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Life span	Nesting period	Realistic	Range of post-emergent female life span: 6-39 days, average life spans: 20-25 days	Post-emergent female life span most important in the context of solitary bee life cycle Data for <i>O. cornuta</i> ; similar range reported for <i>O. lignaria</i> and <i>O. bicornis</i> ; no data for <i>O. cornifrons</i>	(Tepedino and Torchio 1982b; Frohlich and Tepedino 1986; Sugiura and Maeta 1989; Bosch 1994; Bosch et al. 2001; Bosch and Vicens 2005; Bosch and Vicens 2006; Bosch 2008; Sgolastra et al. 2016; Sgolastra et al. 2016) (Tasei 1973; Bosch et al. 2001; Bosch and Vicens 2006; Bosch et al. 2008; Steffan-Dewenter and Schiele 2008; Sgolastra et al. 2019; Wildbienen-Arten (Apidae): alphabetisch)
Reproductive/breeding season	Combination of emergence time and nesting period	General	Emergence in early spring (March – April, earlier/later dependent on temperature/region); reproductive season lasts for the female's adult life span	Temperature dependent; varies by species; reproductive season determined by time of emergence and female post-emergence life span Reported for all 4 species; of the co-occurring species: <i>O. cornuta</i> – early (March); <i>O. bicornis</i> - later (mid April)	(Bosch et al. 2001; Bosch et al. 2008; Steffan-Dewenter and Schiele 2008; Sgolastra et al. 2019; Wildbienen-Arten (Apidae): alphabetisch)
Reproductive frequency	Voltinism	General	Univoltine	No variability in this trait in the model <i>Osmia</i> species	(Bosch et al. 2001; Bosch et al. 2008)
Reproductive output/clutch size	Fecundity	Realistic	Species-specific: 1-35 eggs/female; average: 9-18 eggs/female; <i>O. lignaria</i> : 2-48 eggs/female, average: 21.2; 1-3 eggs/day	Egg laying rate corresponds to nest building rate; declines with female age and reduced resource availability; lifetime fecundity mainly dependent on nesting female life span Data reported for <i>O. lignaria</i> , <i>O. cornuta</i> , <i>O. pumila</i> and <i>O. bicornis</i> ; daily egg/cell production rate reported for <i>O. lignaria</i> and <i>O. cornuta</i> ; no data for <i>O. cornifrons</i>	(Bosch 1994; Goodell 2003; Bosch and Vicens 2005; Bosch and Vicens 2006; Bosch 2008; Bosch et al. 2008; Palladini and Maron 2014; Giejdasz et al. 2016; Sgolastra et al. 2016)

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Egg development time	NA	General-realistic	<i>O. cornuta</i> and <i>O. bicornis</i> : 7-8 days; <i>O. lignaria</i> : 7.1 – 9.8 days (females; males ~1 day shorter)	Temperature-dependent; under laboratory conditions (Tasei: 21 C in <i>O. cornuta</i> and <i>bicornis</i> ; Bosch and Kemp: different temperature treatments) No data for <i>O. cornifrons</i>	(Tasei 1973; Bosch and Kemp 2000; Bosch et al. 2008)
Larval development time	Larval feeding period	General-realistic	<i>O. lignaria</i> : I-IV instar 3.7 – 8.4 days, V instar 6.1 – 13.3 days; <i>O. cornuta</i> and <i>O. bicornis</i> : 24 – 40 days <i>O. lignaria</i> (females, males with slightly shorter development times): cocoon 2.3 – 9.3 days, prepupa 17 – 39.3 days, pupa 19.5 – 48.2 days, orchard: 33.6 days	Temperature-dependent; data from constant temperature regimens applied No data for <i>O. cornifrons</i>	(Tasei 1973; Westrich 1997; Bosch and Kemp 2000; Bosch et al. 2008; Sedivy et al. 2011)
Pupa (post-feeding) development time	NA	General-realistic		Temperature-dependent; data from constant temperature regimens applied (apart from orchard)	(Bosch and Kemp 2000)
Development egg - adult	NA	General-realistic	<i>O. lignaria</i> (females and males in orchard): egg-adult (in-nest) 97.1		
Onset of maturation	NA	General	Shortly after emergence (2-5 days after adult emergence; maturation corresponds to start of nest building); <i>O. lignaria</i> : 2-9 days (average 4.2 days)	Shortly after emergence, exclusively dependent on season/temperature	(Bosch et al. 2008; Sgolastra et al. 2016)
Hatching (eggs)/germination (seeds) rate	NA	Realistic-precise	Background mortality from parasitism/ predation: 11% (range: 5-18%); from developmental failure (unknown reasons): 10% (range: 6-14%); 10-15% (Sedivy et al., small sample size)	Mean across <i>Osmia</i> species; summarizes background mortality prior to overwintering period (egg-pre-emergent adult); Sedivy et al.: <i>O. bicornis</i> and <i>O. cornuta</i> survival to adult stage	(Bosch 1992; Bosch and Vicens 2005; Sedivy et al. 2011)
Immature transition rate (including metamorphosis) <sup>1</sup>	NA	Realistic-precise	Mortality during winter: 5% (range: 0-14%)	<i>O. lignaria</i> ; cocoon survival through emergence	(Bosch and Kemp 2000; Bosch et al. 2010; Sgolastra et al. 2011)
Sex ratio	NA	Realistic	<i>O. cornuta</i> and <i>O. bicornis</i> : 0-1; ~1.6-1.7 males per female (ratio ~0.38-0.59); <i>O. lignaria</i> : 0-1; average female ratio 0.4;	Sex ratio as female offspring per total offspring (reflects sex ratio of emerging bees); decline in female sex ratio with	(Bosch and Vicens 2005; Bosch and Vicens 2006; Seidelmann 2006; Seidelmann

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
			dependent on nesting female age and resource availability	nesting female age and resource availability No data from <i>O. cornifrons</i>	et al. 2010; Giejdasz et al. 2016; Sgolastra et al. 2016
Recruitment rate	NA	NA	NA	Covered by previous characteristics	
Survival rate	NA	General-realistic	From emerging females, 50-75% establish nests; adult female survival rate defined by length of life span	Failure of nest establishment assumed to correspond to mortality	(Bosch and Kemp 2002)
Growth rate	NA	NA	NA	Growth assumed to be directly determined by provisioning size	(Bosch and Vicens 2006)
Provision weight – females	NA	Realistic	<i>O. cornuta</i> : 5.89 x adult (dry weight); <i>O. cornifrons</i> : 8.33 x adult (dry weight); <i>O. lignaria</i> : 3.07 – 3.59 x adult (wet weight)	Neff (2008), Table I; for absolute weights refer to references therein	(Neff 2008)
Provision weight – males	NA			See females	
Body size - females	Body size	Realistic-precise	<i>O. lignaria</i> : 10-11mm length, 2.9mm ITD, 0.107-0.196 g (average: 0.158 g) wet weight; <i>O. cornuta</i> : 12-16mm length, 0.083-0.257g weight (range of averages from 3 study years, nesting females: 0.152-179g); <i>O. bicornis</i> : 10-13mm length, 3.3mm ITD, ~100mg weight; <i>O. cornifrons</i> : 2.9mm ITD	Adult body size; directly correlated with provision weight; smaller bees have a lower chance of emergence	(Westrich 1997; Bosch and Vicens 2006; Bosch et al. 2008; Sgolastra et al. 2016; Sgolastra et al. 2019; Hofmann et al. 2020; Species Osmia lignaria - Blue Orchard Bee; Wildbienen-Arten (Apidae): alphabetisch); discoverlife.org
Body size - males	NA	Realistic-precise	<i>O. lignaria</i> : 9-10mm length, 0.072-0.129 g (average: 0.099 g); <i>O. cornuta</i> : 0.065-0.219g (range of	See females	(Bosch and Vicens 2006; Sgolastra et al. 2016; Hofmann et al. 2020); discoverlife.org

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
			averages from 3 study years: 0.106-0.116 g)		
Seedling emergence; emergence after hibernation; emergence of new generation	Emergence time of females	General	Emergence in early spring (March – April, earlier/later dependent on temperature/ region)  <i>O. lignaria</i> , <i>O. cornifrons</i> , and <i>O.</i> <i>cornuta</i> : males emerge on average 2-4 days ahead of females; <i>O.</i> <i>bicornis</i> : males emerge ~2 weeks before females	Temperature and species dependent; see reproductive/breeding season	see reproductive/breeding season
Protandrous emergence	NA	General		Depends on temperature	(Bellman 1995; Bosch et al. 2008)
Dormancy duration (inactive life stages, e.g., hibernation, soil seed bank)	NA	General	<i>Osmia</i> overwinter as pre-emergent adults; pre-pupal stage also goes through a period of dormancy	Timing defined by nest production, development times and emergence time	(Bosch et al. 2008)

Table 68. Population and spatial characteristics. Data for *O. lignaria*, *O. cornuta*, *O. bicornis* and *O. cornifrons* compiled. NA = Not applicable.

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Density dependence	NA	General	Nest sites limiting, floral resources limiting	Density dependence due to nest site limitation/increased parasitism rate in high nest densities found inconsistently across studies, floral resource limitation hypothesized (but not limited to intra-specific competition)	(Rosenheim 1990; Steffan-Dewenter and Schiele 2008; Dainese et al. 2018; Farzan 2018; Groulx and Forrest 2018)
Population size	NA	NA	NA	Data for unmanaged populations not available	
Spatial Metapopulation structure	NA	NA	NA	No data available for use in model	
Dispersal/migration	NA	NA	NA	Quantitative data on dispersal not available; hard to distinguish from mortality and failure of nest establishment	(Bosch and Vicens 2006; Bosch et al. 2008)
Foraging range	Foraging range	General	0.4 – 1.2 km across Osmia sp.; Hofmann et al., Table 2: <i>O. bicornis</i> : ~0.1 km (max. 0.25 km), <i>O. cornuta</i> : ~0.1 km (max. 0.7 km) Open areas such as parks, agricultural landscapes, etc.; floral resource availability linked to bee abundance	Range appears similar across model species	(Greenleaf et al. 2007; Zurbuchen et al. 2010; Hofmann et al. 2020; Kratschmer et al. 2020)
Habitat features	NA	General-realistic	Europe in temperate climates; introduced to/managed in orchards		(Bellman 1995; Steffan-Dewenter and Schiele 2008; Dainese et al. 2018)
Geographical range	NA	General			(Bellman 1995; Bosch et al. 2008)

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Habitat classification/suitability	Nesting substrate	General	Nest above-ground in pre-existing cavities		(Bosch et al. 2001)

Table 69. External factors. Data for *O. lignaria*, *O. cornuta*, *O. bicornis* and *O. cornifrons* compiled. NA = Not applicable.

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Predation/herbivory	NA	NA	Background mortality from brood parasitism estimated 11% (range: 5-18%)	Brood parasitism assumed constant	(Bosch 1992)
Competition	NA	NA	NA		
Environmental conditions	NA	General	Winter conditions (weather) may influence emergence rate	From laboratory studies; cumulative weather data	(Bosch and Kemp 2000; Bosch and Kemp 2004; Bosch and Vicens 2006; Bosch et al. 2010; Sgolastra et al. 2011; Schenk et al. 2018)
Stressors - pathogens	NA	NA	NA		
Stressors – abiotic, other	NA	NA	NA		
Existing management	NA	General	Management of orchard populations		(Bosch et al. 2008)
Indirect effects (obligatory relationships)	NA	NA	NA		

Table 70. Additional characteristics identified as important for solitary bees and their interactions with their environment. Data for *O. lignaria*, *O. cornuta*, *O. bicornis* and *O. cornifrons* compiled. NA = Not applicable.

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Nesting substrate / strategy	Nesting substrate	General	Above-ground nests in existing cavities		(Bosch et al. 2008)
Nesting material	Nesting material	General	Soil/mud used for cell partitions and nest plugs		(Bosch et al. 2001; Bosch et al. 2008)
Nesting material weight/size	NA	Precise	<i>O. cornuta</i> : Bosch 1994: 110 +/- 30 mg dry weight (4.41 mud loads); Bosch and Vicens 2005: ~90 mg	See Bosch 1994, Table II; note that other mud structures (initial and vestibular partition, terminal plug are larger); Bosch & Vicens 2005: no difference between female and male cells	(Bosch 1994; Bosch and Vicens 2005)
Pollen transport	Pollen transport	General	Abdomen: Megachilidae have hairs (scopa) on the underside of their abdomen for pollen transport, rather than on their legs (like many other bee species)		(Michener 2007)
Flower preference	Flower preference	General	Polylectic; location-specific information on pollen composition of provisions available	Level of flower preference may vary between species; polylecty does not mean that bees forage on all flowers	(Bosch 1994; Bosch et al. 2001; Sedivy et al. 2011; Peters et al. 2016; Ruddle et al. 2018; Ryder 2019; Sgolastra et al. 2019; Bosch et al. 2021; Bednarska et al. 2022)

Characteristic	Trait (from bee trait table, Schmolke et al. 2021)	Complexity level of data	Data summary	Remarks	References
Composition of food provision	NA	General-precise	<i>O. bicornis</i> : average sugar content in control provisions: 39.2+/-4.9% (Ruddle et al. 2018); <a href="#">European Food Safety Authority (EFSA) et al. (2023)</a> : consumption during larval stage: <i>O. bicornis</i> : 91 mg sugar, 80.7-92.5 mg pollen; <i>O. cornuta</i> : 165 mg sugar, 80.7-92.5 mg pollen	Bosch (1994): reports pollen grains per provision; Ruddle et al. 2018: average of 3 samples; average was higher in treatments (45.7+/-17.3%); variability between dates; <a href="#">European Food Safety Authority (EFSA) et al. (2023)</a> : assumption that nectar contains 30% sugar	(Bosch 1994; Ruddle et al. 2018); Ruddle et al. 2018: from data tables (not paper), not reported if by weight or volume; <a href="#">European Food Safety Authority (EFSA) et al. (2023, Table 16)</a> .
Composition of adult food	NA	General	Includes pollen irrespective of female bee age	From gut content of <i>O. cornifrons</i>	(Taniguchi 1956; Cane 2016)

# APPENDIX B

In SolBeePop<sub>ecotox</sub>, weather, floral resource availabilities in the landscape and the concentration of a pesticide in bee-relevant matrices are considered. Environmental conditions influence brood cell production in nesting females. Pesticide exposures can affect survival of post-emergent females and brood (females and males). The environmental conditions and pesticide concentrations are defined by the input file (*input.floral*) that includes nine input time series. They correspond to daily definitions of weather-related foraging opportunities, resource quality from crops and wildflowers, respectively, and the proportion of foraging on either of those resources. The concentrations of pesticides are defined separately for nectar and pollen originating from a treated crop, i.e., the same crop that is defined in the resource quality time series. In addition, the concentration of the pesticide in a direct spray application is defined as well as in nesting materials (soil for soil-nesting bees and bees that use soil or mud for above-ground nest construction and leaves for leaf-cutter bees). The input time series make it possible to summarize the floral resource availability derived from the landscape composition within a species' foraging range. The pesticide exposure depends on the daily pesticide concentrations in bee-relevant matrices and the proportion of use by the bees. Thus, the spatial landscape composition can be captured implicitly in the input to the model. Temporal dynamics related to flower phenology and application timing can be captured on a daily basis. While detailed information about the bee species' foraging preferences and landscape composition can be translated to the input, simplified inputs in the absence of quantitative information can also be generated.

In the following, the content of the input file is described in detail. We provide a description of how an input file can be generated for hypothetical scenarios as well as realistic weather conditions and landscapes. For simulations over multiple years in which conditions are variable between years, an input file for each simulated year needs to be generated. We address how multiple input files can be used by the model using the *MultiYearInput* setting of the model. Citations listed in the Appendix are included in the Reference list.

## Description of the foraging and floral resource input file

The input file to the model defines a time series of daily foraging and floral resource quality values. An input file must contain 366 rows with the first row stating the column headers and the 365 subsequent rows including the daily data. The input is organized in five columns (in the format ".csv") as listed below.

1. "doy" – Day of year as a numerical (1 – 365)
2. "Prop\_foraging\_day" – The proportion of a given day available for foraging. This value reflects the daily weather and can take values between 0 (no foraging due to inclement weather) and 1 (bees can forage the maximum daily duration).
3. "Quality\_crop" – Daily floral resource quality of a flowering, bee-attractive crop. The quality summarizes the distance of the flowering crop from the nesting location and the resource availability within the patch (field). Values can range between 0 (no flowering crop within the

foraging distance of the bee) and 1 (highly attractive flowering crop within short distance from nest the location).

4. “Quality\_nat” - Daily floral resource quality of non-crop wildflower resources within the foraging range of the bee. The quality summarizes the distance of the areas with flowers from the nesting location and the resource availability within the (closest and/or most attractive) areas. Values can range between 0 (no non-crop flowers within the foraging distance of the bee) and 1 (highly attractive flowers within short distance from the nest location).
5. “Prop\_foraging\_crop” – Daily proportion of foraging on crop. The foraging on wildflower (non-crop) resources corresponds to (1 – Prop\_foraging\_crop).
6. “Concentration\_nectar” – Daily concentration of a pesticide in nectar ( $\mu\text{g a.i./g}$ ) from the defined crop (treated flowering, bee-attractive plants which correspond to “Quality\_crop”).
7. “Concentration\_pollen” - Daily concentration of a pesticide in pollen ( $\mu\text{g a.i./g}$ ) from the defined crop (treated flowering, bee-attractive plants which correspond to “Quality\_crop”).
8. “Concentration\_spray” – Concentration of pesticide in direct spray from an application (mg a.i./L = ng a.i./ $\mu\text{L}$ ). The concentration corresponds to the application rate but needs to be given in the stated unit.
9. “Concentration\_nest\_mat” – Daily concentration of pesticide in soil ( $\mu\text{g a.i./g}$ ) used for nesting (soil-nesting bees and bees using soil or mud for above-ground nest construction). The concentration depends on the location of the nests relative to the treated crop and the depth of the nest (for soil-nesting bees). This input time series is unused in simulations of leaf-cutter bees.
10. “Concentration\_leaf” – Daily concentration of pesticide on leaves ( $\mu\text{g a.i./cm}^2$ ) used for lining of brood cells (leaf-cutter bees). This input time series is unused in simulations of soil-nesting bees and bees using soil or mud in nest construction.

*Table 71. Partial example input file (from simulations of the Eurofins 2021 semi-field study with exposures from a dimethoate application). The input file was generated for the simulation of a semi-field study in which floral resources are exclusively available from the flowering crop (oilseed rape) in the net tent (tunnel).*

doy	Prop_foraging_day	Quality_crop	Quality_at	Prop_foraging_crop	Concentration_nectar	Concentration_pollen	Concentration_spray	Concentration.nest.mat	Concentration.leaf
1	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
129	1	1	0	1	0.06525	5.0775	855	0.093466667	0
130	1	1	0	1	0.039006412	3.035326553	0	0.068	0
131	0	1	0	1	0.023318011	1.814516452	0	0.030833333	0
132	1	1	0	1	0.013939493	1.084716882	0	0.020186667	0
133	1	1	0	1	0.008333021	0.648443122	0	0.019253333	0
134	1	1	0	1	0.004981475	0.387638922	0	0.018246667	0
135	1	1	0	1	0.002977923	0.231730323	0	0.014993333	0
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

*In*

**Table 71**, a few example rows of an input file generated for the simulation of a semi-field study (Eurofins 2021 semi-field study with *O. bicornis* and dimethoate exposure; see also Section 7.2). The input file captures a simple landscape with only one resource patch available to the bees for foraging. The resource was a mass-flowering crop (oilseed rape) which was in full bloom during the field phase of the study. The nesting location and the resource were directly adjacent to each other within the net tent (tunnel) installed for the study, and thus, the bees were assumed to a very small travel distance between nest and resource. Although foraging on oilseed rape only may not fully correspond to foraging preferences by *O. bicornis* (Sedivy et al. 2011; Peters et al. 2016; Ruddle et al. 2018; Ryder 2019; Bednarska et al. 2022), we assumed that that availability of floral resources from the crop was optimal within the tunnel, i.e., we assigned Quality\_crop = 1 for all days of the tunnel phase of the study. No wildflowers were present within the tunnel and bees could not fly beyond the tunnel, thus Quality\_nat = 0 for all days and all foraging occurred on crop (Prop\_foraging\_crop = 1 during the tunnel phase). We had daily weather data available for the study location, including maximum air temperature (°C), amount of precipitation (mm) and relative air humidity (%). For *O. bicornis*, we could identify threshold definitions of minimum temperature and maximum humidity suitable for foraging (Seidelmann et al. 2010; Franke et al. 2021). In addition, general threshold definitions for weather conditions suitable for foraging across bee species in blueberry fields (Drummond 2016; Drummond et al. 2017) were used for maximum wind speed and precipitation due to lack of species-specific information (see also file "SolBeePop\_ecotox\_Tables.xlsx", Foraging parameters). Because the information on *O. bicornis* weather-related foraging was limited to thresholds, we took the simplifying assumption that any day with weather conditions within the thresholds for suitable foraging conditions meant that the bees were limited in foraging due to weather during that day, i.e., Prop\_foraging\_day = 1. If any weather condition was beyond a threshold defining suitable conditions for *O. bicornis*, no foraging on that day was assumed, or Prop\_foraging\_day = 0. The tunnel phase of the study started on 23 April or day-of-year (doy) 129 and ended on 26 May (doy 146). Dimethoate was applied as a spray application during hte day on 9 May (doy 129). The concentration of dimehoate in nectar and pollen was estimated from the application rate on the first day (day of spray application) and a kinetic function was applied to estimate the exposure during the rest of the tunnel phase (see Section 7.2.4). The exposure from direct spray was only occurred on the day of application. We assumed that the bees collected the soil used for the construction of brood cell partitions within the treated area, and estimated residues in hte top soil layer using a standard fate model approach (see Section 7.2.4). Leaves are not used as nesting material by *O. bicornis*, and no exposure was assumed from that route. Because no bee activity occurred outside the date range of the tunnel phase, the foraging and floral resource did not need to be defined for all other dates, and daily values of Prop\_foraging\_day, Quality\_crop, Quality\_nat and Prop\_foraging\_crop as well as the columns defining exposure were set to 0. The input file without exposure time series was generated using the R-script "Foraging\_Landscape\_InputSce\_SolBeePop2022.R" which is addressed below (Generating an input file). The exposures were added using a separate script specific to dimethoate exposure assumptions.

Exposures from the input file define the concentrations of a pesticide in nectar and pollen from the treated crop. Thereby, Prop\_foraging\_crop defines the proportion of food originating from the crop, and thus, is exposed. The concentration of the pesticide in the food consumed by the adult bees and in the brood provisions, respectively, are reduced accordingly if Prop\_foraging\_crop < 1. In addition, Prop\_foraging\_crop defines the probability of an individual adult bee to be exposed to direct spray on the day of application (only one application per day can be simulated). Exposure concentrations in

nesting material are assumed to apply to all used nesting material (irrespective of Prop\_foraging\_crop). The ultimate exposure of each individual bee and brood provision depends on the transfer factors defined as model parameters.

The input used for the simulation of a semi-field study is an example for a realistic input generated for a specific study with a very simple landscape. Further analysis of the model will include the representation of realistic landscape scenarios through input files derived from landscape- and species-specific data. The scenarios can be reflected by variability in resource availability or quality (Quality\_crop and Quality\_nat) between days and quality definitions that fall between 0 and 1. The quality of a resource from the perspective of a foraging bee may be driven by multiple factors. The distance between nest location and resource patches has been recognized as important, i.e., affecting brood sex ratio and production rates (Peterson and Roitberg 2006b). Correspondingly, longer foraging times within a flower patch would also be expected to affect reproductive rates of nesting females. Foraging times needed within a patch may be influenced by flower density and time required to extract pollen or nectar from a flower type. Such relationships have been reported for honey bees (Winston 1987) but detailed information is rarely available for solitary bee species.

To represent a realistic landscape, the location of the nesting site should be defined first. The landscape composition around the nesting site can then be categorized whereby the relevant radius around the nest location is defined by the foraging range of the bee species (see Appendix A, Table 56, Table 60, Table 64, and Table 68 for the foraging ranges of the model bee species). If detailed landcover data for the identified relevant area are available, landcovers containing flower species can be identified that could be attractive to the simulated bee species. Patches with high attractiveness to the species occurring in close proximity to the nest location can be assumed to have the highest quality during flowering. The quality of patches can be assumed to decline with distance from the nest location. A simple assumption could be a linear decline in quality with distance whereby the quality reaches 0 at a distance corresponding to the maximum foraging range. A patch at a distance half the foraging range could accordingly be assumed to have a resource quality of 0.5, or Quality\_crop = 0.5 if the patch is a crop or orchard, Quality\_nat = 0.5 if the patch has a (semi-)natural landcover. For a mass-flowering crop, Quality\_crop > 0 during crop flowering, and Quality\_crop = 0 for all other days. Similar assumptions can be applied to patches containing (mixed) wildflowers. However, mixed flower patches generally provide resources over extended time periods to polylectic species. Multiple patches within the foraging range can be combined by using either the average or maximum estimate of floral quality across patches for each day. For instance, if multiple crops attractive to the bee species are present in the relevant area, the closest patch (field) with flowering can be used as proxy for resource quality from crop for any given day. This can be applied to wildflower patches as well.

Alternatively, detailed information on pollen compositions of provisions collected by nesting bees can be used to inform the input. The pollen composition can inform what resources are used by bees on a given day (because each provision can be assumed to be collected within one day, at most over two days). Plant species identified in the provisions can be matched to landcover types in the landscape and the flowering phenology of the plants. In addition, the pollen composition of provisions can indicate whether a species may exploit only one resource on a given day or tend to collect pollen from a range of flower species even if one resource is plentiful.

Note that resource qualities only have to be defined for the date range corresponding to the active season of the simulated bee species. During times in which no bee could be active, daily values can be set to 0.

For the definition of proportional foraging on a given day, more detailed information on the foraging preferences of a species or hourly weather data can be used. For instance, if a species is reported to initiate foraging only if temperatures reach at least 10 °C, hourly weather data could inform whether the entire foraging period of the bee species is available on a given day or temperatures only exceeded the threshold for a proportion of its foraging day. Similarly, precipitation events may be limited to a few hours of the day and still allow foraging for parts of the day. Note that this also requires information about when during the day a species is foraging. Many solitary bee species appear to be foraging for nectar and pollen only during limited times of the daylight hours (Danforth et al. 2019). As for the resource qualities, weather-related foraging suitability (proportion of the day available for foraging) only needs to be defined in the input file during date ranges simulated bees are active (post-emergent bees present). During times in which no bee could be active, daily values can be set to 0.

## Generating an input file

With the model code, we are also providing an R-script (R Core Team 2022) (“Foraging\_Landscape\_InputSce\_SolBeePop2022.R”, Schmolke et al. 2023) that was used to generate study (and weather) specific input files for the simulation of the semi-field studies (see Section 7.1). The script reads in weather data that provides 365 days of daily values for maximum air temperature, amount of precipitation and relative air humidity. No data on wind speeds were available and thus, were not used for the input file generation. The thresholds for minimum temperature for foraging, maximum amount of precipitation and maximum humidity applicable to the study species can be set in the script.

In addition to weather data, the crop flowering dates, and quality can be set as well as for the wildflower resources. The script would need to be extended for generating inputs with variable floral qualities or intermittent floral resource availability. In addition, the script would need to be expanded to definition of exposures as needed.

## Use of multi-year inputs

Simulations of multiple years with the model can be set up to use the same yearly input file for each simulated year or specified input files for each year. If *MultiYearInput* is switched “Off,” the model read in a single input file as described above. The file name of the input needs to be specified on the SolBeePop interface (*input.floral*). The number of years simulated are specified by *Num.repeat.yr*: in each of those years, the same input file is used as daily time series.

Setting *MultiYearInput* to “On” makes it possible to run multiple years with the model, applying a different input file in each simulated year. The input files used are defined in a csv file (comma separated values). An example is provided in Table 72. The file contains 3 columns and at least two rows. The first row states the column headers and is not used by SolBeePop. Each following row lists the name of an input file (following the file format for *input.floral*) and two parameters related to density dependence, *DD.thresh* and *DD.max.cells*. The number of rows in the file corresponds to the number of years simulated by the model (minus the header row). The two density dependence parameters overwrite the values of the same parameters on the interface. The setting of the density dependence

thresholds makes it possible to simulate variability of availability of nesting space between years. Multiple year inputs have not been used in the simulation results presented in this TRACE document.

*Table 72. Example file (List.input.floral) for the simulation of multiple years with SolBeePop in which input times series differ between simulated years. A file in this format is required if MultiYearInput = “On”. Using the example as List.input.floral would result in 10 simulated years.*

Filename	DD.thresh	DD.max.cells
Floral_generic_optimal.csv	250	1000
Floral_generic_Sce2.csv	250	1000
Floral_generic_Sce3_Nomia.csv	250	1000
Floral_generic_optimal.csv	250	1000
Floral_generic_Sce2.csv	250	1000
Floral_generic_Sce3_Nomia.csv	500	2500
Floral_generic_optimal.csv	500	2500
Floral_generic_Sce2.csv	500	2500
Floral_generic_Sce3_Nomia.csv	500	2500
Floral_generic_optimal.csv	500	2500