Supporting Information for: DEBkiss or the quest for the simplest generic model of animal life history

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1 Model summary

Model assumptions in Table 1, model equations in Table 2, and parameters in Table 3.

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1. There are three types of biomass: food, assimilates and structural body components. Each type has a constant composition. They can be converted in each other with a certain constant efficiency. The state variables of the organism are the masses of the structural body, the reproduction buffer for adults, and the egg buffer used by the developing embryo. Total body mass is the sum of structure and reproduction buffer. The reproduction and egg buffer consist of assimilates.
2. The animal has three life stages: an embryo that does not feed but utilises the egg buffer, a juvenile that feeds but does not reproduce, and an adult that reproduces. The embryo starts with an egg buffer of assimilates and negligible structural mass. The first transition (birth) is triggered by the depletion of the egg buffer, and the second transition (puberty) by reaching a critical structural body weight.
3. The maximum feeding rate is proportional to the surface area of the animal. The animal is either searching for food or handling it (with constant handling time), leading to a hyperbolic functional response in the food density (Holling type II).
4. Food is instantly translated into assimilates that are directly used to fuel metabolic processes. Embryos assimilate their egg buffer at the maximum rate for their structural size.
5. The flow of assimilates is split into a constant fraction κ for maintenance and structural growth (the soma), and $1 - \kappa$ for maturation and reproduction. From the κ flow, maintenance costs are paid first. Only structural biomass requires maintenance, which is proportional to its volume. The remainder of this flow is used for growth (with certain efficiency).
6. For adults, the $1 - \kappa$ flow is used to fill the reproduction buffer. For embryos and juveniles, all of the assimilates in this flux are burnt to increase complexity of the organism. At spawning events, the contents of the reproduction buffer are converted into eggs. The part of the buffer that was insufficient to create a single egg remains in the buffer. Transformation of buffer to egg comes with a certain (generally high) efficiency.
7. If feeding is insufficient to pay somatic maintenance costs, the organism first diverts energy from the 1-κ flux of assimilates and from the reproduction buffer. If that is insufficient, structure is converted into assimilates to pay maintenance.

Table 1: The list of assumptions that leads to the DEBkiss model.

Specification of feeding	
Maximum feeding	$J^a_{Xm} = J^a_{Am}/y_{AX}$
Half-saturation	$K = J^a_{Xm}/F^a_m$
Functional response	$f = \frac{X}{X+K}$
Body volume	$L^3 = W_V/d_V$
Feeding	$J_X = f J^a_{Xm} L^2$ (if $W_B > 0$ then $J_X = 0$)
Specification of assimilate fluxes	
Assimilation	$J_A = f J^a_{Am} L^2$ (if $W_B > 0$ then $f = 1$)
Somatic maintenance	$J_M = J^v_M L^3$
Structural growth	$J_V = y_{VA}(\kappa J_A - J_M)$
Reproduction buffer	$J_R = (1-\kappa) J_A$ (if $W_V < W_{Vp}$ then $J_R = 0$)
Assimilate fluxes under starvation ($\kappa J_A < J_M$)	
$J_A > J_M$ or $W_R > 0$	$J_V = 0$ and $J_R = J_A - J_M$ (if $W_V < W_{Vp}$ then $J_R = 0$)
$J_A \leq J_M$ and $W_R = 0$	$J_V = (J_A - J_M)/y_{AV}$ and $J_R = 0$
State variables	
Egg buffer	$\frac{d}{dt} W_B = -J_A$ with $W_B(0) = W_{B0}$ (until $W_B = 0$)
Structural body mass	$\frac{d}{dt} W_V = J_V$ with $W_V(0) \approx 0$
Reproduction buffer	$\frac{d}{dt} W_R = J_R$ with $W_R(0) = 0$
Spawning events	
Number of eggs	$\Delta R = \text{floor}(y_{BA} W_R / W_{B0})$
Reset buffer	$W_R = W_R - \Delta R W_{B0}/y_{BA}$
Continuous reproduction	$R = y_{BA} J_R / W_{B0}$
Derived model results	
Max. structural mass	$W_{Vm} = d_V \left(\kappa J^a_{Am}/J^v_M\right)^3$
Growth rate constant	$r_B = y_{VA} J^v_M / (3 d_V)$
Max. reproduction rate	$R_m = (1-\kappa) J^a_{Am} L^2 y_{BA}/W_{B0}$
Mass at birth	$W_{Vb} = W_{B0} y_{VA} \kappa$ (when $J_M \approx 0$)
Hatching time	$t_b = 3 W^{1/3}_{B0} d^{2/3}_V / (J^a_{Am} (y_{VA}\kappa)^{2/3})$ (when $J_M \approx 0$)
Physical length	$L_w = L/\delta_M$
Total weight	$W_w = W_V + W_R$

Table 2: Model definition and some derived model results. The 'floor' function for the spawning events means rounding to the nearest integer less than the value between brackets.

Symbol	Explanation	Dimension	Sugg. value
	Primary parameters		
F_m^a	Maximum area-specific searching rate	$l_e^3/(l^2t)$	–
J_{Am}^a	Maximum area-specific assimilation rate	$m_a/(l^2t)$	–
J_M^v	Volume-specific maintenance costs	$m_a/(l^3t)$	–
W_{B0}	Assimilates in a single freshly-laid egg	m_a	–
W_{Vp}	Structural body mass at puberty	m	–
y_{AV}	Yield of assimilates on structure (starvation)	m_a/m	0.8 mg/mg (dwt)
y_{AX}	Yield of assimilates on food	m_a/m_f	0.8 mg/mg (dwt)
y_{BA}	Yield of egg buffer on assimilates	m_a/m_a	0.95 mg/mg (dwt)
y_{VA}	Yield of structure on assimilates (growth)	m/m_a	0.8 mg/mg (dwt)
κ	Fraction of assimilation flux for soma	–	0.8
	Conversions		
d_V	Dry-weight density of structure	m/l^3	0.1 mg/mm^3
δ_M	Shape correction coefficient	–	
	Fluxes, states and forcings		
J_A	Mass flux for assimilation	m_a/t	
J_M	Mass flux for maintenance	m_a/t	
J_R	Mass flux to reproduction bufeer	m_a/t	
J_V	Mass flux for structure	m/t	
J_X	Mass flux of food	m_f/t	
W_B	Mass of assimilates buffer in egg	m_a	
W_R	Mass of reproduction buffer in adult	m_a	
W_V	Mass of structural body	m	
X	Food density in the environment	m_f/l_e^3	
	Other output and secondary parameters		
f	Scaled functional response (0-1)	–	
J_{Xm}^a	Maximum area-specific feeding rate	$m_f/(l^2t)$	
K	Half-saturation food density	m_f/l_e^3	
L	Volumetric body length	l	
L_w	Physical body length	l	
r_B	Von Bertalanffy growth rate constant	$1/t$	
ΔR	Number of eggs in a clutch	#	
R	Continuous reproduction rate	$\#/t$	
R_m	Maximum continuous reproduction rate	$\#/t$	
t_b	Time between egg laying and birth	t	
W_{Vb}	Structural body mass at birth	m	
W_w	Physical body weight (total)	m	

Table 3: Explanation of symbols, with dimensions given in mass (m for body, m_a for assimilates, and m_f for food), length (l_e for environment, l for organism), numbers (#), time (t). Suggested values for the yields (apart from y_{AV}) based on the typical values in [8].

2 Derived properties

2.1 Maximum size and growth rate

Note that $L^3 = W_V/d_V$. We fill in the growth equation with the fluxes J_A and J_M, and use the scaled functional response f:

$$\frac{d}{dt}(d_V L^3) = 3d_V L^2 \frac{d}{dt}L = y_{VA}\left(\kappa f J^a_{Am} L^2 - J^v_M L^3\right) \tag{1}$$

$$\frac{d}{dt}L = \frac{y_{VA}}{3d_V} J^v_M \left(f\kappa \frac{J^a_{Am}}{J^v_M} - L\right) \tag{2}$$

At maximum food ($f = 1$) and no stressor effects, we can obtain the von Bertalanffy growth equation, with as parameters the maximum volumetric length (L_m) and the growth rate constant (r_B):

$$\frac{d}{dt}L = r_B(fL_m - L) \tag{3}$$

$$L_m = \kappa \frac{J^a_{Am}}{J^v_M} \quad \text{and} \quad r_B = \frac{y_{VA}}{3d_V} J^v_M \tag{4}$$

We can similarly fill in the equation for the continuous reproduction rate (buffer size reduces to zero), and derive the maximum reproduction rate:

$$R = (1-\kappa) f J^a_{Am} L^2 \frac{y_{BA}}{W_{B0}} \tag{5}$$

$$R_m = (1-\kappa) J^a_{Am} L^2_m \frac{y_{BA}}{W_{B0}} \tag{6}$$

$$R = f R_m \frac{L^2}{L^2_m} \tag{7}$$

2.2 Approximate size and age at birth

Growth of the embryo is given by:

$$\frac{d}{dt}L = \frac{y_{VA}}{3d_V}\left(\kappa J^a_{Am} - J^v_M L\right) \quad \text{with } L(0) \approx 0 \tag{8}$$

If we assume that maintenance losses are negligible in this stage:

$$\frac{d}{dt}L = \frac{y_{VA}}{3d_V} \kappa J^a_{Am} \quad \text{with } L(0) \approx 0 \tag{9}$$

This is not a differential equation anymore, and we can easily solve to:

$$L = \frac{y_{VA}}{3d_V}\kappa J^a_{Am} t \tag{10}$$

$$W_V = d_V \left(\frac{y_{VA}}{3d_V}\kappa J^a_{Am}\right)^3 t^3 \tag{11}$$

$$= \frac{1}{d_V^2}\left(\frac{y_{VA}}{3}\kappa J^a_{Am}\right)^3 t^3 \tag{12}$$

The mass of egg reserve over time is determined by:

$$\frac{d}{dt}W_B = -J^a_{Am}L^2 \quad \text{with } W_B(0) = W_{B0} \tag{13}$$

Filling in the equation for L:

$$\frac{d}{dt}W_B = -J^a_{Am}\left(\frac{y_{VA}}{3d_V}\kappa J^a_{Am}\right)^2 t^2 \quad \text{with } W_B(0) = W_{B0} \tag{14}$$

$$= -(J^a_{Am})^3\left(\frac{y_{VA}}{3d_V}\kappa\right)^2 t^2 \tag{15}$$

Again, this is an ordinary derivative that we can solve to:

$$W_B = W_{B0} - \frac{(J^a_{Am})^3}{3}\left(\frac{y_{VA}}{3d_V}\kappa\right)^2 t^3 \tag{16}$$

$$= W_{B0} - \left(\frac{J^a_{Am}}{3}\right)^3\left(\frac{y_{VA}}{d_V}\kappa\right)^2 t^3 \tag{17}$$

$$= W_{B0} - \frac{1}{d_V^2}\left(\frac{J^a_{Am}}{3}\right)^3 (y_{VA}\kappa)^2 t^3 \tag{18}$$

$$= W_{B0} - \frac{W_V}{y_{VA}\kappa} \tag{19}$$

The egg buffer is finished when $W_B = 0$ and then:

$$W_{B0} = \frac{W_{Vb}}{y_{VA}\kappa} \tag{20}$$

$$W_{Vb} = W_{B0}y_{VA}\kappa \tag{21}$$

This result could also be derived directly; clearly, in the absence of maintenance, y_{VA} and κ determine how the egg buffer is used to make structural biomass. Birth occurs when $W_V = W_{Vb}$ and thus:

$$\frac{1}{d_V^2}\left(\frac{y_{VA}}{3}\kappa J_{Am}^a t_b\right)^3 = W_{B0} y_{VA}\kappa \tag{22}$$

$$t_b^3 = \frac{3^3 d_V^2 W_{B0} y_{VA}\kappa}{\left(y_{VA}\kappa J_{Am^a}\right)^3} \tag{23}$$

$$= \frac{3^3 d_V^2 W_{B0}}{(y_{VA}\kappa)^2 (J_{Am}^a)^3} \tag{24}$$

$$t_b = \frac{3 d_V^{2/3} W_{B0}^{1/3}}{(y_{VA}\kappa)^{2/3} J_{Am}^a} \tag{25}$$

3 Maturity and maturity maintenance

3.1 Adding maturity maintenance

Maturity maintenance in DEB theory is paid from the $1-\kappa$ flux to maintain the development status of the organism. This process can easily be included in DEBkiss in a slightly modified form. In DEB, maturity maintenance is proportional to the cumulative investment in maturity, up to puberty, when it is fixed to the value at puberty. Here, we do not follow maturity, so we cannot link maturity maintenance to that state. As an alternative, we can use structural body volume as a proxy for maturity. We also need additional assumptions about if and how to pay for maturity maintenance under starvation. All other parameters being equal, adding this process leads to less reproductive output and a slightly different shape of reproduction rate versus body size. This effectively yields a model that is (for the feeding life-cycle stages) equivalent to the simplified DEBtox approach [5] when the reserve density goes to zero. For practical applications, it makes sense to include maturity maintenance as a process *a priori* (it can always be set to zero). In the simplest possible model (e.g., for teaching purposes), however, it should be left out. To include maturity maintenance, we need to add some assumptions:

1. Maturity maintenance is proportional to structural volume up till puberty. After puberty, maturity maintenance is fixed to the level at puberty.

2. From the $1-\kappa$ flux of assimilates, maturity maintenance is paid first. The remainder goes to the reproduction buffer.

3. Under starvation, maturity maintenance is paid from the reproduction buffer as long as there is something in the buffer. Maturity maintenance is not paid from structure.

So we obtain for the maturity maintenance flux J_J:

$$J_J = J_J^v L^3 \quad \text{when } W_V < W_{Vp} \tag{26}$$

$$J_J = J_J^v L_p^3 \quad \text{when } W_V \geq W_{Vp} \text{ (note: } L_p^3 = W_{Vp}/d_V) \tag{27}$$

where J_J^v is the volume-specific costs for maturity maintenance. The maturity maintenance flux is withdrawn from the $1-\kappa$ flux, so the reproduction flux becomes:

$$J_R = (1-\kappa)J_A - J_J \tag{28}$$

Under starvation ($\kappa J_A < J_M$), we assume that maturity maintenance is (partly) paid as long as possible, until the organism needs to shrink:

$$J_A > J_M + J_J \text{ or } W_R > 0: \quad J_V = 0 \text{ and for adults } J_R = J_A - J_M - J_J \tag{29}$$

$$J_M + J_J \geq J_A > J_M \text{ and } W_R = 0: \quad J_V = J_R = 0 \text{ and } J_J = J_A - J_M \tag{30}$$

$$J_A \leq J_M \text{ and } W_R = 0: \quad J_V = (J_A - J_M)/y_{AV} \text{ and } J_R = J_J = 0 \tag{31}$$

In principle, J_J^v is a primary parameter that can be fitted to experimental data. However, we can also set it to a 'suggested value', by assuming a link with somatic maintenance. If $\kappa = 0.8$, the remaining flux $1-\kappa$ is 4 times smaller. We can start from the assumption that J_J^v will also be 4 times smaller than J_M^v. In general, let's take:

$$J_J^v = \frac{1-\kappa}{\kappa} J_M^v \tag{32}$$

This is not just an arbitrary choice: in the standard DEB model, linking these maintenance processes in this exact way yields the situation where the cumulative investment in maturity at puberty is independent of the food availability. This is one of the assumptions underlying the 'DEBtox' simplification [5].

To derive the reproduction rate in compound parameters:

$$R = \frac{y_{BA}}{W_{B0}} \left((1-\kappa) f J_{Am}^a L^2 - \frac{1-\kappa}{\kappa} J_M^v L_p^3 \right) \tag{33}$$

$$= \frac{y_{BA}}{W_{B0}} \frac{1-\kappa}{\kappa} J_M^v \left(\kappa f \frac{J_{Am}^a}{J_M^v} L^2 - L_p^3 \right) \tag{34}$$

$$= \frac{y_{BA}}{W_{B0}} \frac{1-\kappa}{\kappa} J_M^v \left(f L_m L^2 - L_p^3 \right) \tag{35}$$

$$R_m = \frac{y_{BA}}{W_{B0}} \frac{1-\kappa}{\kappa} J_M^v \left(L_m L_m^2 - L_p^3 \right) \tag{36}$$

$$R = R_m \frac{f L_m L^2 - L_p^3}{L_m^3 - L_p^3} \tag{37}$$

Adding maturity maintenance (using the suggested link to somatic maintenance) improves the fit to the reproduction data in our case study (Fig. 2), and results in somewhat different parameter estimates (Table 4).

3.2 Maturity in more detail

We can follow the investment into maturity in more detail. This could especially be useful if body size at puberty varies with treatments or between individuals. The investment

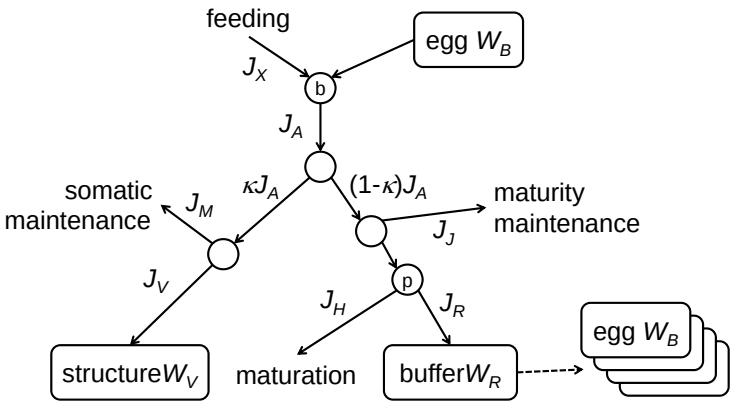

Figure 1: Schematic diagram of the mass flows in the model extended with maturity maintenance (and showing the maturation flux J_H).

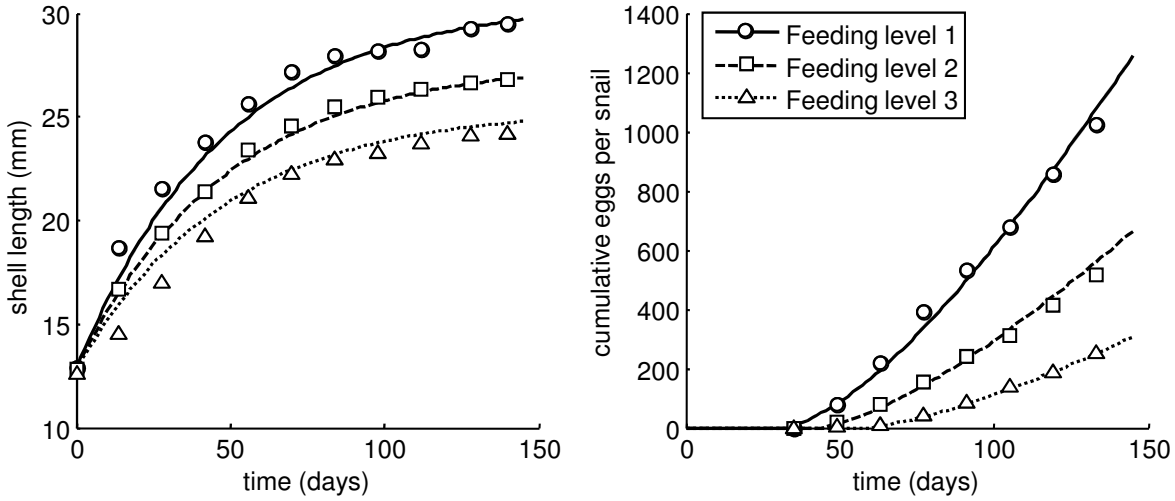

Figure 2: Fits of the DEBkiss model to growth and reproduction data for the pond snail in three feeding regimes [9]. In contrast to the fits in the main text, this is the model extended with maturity maintenance.

Symbol	Add mat. maint.	Also male function	Unit
J^a_{Am}	0.12 (0.11-0.13)	0.14 (0.13-0.16)	mg/mm^2/d
J^v_M	0.0078 (0.0069-0.0088)	0.0078 (0.0069-0.0088)	mg/mm^3/d
W_{Vp}	67 (63-70)	67 (63-70)	mg
y_{BA}	0.95 (n.e.)	0.55 (n.e.)	mg/mg
κ	0.78 (0.76-0.80)	0.67 (0.65-0.69)	–
f_2	0.90 (0.89-0.92)	0.90 (0.89-0.92)	–
f_3	0.83 (0.81-0.85)	0.83 (0.81-0.85)	–

Table 4: Parameter estimates for the fits to the growth and reproduction data for the pond snail (see Figure 2). The following parameters were fixed: $d_V = 0.1$ mg/mm^3, $y_{VA} = 0.8$, $\delta_M = 0.401$, $W_{B0} = 0.15$ mg, $L_w(0) = 12.8$ mm, $f = 1$ for the *ad libitum* feeding level. For the two limiting food levels, f_2 and f_3 are used instead of $f = 1$. The difference between the two fits lies in a different fixed value for y_{BA}.

in maturity can be linked to developmental stages [1], and can be quantified using the cumulative dry mass of assimilates invested in it, W_H. Here, we are starting more general, loosening assumption 1 from the previous section, and taking maturity maintenance proportional to the cumulative investment in maturity:

$$J_H = \frac{d}{dt}W_H = (1-\kappa)J_A - J_J \quad \text{with } J_J = k_J W_H \quad \text{and } W_H(0) \approx 0 \tag{38}$$

where k_J is the maturity maintenance rate coefficient (dimension t^{-1}). Now, k_J is a free parameter, and we can link developmental switches (such as puberty) to a maturity level rather than a fixed structural size. Note that for adults, $J_H = 0$, as this entire flux is used for reproduction after reaching puberty. Under starvation, we can depart from the assumption that investment into maturity continues as long as there is anything left in the $1-\kappa$ branch after paying maturity maintenance.

How can we obtain a fixed size at puberty at different food levels? In that case, structure needs to be a perfect proxy for maturity, or in other words, the maturity density needs to be constant (a similar derivation was presented in [5]):

$$\frac{W_H}{L^3} = W_H^v = \text{constant} \tag{39}$$

Both L^3 and W_H start at a very low value at the start of embryonic development. If the ratio of these two states must remain constant, so their derivatives should also have a constant ratio:

$$\frac{\frac{d}{dt}W_H}{\frac{d}{dt}L^3} = W_H^v \quad \Rightarrow \quad \frac{d}{dt}W_H = W_H^v \frac{d}{dt}L^3 = \frac{W_H^v}{d_V}\frac{d}{dt}W_V \tag{40}$$

Filling in the equations for the two derivatives:

$$(1-\kappa)J_A - k_J W_H = W_H^v \frac{y_{VA}}{d_V}(\kappa J_A - J_M^v L^3) \tag{41}$$

$$(1-\kappa)J_A - k_J W_H = W_H^v \frac{y_{VA}}{d_V}\kappa J_A - W_H^v \frac{y_{VA}}{d_V} J_M^v L^3 \tag{42}$$

For this equality to hold for every pattern of J_A over time, both the factors before the J_A and the subtracted terms must be equal on both sides. Starting with the subtracted terms:

$$k_J W_H = W_H^v \frac{y_{VA}}{d_V} J_M^v L^3 \tag{43}$$

$$k_J = \frac{y_{VA}}{d_V} J_M^v \quad \text{note that } W_H^v = \frac{W_H}{L^3} \tag{44}$$

Thus, k_J needs to have a particular relationship to J_M^v. Next the terms before J_A:

$$1-\kappa = W_H^v \frac{y_{VA}}{d_V}\kappa \tag{45}$$

$$W_H^v = \frac{1-\kappa}{\kappa}\frac{d_V}{y_{VA}} \tag{46}$$

Note that we can multiply Equation 44 and 46 to obtain:

$$k_J W_H^v = \frac{1-\kappa}{\kappa} J_M^v = J_J^v \tag{47}$$

which is exactly the same result as we derived more intuitively in the previous section.

4 Calculating the respiration flux

Respiration can be taken proportional to the total flux of assimilates that is dissipated. The dissipation flux is the sum of the assimilates used for maintenance (somatic and maturity) and maturation, plus the overheads for growth, reproduction and feeding. Introducing an additional subscript 'o' to specify overheads, the total dissipation flux is given by:

$$J_D = J_M + J_J + J_H + J_{Vo} + J_{Ro} + J_{Xo} \tag{48}$$

For a growing organism, the overhead fluxes for growth and reproduction are easily calculated from the yield coefficients, but under starvation conditions, more care is needed. For the growth overheads, we have to distinguish the situation for growth and shrinking separately:

$$J_{Vo} = \begin{cases} (1-y_{VA})J_V & \text{if } J_V \geq 0 \\ -(1-y_{AV})J_V & \text{if } J_V < 0 \end{cases} \tag{49}$$

For the reproduction overheads, when there is no reproduction buffer, the overheads are paid continuously:

$$J_{Ro} = (1 - y_{BA})J_R \tag{50}$$

Note that J_R cannot become negative, unless there is a reproduction buffer. So, for continuous reproduction, we do not have to consider the case of starvation. When there is a reproduction buffer, J_R will be negative when the buffer is used to pay maintenance costs. In that case, there is no transformation, so $J_{Ro} = 0$. We assumed that overhead costs are paid at spawning, so we predict an instantaneous dissipation of an amount of assimilates:

$$\Delta W_D = \frac{W_{B0}\Delta R}{y_{BA}} - W_{B0}\Delta R \tag{51}$$

In practice, the overheads of reproduction will only be a small fraction of the total dissipation flux, so assuming a constant overhead flux J_{Ro} will not radically affect the respiration predictions.

The feeding overheads J_{X0} (also referred to as the heat increment of feeding) are a bit more complex to obtain in the model. The yield coefficient y_{AX} specifies the gain of assimilates on food, but the remainder $(1 - y_{AX})$ is not totally burnt as overheads as it includes the mass of the faeces too. In practice, respiration is often determined in animals that have been starved for a while to allow this component to be ignored.

For embryos, we can use a simpler calculation of J_D, as the entire flux of assimilates that is not fixed in structure has to be burnt:

$$J_D = J_A - J_V \tag{52}$$

5 Extensions for temperature and deviating growth

5.1 Changes in temperature

We can assume that all rate constants (with a dimension that includes 'per time') scale in the same way with temperature. We can use the Arrhenius relationship to scale from a reference temperature T^* to the actual temperature T (both in Kelvin). All physiological rate constants have to be multiplied by:

$$F_T = \exp\left(\frac{T_A}{T^*} - \frac{T_A}{T}\right) \tag{53}$$

where T_A is the Arrhenius temperature in Kelvin. Lika and co-workers [8] suggest a value of 8000 K as typical value.

5.2 Deviating growth curves: V1-stage

Following [7, 1], we can add a V1 acceleration stage after birth, which lasts until 'metamorphosis' at a certain size L_j. V1 morphy implies that feeding and assimilation scale with a volume L^3 instead of a surface L^2. The maximum specific assimilation rate J^a_{Am} needs to be multiplied by a factor δ:

$$\delta = \begin{cases} 1 & \text{if } W_V < W_{Vb} \\ L/L_b & \text{if } W_{Vb} < W_V < W_{Vj} \\ L_j/L_b & \text{if } W_V > W_{Vj} \end{cases} \tag{54}$$

This module adds one parameter ($W_{Vj} = d_V L_j^3$). Note that the parameter value for J_{Am}^a now represents the value for the embryo only; maximum length now becomes L_j/L_b times the L_m calculated from J_{Am}^a for the embryo.

5.3 Deviating growth curves: juvenile food limitation

Following [3], we can take a size-dependent food limitation as hyperbolic function:

$$f = f_0 \left(1 + \frac{W_{Vf}}{W_V}\right)^{-1} \tag{55}$$

where W_{Vf} is the structural body weight at which f is half the value of f_0. Alternatively, one could try the food limitation function of [9]:

$$f = a f_0 \frac{L}{L_m} \quad \text{as long as } L < L_f \tag{56}$$

where a is a dimensionless proportionality constant, and L_f the critical length above which the food limitation disappears.

6 Toxicants

6.1 Adding toxicokinetics

The simplest model for toxicokinetics (TK) is the first-order one-compartment model, where the entire organism is seen as a well-mixed homogeneous compartment. It is possible to account for effects of growth on TK [5]. In the absence of a (considerable) reproduction buffer, we can use the following equations for the scaled (c_V) and unscaled (C_V) internal concentration in a growing organism (see [5]):

$$\frac{d}{dt} c_V = k_e^* \frac{L_m}{L}(c_d - c_V) - \frac{c_V}{W_V}\frac{d}{dt} W_V \tag{57}$$

$$\frac{d}{dt} C_V = k_e^* \frac{L_m}{L}(P_{Vd} c_d - C_V) - \frac{C_V}{W_V}\frac{d}{dt} W_V \tag{58}$$

where c_d is the dissolved concentration in water, P_{Vd} is the partition coefficient between dry weight of structure and water, and k_e^* is the reference elimination rate constant at maximum size. The elimination rate scales with a surface:volume and thus inversely with a length measure (as long as growth is isomorphic). The last term in the equation deals with growth dilution. In the scaled equation, note that $c_V(\infty) = c_d$.

Symbol	Explanation	Dimension	Sugg. value
c_d	Dissolved concentration in water	m_q/l_e^3	–
c_V	Scaled concentration in structure	m_q/l_e^3	–
C_R	Concentration in repro buffer	m_q/m	–
C_V	Concentration in structure	m_q/m	–
C_w	Concentration in whole organism	m_q/m	–
J_{QR}	Flux of chemical with continuous repro	m_q/t	–
k_e	Elimination rate coefficient	$1/t$	–
k_e^*	Reference elimination rate constant	$1/t$	–
P_{Rd}	Partition coeff. repro buffer-water	l_e^3/m_a	–
P_{RV}	Partition coeff. repro buffer-structure	m/m_a	1
P_{Vd}	Partition coeff. structure-water	l_e^3/m	–
P_{wd}	Partition coeff. whole body-water	l_e^3/m	–
v_Q	Mass-transfer coefficient for chemical exchange	l/t	–
W_Q	Mass of chemical in whole organism	m_q	–
W_{QR}	Mass of chemical in repro buffer	m_q	–
W_{QV}	Mass of chemical in structure	m_q	–
δ_Q	Shape correction for chemical uptake	–	
ΔW_Q	Change in mass of chemical at spawning	m_q	–

Table 5: Explanation of symbols, with dimensions given in mass (m for body dwt., m_a for assimilates dwt., and m_q for chemical mass), length (l_e for environment, l for organism), time (t).

Because we now have an explicit mass balance for biomass in DEBkiss, it makes sense to do the same for chemical mass. In this way, we can include the chemical losses due to reproduction (transfer of chemical from mother to the eggs), and the effects due to the build up and emptying of the reproduction buffer. Now, we have to proceed more carefully. Because there are now two types of body mass that change in time in a different (or even discontinuous) way, it makes sense to start following chemical mass W_Q instead of concentrations, and apply strict mass balancing. This has the added benefit that we can even include the test vessel into our mass balance and thus account for the loss of chemical in water due to uptake into the animal. We depart from a series of assumptions:

1. The dynamics of the internal concentration in the whole organism follows one-compartment first-order kinetics, but with parameters that vary over time. To achieve this, chemical exchange between structural biomass and reproduction buffer must be fast relative to exchange with the environment.

2. The exchange flux of chemical with the exposure medium is proportional to the *structural* surface area and inversely proportional to the *total* body weight.

3. The reproduction buffer can have a different affinity for the chemical than structural biomass. The initial concentration in the eggs is the same as the concentration in the reproduction buffer just before spawning.

Total body weight of the animal $W_w = W_V + W_R$. The exchange of the chemical between the environment (dissolved concentrations) and the animal can be seen as a diffusion process. The exchange rate constant (commonly known as the elimination rate, k_e) depends on the surface area for exchange (which is linked to structural volumetric length using a shape corrector δ_Q), the total weight of the animal, and on the mass-transfer coefficient or 'conductance' of the interface for the chemical (v_Q):

$$k_e = d_V v_Q \frac{(\delta_Q L)^2}{W_w} \tag{59}$$

The elimination rate thus depends both on structural weight (we assume the surface for exchange is associated with structural biomass only) and on the total weight, and thus changes over time. For practical purposes, we can introduce a reference value k_e^* to indicate the elimination rate constant for a fully grown adult without reproduction buffer:

$$k_e^* = d_V v_Q \frac{\delta_Q^2 L_m^2}{W_{Vm}} = v_Q \frac{\delta_Q^2}{L_m} \tag{60}$$

which means we can rewrite the actual size-dependent elimination rate as (note that $W_{Vm} = d_V L_m^3$):

$$k_e = k_e^* \frac{d_V L^2 L_m}{W_V + W_R} \tag{61}$$

When there is no buffer ($W_R = 0$), we return to the expression for the elimination rate as used above:

$$k_e = k_e^* \frac{L_m}{L} \tag{62}$$

When we deal with a reproduction buffer, the total weight of the organism will change instantly at spawning. Therefore, it is advisable to follow chemical masses rather than concentrations. The whole organism acts as a one-compartment model:

$$\frac{d}{dt} W_Q = k_e W_w \left(P_{wd} c_d - \frac{W_Q}{W_w} \right) \tag{63}$$

The total partition coefficient P_{wd} is a weighted average of those for structural biomass and the reproduction buffer:

$$P_{wd} = \frac{P_{Vd} W_V + P_{Rd} W_R}{W_w} \tag{64}$$

It is practical to introduce a partition coefficient between the reproduction buffer and structure:

$$P_{RV} = \frac{P_{Rd}}{P_{Vd}} \tag{65}$$

and use that to rewrite the total partition coefficient:

$$P_{wd} = \frac{P_{Vd}W_V + P_{RV}P_{Vd}W_R}{W_w} \tag{66}$$

$$= P_{Vd}\frac{W_V + P_{RV}W_R}{W_V + W_R} \tag{67}$$

Now, it is easily shown how the total partition coefficient differs from the partition coefficient of structure. When $W_R = 0$ or $P_{RV} = 1$, we obtain $P_{wd} = P_{Vd}$.

With the above equations we can model the total chemical mass in the body up to a spawning event. At spawning, the total mass of chemical is instantly reduced by a fraction that equals the fraction of assimilates transferred into the eggs:

$$\Delta W_Q = \frac{W_{B0}\Delta R}{W_R}W_{QR} \tag{68}$$

Note that this implies that the mother's chemical *concentration* will *increase* (slightly) at spawning: the mass that is lost in the overheads of the egg production (as y_{BA} is smaller than 1) does not come with an associated loss of chemical.

To calculate the transfer to eggs, we need access to the chemical mass in the reproduction buffer W_{QR}. To calculate toxicant effects, we need access to the chemical amount in structure W_{QV}. The fraction of the total chemical mass that is in the buffer obviously depends on the mass of assimilates in the buffer, but also on the partition coefficient P_{RV}. We start from the definition of the three internal concentrations:

$$C_w = \frac{W_Q}{W_w} \quad C_V = \frac{W_{QV}}{W_V} \quad C_R = \frac{W_{QR}}{W_R} \tag{69}$$

and the definition of P_{RV}, coupled with the assumption of fast equilibration between buffer and structure:

$$P_{RV} = \frac{C_R}{C_V} = \frac{W_{QR}}{W_R}\frac{W_V}{W_{QV}} \tag{70}$$

Using $W_{QR} = W_Q - W_{QV}$, and some manipulation, we obtain:

$$W_{QV} = W_Q\left(1 + P_{RV}\frac{W_R}{W_V}\right)^{-1} \tag{71}$$

Clearly, when $P_{RV} = 0$ it follows that $W_{QV} = W_Q$. Further, the larger P_{RV} and the larger the buffer relative to structure, the smaller the fraction that W_{QV} forms of the total body mass of chemical. Knowing W_{QV} and W_Q means that we also can calculate W_{QR} as the difference, as well as C_V.

C_V is still the unscaled internal concentration in structure; the equations we presented still include P_{Vd} as a model parameter. It is possible to scale the internal concentrations with P_{Vd} to obtain scaled concentrations c_V. However, as the total partition coefficient P_{wd} varies in time, the interpretation that $c_V(\infty) = c_d$ is lost. A toxicity threshold on c_V thus does not imply a safe water concentration. In practical calculations, we can simply

set $P_{Vd} = 1$, as long as we make sure that the parameters that have a dimension including 'internal concentration' should now be interpreted as 'scaled internal concentration'.

When we can consider reproduction to be continuous, $W_R = 0$ but, for adults, there is still a continuous flux of chemical out of the body with eggs:

$$J_{QR} = RW_{B0}P_{RV}C_V \tag{72}$$

This flux can be subtracted from the changes in concentration as follows:

$$\frac{d}{dt}c_V = k_e^*\frac{L_m}{L}(c_d - c_V) - \frac{c_V}{W_V}\frac{d}{dt}W_V - \frac{RW_{B0}}{W_V}P_{RV}c_V \tag{73}$$

$$\frac{d}{dt}C_V = k_e^*\frac{L_m}{L}(P_{Vd}c_d - C_V) - \frac{C_V}{W_V}\frac{d}{dt}W_V - \frac{RW_{B0}}{W_V}P_{RV}C_V \tag{74}$$

From these equations, it is obvious that the losses due to reproduction can be ignored by taking $P_{RV} = 0$.

6.2 Toxicant effects

The internal concentration can subsequently be linked to any of the primary parameters of the model (see [5, 4]). Following [6], we can use a linear-with threshold (c_0) relationship for the dimensionless stress level on a parameter (in the control, $s = 0$):

$$s = \frac{1}{c_T}\max(0, c_V - c_0) \tag{75}$$

Here, we assume that the dose metric is the scaled internal concentration in structure c_V. The proportionality c_T is called the 'tolerance' concentration. Stress can increase or decrease the value of a parameter p like so:

$$p \to p(1+s) \quad \text{or} \quad p \to p\max(0, 1-s) \tag{76}$$

For some parameters there is room for discussion. Take the yield coefficient for structure on assimilates y_{VA}. A decrease in the yield can be implemented as $y_{VA}(1-s)$. But, if we interpret the effect as an increase in the overhead costs for growth, we should take $y_{VA}/(1+s)$. It all depends on our interpretation of effects. In the past, effects on yields have been implemented as an increase in the overheads [6, 4, 5].

Effects on survival can similarly be linked to the internal concentration, e.g., by using any of the toxicodynamic modules of the GUTS framework [2]. In the stochastic-death case, the hazard rate due to toxic stress (h_Q) is given by:

$$h_Q = b\max(0, c_V - c_{0s}) \tag{77}$$

where c_{0s} is the threshold for effects on survival, and b is a proportionality constant referred to as the 'killing rate'.

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