SolBeePop

Population model for solitary bees in agricultural landscapes

TRACE documentation

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The documentation of the model SolBeePop 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.nlogo), files referred to in this documentation as well as scripts used for model simulations and analysis are available on GitHub: https://github.com/Waterborne-env/SolBeePop

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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.

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. The conceptual model addresses the representation of solitary bee populations based on their ecological traits. The current concept does not include exposure and effects of pesticides but is developed for including theses as future extension.

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.
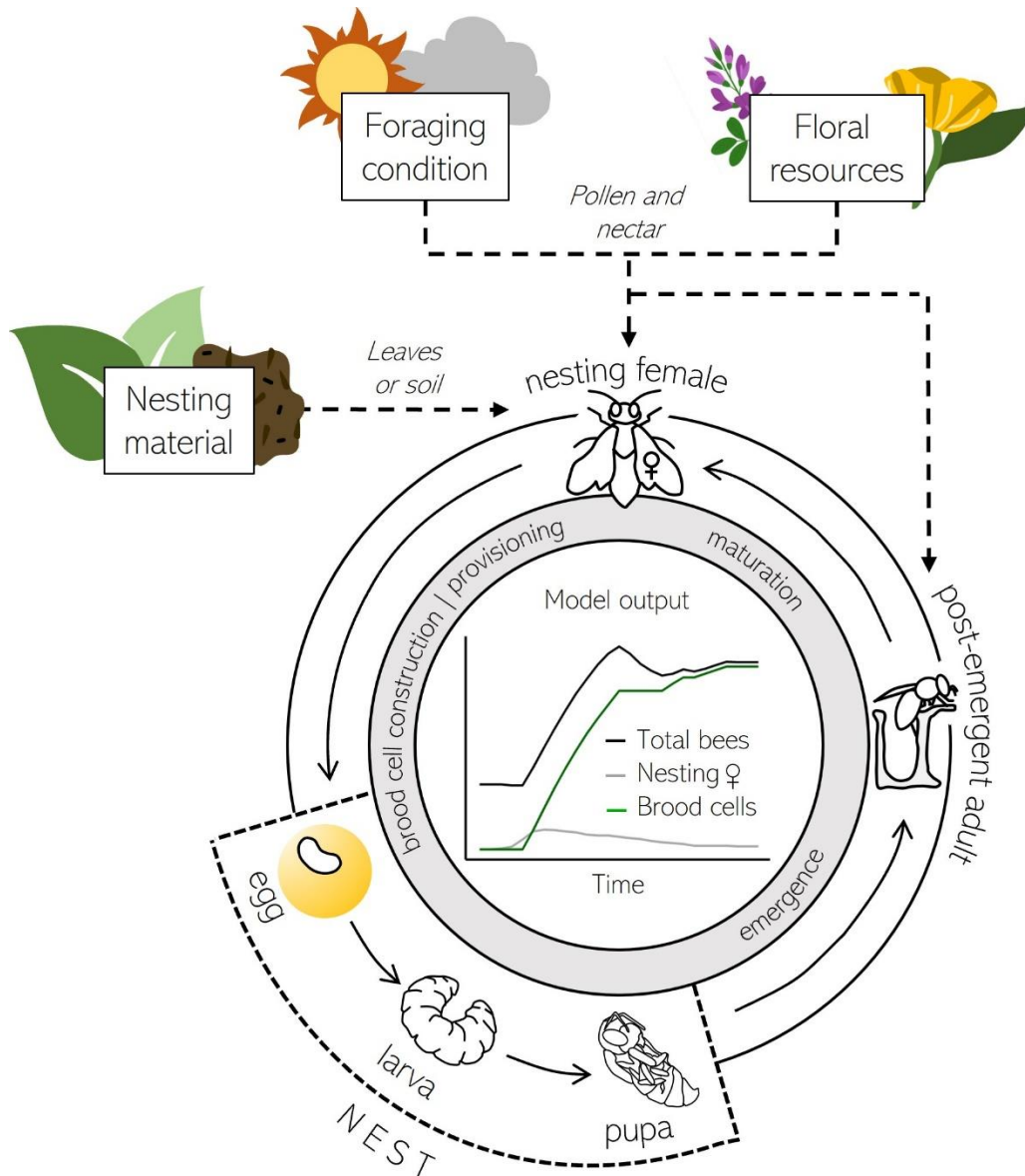
Figure 1. Graphical representation of the completed conceptual model for SolBeePop.

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. 2019). 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.
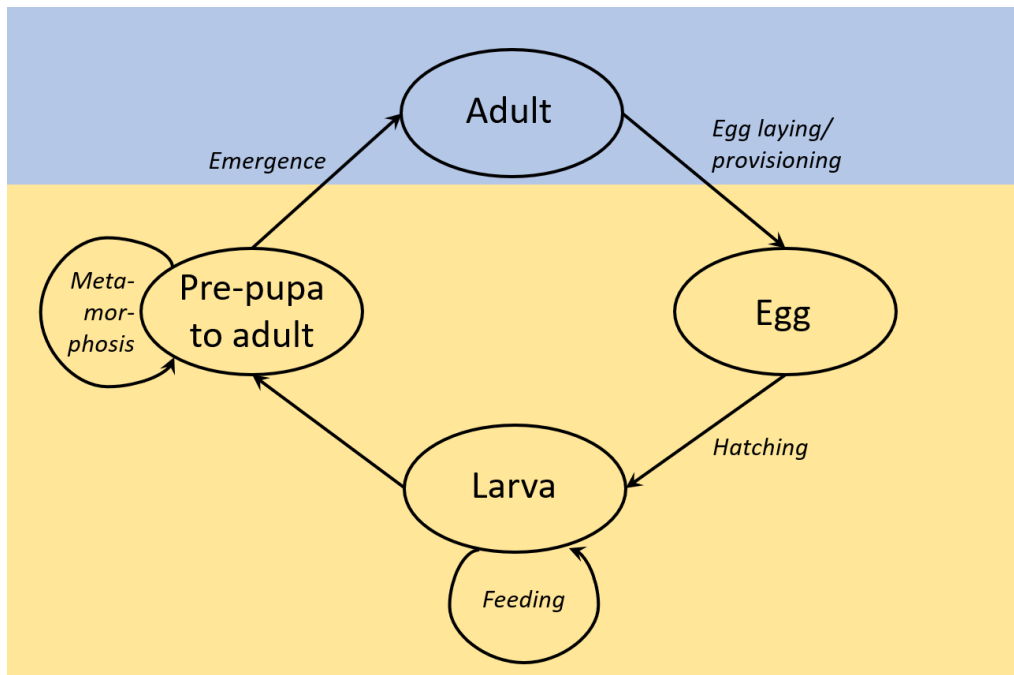
Figure 2. Generalized life cycle representation of solitary bees for the model. The stages from pre-pupa (5ᵗʰ larval instar after the larva ceased feeding) to adult prior to emergence from the nest are combined. Overwintering (dormancy) may occur either in pre-pupal or adult stage, dependent on species. 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).
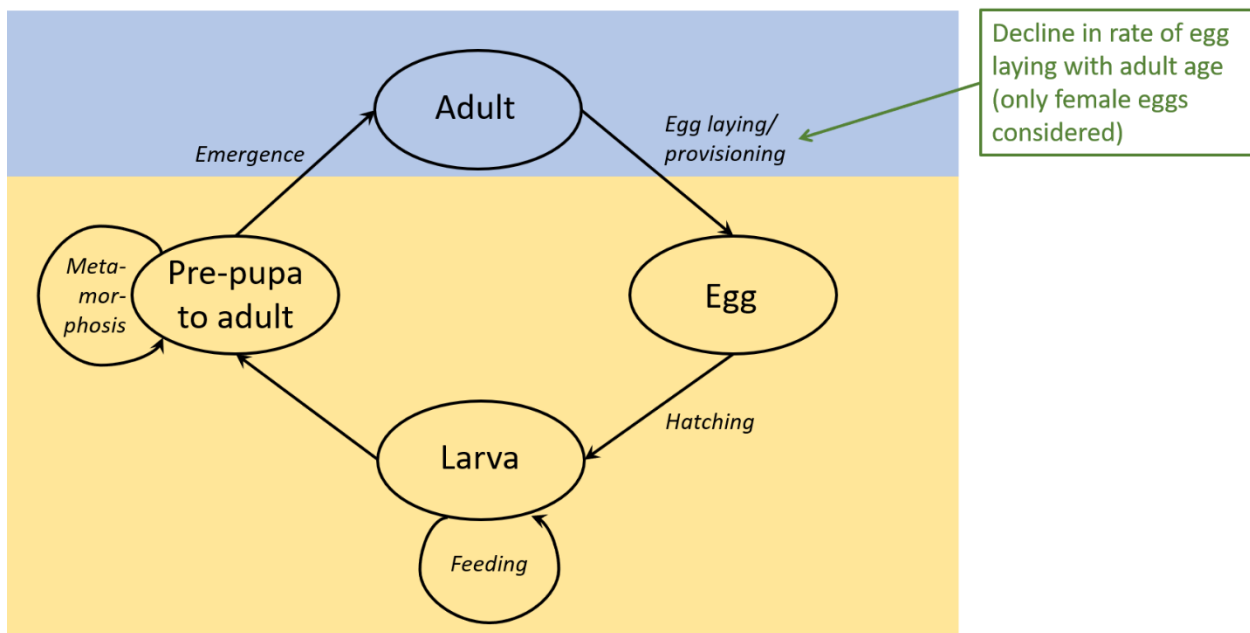
Figure 3. Rate of egg laying is declining with the age of the nesting female.

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

	Question	Yes	No
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 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. For the estimation of the strength of intra-specific competition for floral resources, no specific data are available to inform the model.

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 *other than* migration 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).
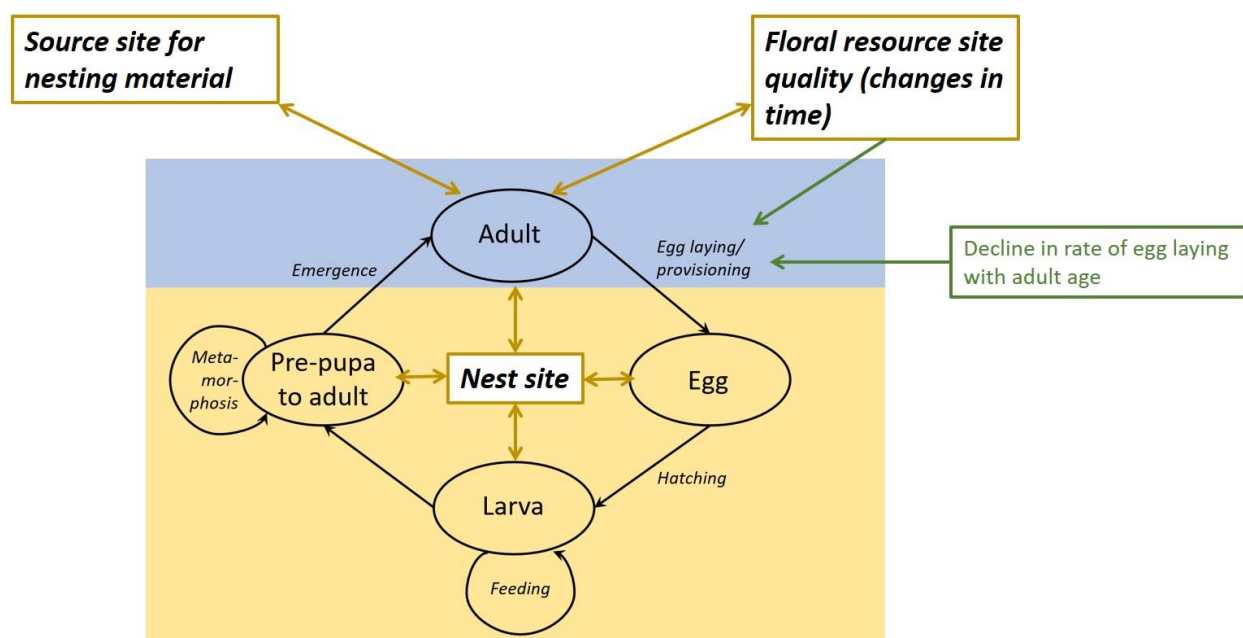
Figure 4. Representation of habitat types used by the solitary bees in the model.

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	
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	Categorical or qualitative impacts to diet could be	

		vital rate estimates to add precision	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

	Question	Yes	No	Remarks
	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 oligolectic 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

The current conceptual model focuses on capturing the life cycle of multiple solitary bees and its interaction with the floral resource availability in the landscape. Exposure and effects of pesticides are not addressed with the current concept.

Temporal Representation

	Question	Yes	No
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. The model was developed to allow the future extension with pesticide exposures via different, species-specific routes and 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*). Post-emergent bees have a daily 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. 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_Tables.xlsx."

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 5th 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.

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 specie 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 (*emerge.doy*) of each simulated bee is chosen from a normal distribution defined by the inputs *day.emerge.f* or *day.emerge.m* (mean emergence day) and *var.emerge.f* or *var.emerge.m* (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, *max.survival.e.f* or *max.survival.e.m* (egg through emergence, model parameter) for females and males, respectively, and the relative provision size, *prov.size.*
Female survival from emergence to first nesting	2.4.1. Life cycle	Females' probability (*emerged.survival*, 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.

Stochastic process	Submodel	Description
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): *sex.ratio* corresponds to the probability of a female offspring.
Foraging decision		If *stoch.crop.forag* 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.

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*). See file SolBeePop_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).

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.maturation*). 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 (5th 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.survivale.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.maturation* 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

> *cell.age = a.cell.age × 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

> *cell.res = a.cell.resource × prov.today + (1 − 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

> *cell.prod = max.cells × cell.age × 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

> *sex.age = a.sex.age × 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

　　　sex.res = a.sex.resource × prov.today + (1 – a.sex.resource)

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

Equation 2.6

　　　sex.ratio = max.f.ratio × sex.age × sex.res

If *cell.prod* ≥ 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

　　　size.age = a.size.age × age.stage + 1

Equation 2.8

　　　size.res = a.size.resource × prov.today + (1 – a.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

　　　prov.size = size.age × size.res

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

Equation 2.10

　　　e = max.survival.e × 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 5.

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

- *DD.max.cells.s*: maximum number of brood cells that could fit (theoretically) into the nesting site.
- *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 5, 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

$$(DD.max.cells.s - DD.thresh.s)/2$$

No reduction in brood cell production rate occurs if the total number of bees in in-nest life stages (*occ.cells*) is below the threshold (*DD.thresh*). If the number of bees in in-nest life stages exceeds the threshold, the factor for the brood cell production rate reduction, *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 5, Bottom). The slope of the logistic function is defined by the input parameter *DD.log.slope*.

Equation 2.12

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

Equation 2.13

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

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.
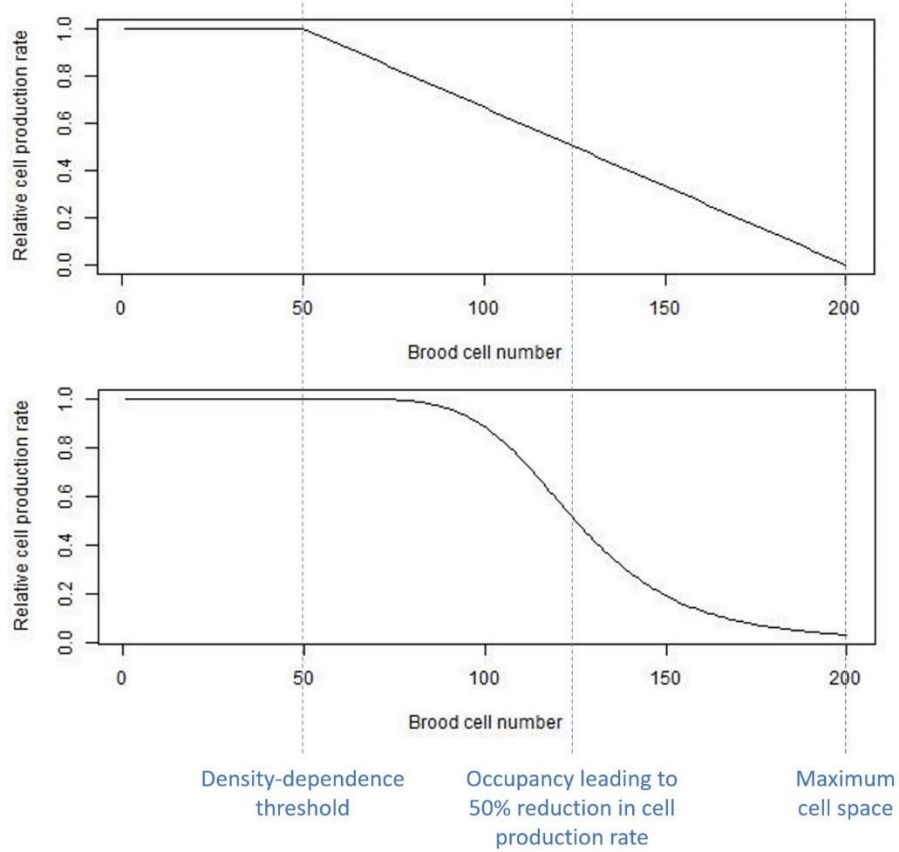
Figure 5. Function shapes for the relationship between brood cell number (number of bee agents in pre-emergent life stages) and the relative reproductive rate of nesting females. Top: linear relationship. Bottom: logistic relationship.

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 6. 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 ± SE) of O. cornuta by study year and half season (data from Bosch and Vicens 2005, Table 1). The proportional difference, Δ brood cells, is calculated as (brood cells (H2) −brood cells (H1))/brood cells (H1).

Study year	Brood cells H1	Brood cells H2	Δ brood cells	Δ age	*a.cell.age*
1994	0.78 ± 0.03	0.61 ± 0.04	-0.218	26	-0.008
1995	0.59 ± 0.03	0.53 ± 0.04	-0.102	25	-0.004
				Average:	-0.006
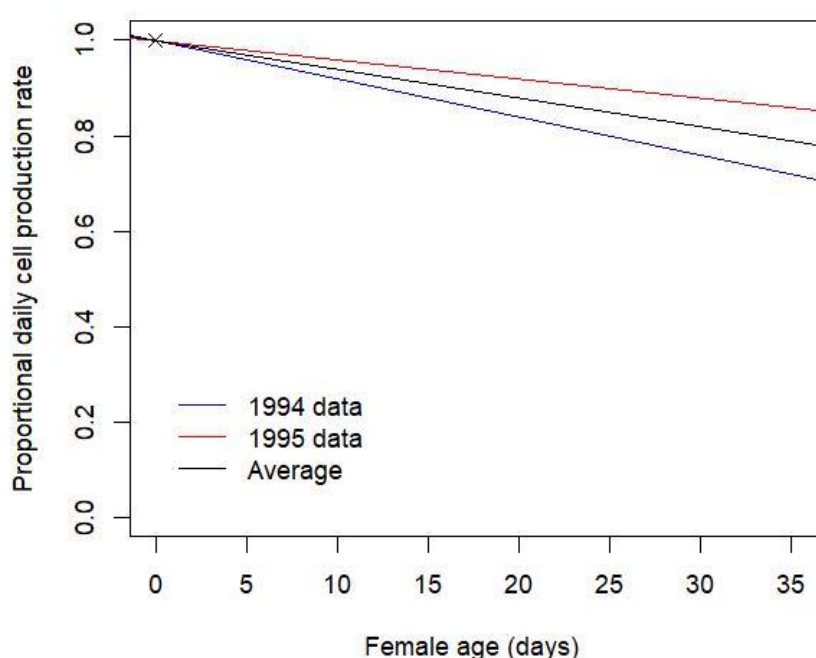
Figure 6. Linear relationship between days into O. cornuta nesting season (corresponding to nesting female age) and production of brood cells/female/day by study year and half season (data from Bosch and Vicens 2005, Table 1). The relationship is assumed to be proportionally declining from the maximum 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.

Equation 3.2   *a.cell.resource = Δ cells / Δ resource*

Equation 3.3   *Intercept = 1 – a.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 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 7, 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 7, 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, Δ 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	Δ brood cells	Δ resource	*a.cell. resource*	Intercept
Goodell 2003	*O. pumila*	Absent	1.16		1.55	0.252	0.296	0.851	0.149
Goodell 2003	*O. pumila*	Present	0.85		1.45	0.414	0.296	1.399	-0.399
Kim 1999	*M. apicalis*	--	1.24 ± 0.08 (SE)		1.58 ± 0.08 (SE)	0.215	0.5	0.43	0.57
Peterson and Roitberg 2006	*M. rotundata*	--	0.20	0.41	1	0.8 (high to low)	0.75 (high to low)	1.07	-0.07
							Average:	0.94	0.063
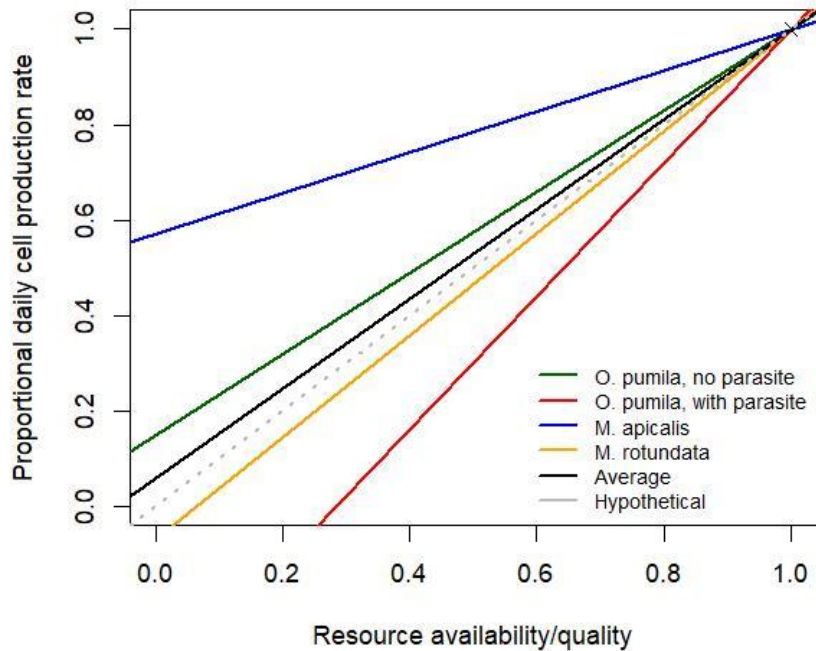
Figure 7. Linear relationship between resource availability (or quality) and production of brood cells/female by study (data for O.pumila from Goodell 2003; data for M. apicalis from Kim 1999; data for M. rotundata from Peterson and Roitberg 2006). The average uses the average steepness across data sets 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 = Δ sex ratio / Δ 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 8 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, Δ 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	Δ sex ratio (f/(f+m))	Δ 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
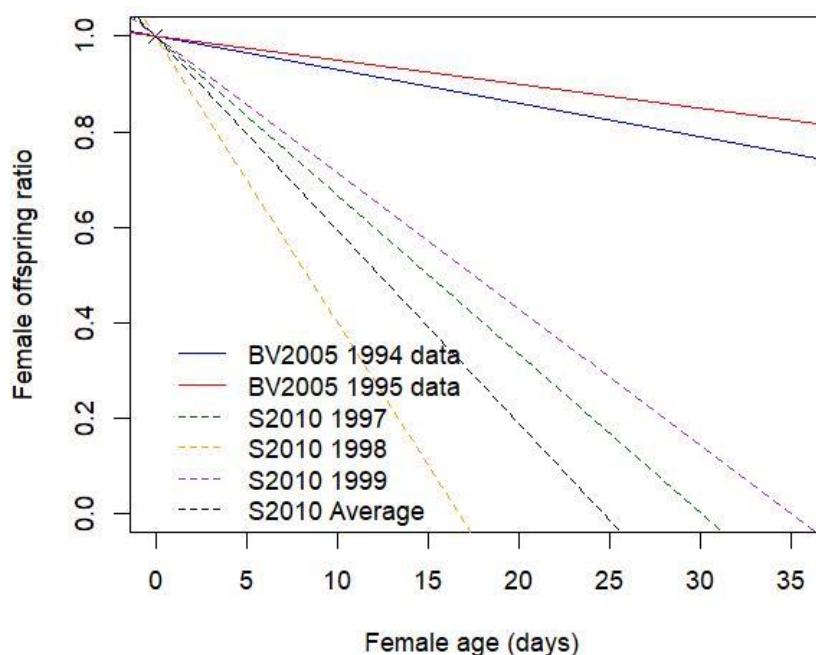
Figure 8. Linear relationship between days into O. cornuta nesting season (corresponding to nesting female age) and ratio of female offspring produced by study year and half season (BV2005, data from Bosch and Vicens 2005, Table 1) and data on O. bicornis from Seidelmann et al. (2010), Table 3 (S2010). 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 ± 0.1 offspring were female in nests 1, declining to 0.3 ± 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 = Δ sex ratio / Δ 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 9 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	*a.sex.resource*	Intercept
0.29 ± 0.09	0.5 ± 0.08	0.21 ± 0.09	0.5	0.42	0.58
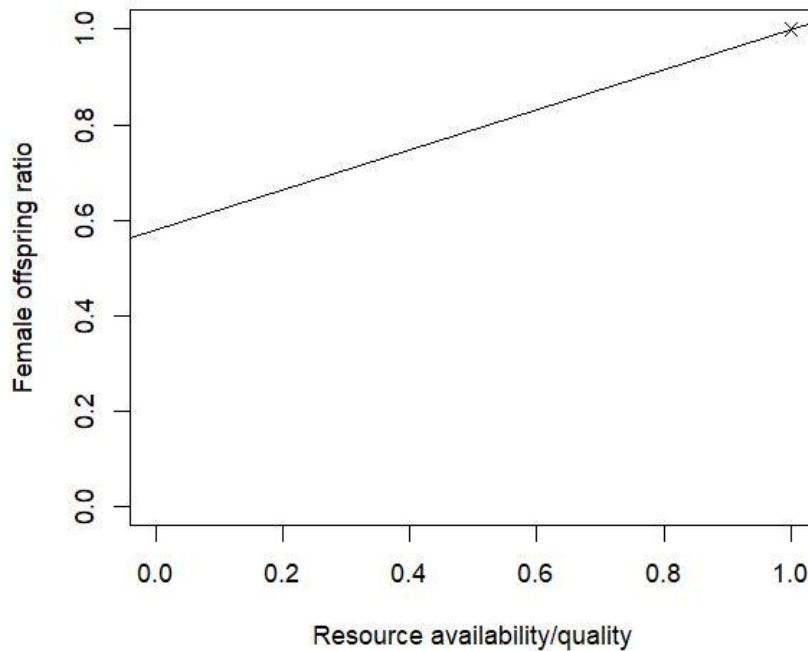
Figure 9. Linear relationship between relative resource availability and ratio of female offspring produced by M. apicalis (data from Kim 1999). The maximum female offspring ratio is assumed to occur under optimal foraging conditions and floral resource availability.

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 10 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 +/- 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 10.

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, Δ 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 ± SE)	H2 (weight in mg; mean ± SE)	Δ size	Δ age (days)	*a.size.age*
BV2005	1994	182.9 ± 2.4	158.9 ± 5.2	-0.126	26	-0.005
BV2005	1995	189.4 ± 4.0	180.1 ± 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
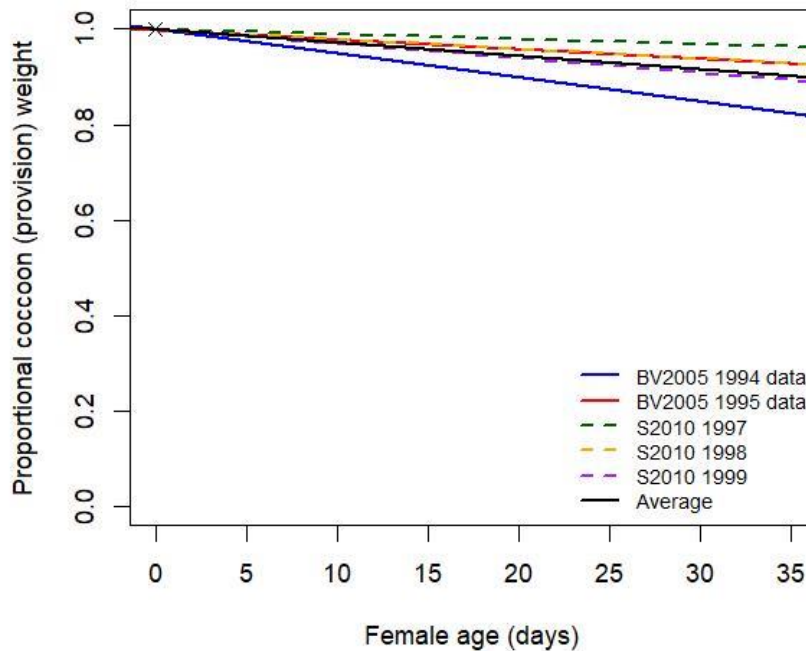
Figure 10. Linear relationship between days into nesting season (assumed to correspond to nesting female age) and female offspring cocoon/provision weight. BV2005: data from the study by Bosch and Vicens (2005) conducted over 2 years with O. cornuta. S2010: data from the study by Seidelmann et al. (2010) 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 11. 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).

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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 Δ size = (high − low)/high.

Female code	Low floral resources	High floral resources	Δ size	Δ 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
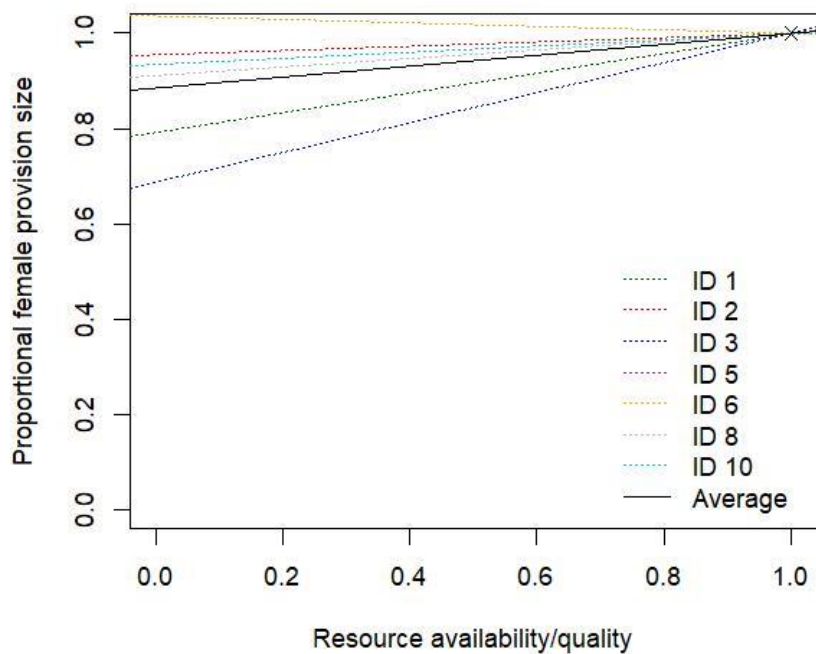
Figure 11. Linear relationship between relative resource availability and proportional provision size provided to female offspring by M. apicalis (data from Kim 1999). The maximum female provision size is assumed to occur under optimal foraging conditions and floral resource availability. The IDs refer 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' (2nd 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' (3rd and 4th 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 12, 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).
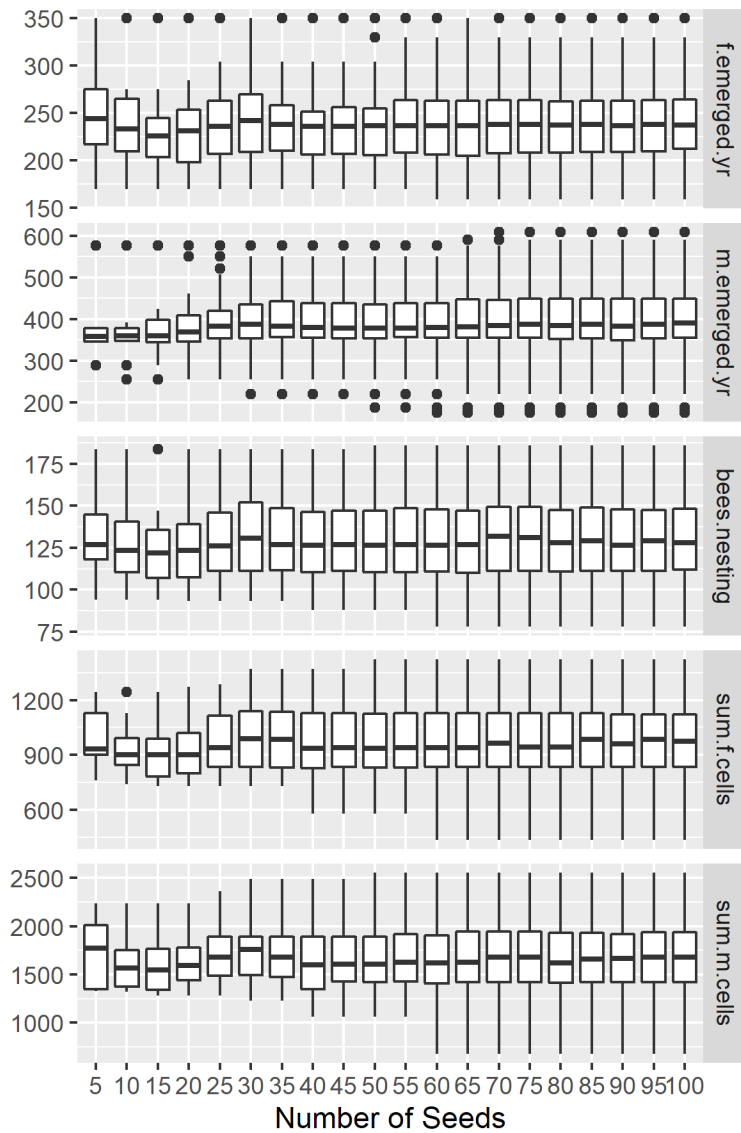
Figure 12. Test of repeat simulations with the SolBeePop model. The number of seeds refers to the number of repetitions conducted with different random number seeds but identical model parameter settings. The median, 25th and 75th percentile range of model outputs due to stochasticity in the model are shown as boxes, the whiskers indicate 1.5 times the interquartile range.

5. MODEL OUTPUT VERIFICATION

The calibration and validation of SolBeePop with *Osmia* semi-field study data is described in Chapter 7. No further systematic model output verification was conducted.

6.   MODEL ANALYSIS

6.1. Analysis of parameter uncertainty (sensitivity analysis)

6.1.1. Methods

The analysis of the model sensitivity 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 sensitivity 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 sensitivity analysis are listed in Table 8, the default parameters and their ranges for *N. melanderi* in Table 9. 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 sensitivity 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 8 and Table 9, including parameters that were not species-specific and were not changed across simulations.

The parameters included in the sensitivity analysis (parameters with a range of values listed in Table 8 and Table 9) 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 8, 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[1] from the parameter space was calculated. Simulations with each of these parameter combinations were repeated 10 times with different random number seeds[2]. Because the species-specific parameters (traits) were expected to interact differently with different scenarios of

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[1] (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 x N_{min}.

[2] 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. See also Section 4.3.

temporal floral resource availability, the sensitivity 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 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 sensitivity 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 sensitivity 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 sensitivity analysis, the six parameters for the reproductive relationships (*a.cell.age, a.sex.age, a.size.age, a.cell.resource, a.sex.resource, a.size.resource*) were used with their ranges determined based on the data across species (see also remarks in Table 8).

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 8. Model parameter values applied in the sensitivity analysis with example species Osmia bicornis. 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	*Osmia bicornis* (default parameter value)	Included in SA	Min value in SA	Max value in SA	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			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	
stoch.crop.forag	FALSE	No	--	--		
Density.dep	FALSE	No				
DD.thresh.s	NA	No				
DD.max.cells.s	NA	No				

Interface parameter name	*Osmia bicornis* (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
DD.funct	NA	No				
DD.log.slope	NA	No				
day.emerge.f	105	No	--	--	Species-specific but not included in the sensitivity analysis. See text.	
var.emerge.f	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)
day.emerge.m	91	No	--	--	Species-specific but not included in the sensitivity analysis. See text.	
var.emerge.m	2	No	--	--	Species-specific but not included in the sensitivity analysis: no data available (see *var.emerge.f*) and male emergence timing does not affect reproductive rates in the model.	
latest.emerge	365	No	--	--	Parameter used for multi-voltine life cycles only; unused if Voltinism = 'univoltine'	
dev.egg	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	
dev.larva	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	
dev.cocoon	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	

Interface parameter name	*Osmia bicornis* (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
t.maturation	3	Yes	1	10	values need to be integers	(Bosch et al. 2008; Sgolastra et al. 2016)
m.life	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	
max.nesting.life	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)
p.max.nesting.life	0.04	Yes	0.01	0.1		Parameter does not correspond to a trait measured in any published study: generic value range applied
max.f.ratio	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)
max.cells	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)
max.survival.e.f	0.74	Yes	0.58	0.89		(Bosch 1992; Bosch and Vicens 2005; Sedivy et al. 2011)

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

Table 9. 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	*Nomia melanderi* (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
Start.day	1	--	--	--		
Species	N.melanderi	--	--	--		
Voltinism	univoltine	--	--	--		
Initial.num.f	100	--	--	--		
Initial.num.m	200	--	--	--		
Initial.stage	cocoon	--	--	--		
Initial.age	200	--	--	--		
RndSeed		see remarks			10 random number seeds per parameter combination	
MultiYearInput	FALSE	--	--	--		
List.input.floral	NA	--	--	--		
Num.repeat.yr	2	--	--	--		
input.floral		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	
stoch.crop.forag	FALSE	--	--	--		
Density.dep	FALSE	--	--	--	Density dependence not included in this analysis	
DD.thresh.s	NA	--	--	--		
DD.max.cells.s	NA	--	--	--		

Interface parameter name	*Nomia melanderi* (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
DD.funct	NA	--	--	--		
DD.log.slope	NA	--	--	--		
day.emerge.f	174	--	--	--	only meaningful to test in the context of floral phenology scenarios	
var.emerge.f	6	Yes	3	9	values need to be integers	Mayer and Miliczky 1998; Vinchesi et al. 2013
day.emerge.m	167	--	--	--		
var.emerge.m	8	--	--	--		
latest.emerge	365	--	--	--	only meaningful to test for facultatively bivoltine life cycles	
dev.egg	2	--	--	--	development times not influential to model outputs (in univoltine life cycles)	
dev.larva	6	--	--	--		
dev.cocoon	20	--	--	--		
t.maturation	1	Yes	1	7	values need to be integers	Bohart and Cross 1955; Johansen et al. 1978
m.life	14	--	--	--	not impactful to model dynamics or outputs (other than number of post-emergent males)	
max.nesting.life	26	Yes	22	30	values need to be integers	Bohart and Cross 1955
p.max.nesting.life	0.04	Yes	0.01	0.1		Not available; generic large range included
max.f.ratio	0.51	Yes	0.35	0.51		Mayer and Miliczky 1998
max.cells	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	*Nomia melanderi* (default parameter value)	Included in SA	Min value in SA	Max value in SA	Remarks	Value ranges based on
max.survival.e.f	0.868	Yes	0.729	0.868	apply the same value to max.survival.e.f and max.survival.e.m	Rust 2006
max.survival.e.m	0.868	see remarks			apply the same value to max.survival.e.f and max.survival.e.m	
emerged.survival	0.544	Yes	0.5	0.75	generic range applied in the absence of data (same range as applied to Osmia)	
a.cell.age	-0.006	Yes	-0.008	-0.004		Bosch and Vicens 2005
a.sex.age	-0.0406	Yes	-0.0599	0		Seidelmann et al. 2010
a.size.age	-0.003	Yes	-0.005	-0.001	Reproductive relationships characterized using data from multiple species (see also Table 8)	Bosch and Vicens 2005; Seidelmann et al. 2010
a.cell.resource	0.94	Yes	0.43	1.4		Kim 1999; Goodell 2003; Peterson and Roitberg 2006
a.sex.resource	0.42	Yes	0	0.6		Kim 1999 (no range; range for testing in SA not supported by data)
a.size.resource	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 10 and Table 11). 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 10. Results of the sensitivity 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.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	-0.004	-0.008			
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		-	-

Table 11. Results of the sensitivity 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.maturation	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 Figure 13, Figure 14, and Figure 15, 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 sensitivity 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.maturation* 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.
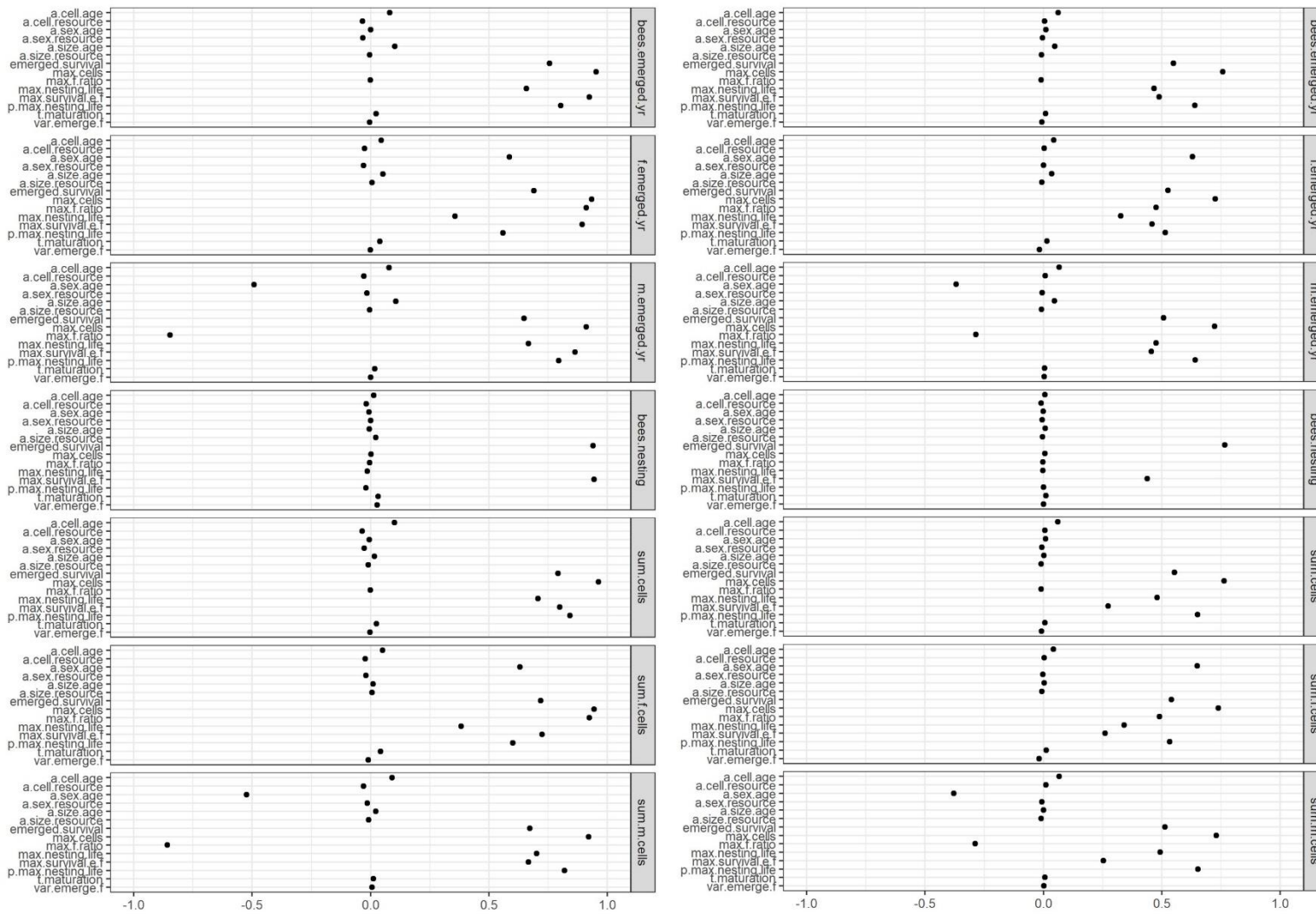
Figure 13. Scenario 1: optimal foraging and floral resource availability. Left: O. bicornis; Right: N. melanderi. Parameters included in the sensitivity analysis and their impact on the model outputs shown as partial rank correlation coefficient (PRCC). Positive PRCCs indicate an increase in the output 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.
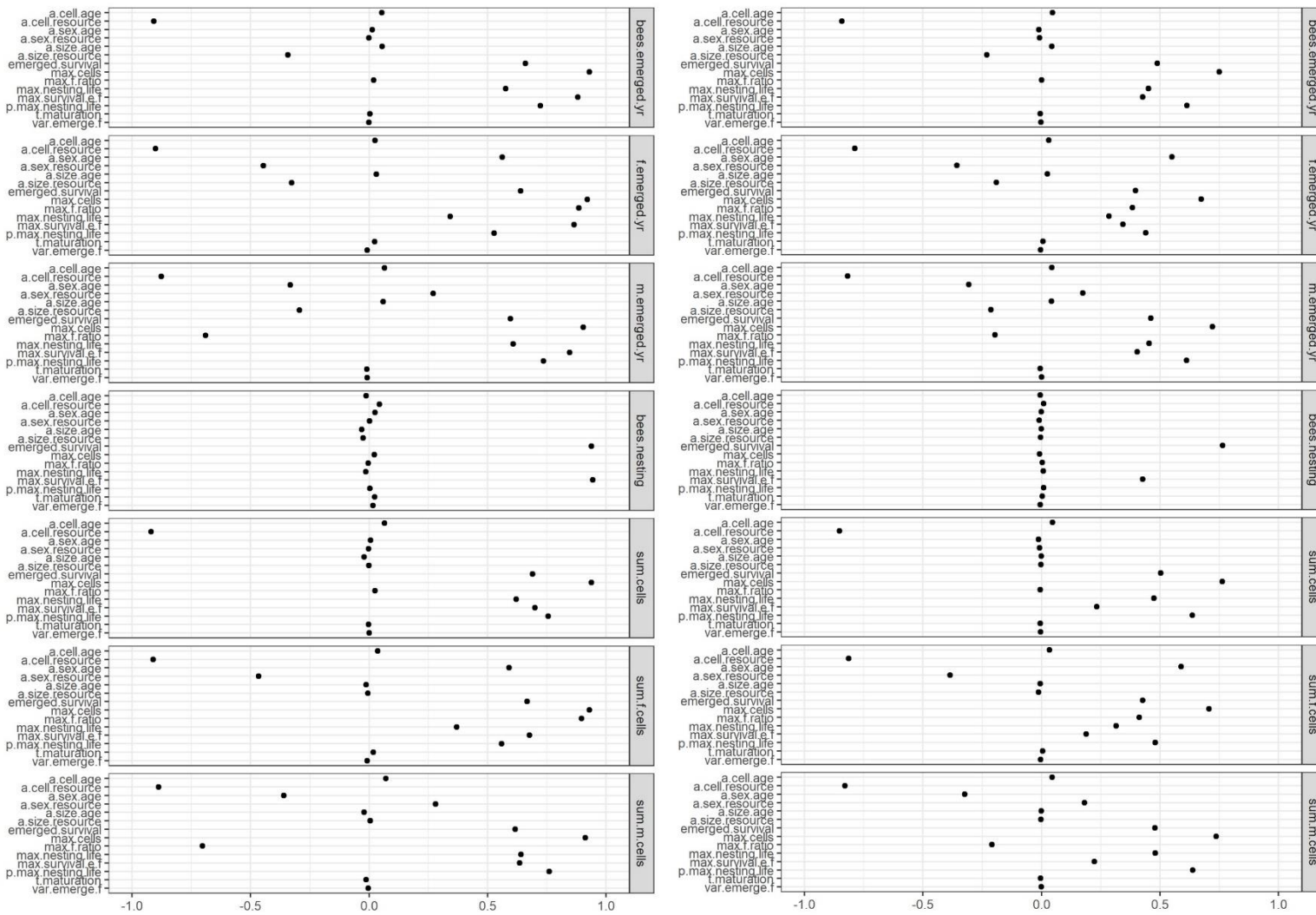
Figure 14. Scenario 2: uniform half-optimal foraging and floral resource availability. Left: O. bicornis; Right: N. melanderi. Parameters included in the sensitivity analysis and their impact on the model outputs shown as partial rank correlation coefficient (PRCC). Positive PRCCs indicate an increase 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.
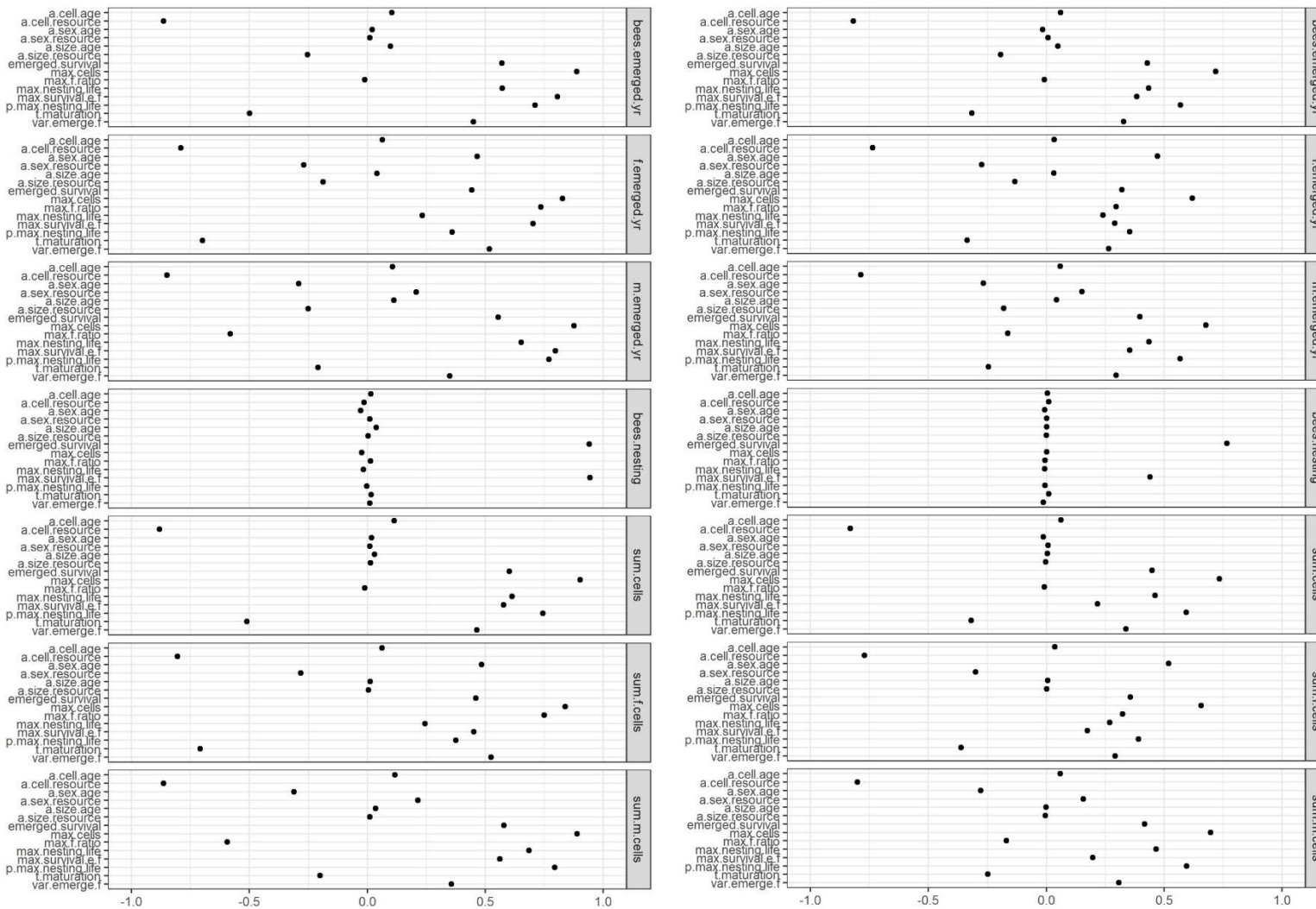
Figure 15. Scenario 3: half-optimal foraging and floral resource availability with a 10-day foraging gap. Left: O. bicornis; Right: N. melanderi. Parameters included in the sensitivity analysis and their impact on the model outputs shown as partial rank correlation coefficient (PRCC). Positive PRCCs 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. 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.

6.2.1. Simulations

Cross-species simulations were conducted using species-specific parameter values as listed in Table 12. 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 12). 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 12. 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	*Osmia bicornis*	*Megachile rotundata*	*Nomia melanderi*	*Eucera pruinosa*
Start.day	1	1	1	1
Species	O.bicornis	M.rotundata	N.melanderi	E.pruinosa
Voltinism	univoltine	univoltine	univoltine	univoltine
Initial.num.f	50	50	50	50
Initial.num.m	75	75	75	75
Initial.stage	cocoon	cocoon	cocoon	cocoon
Initial.age	200	200	200	200
RndSeed	50 different numbers applied (for each repeat simulation)			
MultiYearInput	FALSE	FALSE	FALSE	FALSE
List.input.floral	NA	NA	NA	NA
Num.repeat.yr	30	30	30	30
input.floral	Floral_generic_optimal.csv			
stoch.crop.forag	FALSE	FALSE	FALSE	FALSE
Density.dep	TRUE	TRUE	TRUE	TRUE
DD.thresh.s	250	250	250	250
DD.max.cells.s	2500	2500	2500	2500
DD.funct	linear	linear	linear	linear
DD.log.slope [a]	2	2	2	2
day.emerge.f	105	166	174	212
var.emerge.f	3	3 [b]	6	30
day.emerge.m	91	164	167	202
var.emerge.m	2	2 [b]	8	15
latest.emerge	365	365	365	365
dev.egg	8	3	2	8 [b]
dev.larva	32	9	6	15
dev.cocoon	68	8	20	68 [b]
t.maturation	3	7	1	4
m.life	21	7	14	14
max.nesting.life	36	52	26	36 [b]
p.max.nesting.life	0.04	0.04	0.04	0.04
max.f.ratio	0.59	0.83	0.51	0.7
max.cells	2	2	1	1.65
max.survival.e.f	0.74	0.65	0.868	0.74
max.survival.e.m	0.74	0.65	0.868	0.74
emerged.survival	0.544	0.69	0.544	0.544
a.cell.age	-0.006	-0.006	-0.006	-0.006
a.sex.age	-0.0406	-0.0406	-0.0406	-0.0406

Interface parameter name	*Osmia bicornis*	*Megachile rotundata*	*Nomia melanderi*	*Eucera pruinosa*
a.size.age	-0.003	-0.003	-0.003	-0.003
a.cell.resource	0.94	0.94	0.94	0.94
a.sex.resource	0.42	0.42	0.42	0.42
a.size.resource	0.114	0.114	0.114	0.114

[(a)] Unused parameter: only applies if *DD.funct* = 'log' is chosen

[(b)] No data found for this trait and species; value from *O. bicornis* used

6.2.2. 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 life-time 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).

6.2.3. 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 13; Figure 16). *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 18). 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 13; Figure 17).

Table 13. 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.

	Osmia bicornis	*Megachile rotundata*	*Nomia melanderi*	*Eucera pruinosa*
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
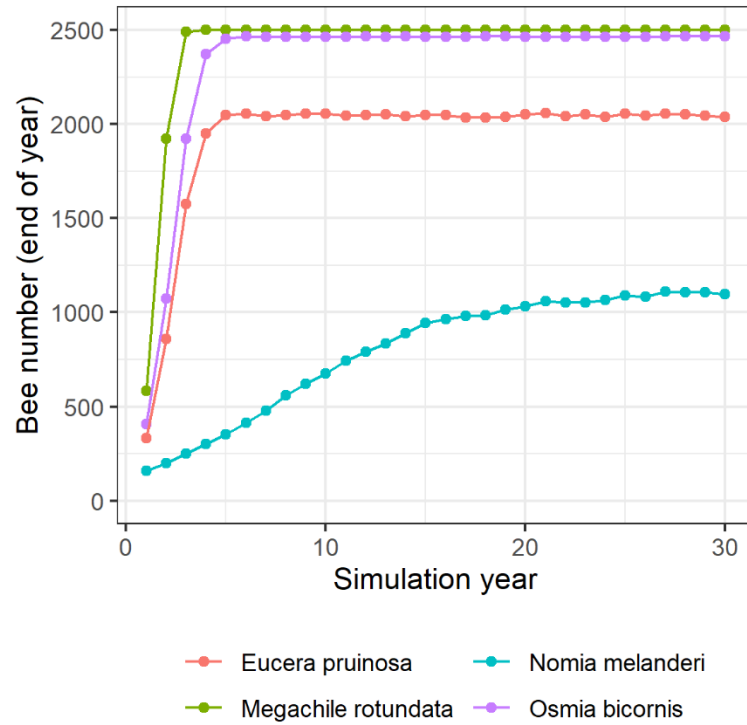
Figure 16. Average total number of bees (brood cells) at the end of each simulated year for the four species. The average of the numbers from years 21-30 are used to calculate the "carrying capacity."
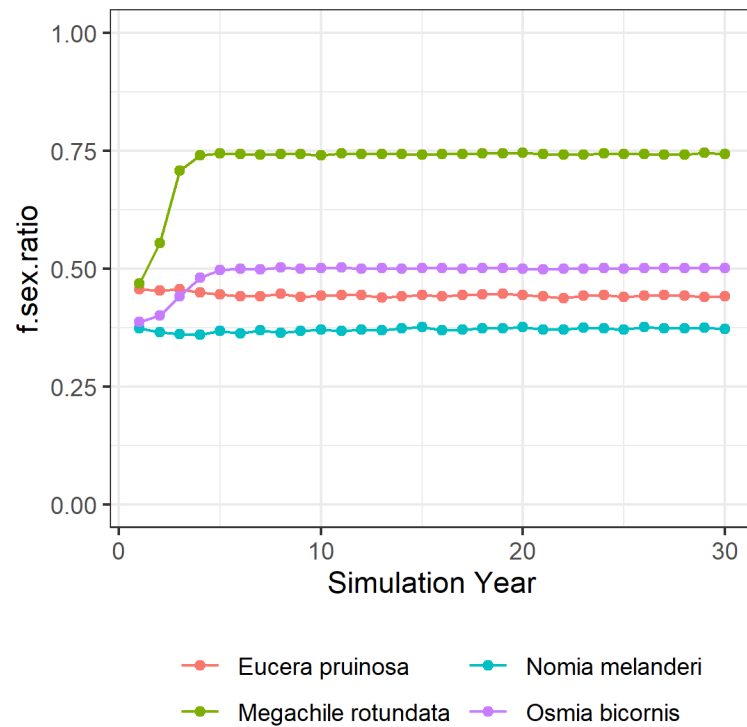
Figure 17. Average female sex ratio (f.sex.ratio) of each year's offspring by species.
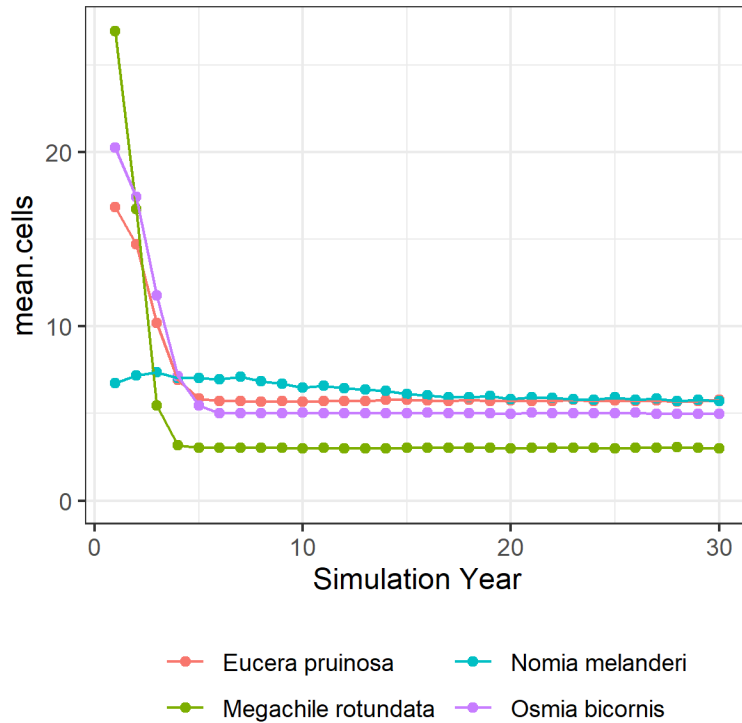
Figure 18. Average number (mean.cells) of offspring (brood cells) produced per nesting female in each simulated year.

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 18). 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 13).

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.

7. MODEL OUTPUT CORROBORATION

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

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 14). 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 19 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 the Celle study produced clearly less brood cells.

Table 14. 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
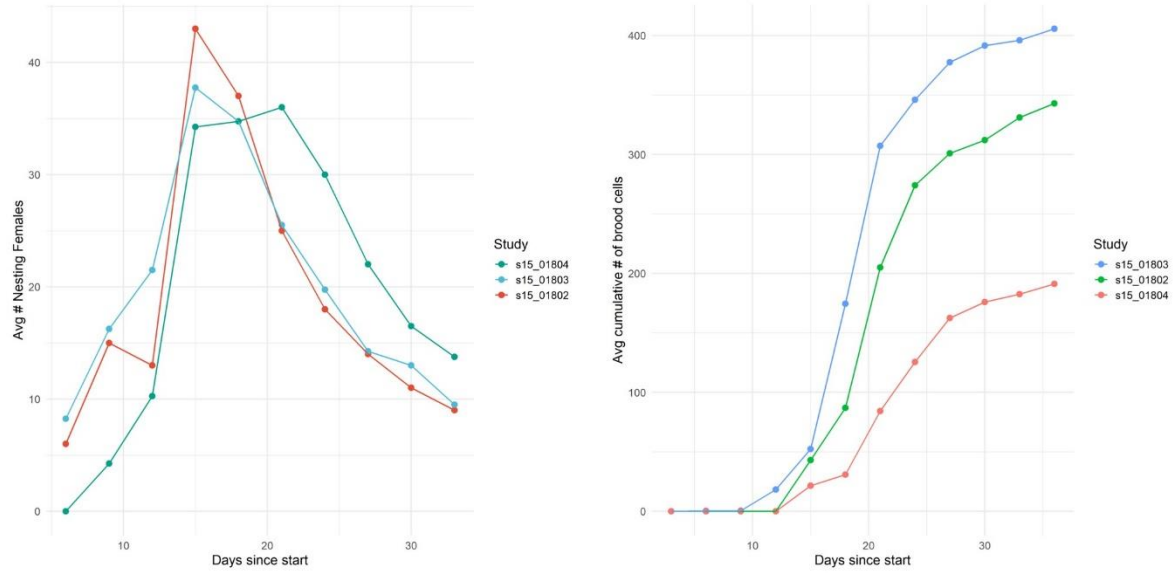
*Figure 19. Data from the three semi-field studies from Ruddle et al. (2018) reported for the tunnel phase. The x-axis shows the days since the release of cocoons into the tunnels for better comparison. **Left**: average number of nesting females observed in the nest blocks. **Right**: average cumulative 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 15.

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 16. 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 17.

Table 15. 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 *O. bicornis* 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 14)
crop.end	End date (Julian day) of crop flowering	Study-specific	Corresponds to the end of the tunnel phase in the studies (see Table 14)
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 *O. bicornis* 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 16. 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 S15-01802	Tübingen S15-01803	Celle S15-01804	Remarks
Start.day	111	113	119	Day of year of cocoon release into the tunnels; see Table 14
input.floral	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 15
day.emerge.f	115, 118	117, 120	123, 126	Early and late emergence scenarios, see text
day.emerge.m	114, 117	116, 119	122, 125	Early and late emergence scenarios, see text
latest.emerge	147	149	155	Day of year of last day in tunnels; see Table 14

Table 17. 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 (*O. bicornis*)	Included in calibration	Min value in calibration	Max value in calibration	Remarks
Start.day	See remarks	--	--	--	Differs between studies (see Table 16)
Species	O.bicornis	--	--	--	
Voltinism	univoltine	--	--	--	
Initial.num.f	60	--	--	--	Number released in all studies
Initial.num.m	90	--	--	--	Number released in all studies
Initial.stage	cocoon	--	--	--	Life stage released in all studies
Initial.age	300	--	--	--	
RndSeed	See remarks	--	--	--	Different random numbers used for each of the 10 repeat simulations
MultiYearInput	FALSE	--	--	--	
List.input.floral	NA	--	--	--	
Num.repeat.yr	2	--	--	--	2 years to capture emergence of F1
input.floral	See remarks	--	--	--	Differs between studies (see Table 16)
Density.dep	FALSE	--	--	--	
DD.thresh.s	1	--	--	--	unused
DD.max.cells.s	1	--	--	--	unused
DD.funct	linear	--	--	--	unused
DD.log.slope	1	--	--	--	unused
stoch.crop.forag	FALSE	--	--	--	
day.emerge.f	See remarks	--	--	--	Differs between studies; two scenarios included in calibration (see Table 16 and text for further explanation)
var.emerge.f	3	Yes	1	7	Standard deviation around the mean emergence date (day of year) of female bees (*day.emerge.f*); parameter range from model analysis applied (Section 6.1)
day.emerge.m	See remarks	--	--	--	Differs between studies; two scenarios included in calibration (see Table 16 and text for further explanation)
var.emerge.m	2	--	--	--	
latest.emerge	See remarks	--	--	--	Differs between studies (see Table 16)
dev.egg	8	--	--	--	

Parameter name	Default value (*O. bicornis*)	Included in calibration	Min value in calibration	Max value in calibration	Remarks
dev.larva	32	--	--	--	
dev.cocoon	68	--	--	--	
t.maturation	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)
m.life	21	--	--	--	
max.nesting.life	36	--	--	--	Excluded from calibration because the tunnel phase was shorter than the maximum life span
p.max.nesting.life	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)
max.f.ratio	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)
max.cells	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)
max.survival.e.f	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)
max.survival.e.m	0.74	see remarks			No separate data for females and males available for survival to emergence: the same value was applied to *max.survival.e.f* and *max.survival.e.m* in the simulations
emerged.survival	1	--	--	--	Based on study data, this parameter is not separable from *max.survival.e.f*
a.cell.age	-0.006	--	--	--	Excluded because it was not impactful in the model analysis (Section 6.1)
a.sex.age	-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)
a.size.age	-0.003	--	--	--	Excluded because it was not impactful in the model analysis (Section 6.1)
a.cell.resource	0.94	--	--	--	Excluded because it was only impactful in the model analysis (Section 6.1) for sub-optimal foraging scenarios
a.sex.resource	0.42	--	--	--	Excluded because it was only impactful in the model analysis (Section 6.1) for sub-optimal foraging scenarios
a.size.resource	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 (see also Section 4.3). 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 14). 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 18 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 18. 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)	$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n}|O_i - P_i|$$ $$\text{NMAE} = \frac{MAE}{\bar{O}}$$	Other names used for the same indicator: relative MAE, MARE	(Bennett et al. 2013; Harmel et al. 2014; EFSA 2018)
Normalized mean square error (NRMSE)	$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(O_i - P_i)^2}$$ $$\text{NRMSE} = \frac{RMSE}{\bar{O}}$$	Indicator is very sensitive to outliers; NRMSE ≤ 0.5 suggested acceptable performance for TKTD models[1] in EFSA (2018)	(Bennett et al. 2013; Harmel et al. 2014; EFSA 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)

[1] 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 19). In Figure 20, 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 19. 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 NRSMEs 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.maturation	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
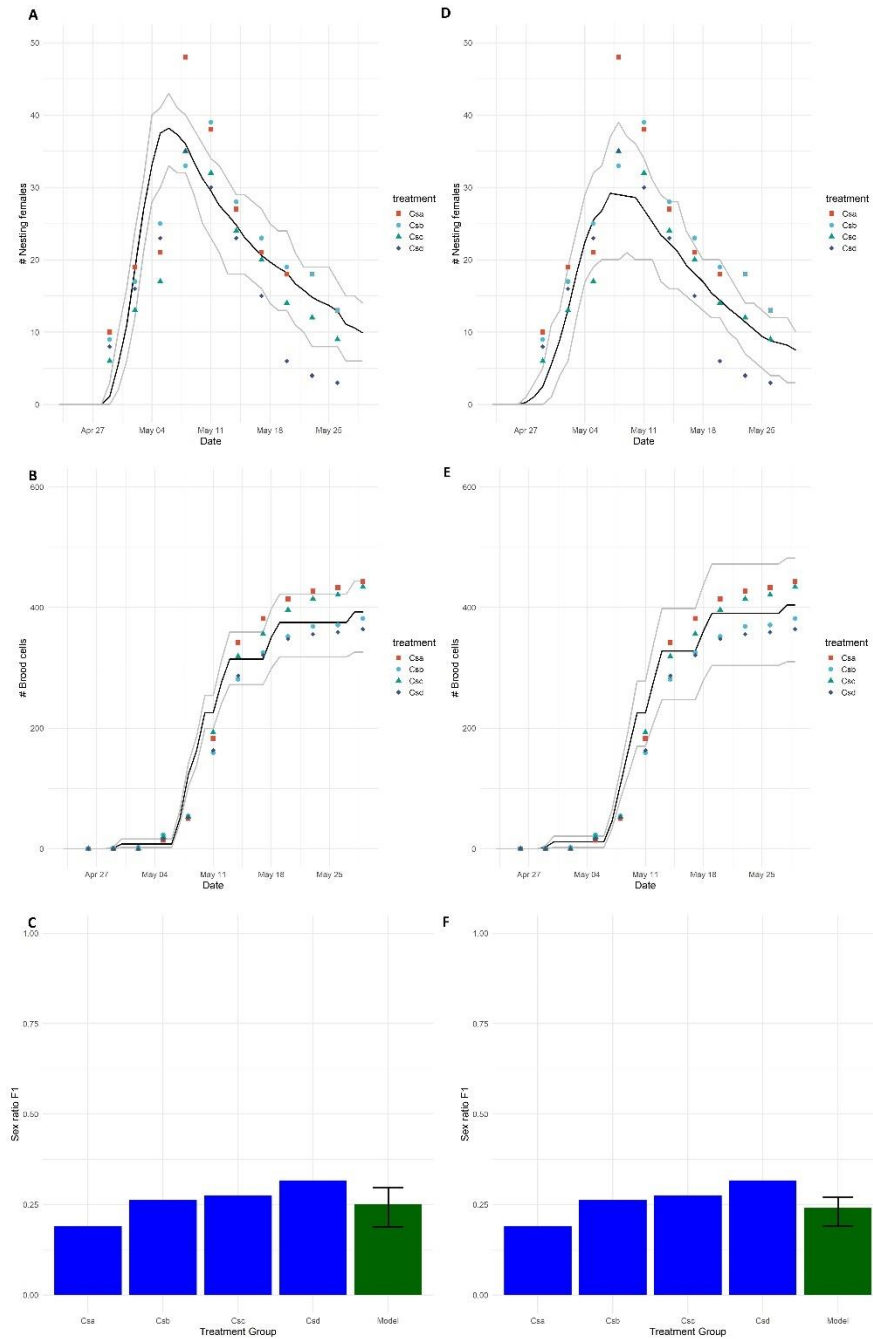
*Figure 20. Best simulations of study **S15-01803** based on the comparison between average simulation outputs (predictions) and average of the four tunnels in the study (observations). Comparison of observed and simulated number of nesting females per day (A, D) and cumulative brood cells produced (B, 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 16). For study S15-01804, the best fits to data are listed based on the early and late emergence scenario (Table 20). In Figure 21, 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 20. 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 NRSMEs 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.maturation*	*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
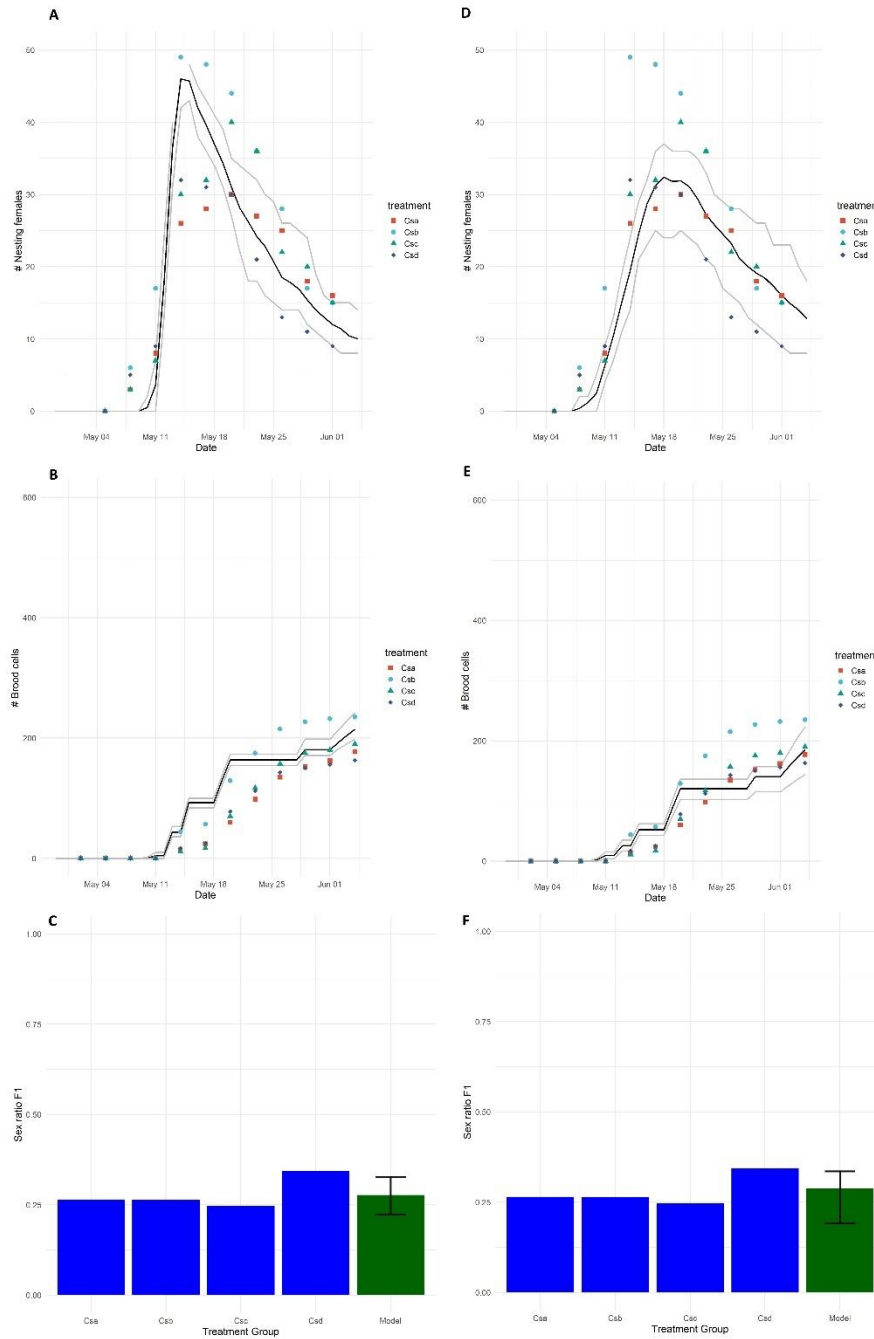
*Figure 21. Best simulations of study **S15-01804** based on the comparison between average simulation outputs (predictions) and average of the four tunnels in the study (observations). Comparison of observed and simulated number of nesting females per day (A, D) and cumulative brood cells produced (B, 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.*

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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 19) 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 21.

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 (NRMSE < 0.5). In Figure 22, 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 21). 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 23. Validation simulations indicate an overestimation of brood cell production compared to observed brood cell production in study S15-01804.

Table 21. 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 NRSMEs 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.maturation*	*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
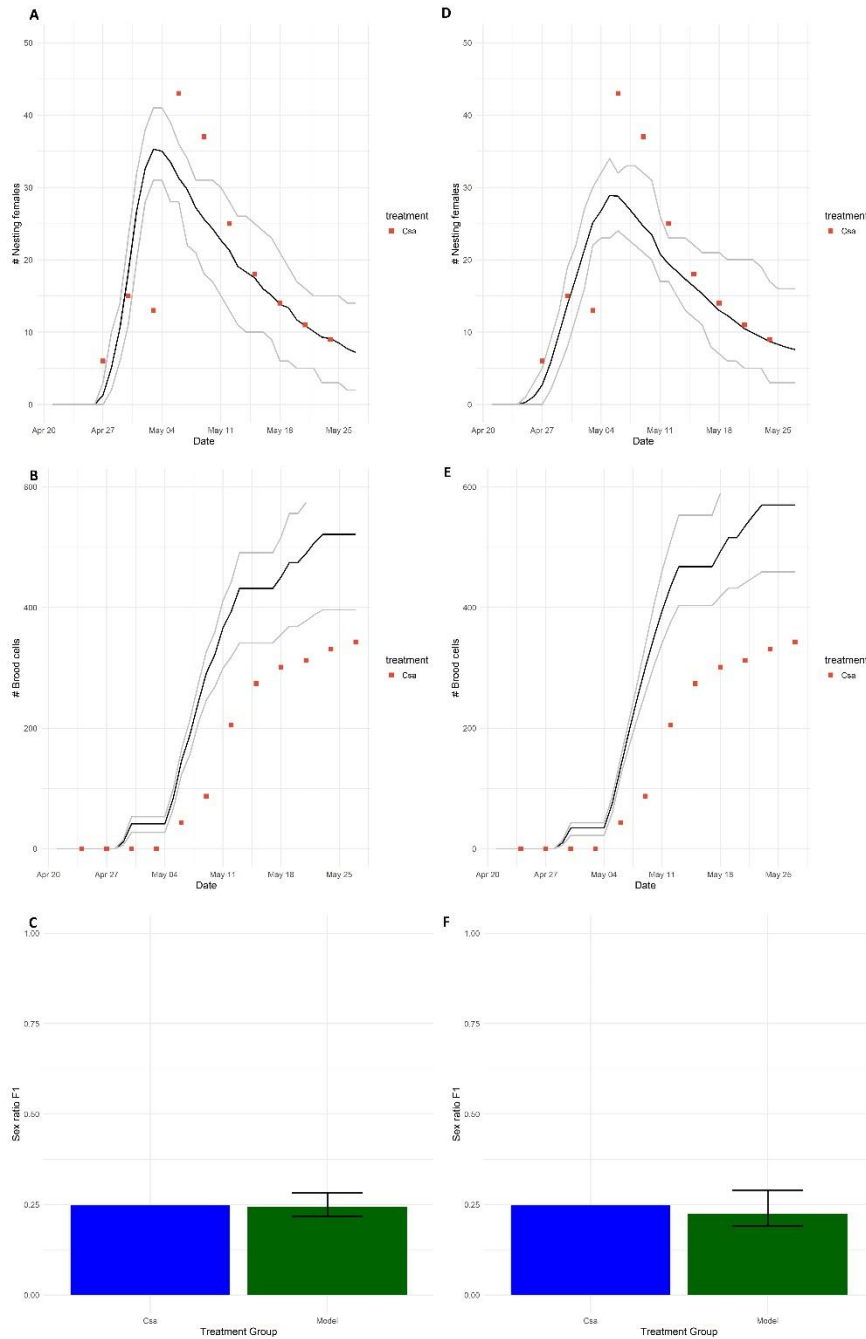
*Figure 22. **Validation simulations of study S15-01802** using the best fits to study S15-01803. Comparison of observed and simulated number of nesting females per day (A, D) and cumulative brood cells produced (B, E) during the tunnel phase of the semi-field study S15-01802. The black lines show the averages 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 that 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 that were the best fit to the late emergence scenario with study S15-01803 (B).*

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*Figure 23. **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 averages 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 that 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 that 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 20) 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 22.

Simulating study S15-01802 with the best fits to S15-01804 results in good representations of the S15-01802 study data in all scenarios (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 24, 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 NRMSE < 0.5 (see Table 22). 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 25, 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 22. 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 NRSMEs 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.maturation*	*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
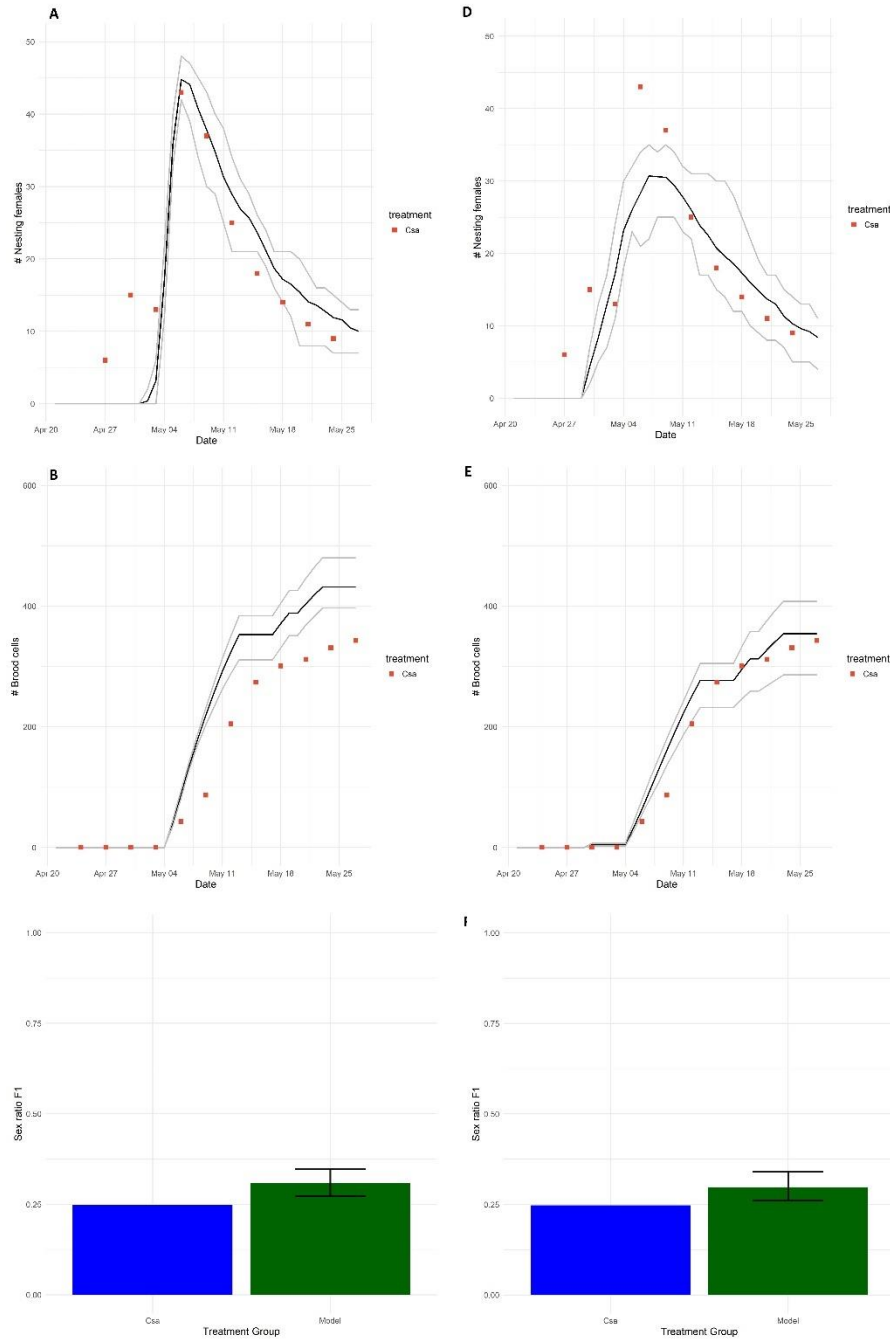
Figure 24. Validation simulations of study S15-01802 using the best fits to study S15-01804. Comparison of observed and simulated number of nesting females per day (A, D) and cumulative brood cells produced (B, E) during the tunnel phase of the semi-field study S15-01802. The black lines show the averages 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 that 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 that were the best fit to the late emergence scenario with study S15-01804 (B).

*Figure 25 **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 that 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 that 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 f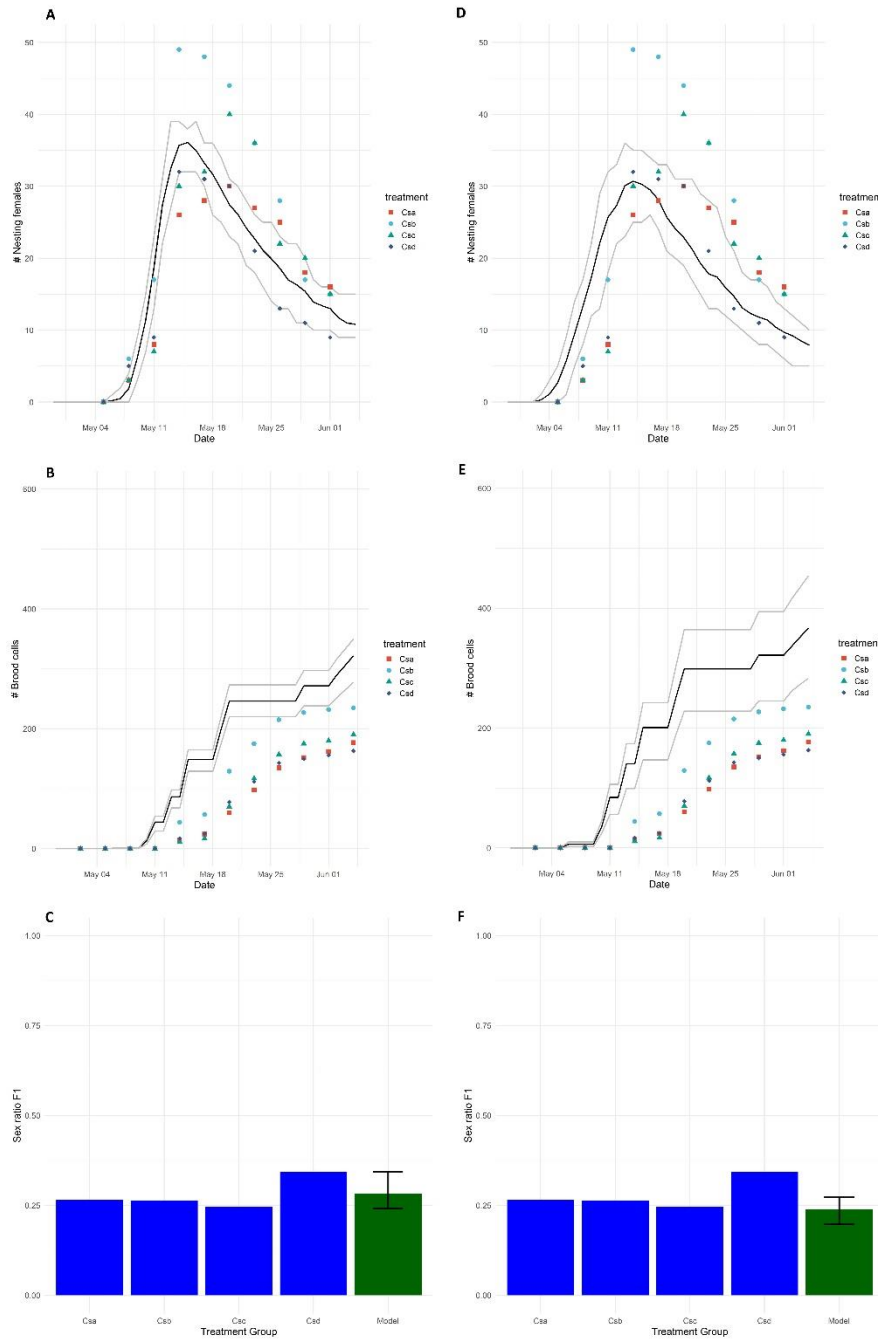rom the three studies indicated that emergence from the released cocoons or the onset of nesting by the released females started at different times (relative to the released date), two temporal emergence scenarios were used in the calibrations.

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 NRSME 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.

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APPENDIX A

In Table 23 through Table 38, 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 23. 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			*No data could be found*	
Larval development time	Larval feeding period	General	15 days	Reported in supplementary information	(Willis Chan et al. 2019)
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			*No data could be found*	
Immature transition rate (including metamorphosis)[1]	NA			*No data could be found*	
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			*No data could be found*	

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 24. 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. 2019)
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		(López-Uribe et al. 2016)
Habitat classification/suitability	Nesting substrate	General	Soil nesting, close to or within pumpkin fields; preference for wet soils, under vegetation (e.g., wet leaves); soil clay content negatively correlated with *E. pruinosa* abundance		(Hurd et al. 1974; Julier and Roulston 2009)

Table 25. 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 26. 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 (± SE) number of [squash] pollen grains in a fully provisioned hoary squash bee nest cell is 62,719.23 ± 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	*No data could be found*	

Data summary for *Megachile rotundata*

Table 27. 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 2nd generation bees)	Temperature dependent; varies by species; can be bivoltine in warmer climates	(Tasei and Masure 1978; Pitts-Singer and Cane 2011; Blattschneiderbienen: Megachile rotundata)[1]
Reproductive frequency	Voltinism	General-realistic	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		(Pitts-Singer and Cane 2011)
Reproductive output/clutch size	Fecundity	General-realistic	Up to 57 eggs/female under ideal conditions; max. 2 eggs/day (Pitts-Singer and Cane); 25-30 eggs/female (Tasei)	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)	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	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)	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)

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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: Megachile rotundata); 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	*M. rotundata* overwinters as pre-pupa (after1-2 generations); no diapause in first generation if bivoltine		(Pitts-Singer and Cane 2011)

[1] Tasei and Masure 1978: *Megachile pacifica = Megachile rotundata*

Table 28. 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: Megachile rotundata)
Geographical range	NA	General-realistic	South and central Europe; introduced to the US for alfalfa pollination		(Blattschneiderbienen: Megachile rotundata)
Habitat classification/suitability	Nesting substrate	General-realistic	Nest above-ground in pre-existing cavities		(Sgolastra et al. 2019)

Table 29. 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 30. 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)		(Michener 2007)
Flower preference	Flower preference	General	Polylectic; provisions mainly composed of alfalfa pollen in bees managed for alfalfa pollination		(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			*No data could be found*	

Data summary for *Nomia melanderi*

Table 31. 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		*No data could be found*	
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		*No data could be found*	
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 32. 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)	(Cane 2008)
Dispersal/migration	NA	NA	NA	Quantitative data on dispersal not available; hard to distinguish from mortality and failure of nest establishment	
Foraging range	Foraging range	General	1.6 - 11.3 km	WA sites suggest shorter flight distances due to proximity to alfalfa fields (Cane 2008)	(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 33. 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 34. 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^3)	Nectar not reported	(Cane et al. 2017)

Data summary for *Osmia*

Table 35. 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 *O. cornuta*; similar range reported for *O. lignaria* and *O. bicornis*; no data for *O. cornifrons*	(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)
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: *O. cornuta* – early (March); *O. bicornis* - later (mid April)	(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 frequency	Voltinism	General	Univoltine	No variability in this trait in the model *Osmia* 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; *O.lignaria*: 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; life-time fecundity mainly dependent on nesting female life span Data reported for *O. lignaria*, *O. cornuta*, *O. pumila* and *O. bicornis*; daily egg/cell production rate reported for *O. lignaria* and *O. cornuta*; no data for *O. cornifrons*	(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	*O. cornuta* and *O. bicornis*: 7-8 days; *O. lignaria*: 7.1 – 9.8 days (females; males ~1 day shorter)	Temperature-dependent; under laboratory conditions (Tasei: 21 C in O. cornuta and bicornis; Bosch and Kemp: different temperature treatments) No data for *O. cornifrons*	(Tasei 1973; Bosch and Kemp 2000; Bosch et al. 2008)
Larval development time	Larval feeding period	General-realistic	*O. lignaria*: I-IV instar 3.7 – 8.4 days, V instar 6.1 – 13.3 days; *O. cornuta* and *O. bicornis*: 24 – 40 days	Temperature-dependent; data from constant temperature regimens applied No data for *O. cornifrons*	(Tasei 1973; Westrich 1997; Bosch and Kemp 2000; Bosch et al. 2008; Sedivy et al. 2011)
Pupa (post-feeding) development time	NA	General-realistic	*O. lignaria* (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 (apart from orchard)	(Bosch and Kemp 2000)
Development egg - adult	NA	General-realistic	*O. lignaria* (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); *O. lignaria*: 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 *Osmia* species; summarizes background mortality prior to overwintering period (egg-pre-emergent adult); Sedivy et al.: *O. bicornis* and *O. cornuta* survival to adult stage	(Bosch 1992; Bosch and Vicens 2005; Sedivy et al. 2011)
Immature transition rate (including metamorphosis)[1]	NA	Realistic-precise	Mortality during winter: 5% (range: 0-14%)	*O. lignaria*; cocoon survival through emergence	(Bosch and Kemp 2000; Bosch et al. 2010; Sgolastra et al. 2011)
Sex ratio	NA	Realistic	*O. cornuta* and *O. bicornis*: 0-1; ~1.6-1.7 males per female (ratio ~0.38-0.59); *O.lignaria*: 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 nesting female age and resource	(Bosch and Vicens 2005; Bosch and Vicens 2006; Seidelmann 2006; Seidelmann et al. 2010; Giejdasz et al.

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	availability No data from *O. cornifrons*	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	*O. cornuta*: 5.89 x adult (dry weight); *O. cornifrons*: 8.33 x adult (dry weight); *O. lignaria*: 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	*O. lignaria*: 10-11mm length, 2.9mm ITD, 0.107-0.196 g (average: 0.158 g) wet weight; *O. cornuta*: 12-16mm length, 0.083-0.257g weight (range of averages from 3 study years, nesting females: 0.152-179g); *O. bicornis*: 10-13mm length, 3.3mm ITD, ~100mg weight; *O. cornifrons*: 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	*O. lignaria*: 9-10mm length, 0.072-0.129 g (average: 0.099 g); *O. cornuta:* 0.065-0.219g (range of averages from 3 study years:	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
			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)	Temperature and species dependent; see reproductive/breeding season	see reproductive/breeding season
Protandrous emergence	NA	General	*O. lignaria*, *O. cornifrons*, and *O. cornuta:* males emerge on average 2-4 days ahead of females; *O. bicornis*: males emerge ~2 weeks before females	Depends on temperature	(Bellman 1995; Bosch et al. 2008)
Dormancy duration (inactive life stages, e.g., hibernation, soil seed bank)	NA	General	*Osmia* 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 36. 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: *O. bicornis*: ~0.1 km (max. 0.25 km), *O. cornuta*: ~0.1 km (max. 0.7 km)	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	Open areas such as parks, agricultural landscapes, etc.; floral resource availability linked to bee abundance		(Bellman 1995; Steffan-Dewenter and Schiele 2008; Dainese et al. 2018)
Geographical range	NA	General	Europe in temperate climates; introduced to/ managed in orchards		(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 37. 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 38. 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	*O. cornuta*: 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	*O. bicornis*: average sugar content in control provisions: 39.2+/-4.9% (Ruddle et al.); EFSA 2022: consumption during larval stage: *O. bicornis*: 91 mg sugar, 80.7-92.5 mg pollen; *O. cornuta*: 165 mg sugar, 80.7-92.5 mg pollen	Bosch (1994): reports pollen grains per provision; Ruddle et al.: average of 3 samples; average was higher in treatments (45.7+/-17.3%); variability between dates; EFSA 2022: assumption that nectar contains 30% sugar	(Bosch 1994; Ruddle et al. 2018); Ruddle et al.: from data tables (not paper), not reported if by weight or volume; EFSA 2022 draft bee RA guidance, Table 14
Composition of adult food	NA	General	Includes pollen irrespective of female bee age	From gut content of *O. cornifrons*	(Taniguchi 1956; Cane 2016)

APPENDIX B

In SolBeePop, weather and floral resource availabilities in the landscape are considered as environmental conditions that influence brood cell production in nesting females. These environmental conditions are defined by the input file (*input.floral*) that includes four input time series, corresponding 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 input time series make it possible to summarize the floral resource availability derived from the landscape composition within a species' foraging range. Thus, the spatial landscape composition can be captured implicitly in the input to the model. Temporal dynamics related to flower phenology 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).

Table 39. Partial example input file. 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_nat	Prop_foraging_crop
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	0	0	0	0
5	0	0	0	0
6	0	0	0	0
7	0	0	0	0
⋮	⋮	⋮	⋮	⋮
119	1	1	0	1
120	0	1	0	1
121	0	1	0	1
122	1	1	0	1
123	0	1	0	1
124	0	1	0	1
125	0	1	0	1
⋮	⋮	⋮	⋮	⋮

In Table 39, a few example rows of an input file generated for the simulation of a semi-field study (see also Section 7.1). 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_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 29 April or day-of-year (doy) 119 and ended on 4 June (doy 155). 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 were set to 0. The input file was generated using the R-script "Foraging_Landscape_InputSce_SolBeePop2022.R" which is addressed below (Generating an input file).

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 24, Table 28, Table 32, and Table 36 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 give 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" on https://github.com/Waterborne-env/SolBeePop) 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.

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 40. 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 40. 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