Appendix B. DEB-IBM model description (ODD). Ecological Archives A024-217-A2.

From: "Limitations of extrapolating toxic effects on reproduction to the population level"

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NetLogo file can be downloaded from http://popecology.wordpress.com/

DEB-IBM: Model Description

The model description follows the ODD protocol for describing individual-based models (Grimm et al. 2006, 2010) and is adapted from Martin et al. (2012).

a) 1. Purpose

The purpose of this model is to explore the population-level consequences of chemical stress on individuals brought about by different physiological modes of actions (PMoAs).

b) 2. Entities, state variables, and scales

The model includes two types of entities, *Daphnia* and the environment. Each *Daphnia* is characterized by four primary state variables, henceforth referred to as DEB state variables: structure (L, unit: mm), which determines actual size, feeding rates, and maintenance costs; scaled reserves (U_E, unit: d.mm^2), which serve as an intermediate storage of energy between feeding and mobilization processes; scaled maturity, (U_H unit: d.mm^2), a continuous state variable which regulates transitions between the three development stages (embryo, juvenile, adult) at fixed maturity levels; and finally a scaled reproduction buffer (U_R, unit: d.mm^2) which is converted into eggs during reproductive events. The term "scaled" in reserves, maturity, and buffer refers to the fact that in this "scaled" version of the model the dimension of energy or mass (either as joule or moles of reserve) are scaled out (see Kooijman et al., 2008 and section 2 of the DEB-IBM User Manual from Martin et al. 2012).

In addition to these DEB state variables, intrinsic variation among individuals is created by including a random component in some of the individuals' eight "DEB-IBM parameters". Each individual has a state variable we refer to as a "scatter multiplier" which is a log-normally distributed number, by which four of the standard DEB parameters are multiplied to get the individual-specific set of DEB parameters (see stochasticity section).

Additionally the model includes an ageing submodel based on DEB theory that includes two state variables, damage inducing compounds ($\ddot{q}$), and damage ($\dot{h}$). The aging process is tightly linked to energetics in that the production of damage-inducing compounds is proportional to mobilization (energy utilization). Damage inducing compounds produce damage and thereby affect survival probability. In addition to directly producing damage, damage inducing compound also can proliferate by inducing their own production (see ageing submodel).

The second entity in the model is the environment, which is defined by food density.

c) 3. Process overview and scheduling

Individuals update their DEB state variables based on a discretized form of the differential equations. At each time step, a set of discrete events may occur. If an organism can no longer pay all maintenance costs (the growth equation becomes negative), individuals cover maintenance costs by burning structure (shrink). If individuals shrink below a specific proportion of their previous maximum body size (crit-mass) they have a high probability of dying (0.35 per day). The second source of mortality is death via ageing. Each timestep individuals have a probability of dying that is proportional to their damage state variable, $\dot{h}$. Finally, mature individuals reproduce at fixed intervals equivalent to the length of a typical molt period for a *Daphnia* (2.8 days). At the reproduction timestep, mature *Daphnia* convert all energy accumulated during the previous molt period to embryos; the number of embryos produced is equal to energy accumulated in the reproduction buffer divided by the cost of producing an embryo (see Reproduction submodel for details).

The following pseudo-code describes the scheduling of events within one timestep of the numerical solution of the model equations (see "go" procedure in NetLogo implementation)

For each individual

      [

      Calculate change in reserves

      Calculate change in length

      If mature

            [Calculate change in reproduction buffer]

      Else

            [Calculate change in maturity]

      Calculate change in ageing acceleration

      Calculate change in hazard

      Starvation mortality

      Ageing mortality

      ]

For the environment

      [Calculate resource dynamics]

For mature individuals

      [

      Update molt-time

      If molt-time >= time-between-molts

          [

          Release offspring created at last molt

          Create embryos from reproduction buffer that will hatch the next brood

          Set molt-time 0

          Set reproduction buffer back to 0

          ]

      ]

Update individual state variables

Update environmental state variables

d) 4. Design concepts

Basic principles

The model is based on the Dynamic Energy Budget theory (Kooijman 1993, 2000, 2010). An

overview of the concepts can be found in Kooijman (2001) or Nisbet et al. (2000). The theory

is based on the general principle that the rates of fundamental metabolic processes are proportional to surface area or body volume and a full balance for mass and energy.

Emergence

The structure and dynamics of the population emerge from the properties of metabolic organization of individuals and indirect interactions of individuals via competition for food.

Adaptation

The framework does not include adaptive behavior; in particular, DEB parameters vary among individuals but remain constant over an individual's lifespan. Consequently, the design concepts "objectives", "learning", "prediction", and "sensing" do not apply to this framework.

Interaction

Individuals interact indirectly via competition for food.

Stochasticity

There are two sources of stochasticity in the model. The first source is intra-specific differences in parameter values. We followed the method outlined in Kooijman (1989) where the surface-area-specific maximum assimilation rate of an individual (referred via index i) is given by multiplying the corresponding species-specific rate $\{\dot{J}_{EAm}\}$ with the individual-specific scatter multiplier, SM_i. The "scatter multiplier" is a log-normally distributed random number with a standard-deviation. However, since DEB-IBM is based on the scaled, not the standard, DEB model where $\{\dot{J}_{EAm}\}$ is scaled out of the model, $\{\dot{J}_{EAm}\}$ is a "hidden" parameter affecting four other scaled and compound parameters. These inter-relationships are described in detail in section 2 of the DEB-IBM User Manual of Martin et al. (2012). For our

simulations we used a value of 0.05 for the standard deviation for the scatter multiplier. The

second source of stochasticity is that all mortality processes are probabilistic.

Observation

Because we were primarily interested in investigating the long-term equilibrium effects of the

various PMoAs we allowed an additional 150-day transitory period. After this transitory

period we determined various population-level characteristics for a period of 300 days. For

each simulation we recorded the percentage of populations surviving, the mean population

biomass, mean population abundance, mean resource density, and the average size of

individuals in the population over the 300-day observation period.

5. Initialization

6. Input data

The framework does not include input data representing external driving processes.

7. Submodels

Calculate change in reserve

The change in energy reserves, U_E, of an individual in a time step is determined by the

difference in scaled assimilation, S_A, and mobilization, S_C, fluxes.

$$\frac{d}{dt}U_E = (S_A - S_C)$$
Eq. B.1

The assimilation flux is given by:

$$S_A = fL^2 \quad \text{where} \quad f = \frac{X}{K+X} \quad \text{for} \quad U_H > U_H^b$$
Eq. B.2

where f, the scaled functional response, is assumed to follow a Holling type II functional response for individuals that have surpassed the maturity threshold for birth, U_H^b, X is prey density, and K the half-saturation coefficient. The mobilization flux is given by:

$$S_C = L^2 \frac{ge}{g+e}\left(1 + \frac{L\dot{k}_M}{\dot{v}}\right) \quad \text{where} \quad e = \dot{v}\frac{U_E}{L^3} \qquad \text{Eq. B.3}$$

where e is the scaled reserve density (falls between 0 and 1, with 1 representing maximum reserve density), g is the energy investment ratio (a compound parameter which is a ratio of the costs to synthesize an unit of structural biomass and the product of the maximum reserve density and the proportion of mobilized energy allocated to the soma, κ), and $\dot{k}_M$ is the somatic maintenance rate coefficient, and $\dot{v}$ is energy conductance (see Martin et al. 2012 for detailed discussion of DEB parameters).

Because embryos do not feed exogenously

$$\text{when } U_H < U_H^b \quad f = 0 \qquad \text{Eq. B.4}$$

the assimilation flux will be zero and the change in reserves is reduced to:

$$\frac{d}{dt}U_E = -S_C \qquad \text{Eq. B.5}$$

Rationale:

DEB theory includes a state variable "reserve" which acts as an intermediate between the feeding and mobilization process. Reserves allow for metabolic memory, i.e. the metabolic behavior of individuals is not solely dependent on the current food availability, but rather the "recent" feeding history of an individual. For example animals can continue to grow for a short period of time when food has been removed from their environment.

Calculate change in maturity

Individuals begin with a maturity level U_H of 0, which increases each time step according to the differential equation:

$$\frac{d}{dt}U_H = (1-\kappa)S_C - \dot{k}_j U_H \quad \text{when} \quad U_H < U_H^p$$

else   Eq. B.6

$$\frac{d}{dt}U_H = 0$$

Transitions between development stages occur at set values of maturity. An embryo which feeds exclusively on reserves becomes an exogenously feeding juvenile when $U_H > U_H^b$ and a reproducing adult when $U_H > U_H^p$. Once puberty is reached, maturity is fixed and energy previously directed towards maturity is now allocated to the reproduction buffer. Before *Daphnia* reach puberty, if mobilized energy is not enough to pay maturity maintenance costs, the maturity flux can become negative, and animals decrease in maturity.

Rationale:

Immature individuals divert mobilized energy from reserve between competing functions of growth and development, with the proportion 1-κ of mobilized reserves allocated to development. Individuals first pay maintenance costs associated with maintaining their current level of maturity (the maturity maintenance rate coefficient, $\dot{k}_J$, multiplied by the current level of maturity, U_H) from the mobilized reserves directed toward development from the mobilized reserves [$(1-\kappa)S_C$]. The remainder represents the increase in development during a timestep.

Calculate change in reproduction buffer

When an individual has reached puberty, energy from the maturity flux is diverted into a reproduction buffer, U_R.

$$\frac{d}{dt}U_R = (1-\kappa)S_C - \dot{k}_J U_H^p \text{ for } U_H > U_H^p$$

else   Eq. B.7

$$\frac{d}{dt}U_R = 0$$

If mobilized energy is not enough to pay maturity maintenance costs, the reproduction buffer flux becomes negative to pay maturity maintenance costs. If the reproduction buffer flux is negative, but there is no energy remaining in the reproduction buffer, maturity maintenance is not paid (U_R cannot be < 0).

Rationale:

This submodel is basically the same as for the "calculate change in maturity" submodel, but is calculated only for mature individuals, whose maturity does not increase. The energy that accumulates in the reproduction buffer in a given time step is the difference between mobilized energy allocated towards reproduction and the fixed maturity maintenance costs.

Calculate change in length

During a timestep energy needed for somatic maintenance costs are paid from mobilized energy allocated for soma. The remainder is converted from reserve to structural length. Under non-starvation conditions:

$$\frac{d}{dt}L = \frac{1}{3}\left(\frac{\dot{v}}{gL^2}S_C - \dot{k}_M L \right) \qquad\qquad \text{Eq. B.8}$$

The parameter κ, which determines the fraction of mobilized energy directed to the soma is not explicit in this formula, however, κ, is in the compound parameter g (see section 2.4 in the User Manual of Martin et al. (2012) for a discussion of compound parameters).

Starvation rules

If mobilized energy allocated towards somatic growth and maintenance is insufficient to pay somatic maintenance costs, growth becomes negative. Essentially the *Daphnia* pay maintenance costs by "burning" their structure. When an individual shrinks below 40% of its previous maximum mass, the individual then has a mortality rate of 0.35 d^{-1}. Additionally when *Daphnia* shrink they retain the assimilation ability of their previous maximum length (Martin et al. in press). Thus:

$$S_A = fL^2_{\max} \qquad\qquad \text{Eq. B.9}$$

where $L_{\max}$ is the maximum length the individual has reached.

We implemented an additional starvation submodel (*Daphnia* still have a high probability of dying if they fall below a critical proportion of their previous mass), where for juveniles, mortality was inversely linked to reserve density, e, which is a time-weighted average of feeding history:

$$\Pr(mortality)d^{-1} = M(1-e) \qquad\qquad \text{Eq. B.10}$$

where M is the reserve-dependent mortality coefficient. In Martin et al. (*in press*), the value of M was estimated to be $0.09\,d^{-1}$.

Rationale:

When mobilized reserves allocated to the soma are insufficient to pay somatic maintenance costs, animals may respond in many ways, which can be represented in DEB, for example by shrinking in structure (see Kooijman 2010 for discussion of starvation strategies). Our implementation of the starvation model assumes that *Daphnia* get 100% of the energy invested in growth back to pay maintenance costs when shrinking.

Reproduction submodel

DEB makes no general assumptions about the reproduction buffer handling rules, and therefore be defined for each species. *Daphnia* release clutches of embryos during the molt, using energy accumulated over the intermolt period. These embryos develop in the brood chamber over the next intermolt period, and are released during the next molt, at which time they begin feeding exogenously. Below we describe how this process is replicated mathematically.

At the timestep where *Daphnia* reach maturity ($U_H = U_H^p$), they set a state variable "molt-time" to 0. In each subsequent timestep the state "molt-time" ticks up by the amount of time transpired until it reaches the parameter "time-between-molts". We estimated the time-between-molts to be 2.8 days from the average time to between reproductive events for individually cultured *Daphnia* kept at 20C. When molt-time >= time-between-molts, the *Daphnia* convert energy accumulated in the reproduction-buffer (U_R) into embryos. The number of embryos produced is given by:

$$N = \left\lfloor \frac{U_R \kappa_R}{U_E^0} \right\rfloor \qquad \text{Eq. B.11}$$

Here κ_R represents the conversion efficiency of the reproduction buffer to the reserves of the embryo which is assumed to be high as both in DEB theory are assumed to have the same

composition. The cost of producing one embryo, U_E^0, is the amount of energy needed to create one offspring that will reach the maturity for birth threshold ($U_H = U_H^b$) with a reserve density, e, equal to 1. This value is dependent on the DEB parameters of a species and is calculated numerically using the bisection method during the setup up procedure. The initial bounds for the bisection method were set to 0 and an unrealistically high number to ensure the true value was contained within the initial bounds. Values of U_E^0 were tested by simulating the embryonic period following the mass balance equations of DEB theory. In DEB theory embryos start out as nearly all reserves, and a very small amount of structure. During the embryonic period, embryos mobilize reserves to grow and gain maturity. The selection criteria for the value of U_E^0 was that embryos were within 5% of a reserve density e = 1 when the maturity threshold for birth was surpassed. With the parameter values used for *Daphnia* in our simulations this corresponded with a length at birth = 0.851 mm. This later value falls well within the range of observed hatching sizes of *Daphnia magna*.

In the simulations, after the calibration of the U_E^0 value we do not simulate the embryonic period. Rather we use the U_E^0 value to determine how many offspring are produced, then in the subsequent molts the number of offspring hatched is equal to the number of embryos produced in the previous molt, and their state variables are set to the values determined in the calibration period (L_b = 0.851, e = 1, $U_H = U_H^b$).

Prey dynamics submodel

Simulations with resource-mediated feedback were conducted in dynamic resource environments where the resource (algae) followed semi-chemostat dynamics, with the change in resource density (X) given by:

$$\frac{dX}{dt} = \alpha(X_{max} - X) - P_X \qquad \text{Eq. B.12}$$

where α is the dilution rate, and X_{max} is the equilibrium density of algae in the absence of predation, and P_X is the predation flux to the *Daphnia* population. In DEB theory, feeding rates scale with surface area (L^2), and *Daphnia* are assumed to follow a Holling type II functional response. Thus the predation flux, summed over all individuals i, is given by:

$$P_X = \sum_i f L_i^2 \{\dot{J}_{XAm}\} \text{ and } f = \frac{X}{X+K} \qquad \text{Eq. B.13}$$

where $\{\dot{J}_{XAm}\}$ is the maximum surface-area-specific ingestion rate and K is the half-saturation coefficient.

Ageing submodel

The basic premise of the DEB aging submodel is that damage inducing compounds are created at a rate proportional to reserve mobilization. Damage inducing compounds induce more damage inducing compounds also at a rate proportional to mobilization. The hazard rate for mortality due to ageing of an individual is proportional to density of the accumulated damage in the body. Additionally, the concentration of both damage inducing compounds and damage are assumed to be diluted via growth. The ageing submodel includes two new parameters: the Weibull ageing acceleration parameter, $\ddot{h}_a$, and the Gompertz stress coefficient, s_G. To reduce the total number of parameters, the equations for damage-inducing compounds, damage and hazard rate are scaled and combined to two ODE's, for "scaled acceleration" ($\ddot{q}$) and hazard rate ($\dot{h}$):

$$\frac{d}{dt}\ddot{q} = (\ddot{q}\frac{L^3}{L_m^3}s_G + \ddot{h}_a)e(\frac{\dot{v}}{L} - \dot{r}) - \dot{r}\ddot{q} \text{ where } \dot{r} = \frac{3}{L}\frac{d}{dt}L \qquad \text{Eq. B.14}$$

$$\frac{d}{dt}\dot{h} = \ddot{q} - \dot{r}\dot{h} \qquad \text{Eq. B.15}$$

Rationale:

In our framework ageing processes are linked tightly to energetics as the production of damage inducing compounds is proportional to mobilization. One interpretation of this assumption is that the production of free radicals or other reactive oxygen species is proportional to the use of dioxygen in metabolic processes. The inclusion of energetics in the ageing process allows differences in ageing of animals in feeding conditions or physiological phenotypes to be explained without altering ageing parameters.

Ecotoxicological effects

Chemical stress was simulated by altering DEB parameter(s) associated with a particular PMoA (Table B1). The stress values used for each PMoA - effect level combination are given in Table B2.

Table B1. Parameters of the DEB-IBM model for *Daphnia magna* (a) and their link to various PMoAs through the stress level (b). Parameter values in combination with environmental conditions determine the magnitude of energy fluxes as governed by a set of coupled differential equations (see ODD model description).

a.

DEB parameters

Symbol	Description	Dimension	Value	PMoA
κ	Fraction of mobilized energy to soma	-	0.678	-
κ_R	Fraction of reproduction energy fixed in eggs	-	0.95	Reproduction costs and embryonic hazard
$\dot{k}_m$	Somatic maintenance rate coefficient	t^{-1}	0.3314	Maintenance costs, growth costs
$\dot{k}_j$	Maturity maintenance rate coefficient	t^{-1}	0.1921	Maintenance costs
U_H^b	Scaled maturity at birth	tL^2	0.1108	-
U_H^p	Scaled maturity at puberty	tL^2	2.555	-
$\dot{v}$	Energy conductance	Lt^{-1}	18.1	-
g	Energy investment ratio	-	10	Growth costs
f	Scaled functional response	-	0-1	Feeding/assimilation

b.

DEB parameters under stress

PMoA	Description	Affected parameter	Stressed value
Feeding stress	Decrease in feeding ability	f	$f_s = f/(1+s)$
Maintenance stress	Increase in maintenance costs	$\dot{k}_m, \dot{k}_j$	$\dot{k}_{M,s} = \dot{k}_M(1+s)$ [*] $\dot{k}_{J,s} = \dot{k}_J(1+s)$
Growth stress	Increase in overhead costs of growth	$\dot{k}_m, g$	$\dot{k}_{M,s} = \dot{k}_M/(1+s)$ [†] $g_s = g(1+s)$
Reproduction stress	Decrease in survival during embryonic period	κ_R	$\kappa_{R,s} = \kappa_R \exp(-s)$

[*]Here we show the assumption that both maturity and somatic maintenance costs are both equally affected, however effects on each parameter independently are also possible.

[†] The growth costs PMoA affects the parameter $[E_G]$, the volume-specific costs of structure. This parameter is indirectly included in the scaled DEB through the two compound parameters and $\dot{k}_m$ and g (see Jager and Zimmer 2012 for details).

Table B2. Stress level, s, for each PMoA required to reduce reproduction relative to the control by 25, 50, 75, 90, and 95% in the OECD *Daphnia* reproduction test (effect level). The relationship between, s and the affected DEB parameter(s) for each PMoA is given in Table S2b. The resulting values of s were then used as inputs for population-level simulations (again, assuming a constant value for s).

Effect level	Feeding	Maintenance	Growth	Reproduction
25%	0.09	0.22	0.36	0.29
50%	0.23	0.50	0.95	0.69
75%	0.48	0.92	2.30	1.39
90%	0.78	1.28	4.65	2.30
95%	0.97	1.44	6.80	3.00

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