DEB based IBM for *Daphnia magna*

User Manual

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Introduction

The purpose of the individual-based model (IBM) is the analysis and prediction of the population dynamics of Daphnia magna under environmental stress, considering the competition for food, adaptive plasticity and crowding, and with special emphasis on chemical exposure. The model has initially been published by Gergs et al. (2014. PLoS ONE 9(3): e91503), and has subsequently been extended to allow simulations for toxicant exposure situations under various assumptions.

Within the IBM, life histories of individual daphnids are represented based on dynamic energy budget (DEB) theory. For each individual, the model quantifies the rates at which food is assimilated into reserves and energy is allocated to structure, the reproductive system and maintenance costs. If supplied with sufficient food, then the individual grows (i.e., increases in structure), matures, and reproduces when reaching puberty. If food is scarce, then the individual may suffer from starvation and survival probability is decreased in a size dependent manner. A second death mechanism considered in the model is aging. In the IBM, individuals may adapt to conditions of low food availability by increasing their food intake rate and changing the energy allocation within the body depending on their reserve density. Furthermore, individuals sense population density and suffer from crowding conditions via decreased food intake and respond by producing fewer but bigger offspring. In the IBM, as in nature, population dynamics emerge from individual-level properties and the interaction between individuals, i.e., the competition for food and space.

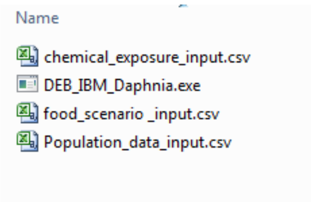
For chemical effect simulations, toxicokinetic-toxicodynamic models (TK-TD) are integrated in the IBM. Moreover, log−logistic concentration response curves (immediate response models) are implemented. To simulate lethal effects in a TK-TD manner, different assumptions of the general unified threshold model of survival (GUTS, Jager et al. 2011. Environ. Sci. Technol. 45, 2529–2540) are implemented in the IBM. To simulate sublethal effects, different physiological modes of actions in a DEB sense, are implemented. See e.g. Jager and Zimmer (2012. Ecological Modelling 225, 74– 81) for details on the stress function and mathematical formulations of the modes of action.

IBM simulations can be carried out to mimic certain experimental conditions or using e.g. default settings for the general exploration of stress situation (e.g. chemical exposure).

System requirements

The executable file of the IBM can be run on Windows computers – no programming environment needs to be installed. The language setting must be chosen in a way that supports the point as the decimal separator and comma-separated columns; e.g. the English language setting is appropriate.

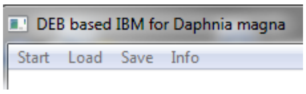
Get started



The executable file folder by default comes with four files, the DEB-IBM executable file (DEB_IBM_Daphnia.exe) and three different input files. Double-clicking the DEB_IBM_Daphnia.exe file opens the user interface of the model. The use interface is explained in the get started section, while the use of the other files are explained in more detail below.

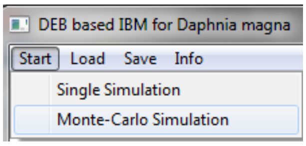
The use interface is organized in three sections:

1) The main ribbon (red square)
2) Model settings (blue square)
3) Model results (green square)

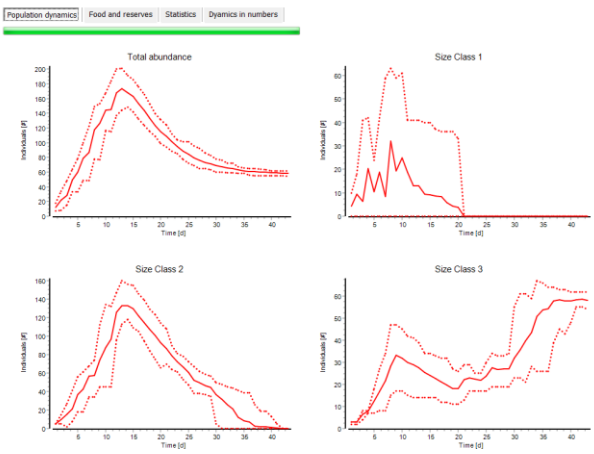


The main ribbon allows to:

1) Run the model (Start)
2) Load population data (details below)
3) Save model results
4) Get some information on version and licensing



Selecting Start→Monte-Carlo Simulations will execute the model multiple times (Compared to Single Simulations where the model is executed only once).

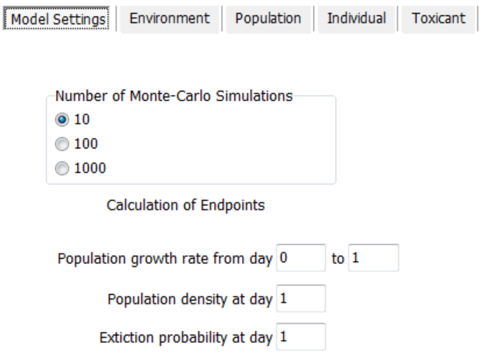


Simulation results are shown in the results section of the user interface e.g. for the total population size and three different size classes within the population (details below). The lines represent the mean as well as the minimum and maximum number of individuals over time.

Model settings

Settings can be adjusted for the aspects of

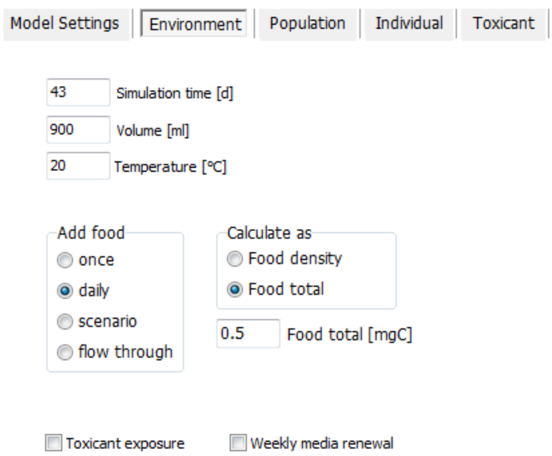
1) (General) model settings
2) Settings of the environment
3) Settings for the population
4) Parameter values for the individual
5) Settings and parameters for chemical exposure (toxicant)



General model settings

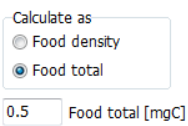
- The number of Monte-Carlo Simulations can be chosen (set to 10 by default)

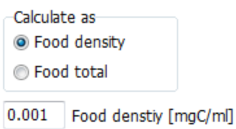
- Three different endpoints are calculated from the (mean) simulation results:
  1) The population growth rate within a defined period
  2) The population density at a predefined simulation day
  3) The extinction probability, i.e. the fraction of populations that went extinct in a given number of Monte-Carlo simulations, on a predefined day



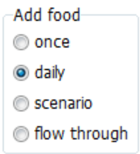
Environment

- Maximum simulation time must be set (43 days by default)
- Volume of the environment is set to 900 ml by default, please note when increasing the volume that the model is validated for laboratory conditions only
- Ambient temperature is set to 20°C by default, the model might not be valid beyond the comfort zone of the species
- Details on the food scenario can be specified (see below)
- Medium can be renewed weekly, i.e. food leftovers are removed on a weekly interval, to mimic laboratory conditions (if checkbox is checked)
- For the simulation of chemical effects the Toxicant exposure checkbox needs to be checked; further settings are defined within the Toxicant settings section

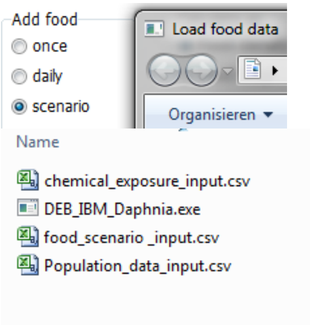




The amount of food can be specified in terms of food density or total food per environmental system.



In the simulations, food can be provided once initially in the simulations, daily, a predefined scenario (other than once or daily), or under flow trough conditions.

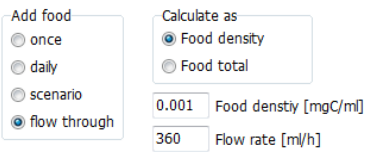


When selecting the scenario based feeding, you will be asked to load a .csv file that contains feeding information.

For instance select the food_scenario_input.csv file.

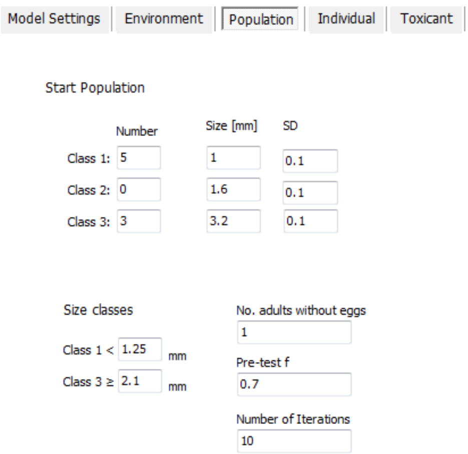
	A	B
1	Day	Food [mgC]
2	0	0.5
3	1	0.5
4	2	0.5
5	3	0.5
6	4	1
7	5	0
8	6	0.5
9	7	0.5
10	8	0.5

In Column A of this file, the time in days is given and Column B bears the information on the total amount of food [mgC]. If changing the file, make sure that information is provided for each of the simulation days, i.e. cross check with the simulation time given in the environmental settings (above).



For the flow through food scenario, the food density in the tank and a flow rate needs to be defined (set to 0.001 mgC/ml and 360 ml/h by default).

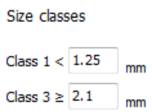
Population



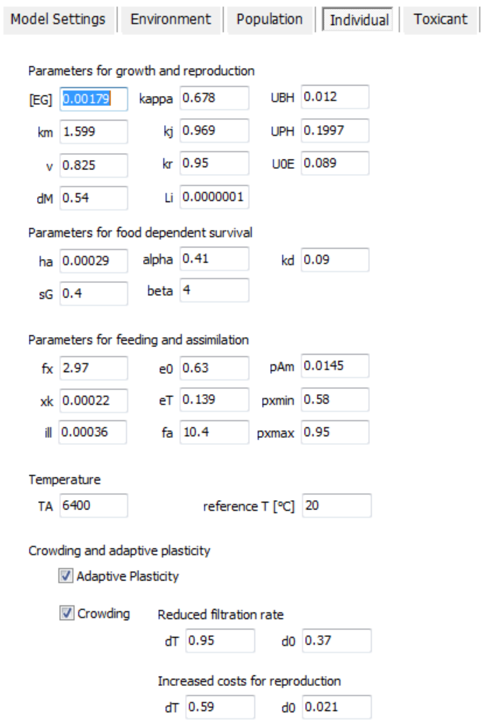
Here, the initial population composition can be set as well as the body sizes for grading the populations into classes.
The initial population structure can be set by giving the number, mean and standard deviation for three classes. These settings are independent of the ones for grading the population into size classes during the simulation.

In addition, the number of adults (i.e. Class 3 in the Start population setting) that do not carry any eggs initially, as well as the scaled functional response prior to the simulations (Pre-test f, e.g. to reflect culture conditions) must be defined.

The Number of Iterations give refer of the number of steps within a day used for the calculation of feeding. An iteration number > 1 decreases the error made in the feeding calculation (e.g. population feeding might temporarily exceed the food availability). There is generally no need for changing the default value.



Three classes for grading the population structure can be defined by setting the upper and lower boundary of Class 1 and Class 3 respectively.

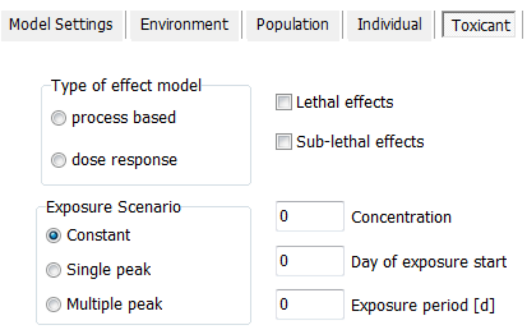


Individual

Sets of parameters are needed to simulate feeding and assimilation, growth and reproduction, survival as well as crowding and and adaptive plasticity.
For the adaptive plasticity it is assumed that at a low reserve density the filtration rate increased and the energy allocation is changed, while for crowding the assumption is that filtration rate is decreased and the cost for reproduction are increased at high population densities. For details see Gergs et al.2014[1]
The rate constants of the model at individual level can be corrected for ambient temperature, where the Arrhenius Temperature T_A determines the slope of the function. The value for T_A has been derived from the add-mypet collection[2].

In general there is no need for changing these parameter values, as this will change the daphnids performance and life history.

[1]PLoS ONE 9(3): e91503. doi:10.1371/journal.pone.0091503)
[2]https://www.bio.vu.nl/thb/deb/deblab/add_my_pet/entries_web/Daphnia_magna/Daphnia_magna_res.html

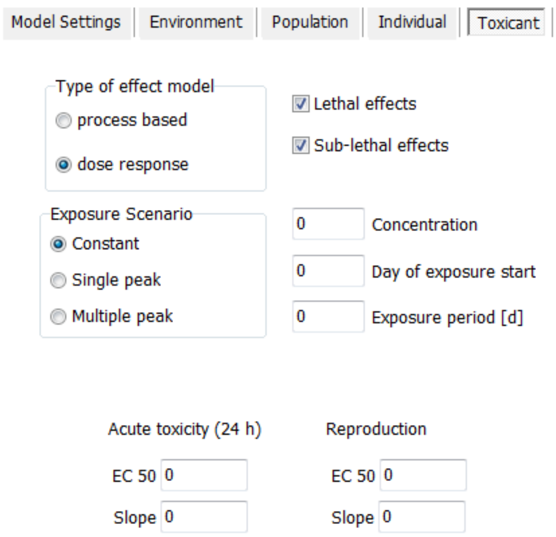


Toxicant

A number of choices need to be made for the simulation of chemical effects. The general type of model, i.e. process base model (TK-TD) or dose response model, needs to be selected as well as the effect type (lethal and/or sublethal).

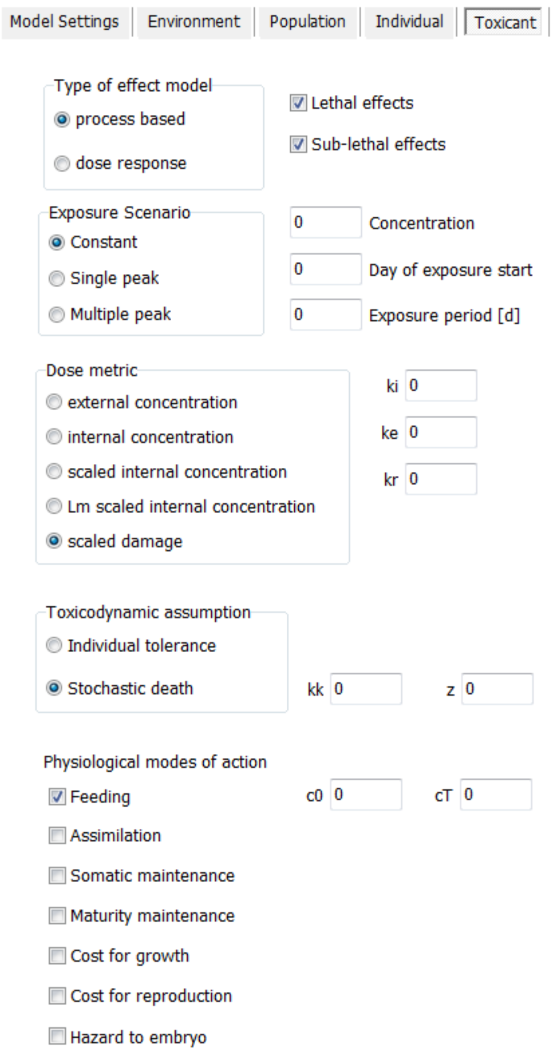
The exposure needs to be defined in terms of the concertation (unit needs to be consistent with effect parameter values) as well as in terms of the scenario, the options are:

1) Constant exposure
2) Single pulse duration determined by the day of exposure start and the duration of the exposure period
3) Multiple-peak scenario as defined in the input file. When selecting this option you are asked to load a .csv file upon model execution (e.g. chemical_exposure_input.csv). Changing the input file works analogous to the food scenario input (above).



For dose-response simulations, the EC50 values as well as the slope of the curve need to specify. Parameter units need to comply with the concertation used for the exposure scenario.

For the acute effects, a certain percentage of the population is randomly removed from the system corresponding to the effect magnitude. For the simulation of sublethal effects, the daphnid's brood size is reduced corresponding to the effect magnitude given by the dose-response curve for a specified concentration.

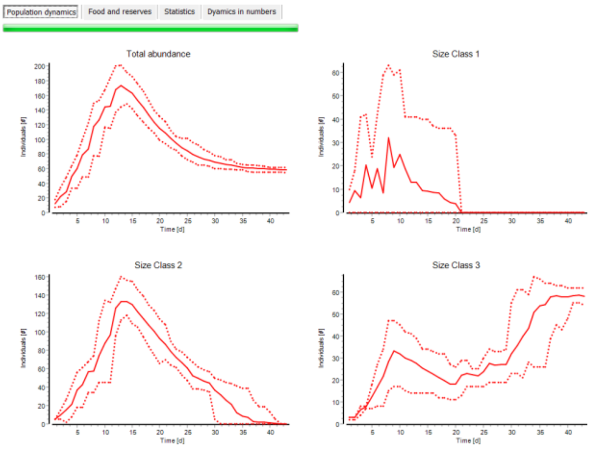


For process based effect modelling, the dose metric needs to be selected and the corresponding parameter values must be specified; for e.g. the scaled damage these are the uptake rate ki, the elimination rate ke, and the damage recovery rate kr, units are [1/d].

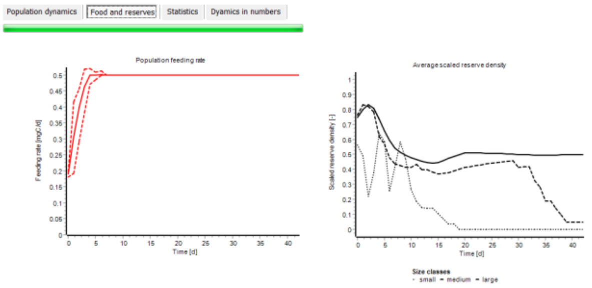
For lethal effects the GUTS toxicodynamic assumption (individual tolerance/stochastic death) needs to be selected and the corresponding parameter values must be specified.

For sublethal effects, select the physiological mode(s) of action and specify the corresponding parameter values.

Model output



When executing Monte-Carlos simulations mean as well as the minimum and maximum number of individuals over time are shown in the population level panel.



The food and reserves panel shows the simulation results for the population feeding rate and the mean scaled reserve density for each of the tree size classes used for grading the population.
This example simulation is done for the default setting of daily feeding of o.5 mgC. Initially, at about day 4 of the simulation the total feeding slightly exceeds the food availability. This error can be further reduced by increasing the number of iterations in the population settings.

Population dynamics | Food and reserves | Statistics | Dyamics in numbers

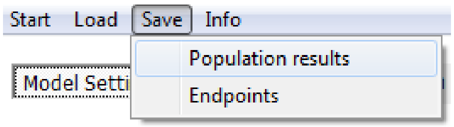
Toxicant Concentration	Population growth rate [1	Population density[#/ml]	Population density max [#	Extinction probability [-]	Mean density[#/ml]
0	1.38629436111989	0.0355555555555556	0.180888888888889	0	0.0993462532299741

The statistics panel shows the results for the different endpoints as specified in the general model settings.

Population dynamics | Food and reserves | Statistics | Dyamics in numbers

Time [d]	Total mear	Total min	Total max	Class 1 me	Class 1 mi	Class 1 ma	Class 2 me	Class 2 mi	Class 2 ma	Class 3 me	Class 3 mi	Class 3 ma	Exti
1	18	7	35	10.1	0	27	5	5	5	2.9	2	3	0
2	26.6	16	38	8.6	0	21	15.1	5	32	2.9	2	3	0
3	32	17	49	5.4	0	21	20.2	9	30	6.4	5	8	0
4	40.9	31	49	8.9	0	26	24.1	9	41	7.9	7	8	0
5	62.1	33	87	21.2	0	52	22.9	0	35	18	7	35	0
6	80	48	105	18	0	46	39.6	15	59	22.4	16	35	0
7	87.7	57	110	8.3	0	31	53.2	30	68	26.2	16	37	0
8	105	78	123	18.4	0	66	55.9	40	66	30.7	17	47	0
9	126.8	77	161	34.8	0	77	59.4	46	80	32.6	23	47	0
10	140.5	106	162	25.8	0	72	82.8	45	128	31.9	22	47	0
11	144.9	115	162	21.2	0	81	93	50	124	30.7	21	46	0
12	162.6	130	194	6.5	0	26	126.6	101	152	29.5	21	44	0
13	161	123	190	6.4	0	25	127.8	96	160	26.8	20	36	0
14	162.8	132	197	6.2	0	25	132	100	167	24.6	19	31	0
15	158.3	127	185	6.1	0	24	129.3	102	157	22.9	18	29	0
16	148.8	120	172	3.6	0	20	124.3	97	151	20.9	15	28	0
17	138.8	110	162	3.1	0	19	115.8	88	140	19.9	14	27	0
18	128.7	100	146	1.8	0	18	108.3	79	128	18.6	14	24	0
19	120.2	98	131	1.7	0	17	100	78	110	18.5	13	24	0
20	111.5	90	125	0	0	0	93.6	72	104	17.9	12	24	0
21	104.4	82	119	0	0	0	86.7	64	102	17.7	12	24	0
22	97.4	77	110	0	0	0	78.1	60	93	19.3	15	25	0

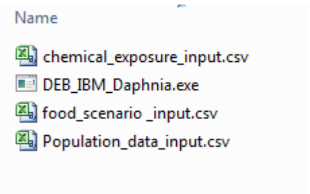
The simulated numbers behind the figures on the population level panel aer listed in the table on the dynamics in numbers panel.



Both the statistics table and the population numbers table can be saved as .csv files.

Always add ".csv" to the file name.

Example application for a specified scenario

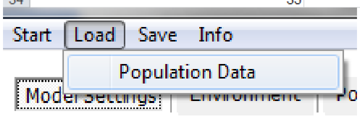


A certain scenario can be run based on the input files for chemical exposure, food scenario and population data input.

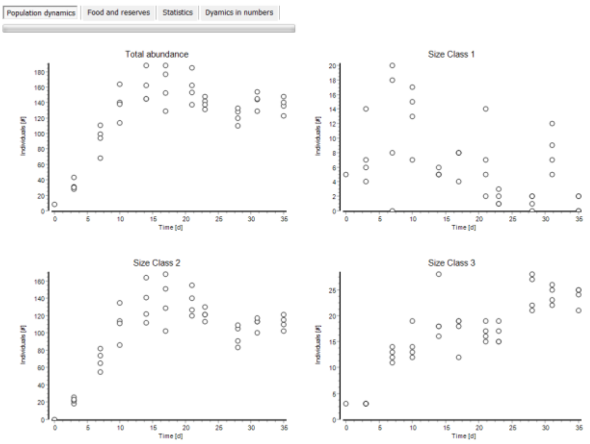
	A	B	C	D	E
1	Test:	Population			
2	Species	Daphnia magna			
3	Temperature [°C]	19			
4	Volume of medium [ml]:	800			
5	Simulation time [d]:	36			
6	Feeding mass [mgC/x]:	0.5			
7	unit x: density or total (0/1)	1			
8	once/daily/scenrio (0/1/3)	1			
9	Initial number of Size class 1	5			
10	Mean length of size class 1 [mm]	1			
11	Standarddeviation of size class 1 [mm]	0.2			
12	Initial number of Size class 2	0			
13	Mean length of size class 2 [mm]	0			
14	Standarddeviation of size class 2 [mm]	0			
15	Initial number of Size class 3	3			
16	Mean length of size class 3 [mm]	3			
17	Standarddeviation of size class 3 [mm]	0.2			
18	Size class 1 < [mm]	1.19			
19	Size class 3 >= [mm]	2.5			
20	Literature	Gergs et al			
21	Test Item	Control			
22	Concentration [µg/l]	0			
23	Day	Class 1	Day	Class 2	Day
24	0	5	0	0	
25	3	7	3	18	
26	7	18	7	82	
27	10	17	10	135	
28	14	6	14	164	
29	17	8	17	168	
30	21	14	21	155	
31	23	3	23	130	
32	28	2	28	105	
33	31	7	31	100	
34	35	0	35	102	

The population data input file has two sections: lines 1-22 contain information on the model settings, beyond line 23 population data can be entered for a model comparison.

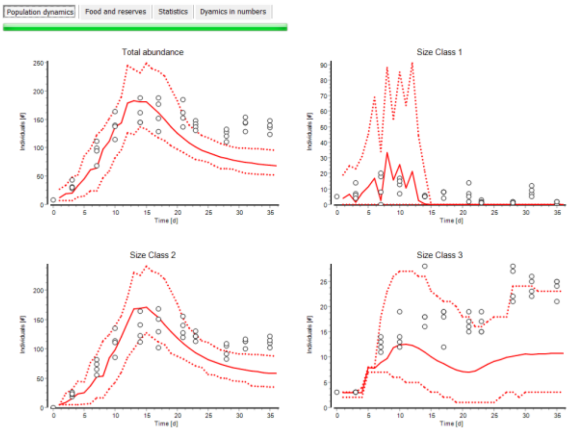
The settings can be also run without entering any population data. Please note that while the actual numbers (e.g. in row B of the settings section) can be changed; the overall structure order of appearance etc. must remain untouched.



The population input file can be loaded via the main ribbon.

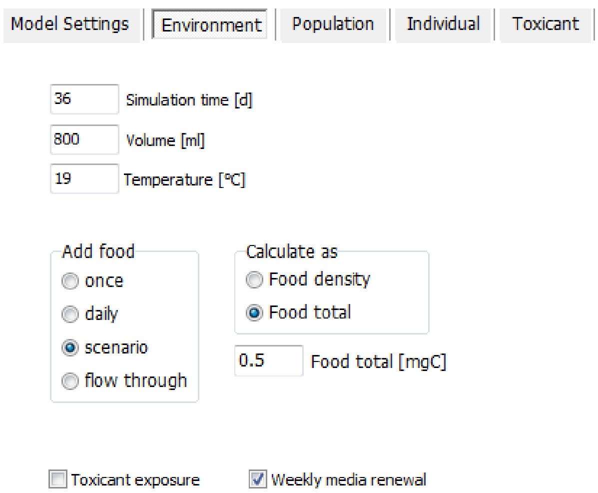


The population data will be shown as white circles in the figures of the results panel. Also the model settings for the population and the environment will be updated based on the information provided in the input file.



When executing the Monte-Carlos simulations, the results will be shown in the same graph allowing for a direct comparison of model results and data.

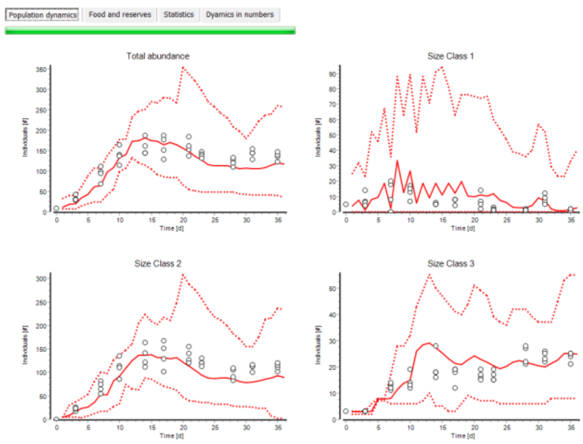
In this example, the model predicts the initial population dynamics and size structure of the population well, but the data in the later part of the experiment is not well matched.



Note that the food scenario is set to daily by default. In the population experiment used for this example, the feeding regime deviates from this assumption.

Deviating food scenarios can be loaded from food input files, therefore, choose “scenario” from the add food list and after starting the model simulation choose an input file.

In the example experiment, the medium was renewed on a weekly basis; this can be accounted for by checking the corresponding box.



Accounting for the above deviations from the model default settings allows for a good prediction of the empirical population dynamics under these conditions.