Vrije Universiteit
Biological laboratory

De ontwikkeling van een dynamisch energie budget en bioaccumulatie model

deel 1, SAWES nota 91.03: achtergrond document

Opdrachtgever: Rijkswaterstaat, Dienst Getijdewateren
Uitvoerder: Vrije Universiteit Amsterdam
Periode: 01/05/89 - 31/12/90

Voorwoord

In de periode 01/05/89 tot 31/12/90 heeft de Vrije Universiteit Amsterdam (VUA) in opdracht van de Dienst Getijde Wateren van Rijkswaterstaat (RWS/DGW) in het kader van het project SAWES (systeemanalyse Westerschelde) onderzoek uitgevoerd naar modelvorming voor het opname/eliminatie gedrag van xenobiotika in dieren in de Westerschelde. In het bijzonder betrof het zware metalen, PCB's, mosselen (*Mytilus*) en de wadpier (*Arenicola*).

Het doel van het onderzoek was een theoretische achtergrond te geven voor de samenhang tussen concentraties van xenobiotica in water en weefsel zoals die in de Westerschelde worden gemeten. Deze inzichten zouden worden vertaald in een model, dat onder het programma SENECA van RWS/DGW als module moest kunnen doorgerekend worden. De noodzaak van het onderzoek werd duidelijk op grond van een voorstudie van Drs.R.J.F. van Haren, uitgevoerd bij RWS/DGW, waarbij bleek dat een klassiek één-kompartimenten model ontoereikend was om de bestaande metingen aan mosselen in te passen. De oorzaak werd gezocht in het fysiologisch gedrag van mosselen, dat een duidelijke seizoens-periodiciteit doorloopt, hetgeen ondermeer terug te vinden is in grote fluctuaties van het lipide gehalte.

Het onderzoek werd uitgevoerd door Drs.R.J.F. van Haren, in de periode 01/05/89-31/08/90, en Hr.H.E. Schepers, in de periode 01/09/89-31/12/90, onder leiding van Prof.Dr.S.A.L.M. Kooijman. Het project werd vanuit RWS/DGW begeleid door een commissie waarin de volgende mensen zitting hadden: Drs.J. van der Meer (projectleider eerste half jaar), Drs.J. Marquenie (eerste paar maanden), Mw.Drs.J.van Buuren (eerste periode), Dr.B.van Eck (volle periode, projectleider na eerste half jaar), Ir.J.P.G. van de Kamer (tweede periode), Drs.J. Schobben (tweede periode).

De probleemstellingen van de verschillende deelonderwerpen en de resultaten zijn neergelegd in de volgende manuscripten

- Application of a one-compartment toxico kinetic model to artificial and environmental contaminated marine mussels (*Mytilus edulis*) in the Werstern Scheldt. Dit is het rapport op grond waarvan besloten is tot aanvullend onderzoek en wat als referentie dienst doet voor het op fysiologische processen gebaseerde model.

- Energy Budgets can explain body size relations. Dit artikel verscheen in *J. Theor. Biol.* **121** (1986): 269-282. Het is op verzoek van RWS/DGW toegevoegd omdat het de theorie geeft voor de opname en gebruik van energie bij dieren in het algemeen, die het mogelijk maakt verschillende soorten op basis van parameterwaarden te vergelijken en de waarden, als eerste benadering, in elkaar om te rekenen op grond van de lichaamsgrootte.

- Application of a dynamic energy budget model to *Mytilus edulis* (L.). Dit concept-artikel zal na bijschaving en commentaar van specialisten worden aangeboden aan *Functional Ecology*. Het bevat de model formulering, de toetsing en de parameter schattingen van het physiologisch model voor de mossel.

- Animal energy budgets affect the kinetics of xenobiotics. Dit artikel is verschenen in *Chemosphere* **21** (1990) 681-694. Het bevat de model formulering van het opname-eliminatie gedrag van xenobiotica

- Energetics affect xenobiotic kinetics in *Mytilus edulis* (L.). Dit concept-artikel zal na bijschaving en commentaar worden aangeboden aan een nog nader vast te stellen tijdschrift. Het bevat de toetsing van het opname-eliminatie model, gecombineerd met het fysiologisch model op mosselen.

  - De parameters van het DEB model voor de wadpier *Arenicola marina* in relatie tot die van de mossel *Mytilus edulis*

- Effects of feeding conditions on toxicity for the purpose of extrapolation. Dit artikel zal verschijnen in *Comp. Biochem. Physiol.* Het staat buiten het contract en moet gezien worden als een "toegift", ten einde zichtbaar te maken welke rol de gedane modelvorming kan spelen in toegepast eco-toxicologisch onderzoek. Het gaat in op de relatie tussen opname en effecten. Het kan een basis zijn voor mogelijk vervolg onderzoek.

- Computer handleiding voor de bij RWS/DGW geïnstalleerde software die onder SENECA draait om de modelvoorspellingen door te rekenen. De verdere "calibratie" en toepassing op andere diersoorten zoals de bot, zal door Drs.J. Schobben worden uitgevoerd.

APPLICATION OF A ONE-COMPARTMENT TOXICO KINETIC MODEL TO ARTIFICIAL AND ENVIRONMENTAL CONTAMINATED *MARINE MUSSELS (Mytilus edulis).* IN THE WESTERN SCHELDT

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1. Introduction

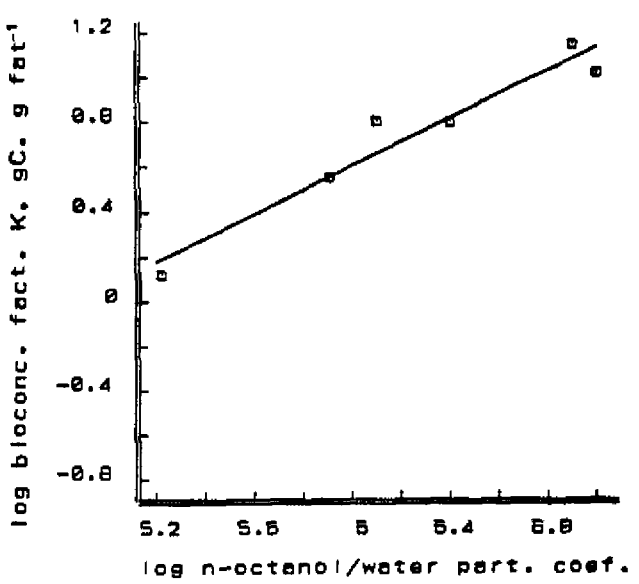
The Western Scheldt in the Dutch Delta area is a polluted ecosystem by heavy metals and organic micropollutants. Main source for xenobiotics entering the Scheldt estuary is the river Scheldt itself.

Marine mussels, *Mytilus edulis*, reflect to some extent in their tissues the external xenobiotic concentrations. Monitoring programs as the Mussel Watch are based on this phenomenon (Goldberg, 1975, 1986).

The Dutch Government started in 1987 the SAWES project to investigate the distribution and behaviour of contaminating substances in the Scheldt estuary and its organisms. The final result will be a Water Quality model which relates discharges and loads to chemical distribution of the contaminating compounds in water, sediments and organisms. In this paper some results are shown on the analysis of the uptake / elimination kinetics of xenobiotics in mussels with the simplest possible model, the one-compartment model, which has also the advantage that it is frequently used (Opperhuizen 1986).

In section 3 the 1-compartment model is applied to laboratory and field conditions in order to estimate the parameters of this model. The influence of energy dynamics and size on the accumulation and elimination of xenobiotics cannot be handled with the ordinary 1-compartiment models as presented in section 2. A discussion and deriviation of a uptake / elimination model which do account for changing physiological rates is presented in Kooijman & van Haren (1990). A comparison of the 1-compartment model and the physiological uptake / elimination model is discussed in Schepers et al, 1991.

Figure 1 K vs K_{ow} for PAH's.
(from estimates -see appendix)



2. One compartment model

The one-compartment accumulation / elimination model is widely used in toxico kinetic studies (Bruggeman,1983; Opperhuizen,1986). For an extensive discussion on special properties of this model see Opperhuizen 1986. The model is:

$$Q' = k\,c(t) - \frac{1}{\tau}Q \qquad \text{given } Q_0 \qquad (2.1)$$

With Q is the concentration in the organism, c(t) is the compound concentration in water, k uptake constant τ and elimination time. When the mussel is in equilibrium, the product $k\tau$ can be interpreted as the bioconcentration factor K. Equation 2.1 can be solved when c(t) is constant and rewritten with $K=k\tau$, which results in:

$$Q(t) = Q_0 e^{-t/\tau} + Kc(1 - e^{-t/\tau}) \qquad (2.2)$$

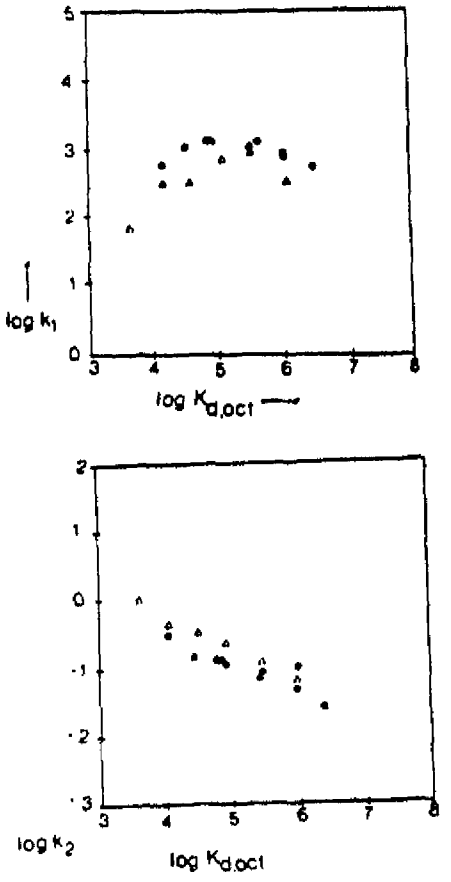


Figure 2(from Opperhuizen)
Dependence of k_1 and k_2 on K_{ow}.

The uptake constant k, can be interpreted in terms of membrane permeation with a diffusion type of kinetics (van Haren et al, 1990).
In bioaccumulation studies the *n*-octanol-water partition coefficient is most often used as an indicator for the bioavailable fraction (see e.g. Geyer et al, 1982; Esser, 1986, Opperhuizen, 1986 and Malhot & Peters, 1988). Between aqueous solubility and octanol-water partition coefficients exists clear empirical relationships (Miller et al, 1985). In figure 1 the bioconcentration factor K is plotted against octanol water partition coefficients.See fig.2 for plots of the dependence of k (called k_1 in the legend) and $1/\tau$ (called k_2 in the legend) on the K_{ow}. (from Gobas et. al. 1986). Recall that the bioaccumulation factor $K = k_1 / k_2$. Fig 2 shows that k_1 is almost independent of the k_{ow} and k_2 decreases as a function of the k_{ow}, thus K will increase (fig 1) with the k_{ow}.

When the mussel is in equilibrium with surrounding water and there is no significant trend in external concentrations c, during a time interval T ($T > 3\tau$), the bioconcentration factor K can be interpreted as the equilibrium fraction of xenobiotics taken up from the ambient water. Fig. 3 shows how K (the slope of the line) is estimated from data for cadmium and chromium.

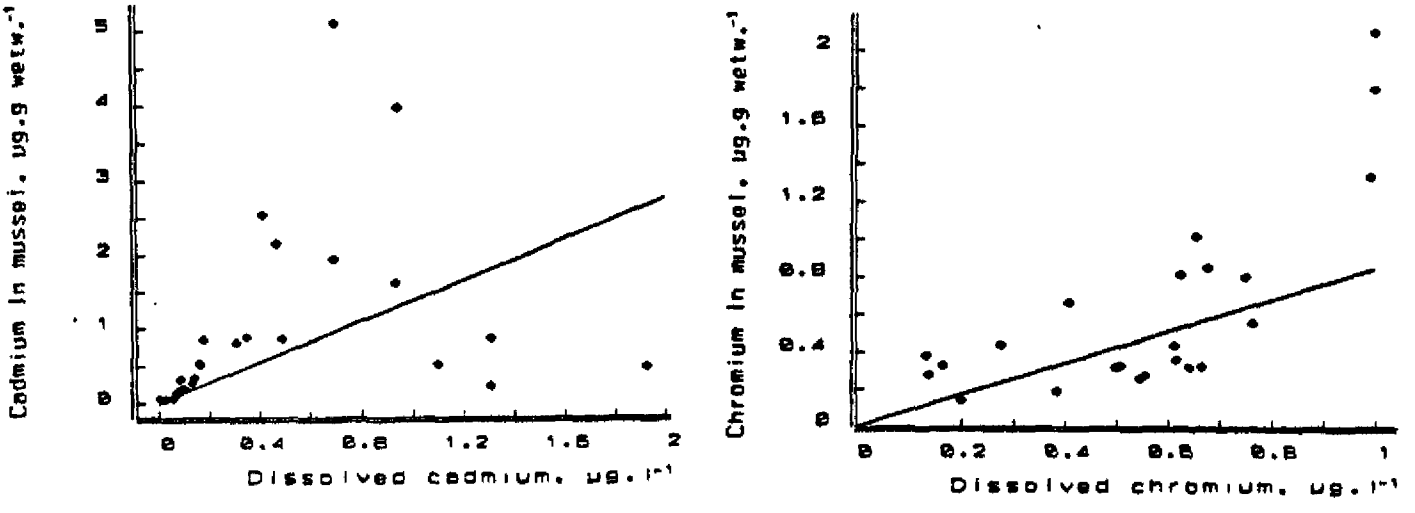


Figure 3 Estimation of Bioconcentration factor K for Cadmium and Chromium.

3 Estimation of the parameters of the one - compartment model

The parameters of the 1-compartment model are estimated by means of a least squares criterion, fitting accumulation / elimination curves from laboratory experiments or active biomonitoring programs in field. The results for each pollutant component are given in the appendix. In Table 1 all estimates for both metals and organic micro pollutants.are listed together with parameter values from the literature.

3.1 Metals

The estimations for metals are carried out with the experimental data of Adema (1981). The estimated parameters are listed in Table 1. The estimated values of the biological halflife $T_{1/2}$ ($= \tau \ln 2$), are compared with other estimates from literature, see Table 1. The biological halflifes for Cd, Cu and Zn are within the parameter range found by others. Large differences of at least one order of magnitude, between reported halflifes for Cd are conspicuous. According to Borchardt (1983) Cd elimination might be increased with decreasing food availability. This trend contradicts our findings ($T_{1/2} \approx 16$ days) of fast elimination rates for Cd under conditions of starvation. At this moment no explanation is available.

The bioconcentration factor K, reflects the partition of the pollutant compound over organism and water. K values can be compared when the physiological conditions of the mussels are equal. Estimated bioconcentration factors K, for mussels in the field, based on yearly mean environmental and tissue pollutant concentrations can be seen in figure 3. The estimated K for Cd in the field is a factor of two higher than the estimated K in the laboratory. For Cr we see a factor of four. This difference might be caused by different metal speciation in field and laboratory due to different chemical characteristics of water and the slib which influence concentrations of ionic or chloride complex fractions of metals, see also van Haren et al (1990). Reported bioconcentration factors for Cd in field based on mussel dry weight are 10000 - 20000 (Talbot, 1985; Cossa 1988). Assuming a dry weight fraction of 15%, our estimated bioconcentration factor of Cd based on field measurements is 9200.

The essential metals Cu and Zn appeared to be independent of environmental Cu or Zn concentrations. Figure 4 (left) shows that there is a Cu concentration in the organism even when the concentration in the water is zero. The same is true for Zinc.(fig. 4, right) An internal mechanism of regulation might be the reason for this phenomenon (Amiard et al, 1987). The site of regulation is probably located in lysosomes in kidney cells (George & Pirie, 1980; George, 1980). The recent discovery of an unique low molecular weight (around 1000 dalton) zinc-binding ligand in the kidney (Lobel, 1989) corroborate these findings. Comparison of bioconcentration factor for essential metals is therefore useless.

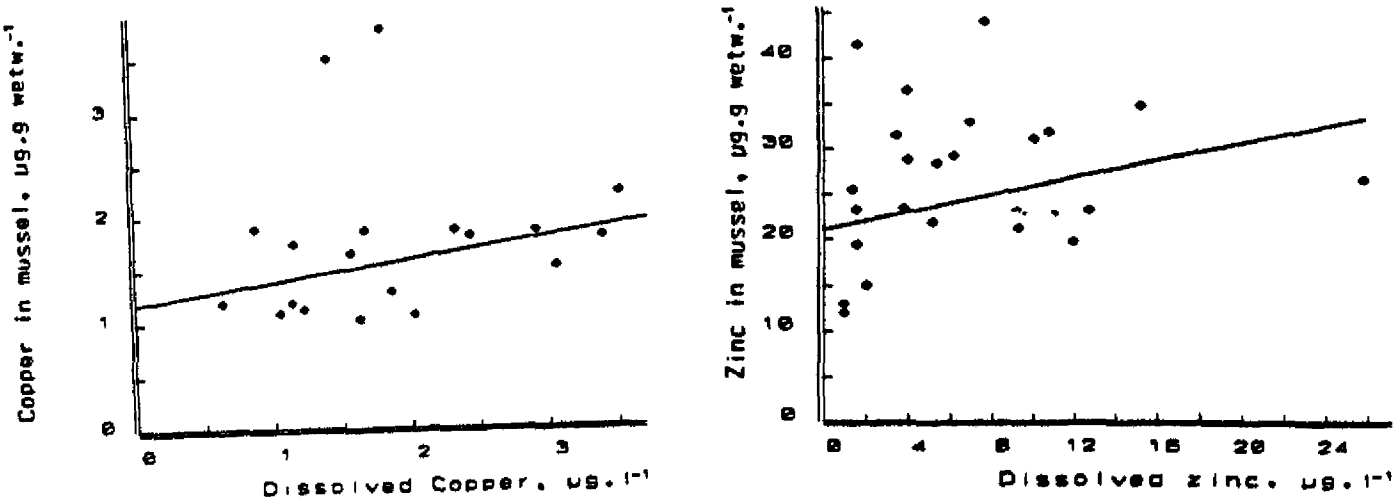


Figure 4: Internal concentration vs external concentration for Copper (left) and Zinc (right) 'in equilibrium' A clear intercept with the y-axis means that some internal regulation for these trace metals exists, which is not incorporated in the model.

3.2 Organic micro pollutants

Estimation of the parameters of the 1-compartment model for organic compounds are carried out with transplantated mussels along a pollution gradient in field. Unfortunately the site of origin of the transplantated mussels was more polluted then the pollution gradient itself, so a nett elimination occurred with a rate dependent on the environmental compound concentrations (NOSPEC, 1989).

The mean environmental compound concentrations which are used as input for the model, are expressed on the fraction organic carbon of the suspended matter. The measured particulate adsorbed pollutant concentrations are more reliable then the measured dissolved pollutant concentrations (NOSPEC 1989). For this reason alone we prefer to use particulate adsorbed concentrations (g metal per g Carbon (C)). Physiological changes due to differences in feeding conditions in time are removed by expressing the internal compound concentrations on the fat content of the mussel. In this way we obtain a bioconcentration factor K with dimensions $gC.gfat^{1}$ which differ in dimensions from most other studies.

The compounds B(a)P and B(b)F give in figure 1 an underestimation of K when compared with the other compounds. Biotransformation of B(a)P and B(b)F might be the reason for the observed deviation. At least for B(a)P it is shown that biotransformation in *Mytilus* occurs (Livingstone et al,1989) at considerable rates, in vitro estimated to be 1.1 $\mu g.d^{-1}$ in gills (gill tissue dry weight 0.1 g; mussel 6-7 cm; temp. 29° C).

More estimates however of the bioconcentration factor K are necessary for obtaining a reliable empirical relationship between K and octanol water partition coefficients.

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5.Appendix
CADMIUM IN MYTILUS EDULIS, ADEMA 1981.

Least squares fit of cadmium concentration in mussel based on dissolved cadmium in natural Oosterschelde water (Dutch Delta area).
Laboratory experiments performed in contineuos flow systems with following specifications (Adema, 1981, report TNO, MD-N&E 81/3):

- temperature: 15° C
- salinity: 28 °/00
- pH: 8
- flow velocity: 237 - 242 l.per 24 hours
- length mussel: 4 - 5 cm

Fitted model, :

$$Q(t) = Q(0)\, e^{-t/\tau} + cK(1 - e^{-t/\tau})$$

with:

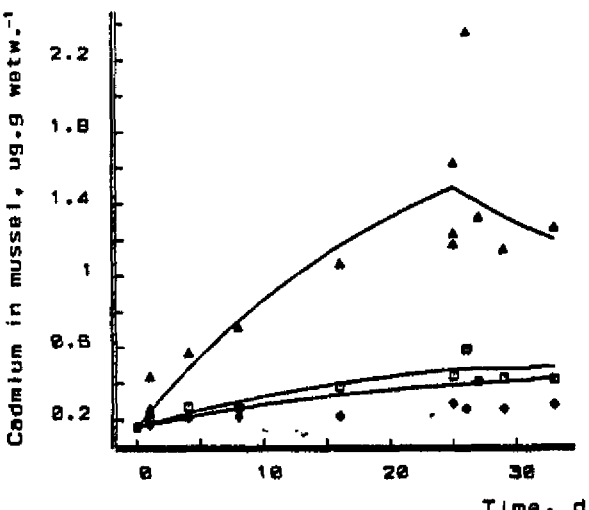
Q	concentration in mussel (µg.g wetw.$^{-1}$)
t	time, d
τ	elimination time constant, d
K	concentration factor, (l.g wetw.$^{-1}$)
c	dissolved concentration, (µg.l^{-1})

Three exposure regimes with the following mean dissolved concentrations:

none:	0.8	µg.l^{-1}	(between 0.01 - 2.2 µg.l^{-1})
low:	1.0	µg.l^{-1}	
high:	3.4	µg.l^{-1}	

Due to the high variance in the none and low exposures, a weighted simultaneous least squares fitted procedure is carried out. Weight coefficients resp. 0.3, 0.6 and 1 for accumulation, 0.3, 0.5 and 1 for elimination.

	estimates	standard deviation	dimension
K	0.636	0.121	l.g wetw.$^{-1}$
τ	22.9	9.03	d



Simultaneous least squares fitted accumulation / elimination curves, respectively 25 and 8 days, of cadmium concentration in mussel after aqeous exposure to three different cadmium concentrations.

CHROMIUM IN MYTILUS EDULIS, ADEMA 1981.

Least squares fit of chromium concentration in mussel based on dissolved chromium in natural Oosterschelde water (Dutch Delta area).
Laboratory experiments performed in continuous flow systems with following specifications (Adema, 1981, report TNO, MD-N&E 81/3):

- temperature: 15° C
- salinity: 28 °/00
- pH: 8
- flow velocity: 237 - 242 l.per 24 hours
- length mussel: 4 - 5 cm

Fitted model, :

$$Q(t) = Q(0)\, e^{-t/\tau} + cK(1 - e^{-t/\tau})$$

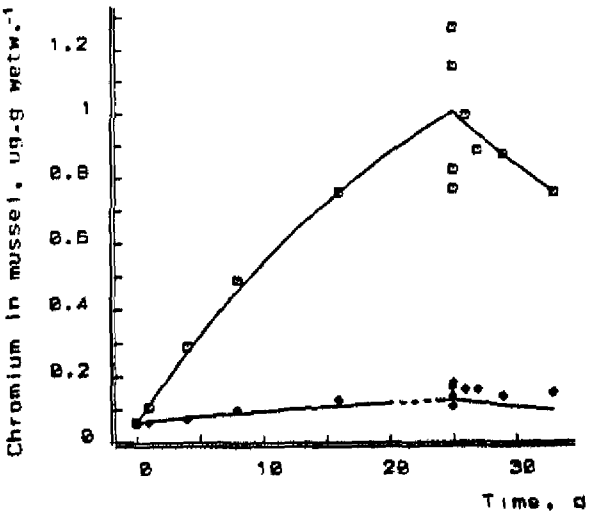
with:

Q	concentration in mussel ($\mu g.g\ wetw.^{-1}$)
t	time, d
τ	elimination time constant, d
K	concentration factor, ($l.g\ wetw.^{-1}$)
c	dissolved concentration, ($\mu g.l^{-1}$)

Two exposure regimes with the following mean dissolved concentrations:

low:	1.0	$\mu g.l^{-1}$
high:	9.4	$\mu g.l^{-1}$

	estimates	standard deviation	dimension
K	0.179	0.0304	$l.g\ wetw.^{-1}$
τ	28.3	8.38	d



Simultaneous least squares fitted accumulation / elimination curves, respectively 25 and 8 days, of chromium in mussel after aqueous exposure to two different (dissolved) chromium concentrations.

ZINC IN MYTILUS EDULIS, ADEMA 1981.

Least squares fit of zinc concentration in mussel based on dissolved zinc in natural Oosterschelde water (Dutch Delta area).
Laboratory experiments performed in continuous flow systems with following specifications (Adema, 1981, report TNO, MD-N&E 81/3):

- temperature: 15° C
- salinity: 28 °/00
- pH: 8
- flow velocity: 237 - 242 l.per 24 hours
- length mussel: 4 - 5 cm

Fitted model,:

$$Q(t) = Q(0)\, e^{-t/\tau} + cK(1 - e^{-t/\tau})$$

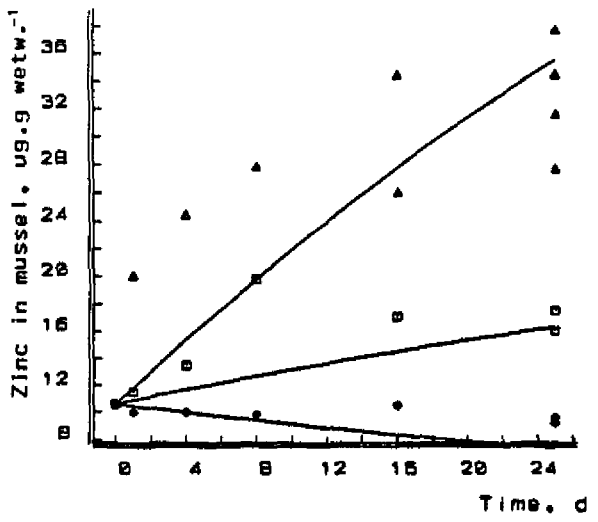
with:

Q	concentration in mussel (µg.g wetw.$^{-1}$)
t	time, d
τ	elimination time constant, d
K	concentration factor, (l.g wetw.$^{-1}$)
c	dissolved concentration, (µg.l^{-1})

Three exposure regimes with the following mean dissolved concentrations:

none:	2.9	µg.l^{-1}
low:	48	µg.l^{-1}
high:	146	µg.l^{-1}

	estimates	standard deviation	dimension
K	0.552	0.259	l.g wetw.$^{-1}$
τ	56.6	37.9	d



Simultaneous least squares fitted accumulation / elimination curves, respectively 25 and 8 days, of zinc in mussel after aqueous exposure to three different (dissolved) zinc concentrations.

COPPER IN MYTILUS EDULIS, ADEMA 1981.

Least squares fit of copper concentration in mussel based on dissolved copper in natural Oosterschelde water (Dutch Delta area).
Laboratory experiments performed in continuous flow systems with following specifications (Adema, 1981, report TNO, MD-N&E 81/3):

- temperature: 15° C
- salinity: 28 °/00
- pH: 8
- flow velocity: 237 - 242 l.per 24 hours
- length mussel: 4 - 5 cm

Fitted model, :

$$Q(t) = Q(0)\, e^{-t/\tau} + cK(1 - e^{-t/\tau})$$

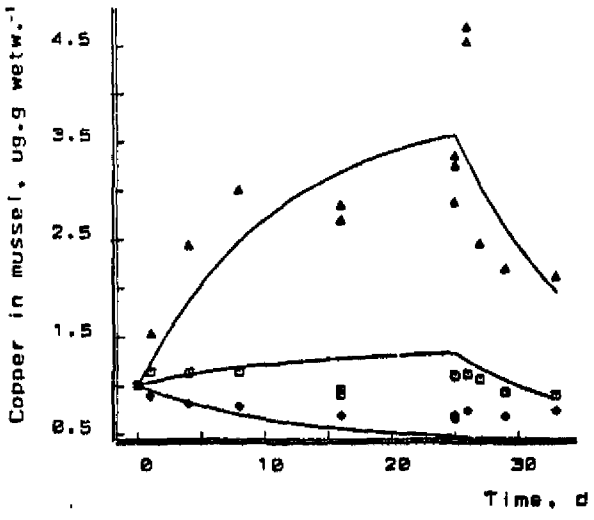
with:

Q	concentration in mussel (µg.g wetw.$^{-1}$)
t	time, d
τ	elimination time constant, d
K	concentration factor, (l.g wetw.$^{-1}$)
c	dissolved concentration, (µg.l^{-1})

Three exposure regimes with the following mean dissolved concentrations:

none:	0.9	µg.l^{-1}
low:	3.0	µg.l^{-1}
high:	8.5	µg.l^{-1}

	estimates	standard deviation	dimension
K	0.456	0.0235	l.g wetw.$^{-1}$
τ	11.2	2.41	d



Simultaneous least squares fitted accumulation / elimination curves, respectively 25 and 8 days, of copper in mussel after aqueous exposure to three different (dissolved) copper concentrations.

PCB52 IN MYTILUS EDULIS, NOSPEC DATA spring 1986.

Least squares fit of concentration of PCB52 in mussel based on PCB52 in suspended matter expressed on its organic carbon content (ng.gC^{-1}).
Input concentration c = Ec(t)
Fitted model, :

$$Q(t) = Q(0)\, e^{-t/\tau} + cK(1 - e^{-t/\tau})$$

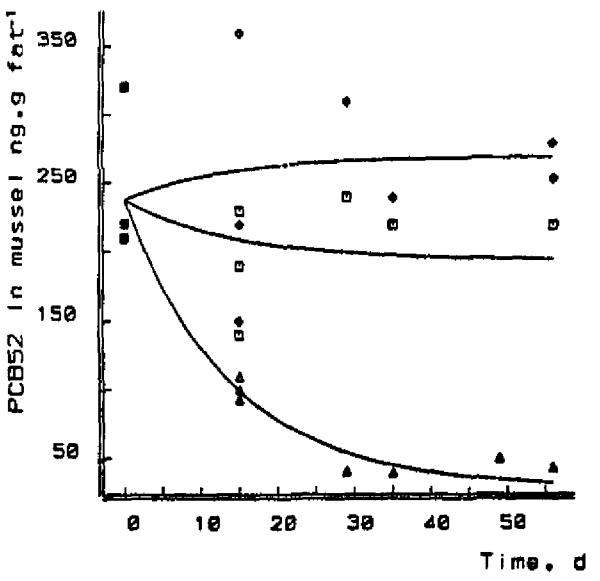
with:

Q	concentration in mussel (ng.g fat^{-1})
t	time, d
τ	elimination time constant, d
K	concentration factor, (gC.g fat^{-1})
c	concentration on suspended matter, (ng.gC^{-1})

Estimates based on following mean input concentrations, ng.gC^{-1}:

	mean	standard deviation
$c_{2\ km}$	28.1	16.5
$c_{10\ km}$	17.5	12.5
$c_{60\ km}$	4.9	3.7

	estimate	standard deviation	dimension
Q(0)	237.6	12.5	ng.g fat^{-1}
K	6.4	0.4	gC.g fat^{-1}
τ	13.9	3.9	d



Simultaneous least squares fitted concentrations in mussel at Noordwijk, coastal distances are 2, 10, 60 km, with input concentrations c = Ec(t), ng.gC^{-1} suspended matter.

PCB153 IN MYTILUS EDULIS, NOSPEC DATA spring 1986.

Least squares fit of concentration of PCB153 in mussel based on PCB153 in suspended matter expressed on its organic carbon content ($ng.gC^{-1}$).

Input concentration $c = Ec(t)$

Fitted model, :

$$Q(t) = Q(0)\, e^{-t/\tau} + cK(1 - e^{-t/\tau})$$

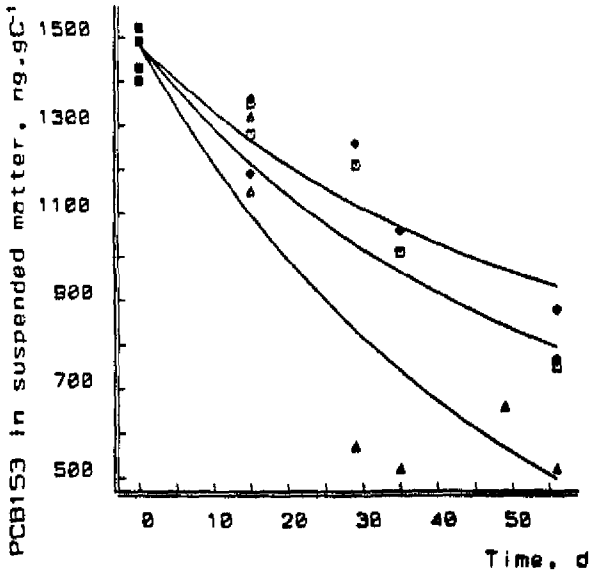
with:

Q	concentration in mussel ($ng.g\ fat^{-1}$)
t	time, d
τ	elimination time constant, d
K	concentration factor, ($gC.g\ fat^{-1}$)
c	concentration on suspended matter, ($ng.gC^{-1}$)

Estimates based on following mean input concentrations, $ng.gC^{-1}$:

	mean	standard deviation
$c_{2\ km}$	49.3	32.0
$c_{10\ km}$	35.3	16.3
$c_{60\ km}$	5.0	3.8

	estimate	standard deviation	dimension
Q(0)	1482.5	29.6	$ng.g\ fat^{-1}$
K	14.1	2.0	$gC.g\ fat^{-1}$
τ	46.9	5.0	d



Simultaneous least squares fitted concentrations in mussel at Noordwijk, coastal distances are 2, 10, 60 km, with input concentrations $c = Ec(t)$, $ng.gC^{-1}$ suspended matter.

B(a)P IN MYTILUS EDULIS, NOSPEC DATA spring 1986.

Least squares fit of concentration of B(a)P in mussel based on B(a)P in suspended matter expressed on its organic carbon content ($ng.gC^{-1}$).
Input concentration c = Ec(t)
Fitted model, :

$$Q(t) = Q(0)\, e^{-t/\tau} + cK(1 - e^{-t/\tau})$$

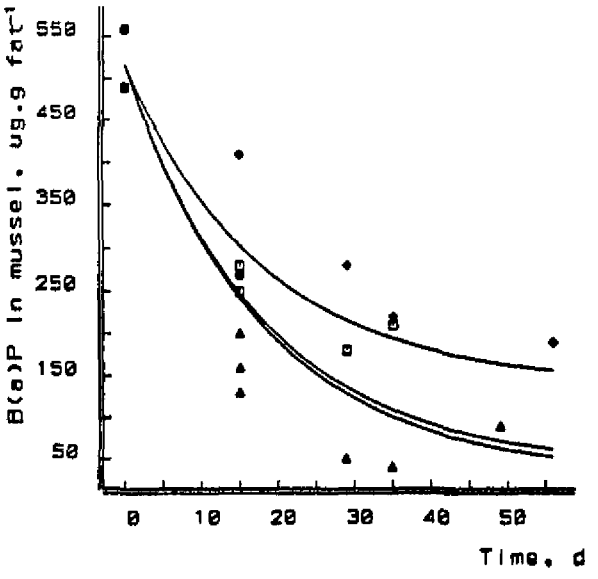
with:

Q	concentration in mussel ($ng.g\ fat^{-1}$)
t	time, d
τ	elimination time constant, d
K	concentration factor, ($gC.g\ fat^{-1}$)
c	concentration on suspended matter, ($ng.gC^{-1}$)

Estimates based on following mean input concentrations, $ng.gC^{-1}$:

	mean	standard deviation
$c_{2\ km}$	249.8	98.4
$c_{10\ km}$	868.3	712.9
$c_{60\ km}$	190.1	118.2

	estimate	standard deviation	dimension
Q(0)	517.1	29.9	$ng.g\ fat^{-1}$
K	0.161	0.0765	$gC.g\ fat^{-1}$
τ	18.0	3.62	d



Simultaneous least squares fitted concentrations in mussel at Noordwijk, coastal distances are 2, 10, 60 km, with input concentrations c = Ec(t), $ng.gC^{-1}$ suspended matter.

FluA IN MYTILUS EDULIS, NOSPEC DATA spring 1986.

Least squares fit of concentration of FluA in mussel based on FluA in suspended matter expressed on its organic carbon content ($ng.gC^{-1}$).
Input concentration c = Ec(t)
Fitted model, :

$$Q(t) = Q(0)\, e^{-t/\tau} + cK(1 - e^{-t/\tau})$$

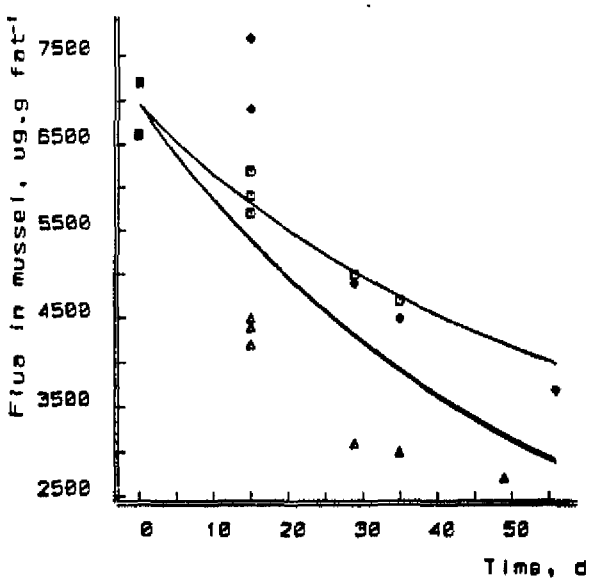
with:

Q	concentration in mussel ($ng.g\ fat^{-1}$)
t	time, d
τ	elimination time constant, d
K	concentration factor, ($gC.g\ fat^{-1}$)
c	concentration on suspended matter, ($ng.gC^{-1}$)

Estimates based on following mean input concentrations, $ng.gC^{-1}$:

	mean	standard deviation
$c_{2\ km}$	673	167
$c_{10\ km}$	1928	857
$c_{60\ km}$	711	349

	estimate	standard deviation	dimension
Q(0)	6951	313	$ng.g\ fat^{-1}$
K	1.33	0.830	$gC.g\ fat^{-1}$
τ	50.2	12.5	d



Simultaneous least squares fitted concentrations in mussel at Noordwijk, coastal distances are 2, 10, 60 km, with input concentrations c = Ec(t), $ng.gC^{-1}$ suspended matter.

Table 1

Least squares estimated bioconcentration factors, K, and biological halflives, $T_{1/2}$, with their standard deviations between brackets of anorganic and organic pollutant compounds in *Mytilus edulis*, under non-equilibrium conditions. For metals Adema (1981) is used and for organic micropollutants NOSPEC (1987) is used. For Cd and Cr the bioconcentrationfactors K, under equilibrium field conditions are printed cursive (data from Dutch contribution to ICES/JMG and kindly provided by the Ministry of Public Workd and Transport.
Model applied is: $Q(t) = Q_0 e^{-t/\tau} + cK(1 - e^{-t/\tau})$, with $T_{1/2} = t \ln 2$.

PAH's are benzo(a)pyrene B(a)P; benzo(b)fluoranthene, B(b)F; fluoranthene, FluA; chrysene, Chr Polychlorobiphenyls are named according to their IUPAC numbers.
$\log(K_{ow})$are resp.: 6.1, 6.4, 7.0, 6.9; Shiu & Mackay,1986;
6.5, 6.57, 5.22, 5.91; Hawker & Connell, 1986)

	Bioconcentration factor, K l.g wet weight^{-1}	Biological halflife, (d) $T_{1/2}$ this article	$T_{1/2}$ other articles	references
Metals				
Cd	0.636 (0.121)	15.8 (6.26)	*M.edulis*: 14-29; 300; 96-190;	(Scholz, 1980; George, 1980; Borchardt, 1983;
	1.38 (0.371)		14-35	Kock & Groenewoud, 1985)
			M.galloprovinciales: 21; 125	(Majori et al, 1973a; Viarengo et al, 1985)
Cr	0.179 (0.0304)	19.6 (5.81)		
	0.851 (0.136)			
Zn	0.552 (0.259)	3[illegible].2 (26.3)	*M.edulis*: 1.3-60; >50	(George, 1980; George et al, 1980)
			M.californianus: 76	(Young et al, 1976)
Cu	0.456 (0.0235)	7.76 (1.67)	*M.galloprovinciales*: 4; 9-10	(Majori et al, 1973b; Viarengo et al, 1985)
Organic compounds				
	K, (g.Cg fat^{-1})			
PCB52	6.4 (0.4)	9.63 (2.7)	*M.edulis*:	
			M.smaragdinus: 5.5	(Tanabe et al, 1987)
			(*Perna veridis*)	
PCB153	14.1 (2.0)	32.5 (3.47)	*M.edulis*: 11.1-12.1; 45.6	(Kock & Groenewoud, 1985; Pruell et al, 1986)
			M.smaragdinus: 8.8	(Tanabe et al, 1987)
B(a)P	0.161 (0.0765)	12.5 (2.51)	*M.edulis*: 15.4	(Pruell et al, 1986)
FluA	1.33 (0.830)	34.8 (8.66)	*M.edulis*: 29.8; 7.6 -11.1	(Pruell et al, 1986); McLeese & Burridge,)
*PCB118	6.3 (0.5)	27.8 (2.84)	*M.smaragdinus*: 6.8	(Tanabe et al, 1987)
*PCB138	10.5 (1.4)	32.6 (3.26)	*M.edulis*: 8.3-11.8	(Kock & Groenewoud, 1985)
			M.smaragdinus: 8.3	(Tanabe et al, 1987)
*B(b)F	0.203 (0.112)	16.0 (1.97)	*M.edulis*: 16.9	(Pruell et al, 1986)
*Chr	3.60 (1.52)	55.0 (49.0)	*M.edulis*: 14.2	(Pruell et al, 1986)

* Not presented as a figure.

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Energy Budgets Can Explain Body Size Relations

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The size-dependence of some 20 physiological variables has been derived from a rather simple model for energy budgets. This nine parameter model is based on detailed observations on the growth and reproduction at varying food densities, and has the state variables size and storage. The size-dependence of some variables works out to be different for animals of the same species as opposed to animals of different species. The reproductive rate, for instance, tends to increase with size for animals of the same species, but to decrease with size for animals of different species. This is because the parameter values are constants within a species, but vary in a size dependent manner for animals of different species. Although growth at constant food density is assumed to be of the von Bertalanffy type, and routine metabolism to be proportional to size, respiration turns out to be about proportional to size to the power 3/4, both within and between species. The value of about 3/4 has frequently been found, but it has always been thought to be incompatible with von Bertalanffy growth.

1. Introduction

he aim of this paper is to show that, starting from assumptions on the quantitative spects of energy budgets, we can derive in a systematic manner the way in which ıany physiological and ecological variables, such as ingestion, growth and reproduc-on, depend on body size. These types of relations have recently come to the ›refront, (McMahon & Bonner, 1983; Peters, 1983; Schmidt-Nielsen, 1984; Calder, 984) and are used to predict, e.g., food chain efficiencies in ecology. Body size :lations are invariably taken to be of the allometric type, i.e. $Y = aW^b$, where the arameters a and b are estimated by linear regression in a log–log plot of the ependent variable Y against body size W. The parameter b has become particularly opular, and will be called the scaling parameter. Apart from heat production, only :levant for endotherms, the most important body size relation concerns respiration, e. rate of oxygen consumption or carbon dioxide production, where the scaling arameter has the value 0·66 for unicellular organisms, 0·88 for ectotherms, and ·69 for endotherms, (see Phillipson, 1981). The exact value of the scaling parameter iffers among authors who take their data from the literature. The variations are ue in part to differences in the species included and in the experimental conditions nder which respiration rates were measured. For crustaceans Vidal & Whitledge 1982) quote values of 0·72 and 0·85, and Conover (1978) gives 0·74. If the regression overs a great many species, from bacteria up to elephants, the scaling parameter

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is found to be 0·75, an almost magic number in scaling relations. Since it is less than unity, it has often been concluded that large animals use energy more efficiently than small ones, even though this has not been substantiated for ectotherms. An implied assumption in this conclusion is, however, that respiration rate corresponds to routine metabolic rate, which includes energy investment in the reconstitution of enzymes and membranes and in routine movements, but not in growth, reproduction, digestion and differentiation. We shall see that this assumption does not hold in the following simple model for energy budgets. Together with routine metabolism energy investments in the other processes mentioned prove to contribute substantially to respiration rate. The model is formulated in terms of the state variables size and energy storage as functions of fluctuating food density. The relevance of the model has been checked for the water flea *Daphnia magna* (Kooijman & Metz, 1984), and Kooijman (1986*a*) on the basis of a wide variety of experimental data and for egg development in fish and birds (Kooijman, 1986*b*). Only a minor part of the data will be considered in this paper for illustrative purposes. We shall confine the discussion to ectotherms. For the extension of the model to endotherms, see Kooijman (1985). Here we shall first derive the model on the basis of a set of assumptions, and then consider scaling relations within and between species.

2. Energy Budgets

The energy budget model is based on the assumptions listed in Table 1. It regards an animal as an input–output system, as illustrated in Fig. 1, with state variables

TABLE 1

Assumptions of the energy budget model

1. Energy utilized for maintenance $\dot{M}$, for growth $\dot{W}$, and for reproduction or differentiation is at the expense of stored energy.
2. For given size, the size-specific storage and its dynamics do not depend on any partitioning rule for energy utilized.
3. Maintenance energy is proportional to size: $\dot{M} = \dot{\zeta} W$.
4. A unit increase in size consumes a fixed amount η of energy.
5. Assimilation $\dot{A}$ is proportional to ingestion $\dot{I}$: $\dot{A} = \dot{I}[\dot{A}_m]/[\dot{I}_m]$.
6. Ingestion starts at birth size W_b, so $\dot{I} = 0$ for $W < W_b$.
7. For $W > W_b$, ingestion is proportional to $W^{2/3}$: $\dot{I} = [\dot{I}_m] f W^{2/3}$, where f is a function of food density, defined on $(0, 1)$.
8. The scaled functional response f depends hyperbolically on food density X: $f = X/(K + X)$, where K is a constant.
9. Differentiation stops and reproduction starts at size W_j.
10. Initially, size and storage are $(0, S_0)$, where the initial egg storage, S_0, is a number such that no assumption is violated.
11. The animal dies as soon as assumption 3 has to be violated.
12. At constant food density, growth $\dot{W}$ is of the von Bertalanffy type after birth, i.e. $\dot{W} = \dot{\rho} W^{2/3} - 3\dot{\gamma} W$, where $\dot{\rho}$ and $\dot{\gamma}$ are positive and constant.
13. At constant food density, the ultimate size, W_∞, is proportional to f^3.
14. At constant food density, $1/\dot{\gamma}$ is linear in f.
15. Energy expenses on growth are non-decreasing with increasing size-specific storage for an animal of a certain size.

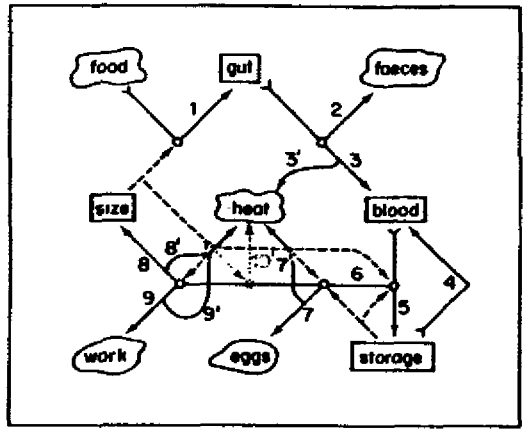

FIG. 1. Energy flow through an animal. Rates: 1. ingestion, 2. defecation, 3. assimilation, 4. mobilization, 5. demobilization, 6. utilization, 7. reproduction, 8. growth, 9. maintenance, 10. heating (only in endotherms). Symbols: → energy flow, ⇢ information flow, ○ decision valve, ' heat loss rate, □ state variable, ⌐¬ source or sink.

size, W, and storage, S. The basic idea is that:

—the tissue cells use energy, which is distributed by the blood at a rate that depends on the energy content of the blood.
—the blood circulates through the body at a rate that is high with respect to the change in the energy content of the blood.
—the mechanism that determines the energy content of the blood (which will be low, anyway) only depends on the energy content of the blood and on the amount of energy kept in storage in certain tissues (which may be considerable).

This process is summarized in assumption 1.

Two key assumptions are that food intake is proportional to surface area, so to $W^{2/3}$, and that growth is of the von Bertalanffy type (assumptions 7 and 12 in Table 1). The validity of the assumptions is illustrated in Figs 2 and 3 for *Daphnia magna*. These two results pose a fundamental problem for any detailed quantitative description of the energy budget. Observations on these daphnids reveal that individuals larger than 2·5 mm produce young at each moult, and that the amount of energy involved in this process is quite substantial (see Kooijman, 1986*a*). Since there is no significant reduction in growth (Fig. 3), nor any notable increase in food intake (Fig. 2) around 2·5 mm, we are faced with the problem of the destination of an energy flow in animals less than 2·5 mm, which corresponds to the energy spent on reproduction in larger animals. This is the basis of assumption 9, where this destination is called differentiation. It is a direct consequence of the assumption 3 that routine metabolic rate is proportional to size W. The basis of this assumption is two-fold. First we have the results of Smith (1957) and Vleck *et al.* (1980) that respiration in eggs of fish and birds is well described by a weighted sum of size and observed growth of the embryo (these results are more conclusive than results for

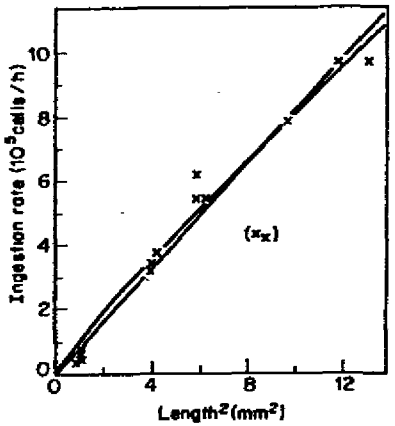

FIG. 2. Measured ingestion rate $\dot{I}$ of *Chlorella pyrenoisoda* cells as a function of body length L of *Daphnia magna* at 20°C and 10^5 cells per ml. The measurements are based on counts of resin particles (±5 μm ϕ) in resuspended faeces of individual daphnids by means of laser optics. The concentration of resin particles is 4 to 7 times 10^3/ml. The function $\dot{I} = \dot{a}L^b$ has been fitted by least squares. The value obtained for $b = 1{\cdot}81$ (95% c.i.: 1·59, 2·03), not significantly different from 2. this leads to $\dot{I} = \dot{a}L^2$ with $\dot{a} = 0{\cdot}81$ (95% c.i.: 0·76, 0·85) cells/(h × mm^2).

animals after birth, because the (relative) size increase is much larger before birth than after, and because the interpretation of respiration data before birth is not complicated by the process of feeding and reproduction). The second basis for the assumption that routine metabolic rate is proportional to size is that only if it is so, can the scaling parameter for the respiration rate be somewhere between 2/3 and 1. This will be clarified in the next section.

In the appendix, it is shown how the change in the state variables, size W and size-specific storage $[S]$, can be derived from the assumptions given in Table 1, the

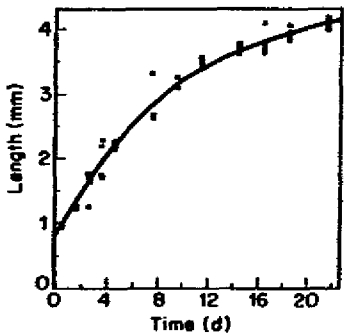

FIG. 3. The measured change in length L in individuals of *Daphnia magna* at 20°C, in 40 ml, supplied with 10^8 cells of *Scenedesmus subspicatus* a day. The curve is of the von Bertalanffy type: $L(t) = L_\infty - (L_\infty - L_0)\,e^{-\dot{r}t}$, where L_0, L_∞ and $\dot{r}$ are parameters and t the time.

result being

$$\dot{W} = \{(W^{2/3}[\dot{A}_m][S]/[S_m] - W\dot{\zeta}/\kappa)/([S] + \eta/\kappa)\}_+$$

$$[\dot{S}] = [\dot{A}_m]W^{-1/3}\{(W \geq W_b)X/(K+X) - [S]/[S_m]\}$$

where X is food density, the dots indicate rates or derivatives with respect to time and $(W \geq W_b)$ has a value of 1 or 0 if true or false. The parameters, which are assumed to be constants for a species in a constant environment (apart from, possibly, a fluctuating food density), are described in Table 2. The initial size is a model parameter, W_b and the size-specific storage at birth has to be equal to that of the mother at the moment of egg formation, if it is to be consistent.

TABLE 2

Parameters of the energy budget model

Symbol	Dimension	Interpretation	Symbol	Dimension	Interpretation
W_b	length^3	Birth size	κ		Proportion of utilized energy channelled to growth and routine metabolism
K	biomass · length^{-3}	Food density resulting in half the max. input	$\dot{\zeta}$	energy · length^{-3} · time^{-1}	Size specific routine metabolic rate
$[\dot{I}_m]$	biomass · length^{-2} · time^{-1}	Surface area specific maximum ingestion rate	η	energy · length^{-3} ·	Energy requirement for a unit increase in size
$[\dot{A}_m]$	energy · length^{-2} · time^{-1}	Surface area specific maximum assimilation	$[S_m]$	energy · length^{-3}	Size specific maximum storage

In Kooijman (1986*a*), the energy content of an egg has been derived on basis of the assumptions given in Table 2. This is necessary for the calculation of the reproduction rate, i.e. the energy channelled into reproduction ($(\kappa - 1)$ times the utilization rate in situations of growth), divided by the energy investment per egg.

The energy content of the gut has not been modelled as a state variable, because its relaxation time is assumed to be small with respect to that of the storage. This seems to be reasonable for animals like daphnids, in which the gut residence time at 20°C can be as short as 20 min. For animals with a large stomach, this assumption may not be appropriate, but the model would still apply in comparing different but constant food inputs.

The state variable energy content of blood only appears implicitly in assumption 1 because of its low energy capacity and small relaxation time. For the purpose in hand, we only have to deal with the utilization rate, and not with the mobilization and demobilization rates indicated in Fig. 1. Substitution of the equations for the assimilation rate and the storage change rate from the appendix, shows that the

utilization rate in situations of growth equals

$$\dot{C} = \{([S]/[S]+\eta/\kappa)\}\{W^{2/3}(\eta/\kappa)[\dot{A}_m]/[S_m]+W\dot{\zeta}/\kappa\}.$$

This equation will be used in the next section.

The different types of energy losses in the form of heat indicated in Fig. 1 are supposed to be fixed fractions of the energy flows involved. (This is in contrast to endotherms, where there is also another type energy drain to heat production for the purpose of heating the body. This flow rate is an order of magnitude larger (see Kooijman, 1986*a*).) Therefore there is no need to model them explicitly. They only show up in the values of the parameters. The parameter η, for instance, will be larger than the energy released in the decomposition of a unit of body tissue, partly because of its entropy or "information content", and partly because of the heat loss involved in growth.

Energy losses in movements have not been modelled explicitly here. In fact they are considered to be negligible as compared with the other energy flows. If they do not happen to be negligible, it may be that average energy losses in movements can be written as a weighted sum of size and surface area. In that case, the formulas do not change, but only the parameter values of $\dot{\zeta}$ and $[\dot{A}_m]$, which increase and decrease, respectively.

The present paper does not deal with the estimation of parameter values from experiments (this is dealt with in Kooijman, 1986*a*), but some remarks on the von Bertalanffy growth curve might be appropriate here. There is a lot of literature showing that von Bertalanffy growth curves fit experimental data on a wide variety of species very well. This is in itself remarkable because most of them concern data on animals in field situations, where food density is usually not constant nor abundant. Computer simulation studies which will be reported elsewhere show the energy storage, as introduced here, flattens out rather wild fluctuations in food density. This (partially) explains the fit.

First, we will consider how a number of variables depend on size within a species, and, secondly, how they do so between species.

3. Body Size Relations in Animals of the Same Species

Energy is normally stored in the form of carbohydrates, proteins and, especially, lipids. The utilization of the energy involves oxygen consumption and a carbon dioxide production. In animals with empty guts, ($\dot{A}=0$), the respiration rate therefore corresponds to the utilization rate in previous section. As shown in Table 3, at constant food density, it can be written as a weighted sum of $W^{2/3}$ and W, which can appear almost linear in a log–log plot with a slope somewhere between 2/3 and 1 (Fig. 4). Although we have assumed that routine metabolic rate increases linearly with size, the increase in respiration rate with size is less steep, owing to the decreasing amount of energy invested in growth and reproduction. In the case of ectotherms, there is no reason to believe that these flows are negligible in short term measurements of respiration rates. Although the actual size increase during this measurement may be negligible, the energy invested in (the overhead of) this increase may not. In endotherms, routine metabolism, including heat production, dominate. (An endotherm eats ten times as much as an ectotherm of comparable size (Farlow, 1976).) It follows that large endotherms are more efficient than small ones, because they lose relatively less energy in cooling. The routine metabolic rate being proportional to size, the fact that the scaling parameter of the respiration is less than one does not necessarily imply that large ectotherms are more efficient users of energy than small ones, and we should seriously consider the possibility that they are not.

In the literature, it has been observed several times that there exists a negative correlation between the von Bertalanffy growth parameter $\dot{\gamma}$ and the ultimate size; see e.g. Duineveld & Jenness (1984). This observation has been used by Knight (1968), to assault the von Bertalanffy model as a reasonable model for growth. In order to remove this correlation, Gallucci & Quin (1979) suggested the transformation $3\dot{\gamma} = kW_\infty^{1/3}$. In the appendix, the ultimate size at constant food density is found

TABLE 3

Some quantities Y expressed as a function of size W and the best fitting scaling parameter b in the allometric equation ln Y = a + b ln W. Where this relation is not strictly linear, the maximum range for b is indicated

Quantity	Equation	Scaling parameter: within species	Scaling parameter: between species
Max ingestion rate	$\dot{I}_m = [\dot{I}_m]W^{2/3}$	2/3	1
Max filtering rate	$\dot{F}_m = [\dot{I}_m]W^{2/3}/K$	2/3	2/3
Saturation constant	$K = \dot{I}_m/\dot{F}_m$	0	1/3
Max assimilation rate	$[\dot{A}_m]W^{2/3}$	2/3	1
Routine metabolic rate	$\dot{\zeta}W$	1	1
Threshold food density	$KW^{1/3}/([\dot{A}_m]/\dot{\zeta} - W^{1/3})$	$\geq 1/3$	1/3
Thresh. ingestion rate	$W\dot{\zeta}[\dot{I}_m]/[\dot{A}_m]$	1	1
Max size	$W_m = (\kappa[\dot{A}_m]/\dot{\zeta})^3$	0	1
Max storage	$[S_m]W$	1	4/3
Threshold storage	$W^{4/3}\dot{\zeta}[S_m]/[\dot{A}_m]$	4/3	4/3
Max starvation time	$W^{1/3}([S_m]/[\dot{A}_m])\ln\{[\dot{A}_m]/(\dot{\zeta}W^{1/3})\}$	−1/3 to 1/3	1/3
Abundance	(max/threshold ingestion)$^{-1}$	−1 to −2/3	−1
Max growth rate	$(4/27)W_m(\dot{\zeta}/\kappa)/([S_m]+\eta/\kappa)$	0	2/3
Max respiration rate	$\dot{C}_m = (W^{2/3}W_m^{1/3}\eta/\kappa + W[S_m])\dot{\zeta}/(\eta+\kappa[S_m])$	2/3 to 1	2/3 to 1
Birth, adult size	W_b, W_j	0	1
Min pre-reprod. period	$J = (3/\dot{\zeta})(\eta+\kappa[S_m])\ln\dfrac{W_m^{1/3}-W_b^{1/3}}{W_m^{1/3}-W_j^{1/3}}$	0	1/3
Max egg storage	$S_0 = W_b[S_m]\{1-1/4(W_b/W_m)^{1/3}\}^{-3}$	0	4/3
Min water loss in eggs	$S_0 - W_b[S_m]$	0	4/3
Min incubation time	$\dfrac{3\kappa}{2\dot{\zeta}}[S_m]^{3/4}\left(\dfrac{S_0}{W_m}\right)^{1/4} \times\left(\dfrac{1}{2}\ln\dfrac{v^2+v\sqrt{2+1}}{v^2-v\sqrt{2+1}}+\arctan\dfrac{v\sqrt{2}}{1-v^2}\right)$ where $v=\{4(W_m/W_b)^{1/3}-1\}^{-1/4}$	0	1/3
Max reproductive rate	$\dot{R}_m = (1-\kappa)\dot{C}_m/S_0$	2/3 to 1	−2/3 to −1/3
Max pop. growth rate	$\dot{R}_m/(1+\dot{R}_m J)$	—	−2/3 to −1/3

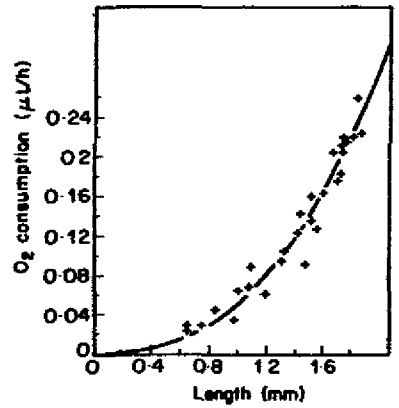

FIG. 4. Respiration rate of *Daphnia pulex* with few eggs at 20°C as a function of length. Data are from Richman (1958, Table 5). The fitted curve is $0{\cdot}0336L^2+0{\cdot}01845L^3$, and is indistinguishable from the curve $0{\cdot}0516L^{2{\cdot}437}$.

to be $W_\infty=(f\kappa[\dot{A}_m]/\dot{\zeta})^3$. Substitution in the expression found for $\dot{\gamma}$ gives $(3\dot{\gamma})^{-1}=\eta/\dot{\zeta}+W_\infty^{1/3}[S_m]/[\dot{A}_m]$. Apart from $\eta/\dot{\zeta}$, which has a small numerical value (Kooijman, 1986*b*), the proposed transformation indeed renders $\dot{\gamma}$ independent of $W_\infty^{1/3}$. Based on the present model, this dependence is caused by the dynamics of stored energy, and it by no means detracts from the von Bertalanffy model as a model for growth at a constant food density. (The parameter $\dot{\zeta}/\eta$ can be shown to the so-called maintenance rate constant, which appears only in the microbial literature, but which deserves wider attention (see Kooijman, 1986*b*). There are indications that the maintenance rate constant increases in the sequence bacteria, daphnids, fish and birds, and decreases in the sequence bacteria and algae, suggesting lines of evolutionary development.)

The reasoning set forth in the previous section has many additional consequences. We shall briefly consider starvation processes, because these are ecologically interesting. Suppose that an animal experiences a period of starvation after a period of constant food supply. From the storage balance equation for the dynamics of the size-specific storage, together with growth being zero, we see that the storage decreases exponentially until the utilization rate equals the routine metabolic rate. Any further decrease in storage would cause death by starvation. When the animal is about to die, we can calculate the minimum storage, the time to death by starvation and the threshold food density (see Table 3), i.e. the food density at which the animal is just able to survive for a long period, (or $\dot{A}=\dot{C}=\dot{M}$, growth and reproduction being zero), as functions of the parameters and the size of the animal. The threshold food density is a hyperbolic function in $W^{1/3}$. Therefore, small animals can survive at food densities at which large ones cannot. Since size tends to increase with age, (which trivially holds at constant food density), the average age of the population decreases in periods at the beginning of starvation. The effect of a temporary drop in food density reflected in the time until death by starvation depends

ones tend to die a little earlier than the small ones, but the differences are slight. This has been verified experimentally (Kooijman, 1986*a*). As we shall see, this behaviour constrasts with that of animals of different species.

From the energy preservation law it follows that the energy spent on reproduction equals $\dot{C}-\dot{M}-\eta\dot{W}$. Substitution of the energy investment in growth shows that the reproductive rate is simply related to the utilization rate, viz. $(W\geq W_j)(1-\kappa)\dot{C}/S_0$ in the growth region of the state space and $(W\geq W_j)(\dot{C}-\dot{M})/S_0$ in the no-growth region, $(W\geq W_j)$ taking the values 1 or 0 if true or false, and S_0 being the initial storage, i.e. the energy investment per young. The expression for S_0, given in Table 3 is derived in Kooijman (1986*b*). As storage at birth is in assumption 12 laid down to be $S_b=[S_m]fW_b$ for a mother feeding at (constant) input level f, the energy consumed during the egg stage, $W<W_b$, equals S_0-S_b. In animals like birds, this use of energy corresponds to the loss of water in eggs, because the metabolic degradation of yolk, releases water that would drown the chicken if it did not evaporate. This water includes water arising from the metabolism of energy-rich chemicals, as well as water deriving from the watery matrix in which these chemicals, are embedded for the purpose of degradation and transport. The observation that loss of water from bird eggs corresponds to the use of energy, and so with S_0-S_b will be used in the next section. The derivation of the incubation time is given in Kooijman (1986*b*). In the growth region of the state space, the reproduction rate is thus proportional to the utilization (or respiration) rate. So their size dependences are similar. See Kooijman (1984) for a test against experimental data.

The pre-reproductive period at constant food density is obtained from the inverse function of size as a function of age, which is a rather simple function due to the von Bertalanffy growth from size W_b (see Kooijman, 1986*a*).

4. Body Size Relations in Animals of Different Species

Within a species, the nine parameters listed in Table 2 are assumed to be constant in a constant environment (apart from, possibly, a fluctuating food density). This is because the energy budget model is basically a model for growth. Any change in the parameter values would immediately result in a violation of one of the assumptions (in particular of assumption 12). The maximum size W_m an individual can reach (at a high age and with an abundance of food), can be written as a function of three parameters (see Table 3). Species that differ in this maximum size therefore have to differ in one or more of these three parameters. Consistent with the basic model formulation, we shall assume that the size specific routine metabolic rate and the fraction of the utilization rate channelled into differentiation or reproduction do not depend on the (maximum) size. This implies that the parameter for the assimilation, $[\dot{A}_m]$, scales with $W_m^{1/3}$. The maximum assimilation rate itself, which is given by $[\dot{A}_m]W^{2/3}$ (see Table 3) therefore scales with W_m, so the scaling parameter is 1.

Since the ingestion rate is assumed to be proportional to the assimilation rate, the ingestion rate also scales with W_m. Farlow (1976) gives a scaling parameter of

rate as well as the threshold value scales with W_m, so we may expect the abundance of species of body size W_m to scale with W_m^{-1}, very nearly what was found by Peters (1983). For filter feeders, where filtering rate $\dot{F}$ is ingestion rate $\dot{I}$ divided by food density so that $F=[\dot{I}_m]W^{2/3}/(K+X)$, the shape parameter K of the Holling functional response can be interpreted as the quotient of maximum ingestion rate and maximum filtering rate, i.e. in absence of food so that $K=\dot{I}_m/\dot{F}_m$. If the filtering rate is dependent on the surface area of the filtering apparatus, it scales with $W_m^{2/3}$ (see Brendelberger & Geller, 1985), so the shape parameter scales with $W_m^{1/3}$ and the threshold food density with $W_m^{2/3}$. This means that a constant environment tends to select for small species, because they are able to outcompete the large ones. Fluctuating environments, on the other hand, tend to select for large species because the time until death by starvation scales with $W_m^{1/3}$. (Threlkeld (1976) found a scaling parameter of 1/4, but 1/3 also fits the data well.) In contrast to what has been found in the previous section for animals of the same species a large specimen of a large species is thus better equipped to survive a period of food shortage than a small specimen of a small species. Brook & Dodson (1965) observed that in the absence of predators, the larger species of zooplankton dominate. On basis of the present theory, the explanation does not lie in the size dependence of the threshold food density as they suggested (because this would operate the other way round), but in the length of periods during which no animal can find sufficient food. This has been confirmed experimentally by Goulden & Hornig (1980).

In order to couple the maximum storage capacity to the maximum energy intake, we assume that the size-specific maximum storage, $[S_m]$ scales with the parameter $[\dot{A}_m]$, i.e. with $W_m^{1/3}$ and that the birth size as well as the size at the end of the pre-reproductive period scales with W_m. These two assumptions complete the scaling relations for the parameters of the energy budget model collected in Table 2. We can now derive expressions for a variety of observable quantities such as maximum growth and minimum pre-reproductive period, write them as functions of the parameters and size and judge how they would behave in a log–log plot against size. In making this judgement, we must remember that the parameters are constants within a species, but allometric functions of size between species. Some of the expressions for the quantities collected in Table 3 then result in proper allometric functions, and so they are linear in a log–log plot against size. Some of the other expressions are not quite linear, but only approximately so (see legend to Fig. 4). In that case the maximum possible range of the scaling parameter is indicated in Table 3, if one nevertheless wishes to fit a linear relationship (in deference to tradition in biological literature). When comparing the results with data from the literature, we should bear in mind that, if the energy budget model really holds, the reported values for the scaling parameter should fall somewhere in this range, depending on the species included. From an analysis of the equations given in Table 3, it follows that the respiration rate scales with about $W_m^{3/4}$, as we also found within a species, a result that has frequently been found (see introduction). It also follows that maximum growth scales with $W_m^{2/3}$, which fits Calow & Townsend's data (1981) very well, that the minimum pre-reproductive period scales with $W_m^{1/3}$, which very

per young, which correspond to egg size, scales with $W_m^{4/3}$ in ectotherms; that the water loss from bird eggs scales with $W_m^{4/3}$, i.e. with (egg size)^1; as found by Rahn *et al.* (1979), that incubation time scales with $W_m^{1/3}$, i.e. with (egg size)$^{1/4}$; as found by Rahn *et al.* (1974) and by Kooijman (1986*b*); and that maximum reproductive rate scales with $W_m^{-1/3}$, the exponent being close to the value of $-1/4$ given in e.g. Peters (1983), (in view of the data). It is interesting to note that, the maximum reproductive rate $\dot{R}_m$ decreases with increasing species size, not, as many authors have suggested, because size-specific routine metabolic rate, but size-specific storage depends on size. The same holds for the duration of the pre-reproductive period, which increases with species size. Since only the age of the mother when she gives birth for the first few times is relevant in the population growth rate and the duration of the pre-reproductive period J is small, and reproduction once started, soon reaches its maximum rate, the population growth rate can be approximated by $\dot{R}_m/(1+\dot{R}_m J)$, and consequently scales with $W_m^{-1/3}$. Considering the proliferation in microbial populations, we can assume that division occurs at given cell size (see Kooijman, 1986*a*). The division interval then corresponds to the expression given for the pre-reproductive period. Since the population growth rate is inversely proportional to the duration of this interval, it scales with $W_m^{-1/3}$. This fits the protozoa data of Fenchel (1974) well, who gave a scaling parameter of $-1/4$. Basic feature of this scaling is that ingestion rate is proportional to the surface area $W_m^{2/3}$. This appears to be particularly relevant for ciliates feeding by phagocytosis, but perhaps less so for bacilli, which change their shape during growth, because the rod diameter remains constant. In the latter case, the population growth rate is independent of cell size and ingestion rate scales with size. This relates to the findings of Banse (1976, 1982) who found a scaling parameter of $-1/4$ and 0, respectively.

Conclusions

Central to the reasoning outlined above are the Holling functional response, the diagram of Fig. 1, and the von Bertalanffy growth equation (von Bertalanffy, 1934). Though popular several decades ago, this growth equation has lost a great deal of its appeal, primarily owing to the observed scaling of respiration rate with body size. This argument does not appear to be a valid one; the scaling parameter of the respiration rate is smaller than that of the routine metabolic rate owing to less and less energy being invested in growth and reproduction with increasing size. The reason lies in the assimilation rate scaling with surface area for animals of the same species. In the considerations given above, I have not attempted to predict the value of the scaling parameter in body size relations correctly to two decimal places. Such an attempt at accuracy is bound to fail, because of the many biological exceptions to general tendencies in body size relations, and because body size relations are not necessarily of the allometric type. With reference to the aim of this paper, the gist of the reasoning is, in fact, that many of the relations between physiological variables and body size can be predicted simultaneously from an elementary knowledge of energy budgets. I have not devised my energy budget model to explain body size relations correctly, but to describe detailed observations of the feeding, growth and

reproduction behaviour of daphnids. In explaining body size relations, storage considerations have proved to be more essential than has been recognized. These relations work out to be different for animals of the same species than for animals of different species. The most striking divergence is in the reproductive rate and in the starvation time. The energy budget model suggests that the environment selects for body size as a compromise between, on one hand, small, because small animals can better survive low food densities and, on the other, large, because large animals can better survive periods of starvation. If starvation periods last too long, however, the population numbers will follow the fluctuations in food density more closely. In that case, the environment will select for small species because of their large population growth rate. Conversely, the model indicates that there is an optimum relation of body size to the time scale in which fluctuations in food density take place.

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APPENDIX

Derivation of the Energy Budget Model

The change of the state variables, size and W and size-specific storage $[S]$ can be derived from the assumption listed in Table 1 as follows.

The energy channelled into differentiation or reproduction (cf. assumption 9) can (always) be written as a fraction $1-\kappa(W,S)$ of the utilization rate $\dot{C}$. This fraction may be a complicated function of the state variables. So the fraction channelled into maintenance plus growth equals $\kappa(W,S)\dot{C} = \dot{M} + \eta\dot{W}$, where the maintenance, $\dot{M}$, is given by $\dot{M} = \dot{\zeta}W$, and $\dot{W}$ stands for growth, i.e. the change in size, W. Assumption 1 states that the utilization rate, $\dot{C}$, equals $\dot{C} = \dot{A} - \dot{S}$, where $\dot{S}$ is the change in storage, S, and the assimilation rate, $\dot{A}$, is proportional to the ingestion rate, $\dot{I}$ (assumption 5), which is given by assumptions 6, 7, and 8. So we have $\dot{A} = [\dot{A}_m] f W^{2/3}$. On the basis of assumption 8, this type of ingestion rate is known as the Holling functional response (see Holling, 1959).

At constant food density X, the storage after birth can be written as a function, S^*, of size, W, and the scaled input $f = X/(K+X)$ (see assumption 8), so $\dot{S}^* = \dot{W}\,\partial S^*/\partial W$. Substituting this and the von Bertalanffy growth, $\dot{W} = \dot{\rho}W^{2/3} - 3\dot{\gamma}W$ given in assumption 12, in the equation obtained above, $\kappa(W,S)(\dot{A}-\dot{S}) = \dot{\zeta}W + \eta\dot{W}$, we can solve $\partial S^*/\partial W$, obtaining

$$\partial S^*/\partial W = (f_1 + g_1 W^{1/3})/(f_2 + g_2 W^{1/3}), \text{ with } f_1 = [\dot{A}_m] f - \dot{\rho}(f)\eta/\kappa;\ f_2 = \dot{\rho}(f);$$

$$g_1 = -\dot{\zeta}/\kappa + 3\dot{\gamma}(f)\eta/\kappa \quad \text{and} \quad g_2 = -3\dot{\gamma}(f).$$

From assumption 2 we have that the size-specific storage, $[S] = S/W$, is independent of the partitioning rule κ, so $\partial^2 S^*/(\partial\kappa\,\partial W) = 0$ for all values of W. For primes denoting derivation with respect to κ considered as a function of time we have that

$$\frac{\partial^2 S^*}{\partial W\,\partial\kappa} = \frac{f_1' f_2 - f_1 f_2' + (f_1' g_2 + f_2 g_1' - f_1 g_2' - f_2' g_1) W^{1/3} + (g_1' g_2 - g_1 g_2') W^{2/3}}{(f_2 + g_2 W^{1/3})^2}$$

has to vanish for all values of W, from which it follows that $(f_1/f_2)' = 0$ and $(g_1/g_2)' = 0$. This gives

$$\dot{\rho}'(f) = \dot{\rho}(f)^2\eta/([\dot{A}_m]\kappa^2) \quad \text{and} \quad (3\dot{\gamma}(f))' = (3\dot{\gamma}(f))^2\eta/(\kappa\dot{\zeta}) - 3\dot{\gamma}(f)/\kappa.$$

Solution of these differential equations gives $\dot{\rho}(f) = [\dot{A}_m] f/(\eta/\kappa + \partial S^*/\partial W)$ and $3\dot{\gamma}(f) = (\dot{\zeta}/\kappa)/(\eta/\kappa + \partial S^*/\partial W)$. Since $\dot{\rho}$ and $\dot{\gamma}$ are independent of size W, and so the ultimate size W_∞, which from $\dot{W} = 0$ is given by $W_\infty^{1/3} = \dot{\rho}/(3\dot{\gamma}) = [\dot{A}_m] f\kappa/\dot{\zeta}$, we have that κ is independent of size. From assumption 13 we also have that κ is independent of f, so κ is the same for different constant food densities. Since $\dot{\rho}$ and $\dot{\gamma}$ are independent of size, we also have that $\partial S^*/\partial W$ is independent of size, W, so S^* has the form $S^* = h(f) + g(f)W$. Assumption 1 states that growth utilizes stored energy, not directly assimilation energy. Therefore $\partial S^*/\partial W$, which is equal to $g(f)$, in $\dot{\rho}$ and $\dot{\gamma}$ has to be replaced by $S^*/W - h(f)/W$, which is only independent of f and W for $h(f) = 0$. So we have $S^* = g(f)W$ or $[S^*] = g(f)$ for $[S^*] = S^*/W$. In accordance with assumption 1 f in $\dot{\rho}$ has to be written as a function of S, so f is

replaced by $g^{-1}([S^*])$, where g^{-1} is the inverse function of g, i.e. $g^{-1}(g(f))=f$. We now obtain

$$\dot{W}=\dot{\rho}W^{2/3}-3\dot{\gamma}W=\{W^{2/3}[\dot{A}_m]g^{-1}([S^*])-W\dot{\zeta}/\kappa\}/(\eta/\kappa+[S^*]).$$

Growth depends on stored energy, S^*, as the only variable that is changing (it changes even when food density is constant), and it does so on its momentary value and not on earlier ones. We can therefore drop the asterisk and apply the equation for growth in situations of fluctuating food density. If however, the food density is fluctuating, the state variables can attain values they cannot attain at constant food density. These values correspond to growth becoming negative in the equation above. Assumption 15 in fact means that, in those situations, priority is given to differentiation or reproduction over growth, which ceases. The dynamics of the size-specific storage, $[\dot{S}]=\dot{S}W-S\dot{W}/W^2$, is now found from the balance equation, $\dot{S}=\dot{A}-\dot{C}$, to be $[\dot{S}]=[\dot{A}_m]W^{-1/3}\{f-g^{-1}([S])\}$.

Assumption 14 states that $1/\dot{\gamma}$ is linear in f, so g is proportional to f, say $g(f)=[S_m]f$, which implies that g^{-1} is proportional to $[S]$ and vice versa. In other words: the size-specific storage obeys a simple first-order process if and only if $1/\dot{\gamma}$ is linear in f. To summarize the final result, we have that the change of the state variables is given by

$$\dot{W}=\{(W^{2/3}[\dot{A}_m][S]/[S_m]-W\dot{\zeta}/\kappa)/([S]+\eta/\kappa)\}_+$$

$$[\dot{S}]=[\dot{A}_m]W^{-1/3}\{(W\geq W_b)X/(K+X)-[S]/[S_m]\}$$

where $(W\geq W_b)$ has value 1 or 0 if true or false, in accordance with assumptions 6 and 5. The model would be much simpler to derive if we assumed that κ is constant, in which case we can drop assumption 12 that growth at constant food density is of the von Bertalanffy type. The reason for not doing this lies in the experimental testing of the assumptions. It is very difficult to measure the different energy flows to growth, maintenance and reproduction directly. Among other things, we have to disentangle the heat losses involved in these processes and measure other forms of overheads (see text).

Application of a dynamic energy budget model to *Mytilus edulis* (L.)[1]

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Abstract. Filtering, ingestion, assimilation, respiration, growth and reproduction of the blue mussel *Mytilus edulis* were sucessfully described in terms of a dynamic energy budget (DEB) model, which previously had been applied successfully to a variety of other species. Parameters of the DEB model, estimated for laboratory situations, were applied to field data. The varying growth rates in the field could be described by taking account of changes in food density and quality, and temperature, on the basis of the Arrhenius relation. The concept Scope For Growth is discussed and interpreted in terms of the DEB model. The energy conductance is found to be close to the mean of many species: 1.64 $mm.d^{-1}$ at 15°C.

Key-words: Energy budget, *Mytilus edulis*, feeding, growth, starvation, reproduction, energy conductance

Introduction

The dynamics of the energy budget of *Mytilus edulis* (L.) are of interest for several reassons. It is an important species in estuarine environments. This calls for a close analysis of its role in terms of energetics. It is commercially yielded, so it is useful to elaborate harvesting programs that can be maintained for long periods. Also, the species is used as a monitor organism for environmental pollution. The uptake and elimination behaviour of xenobiotics, especially the lipophyllic ones like PCB's, depend on feeding conditions, and so on energetics (Lassiter & Hallam, 1988, Kooijman & van Haren, 1990). Results of environmental monitoring programs such as the "Mussel Watch Program" (Goldberg, 1975) are therefore difficult to interpret without a toxico-kinetic model based on physiology which can handle fluctuating conditions in the environment.

Modelling physiological energetics in *M. edulis* is usually based on the widely applied Scope For Growth (SFG) concept and allometric relations be-

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tween body size and physiological rates (Bayne, 1976; Bayne & Newell, 1983; Verhagen, 1983; Baretta & Ruardy, 1985; Klepper, 1989). The SFG concept is based on the energy balance of a mussel in steady state conditions. The amount of energy gained by the individual under such conditions equals the amount of energy lost due to maintenance, growth and reproduction . The SFG is the difference between energy gained by feeding and energy lost by respiration (supposedly a measure of maintenance). When this difference is positive energy is available for growth and reproduction, when it is negative, there is a (dry) weight loss due to the utilization of energy reserves (Bayne & Newell, 1983).

One problem with this approach is that it does not distinguish storage of energy reserves (*i.e.* lipids, glycogen) from 'structural biomass' in its standardization for body weight. The basic difference is that storage materials do not require maintenance and are readily available for use for maintenance, growth and reproduction. Structural biomass on the other hand does require maintenance, *i.e.* energy used for recycling of proteins, regulation of chemical composition and circulation. It is not as readely available as an energy source for production. Another problem in the application of SFG concerns the interpretation of respiration rates. Although measurements of the energy balance of a particular individual take such a short period that the change in size is negligibly small, the energy invested in growth can be substantial. So part of the respiration measured with a standard conversion to energy is connected with growth, while in the SFG, it is fully assigned to maintenance. This problem can be solved by using a dynamic energy budget (DEB) model, which considers an individual as an input- output system with size and stored energy as state variables.

The purpose of the present paper is to show how the DEB model can be apllied to *M. edulis.* Originally, the model was developed for *Daphnia magna* Straus (Kooijman, 1986 a, Evers & Kooijman, 1989) and sucessfully applied to *Lymnaea stagnalis* (L.) (Zonneveld & Kooijman, 1989) and micro– organisms (Kooijman *et al.*, 1991). It permits the description of embryo development (Kooijman, 1986c, Zonneveld & Kooijman, 1991), growth (Kooijman, 1988) and body size scaling relations (Kooijman, 1986b, 1988). Ross & Nisbet (1990) argued that it is necessary to modify the model to obtain consistency with published data on mussel physiology. We reanalyzed these data and used additional ones to test the unmodified DEB model. We will first present a brief description of the model and consider the different

processes which are relevant for the energetics. Subsequently we will test it against data from the literature and some unpublished data.

The DEB model

We will restrict the present discussion to the post-larval stage, which can be splitted into a juvenile stage which cannot reproduce and an adult one. In these stages, the mussel does not change its shape to any significant extent. The chemical composition of the structural biomass and of stored materials is taken to be constant. A list of frequently used symbols is given in Table 1

Two state variables, volume, W (lenght^3), and storage, S (energy) are distinguished. The choice for storage as a state variable is motivated by the observation that animals undergoing a sharp change in food density adapt only gradually to a new growth rate. This implies that there is an energy buffer (Kooijman, 1986a); see also the section on growth.

Uptake is assumed to follow a type II Holling functional response and is taken proportional to surface area (of the filtering apparatus and/or gut), so the ingestion rate is

$$I = \{I_m\} f W^{2/3} \text{ with } f = X/(K+X) \tag{1}$$

where X is the food density, K the saturation constant and $\{I_m\}$ the maximum surface area–specific ingestion rate. The filtering rate is $F = I/X$, on the assumption that there is complete retention of particles. The maximum filtering rate is thus $W^{2/3}\{I_m\}/K$. If the digestive system remains filled with processed food, and has a capacity of V, the gut passage time is V/I (Evers & Kooijman, 1989). The food-energy conversion is taken to be constant, $\{A_m\}/\{I_m\}$, so the assimilation energy, *i.e.* the total energy input, equals $\{A_m\} f W^{2/3}$, where $\{A_m\}$ is the maximum surface area–specific assimilation rate. The incoming energy adds to the reserves. When expressed as density, $[S] = S/W$, so energy reserve per volume of body, the reverves follow a first order process. The relaxation time is taken proportional to length, so that

$$\frac{de}{dt} = v W^{-1/3}(f - e) \tag{2}$$

where $e = [S]/[S_m]$, where $[S_m]$ is the maximum storage density and $v = \{A_m\}/[S_m]$ is the energy conductance (length.time^{-1}). The rate at which

Table 1: Variables, primary and compound parameters

symbol	dimension	interpretation
variables		
t	time	time
X	weight.length^{-3}	food density
W	length^3	body volume
S	energy	energy storage
e	energy.length^{-3}	scaled energy storage density: $S/[S_m]W$
R_c	energy	cumulated energy investment into reproduction
primary parameters		
W_b	lenght^3	volume at birth
W_j	length^3	volume at start reproductive stage
K	weight.lenght^3	saturation constant
$\{I_m\}$	weight.length^{-2}.time^{-1}	maximum surface area–specific ingestion rate
$\{A_m\}$	energy.length^{-2}.time^{-1}	maximum surface area–specific assimilation rate
$[S_m]$	energy.length^{-3}	maximum storage density
ζ	energy.length^{-3}.time^{-1}	volume–specific maintenance costs per unit of time
η	energy.length^{-3}	volume–specific costs for growth
κ		fraction of utilized energy spent on maintenance plus growth
compound parameters		
v	length.time^{-1}	energy conductance: $\{A_m\}/[S_m]$
m	time^{-1}	maintenance rate constant: ζ/η
a		energy investment ratio: $\eta/\kappa[S_m]$

energy is utilized from the storage, is

$$C = -\left.\frac{dS}{dt}\right|_{f=0} = [S_m]\left(-\left.\frac{de}{dt}\right|_{f=0} W - e\frac{dW}{dt}\right)$$
$$= e[S_m]\left(vW^{2/3} - \frac{dW}{dt}\right) \quad (3)$$

A fixed fraction κ of the utilized energy is spent on growth plus maintenance. The latter quantity is taken to be proportional to volume, ζW. So $\kappa C = \zeta W + \eta\frac{dW}{dt}$, where η is the volume-specific costs for growth. Substitution gives

$$\frac{dW}{dt} = \frac{W^{2/3}ev - Wam}{e+a} \quad (4)$$

where the dimensionless investment ratio, $a = \eta/\kappa[S_m]$, and the maintenance rate coefficient, $m = \zeta/\eta$ are compound parameters. Growth ceases when the energy reserves drops below $e = W^{1/3}ma/v$.If the food density is constant long enough, (2) states that e tends to f and remains constant as well. This turns (4) into the well known von Bertalanffy growth equation, having the solution

$$W(t) = \left(W_\infty^{1/3} - (W_\infty^{1/3} - W_0^{1/3})e^{-\gamma t}\right)^3 \quad (5)$$

where $W_\infty^{1/3} = f\kappa\{A_m\}/\zeta$ is the ultimate volume$^{1/3}$ and $\gamma = (3/m+3W_\infty^{1/3}/v)^{-1}$, the von Bertalanffy growth rate. The maximum volume$^{1/3}$ is thus $W_m^{1/3} = \kappa\{A_m\}/\zeta$, which can only be reached at prolonged exposure to abundant food. The von Bertalanffy growth rate is then minimal and equals $\frac{m}{3}\frac{a}{1+a}$.

Back substitution of (4) into the storage utilization rate (3) gives

$$C = \frac{ea[S_m]}{e+a}\left(vW^{2/3} + mW\right) \quad (6)$$

In the absence of feeding and digestion, respiration is taken to be proportional to this utilization rate.

The maximum starvation time, *i.e.* the time until death by starvation, is found by setting the utilization rate in (2) equal to the maintenance rate for $f = 0$. Neglecting the small size increase, for a well-fed individual, we arrive at a starvation time of $\frac{W^{1/3}}{v}\ln\frac{W_m^{1/3}}{\kappa W^{1/3}}$.

The energy drain to development plus reproduction equals $(1-\kappa)C$. The maintenance of a certain degree of maturation is taken to be $\frac{1-\kappa}{\kappa}\zeta \min(W, W_j)$. This choice, which is an alternative way of defining κ, makes the costs of development independent from the feeding conditions. The implication is that the cumulative energy drain to reproduction in adults, *i.e.* in individuals of a body volume larger than W_j, amounts to

$$R_c(t_1,t) = \int_{t_1}^{t} \frac{1-\kappa}{\kappa} \frac{e(s)}{e(s)+a} \eta(vW(s)^{2/3}+mW(s))\,ds - \frac{1-\kappa}{\kappa}\zeta(t-t_1)W_j \quad (7)$$

When the energy reserves would no longer suffice for maintenance, *i.e.* when $e < amW^{1/3}/v$, growth will cease, so that $\frac{dW}{dt} = 0$. The cumulated energy drain to reproduction in animals that continue to allocate energy to reproduction under these circumstances becomes

$$R_c(t_1,t) = \int_{t_1}^{t} (e(s)\{A_m\}W(s)^{2/3} - \zeta W(s))\,ds - \frac{1-\kappa}{\kappa}\zeta(t-t_1)W_j \quad (8)$$

In animals like *Mytilus*, the energy feeding the drain to reproduction accumulates during the non-reproductive seasons inside the animal, but it is assumed to be not metabolically available for other purposes. Reproduction is upon some internal or external stimulus. For the calculation of the actual reproduction, the cumulated energy has to be divided by the energy investment into a single sperm or egg. See Kooijman, 1986c, Zonneveld & Kooijman, 1991 for expressions of these costs on the assumptions that the initial embryo volume is negligibly small and that the energy density at hatching equals that of the mother at egg formation. At spawning, we assume a reset of R_c to zero.

Size

Frequently used measures of size of mussels are shell length, wet weight, dry weight and ash free dry weight. For animals like mussels, wet weight, W_w, relates in a simple way to body volume, assuming a constant specific density close to $d = 1$ g/cm^3. The rationale is that storage compounds replace water (Pieters *et al.*, 1979) and have about the same specific density. For isomorphs, shell length relates to volume as $\alpha L = W^{1/3}$, where α is called the shape coefficient. Fig. 1 confirms this relation. The data represented imply that the shape coefficient $\alpha = 0.333$ (SD 0.097) g$^{1/3}$.cm^{-1}. Kooijman (1988) estimated a shape coefficient of 0.394 based on the intra shell volume.

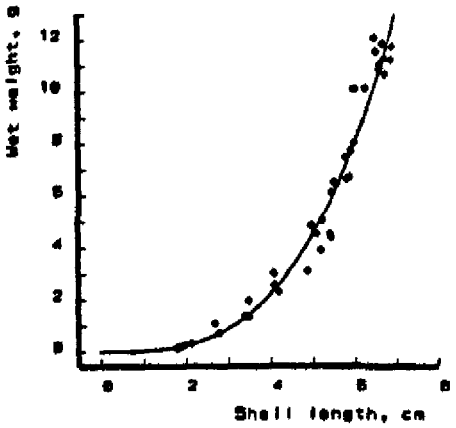

Figure 1: The relation between fresh (wet) weight, W_w, and shell length, L. Data from Borchardt (1985); Pieters *et al.* (1979); Dutch contribution to ICES, Copenhagen. The least squares fitted curve is $W_w = d(\alpha L)^3$ with d=1 g/cm^3, α^3 = 0.03692 (SD 7.59 10^{-5}). It is does not differ significantly from the best fitting allometric one $W = 0.02774L^{3.157}$ on the basis of the likelihood ratio test (p =0.096).

The advantage of length above wet weight is that it allows an easy and accurate measurement which is not destructive. Dry weight or ash free dry weight of the soft parts is a weighted sum of volume, W, storage materials, S, and cumulated reproductive material, R_c. Both latter compounds vary with habitat and season (Pieters *et al.*, 1979; Zandée *et al.*, 1980). Dry weights of the soft parts of a 4.0 cm *M. edulis* take values as extreme as 130 mg and 630 mg, and beyond (Jørgensen, 1976).

The largest mussels found in nature tend to occur in subarctic and arctic regions because of the high food densities. Thiesen (1973) and Thompson (1984) report mean shell lengths of 9.2 and 9.4 cm in Greenland and Newfoundland respectively. Thiesen reports shell lengths exceeding 9.2 cm. Unfortunately he gave no actual lengths because these shells went lost during the meal. The theoretical maximum will doubtless be higher, because plankton densities fall in winter.

Temperature

Acute and long-term responses of *M. edulis* to temperature changes have been described by several authors; for a review see Bayne (1976, p 141). Knowledge of long term-temperature responses is needed for comparing experiments carried out under different temperature regimes. The long-term temperature response is also needed for applying the model to field conditions with seasonally fluctuating temperatures.

The way rates depend on temperature is usually well described by the Arrhenius relation within a species-specific tolerance range (Kooijman, 1988). In *M. edulis* the range is 5-20°C (Widdows & Bayne, 1973; Widdows, 1973a,b).

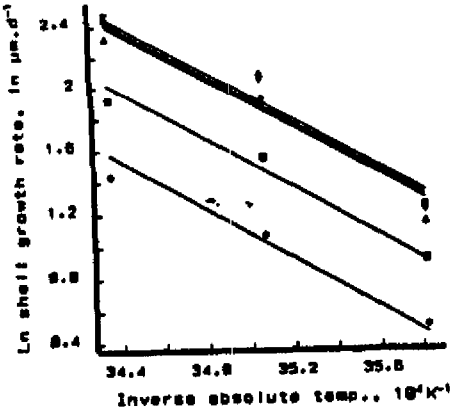

Figure 2: Arrhenius plot for length growth rates of juvenile mussels at 2, 5, 10, 20 and 40 cells *Dunaliella*/μl. Data from Sprung (1986). The Arrhenius temperature is 7579 (SD 167) K.

At lower temperatures, the actual rates are lower than expected because the animal remains in a kind of resting phase until the temperature rises again. At higher temperatures, animals usually die. Lethal temperatures for *M. edulis* vary from 27°C to 40°C as a function of the exposure regime (Bayne, 1976 p181)

The Arrhenius temperature is estimated using growth rates of larval shell length; see Fig.2. We assume that, as a first approximation, all physiological rates are affected in the same way with deviations at temperatures exceeding 20°C. This may be caused by irreversible effects of temperature on the filtration rates. Nielsen (1988) reports decreasing growth rates of juvenile mussels with increasing temperatures, which is in contrast with the expected increasing growth rates of mussel larvae, see Fig.2. The explanation might be in the depletion of food for the juveniles at higher temperatures due to elevated metabolic rates.

Results of Widdows (1978a) and Widdows *et al.* (1979) suggest that there is no long-term effect of temperature on filtration rates of *M. edulis* when rates are corrected to a standard weight of 1 g dry weight. However, during the season, food tends to covary with temperature, so does the reserves and thus the dry weights. Standardization on the basis of dry weights therefore obscures the effect of temperature. For this reason an Arrhenius temperature correction is applied to filtering rates as well, the Arrhenius temperature being $T_A = 7600$ K. The rate at absolute temperature T_1 is thus obtained from that at T_0 according to $v_{T_1} = v_{T_0} e^{T_A(1/T_0 - 1/T_1)}$.

Food

Since energy uptake depends on food availability and quality, some remarks on food for mussels are in order, because it is hard to characterize.

Suspended particles in natural conditions are mixtures of organic and inorganic compounds which vary in size. If larger than 4 μm in diameter, they are fully retained by *M. edulis* whereas a 50% retention is reported for

particles of 1 μm in diameter (Vahl, 1972; Møhlenberg & Riisgård, 1978). Particles less than 1μm are poorly utilized (Wright *et al.*, 1982; Gorham, 1988). Field monitoring programs frequently use the 0.45 μm mesh sieve to distinguish 'dissolved' from particulate or suspended matter (SM). This criterion is also used in the following sections. Thus *M. edulis* will be able to retain most of the particulate matter suspended in the water column.

Particulate organic matter (POM, defined as SM minus its ash weight) is the major food component for *M. edulis*. Laane *et al.* (1987) distinguish a refractory fraction which can not be utilized by metazoans. The non-refractory fraction of POM mainly consists of phytoplankton and detritus. POM in estuaries originates from autochtonous production and allochtonous sources, *vs* rivers and coastal waters. The detritus concentration in estuaries and coastal waters far exceeds the concentration of phytoplankton (Laane *et al.*, 1987). Rodhouse *et al.* (1984) explained high length growth rates of *M. edulis* in winter by allochtonous detritus input into the estuary.

The nutritive value of POM can be estimated by the protein, carbohydrate and lipid contents (Widdows *et al.*, 1979; Laane *et al.*, 1987). The nutritive value expressed as energy per mg SM varies considerably amoung estuaries and seasons. Typical yearly ranges are 22.2-24.8 J.mg SM^{-1} (Lynher estuary, U.K., Widdows *et al.*, 1979), 0.29-15.9 J.mg SM^{-1} (Gironde, France, Laane *et al.*, 1987), 0.18-5.9 J.mg SM^{-1} (Ems-Dollard estuary, the Netherlands, Laan *et al.*, 1987). The nutritive fraction of SM follows a seasonal cycle, similar to that recorded for percentage ash- free material of SM (Widdows *et al.*, 1979). The POM concentration in water can be used as a measure of food energy for *M. edulis* after conversion of POM to its mean energy equivalent of 20.3 J.mg POM^{-1} (Bayne, 1987).

Feeding, ingestion and assimilation

High SM concentrations (> 5 $mg.l^{-1}$, Widdows *et al.*, 1979; 3.2-7.4 $mg.l^{-1}$, Bayne *et al.*, 1989) induce the production of pseudofaeces, consisting of material cleared from suspension but rejected by the mussel before ingestion. Selection for the digestible fraction of SM is demonstrated by Kiørboe *et al.* (1980), who used mixtures of resuspended sediments with cultured algae in their experiments. However, Foster-Smith (1975b) and Widdows *et al.* (1979) found no selection. The labial palp plays a rôle in sorting incoming material, which is conveyed to the mouth or to the rejection tracts (Bayne,

1976 p143-144). Thiesen (1982) has shown that palp size increases with increasing SM concentrations in water. He suggests that large palp size is an adaption to live in turbid waters.

Food intake is a function of body size, particle concentration, and pseudofaeces production (Winter, 1978). A retention efficiency of 100% for POM is assumed in the DEB model. This is realistic under most field conditions. We also assume that the fraction of POM in pseudofaeces is negligibly small. Filtration and ingestion rates are closely related for food densities low enough to prevent pseudofaeces production. At such densities, all the filtered material is ingested.

Foster-Smith (1975) found that the square root of the gill area is proportional to shell length. Fig.3 shows that filtering rate is proportional to squared length. Since no pseudofeaces occurred, ingestion is likely to be proportional to squared length as well. Winter (1977) and Møhlenberg & Riisgård (1979) reported scaling parameters for wet weights of 0.73 at constant food density of 40 10^6 cells.l^{-1} and 0.66 at different food densities. In Winters' review (1978) scaling parameters are reported to vary between 0.27 and 0.82 for dry weights.

At high food densities, the food handling organs (cirri, gill filaments, mucus strings, labial palp and gut) become saturated. Foster-Smith (1975), Riisgård & Møhlenberg (1979) and Riisgård & Randløv (1981) observed decreasing filtration rates at increasing food densities. This decrease has obviously the function of providing the ingestive system with limited amounts of food it can handle. Fig.4 shows the fitted filtration rates at four different shell lengths as a function of food density. The rates are corrected to 15°C.

In very dilute suspensions *M. edulis* ceases filtering (Bayne, 1976 p139). Riisgård & Randløv (1981) reported a threshold food concentration of 1.5 10^6 *Phaeodactylum tricornutum* cells.l^{-1}, below which no filtration occurs due to shell closure. After a period of 24 days at a constant low or high food level, *M. edulis* reacts within an hour to changes in algal concentrations by opening or closing its shell.

Fig.5 shows the ingestion rate as function of food density at different shell lengths. It suggests that the maximum ingestion rate equals the threshold SM concentration of 7.43 mg.l^{-1} at which pseudofaeces production starts. This amounts to 1.8 mg POM.h^{-1} for a 2.5 cm mussel at 14°C (Bayne *et al.*, 1989), which is close to the calculated value of 1.64 mg POM.h^{-1} based on the fitted curves in Fig.5. So the assumption of 100% sorting efficiency

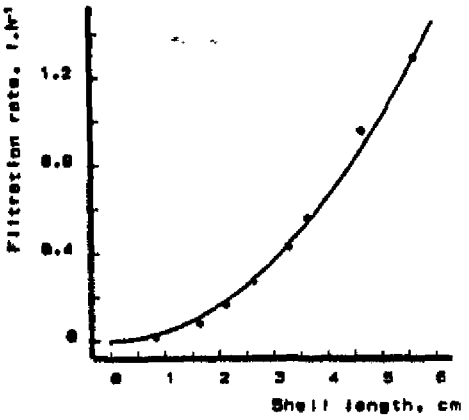

Figure 3: The filtration rate as function of shell length, L, at constant food density (40 10^6 cells.l^{-1} *Dunaliella marina*) at 12°C. Data from Winter 1973. The least squares fitted curve is $\{F\}(\alpha L)^2$, with $\{F\}$= 0.041 (SD 6.75 10^{-4}) l.h^{-1}.cm^{-2}, which is does not differ significantly from the best fitting allometric one $0.039L^{2.03}$ on the basis of the likelihood ratio test (P =0.66).

is corroborated by these results. Fig.6 confirms that the gut passage time is inversely related to ingestion rate, which implies that the food loading of the digestive system remains constant.

The assimilation efficiencies of food in the gut are usually calculated by the method of Conover (1966), *i.e.*:$\frac{F-E}{(1-E)F}$, where F is the ratio of ash free dry weight and dry weight of the ingested food and E that for faeces. This method is based on the assumption that the ash fraction is not assimilated. Other methods are based on incorporation of ^{14}C atoms in tissue or on the difference of energy content of food and faeces.

Some authors argue that the assimilation efficiency depends on food density (Bayne, 1976 p457) or ingestion rate (Foster-Smith, 1975b; Borchardt, 1985). When data from several sources are combined, these dependencies are not obvious, see Fig.7. The presented assimilation rates were obtained by multiplication of the assimilation efficiency of Conover with the ingestion rate and the 'mean' energy equivalent of POM. This leads to an average food–energy conversion of $\{A_m\}/\{I_m\}$ = 11.4 J.mg POM^{-1}, which is 0.56 times the 'mean' energy equivalent of POM.

Respiration and maintenance

The oxygen consumption rate as function of length at constant food densities is shown in Fig.8. On the basis of the DEB model, we expect a proportionality of the oxygen consumption rate to $W + W^{2/3}v/m$, which closely resembles frequently postulated one to $W^{0.75}$ (Kooijman, 1986a, Evers & Kooijman, 1989). The scaling parameter for *M. edulis* varies between 0.595 and 0.930 at different temperatures and dry weights (Bayne, 1976 p161). Hamburger

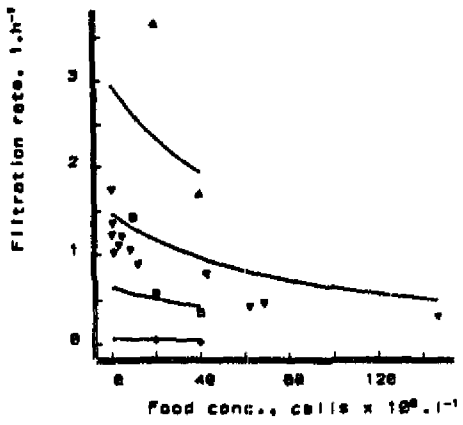

Figure 4: The filtration rate, F, as function of food density, X, for different shell lengths, L. Rates are corrected to 15°C and shell lengths are (from bottom to top) resp. 0.85, 2.65, 4 and 5.65 cm. Data from Winter (1973) and Schulte (1975) (4 cm only). The simultaneously least squares fitted curves are $F = \frac{\{F_m\}(\alpha L)^2}{1+X/K}$, with $\{F_m\}$ = 0.83 (SD 0.098) l.cm^{-2}.h^{-1} and K = 76 (SD 42) 10^6 cells.l^{-1}.

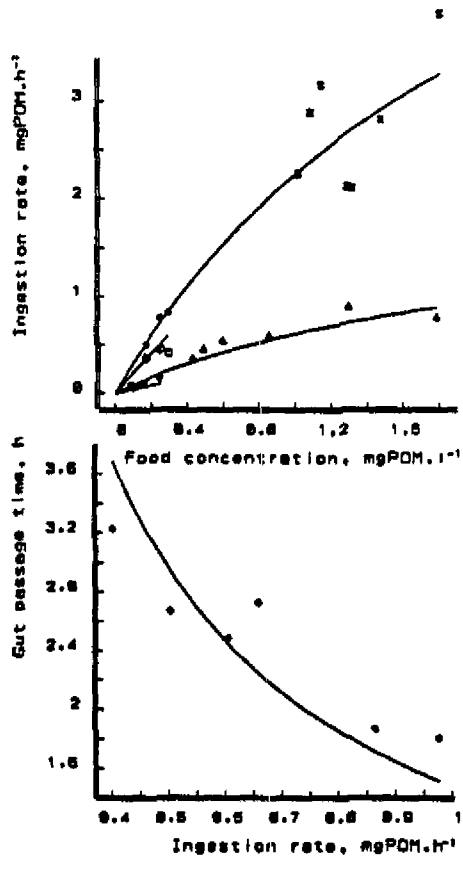

Figure 5: The ingestion rate, I, as function of food density, X, for different shell lengths, L. Food is added as mixtures of algae or organic matter with silt (anorganic particles). Rates are corrected to 15°C and the shell lengths are resp. (from bottom to top) 1.75, 2.5, 4.25, 4.8 and 4.8 cm, data from resp. Kiørboe *et al.*, (1981); Bayne *et al.* (1989); Bayne *et al.* (1987) and Smaal *et al.* (1988). The simultaneously least squares fitted curves are $I = \{I_m\}(\alpha L)^2 X/(K+X)$, with $\{I_m\}$ = 3.0 (SD 1.0) mg POM.cm^{-2}.h^{-1} and K = 2.4 (SD 1.3) mg POM.l^{-1}.

Figure 6: The gut passage time as a function of ingestion rate for a 2.5 cm mussel feeding on a mixture of *Isochrysis galbana*, *Phaeodactylum tricornutum* and ashed silt at 14°C. Data from Bayne *et al.* (1989). The least squares fitted curve is $T = V/I$, with V = 1.48 (SD 0.077) mg POM.

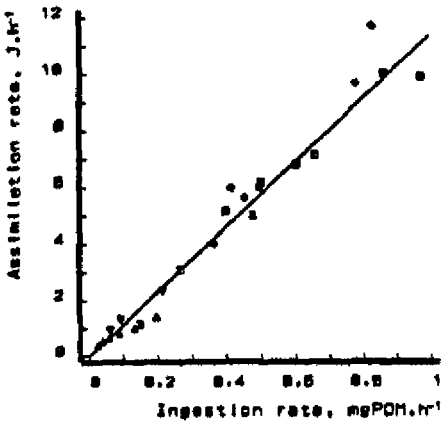

Figure 7: The assimilation rate as a function of ingestion rate for mussels ranging from 1.75 to 5.7 cm. Data from Bayne *et al.* (1987); Bayne *et al.* (1989); Borchardt (1985); Kiørboe *et al.* (1981) and Hawkins & Bayne (1984). All rates are corrected to 15°C. The fitted line is $A = I\{A_m\}/\{I_m\}$ with $\{A_m\}/\{I_m\}$ = 11.4 (SD 0.29) J.mg POM^{-1}.

et al. (1983) found a scaling parameter of 0.903 for veliger larvae and 0.663 for adult mussels. They based their calculations on dry weight instead of wet weight or shell length which bias the estimation of the scaling parameters by the fact that energy reserves do contribute substantially to dry weights, while not requiring energy for maintenance.

Three different levels of oxygen consumption rate of *M. edulis* have been empirically indentified by Thompson & Bayne (1972) in relation to changes in food density. The standard oxygen consumption rate is defined in the absence of food when the oxygen consumption rate declines to a steady state. The active oxygen consumption rate is reached when a starved mussel is fed. Between the limits of standard and active oxygen consumption rates the mussel can show several routine oxygen consumption rates (Bayne, 1976). Thompson & Bayne (1974) showed that the oxygen consumption rate depends hyperbolically on the ingestion rate. This is consistent with the DEB model, if the contribution of ingestion and digestion to respiration is negligible. Substitution of (1) into (6) leads to $V_{O_2} = \frac{V_s I}{W} \frac{W^{1/3}+v/m}{IW^{-2/3}+a\{I_m\}}$ where the proportionality constant V_s (ml O_2.h^{-1}) stands for the standard oxygen consumption rate. This is so because a prolonged ingestion rate of $\{I_m\}WW_m^{-1/3}$ just balances the maintenance costs $W\zeta/\kappa$. At maximally prolonged ingestion, when $I = \{I_m\}W^{2/3}$, the oxygen consumption rate thus becomes $V_{O_2} = V_s\frac{1+W^{-1/3}v/m}{1+a}$. This corresponds with the active oxygen consumption rate of Thompson & Bayne (1972). In Fig. 9 the oxygen consumption is related to ingestion for mussels of different sizes. The estimated parameters are not very useful because a slight deviation in the shell lengths causes a large deviation in the parameter estimates.

After the cessation of growth, oxygen consumption, V_{O_2}, during starvation

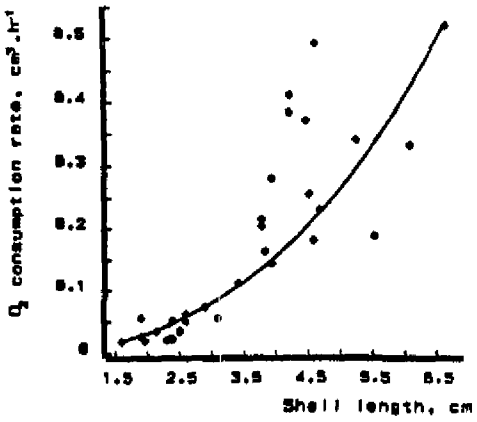

Figure 8: The oxygen consumption rate as function of shell length, L, at constant food density at 15°C. Data from Kruger (1960). The least squares fitted curve is $V_{O_2} = w(L^3 + \frac{v}{m}L^2)$ with $w = 0.022$ (SD 0.0074) $cm^3.cm^{-3}.h^{-1}$ and $\frac{v}{m} = 26.5$ (SD 14.8) mm.

is proportional to the energy spent on maintenance plus reproduction. It decreases exponentially at a rate proportional to body length (Kooijman, 1986b; Evers & Kooijman, 1989) in animals that do not change their storage dynamics and continue to allocate energy to reproduction :

$$V_{O_2}(t) = \{V_0\}W^{2/3}\exp\{-vtW^{-1/3}\} \tag{9}$$

where $\{V_0\}$ is the proportionality constant (ml $O_2.cm^{-2}.h^{-1}$) which depends on the food history at the start of the experiment. The scaled oxygen consumption rate as a function of starvation time at two different body sizes is shown in Fig.10. The estimated value of the energy conductance v at 15°C, 0.24 (SD 0.048) $mm.d^{-1}$ is close to the value of 0.22 (SD 0.018) $mm.d^{-1}$ estimated with data of decreasing lipid weights during starvation (Adema, 1981).

Growth

Age is usually determined in the field on the basis of rings in the shell (Lutz, 1976; Richardson, 1989), size frequencies (*e.g.* Bayne & Worral, 1980), or it is known in experimental setups (*e.g.* Kautsky, 1982). When food density is constant or when food is abundant, the von Bertalanffy growth curve (5) should fit. The fit is mostly satisfying, see Fig. 11 and Tab.2. This implies that the yearly means of food density and temperature remain more or less constant at the sites of sampling (exposed rocky shores in Yorkshire, U.K., Seed, 1969).

Sigmoid growth curves, like the Gompertz growth curve, sometimes fit available data better (Thiesen 1973; Bayne & Worral, 1980). Variations in food density and/or temperature affect growth such that the solution of (2) and (4) can take almost any shape (Kooijman, 1988). Kautsky (1982) measured the mussels individually in cages (ø10 cm) at a depth of 15 m in

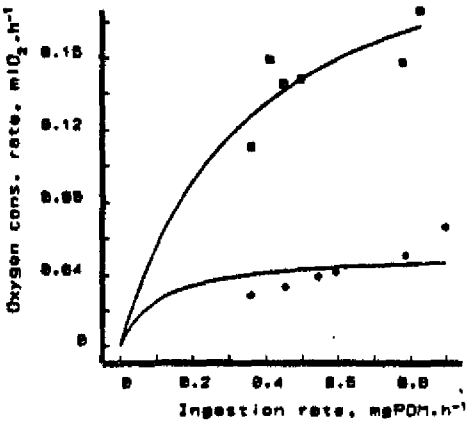

Figure 9: The oxygen consumption rate as function of ingestion rate, I, for the shell lengths, L, 2.5 and 4.5 cm. Data from Bayne *et al.* (1987, 1989). The simultaneously least squares fitted curves are $V_{O_2} = \frac{V_s I}{(\alpha L)^3} \frac{\alpha L + v/m}{I(\alpha L)^{-2} + a\{I_m\}}$ with $V_s(\alpha L)^{-3}$= 0.056 (SD 0.025) ml O_2.h^{-1}, v/m= 5.3 (SD 6.5) mm, $a\{I_m\}$ = 0.16 (SD 0.07) mg POM.cm^{-2}.h^{-1}.

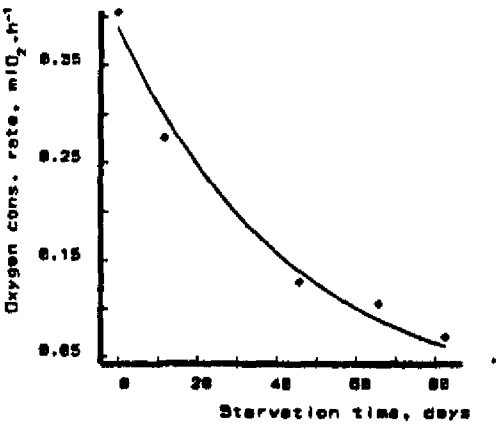

Figure 10: The oxygen consumption rate and the carbohydrate weight in starving 4.5 cm mussels at 15°C. Data from Bayne & Thompson (1970). The least squares fitted curves are $V_{O_2}(t) = V_0 e^{-vt/\alpha L}$, with V_0 = 0.39 (SD 0.014) ml O_2.h^{-1} and v = 0.34 (SD 0.026) mm.d^{-1} and $W(t) = W_0 e^{-vt/\alpha L}$, with W_0=23.4 (SD 1.18) mg and v= 0.25(SD 0.026) mm.d^{-1}.

the Baltic at $7°/_{oo}$. These data, see Fig. 12, clearly show the annual cycle in growth. Assuming that the rates depend on temperature in an Arrhenius way and that the change in food density is slow enough to approximate the energy reserves with $e = f$, (4) can be used to reconstruct the (not measured) food density. So, the predicted length is found from

$$\frac{d}{dt}L = \frac{(L_m f(t) - L)_+}{3(f(t)+a)} a m_{15} (T(t) > T_0) e^{T_A(\frac{1}{288} - \frac{1}{T(t)})} \tag{10}$$

where m_{15} denotes m at 15°C. We used cubic spline functions to descibe $f(t)$ and $T(t)$. The reconstruction of $f(t)$ from the length–time data then amounts to the estimation of the knot values at chosen time points. In view of the scatter, which increases in time in the upper size class in the original data, the fit is acceptable. This illustrates that there is no need to modify (4) to describe sigmoid growth curves. The von Bertalanffy growth rate at $f = 1$ is 0.42 y^{-1} at 15°C on the basis of the parameter values given in Fig. 12.

Strömgren & Cary (1984) found decreasing shell length growth rates during starvation. This can be described by (2) and (4). During the experiment, the mussels in the range of 12-22 mm grew 0.75 mm. When we neglect the change in length, (2) gives $e(t) = e_0 \exp\{-\frac{vt}{aL}\}$. Substitution into (4) gives $\frac{dL}{dt} = \frac{v\exp\{-\frac{vt}{aL}\} - aLm\frac{a}{e_0}}{3a(\exp\{-\frac{vt}{aL}\} + \frac{a}{e_0})}$. Fig. 13 shows a good fit. The parameter values loose a bit of their value by the broad length range of the mussels and the way they are selected for measurement.

We finally consider growth in situations where temperatures and food availabilities changed and have been measured; see Fig. 14. A length data set of *M. edulis* is chosen from the available data in the Oosterschelde (Dutch Delta area). The predicted shell lengths as function of time is shown, based on a conversion of 0.4 mg POC.mg POM^{-1}, see Fig 15.

The deviation of the measured shell lengths from the prediction approximately amount to a factor of 2. This deviation is mainly caused by differences in food qualities between laboratory and field. The energy content of algae cultured in the laboratory is generally lower than from those grown in the field. It is difficult to mimic the nutritive quality of POM in the laboratory unless fresh seawater is used. Values of the saturation constant K and the energy conductance v are affected by differences in food quality. When a free fit of these parameters is allowed, the length growth curve fits satisfactorily

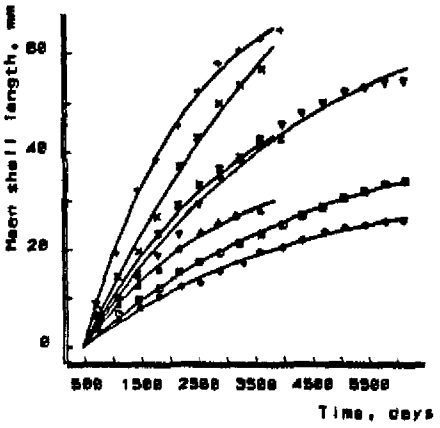

Figure 11: The von Bertalanffy growth curves fitted to length-time data, as reported by Seed (1969) on itertidal North Sea mussels. The parameter values are listed in Table 2.

with the measured shell lengths. The adjusted parameter value for the saturation constant K is 1.69 (SD 0.628) mg POC.l^{-1} (which is equivalent to 4.23 mg POM.l^{-1}) and for the energy conductance v is 0.73 (SD 0.052) mm.d^{-1} at 15°C. The calculated maximal shell length, maximum starvation time and threshold food densities are now 42.1 cm, 36.3 days for a 3 cm mussel and 0.18 mg POM.l^{-1} for a 1.8 cm mussel, respectively. Although the measured shell lengths are well described, the predicted maximal length is probably too high.

Reproduction and spawning

Seed (1969a) reports lengths of fully mature mussels of 6-7 mm in areas of rapid growth and lengths of 2 mm in areas of exceptionally slow growth. Kautsky (1982b) reports that maturity in the slowly growing Baltic *M. edulis* is reached at sizes smaller than 6 mm. Zonneveld & Kooijman (1989) observed that the size at first maturity in the pondsnail *L. stagnalis* depends on day-length. Simultaneous changes in growth and reproduction could be used to deduce that day length only affects the partition coefficient κ and so the energy available for maturation.

M. edulis has a pronounced annual cycle for gametogenesis with one or several spawnings in spring and summer (Bayne, 1976 p22). The annual cycle is usually described by discrete stages of gonad development, *viz.* resting stage, the ripe gonad and the spawning gonad. Observations by Zandée *et al.* (1980) and Pieters *et al.* (1980) showed that energy investment into spawning is a continuous process. They found that the lipid level in mantle

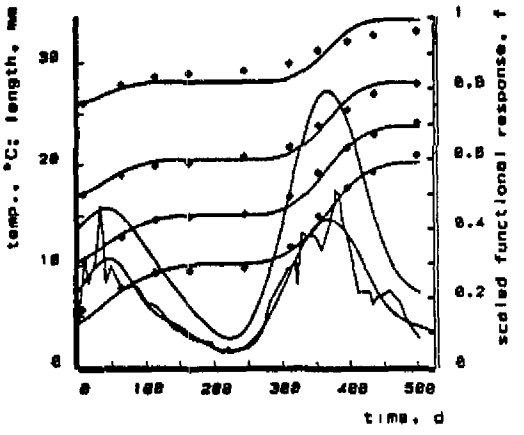

Figure 12: The reconstruction of food density since 1 august from mean length–time data as reported by Kautsky (1982), given a cubic spline description of the measured temperature. Initial lengths were 4.3, 10.4, 17 and 26 mm. Parameters: $L_m = 100$ mm, $a = 0.13$, $m_{15} = 0.03$ d^{-1}, $T_A = 7600$ K.

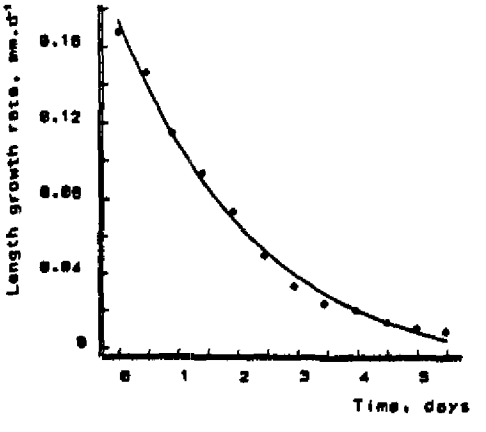

Figure 13: The growth rate in starved mussels at 21.8°C. Data from Strömgren & Cary (1984). The fitted curve is $\frac{d}{dt}L = \frac{ve^{-\frac{wt}{aL}} - \frac{a}{e_0}maL}{3\alpha(e^{-\frac{wt}{aL}} + \frac{a}{e_0})}$, with the shape coefficient $\alpha = 0.333$ and $L = 1.7$ cm. The least squares estimates were $\frac{a}{e_0} = 12.59$ (SD 1.21), $m = 2.36$ (SD 0.99) 10^{-3} d^{-1} and $v = 2.52$ (SD 0.183) mm.d^{-1}.

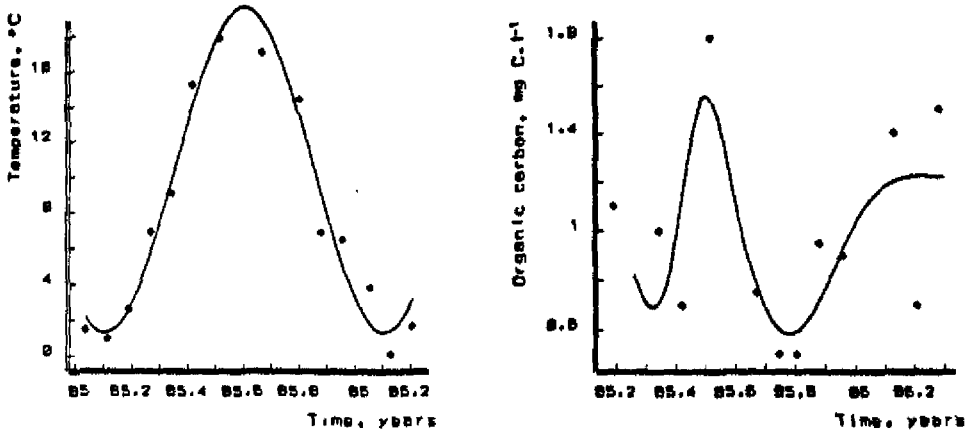

Figure 14: The measured temperature (left) and POC concentrations (right) in the Oosterschelde estuary (near the Storm Surge Barrier) during 1985 and 1986. Data from the Ministry of Public Works and Transport, Tidal Division. The curves are a least squares fitted sinus and a cubic spline

Figure 15: Predicted and fitted shell lengths in the Oosterschelde estuary during 1985 and 1986 based on measured temperature and POC concentration. Data from the Ministry of Public Works and Transport, Tidal Division. The predicted parameters based on laboratory results were K= 0.95 mg POC/l, v_{15}=0.27 mm/d, a=1.03 and $m_{15}a$= 0.0052 d^{-1}. The deviating least squares estimated parameters were K= 1.15 (SD 0.38) mg POC/l and v_{15}=0.59 (SD 0.07) mm/d.

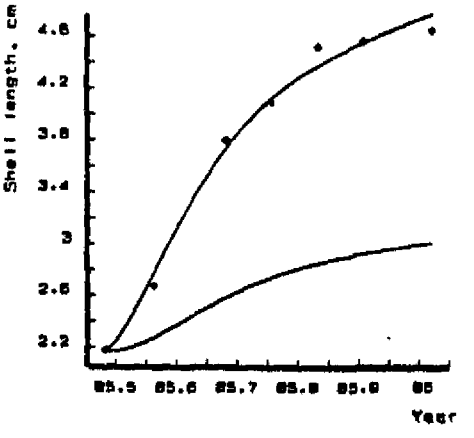

Table 2: Ultimate shell lengths and von Bertalanffy growth rates (with SD).

source	sample method†	temp. °C	L_∞ cm	γ d^{-1}
Rodhouse *et al.* (1984)	c	11	9.60 (0.157)	$2.95\ 10^{-4}$ ($1.13\ 10^{-5}$)
	c	11	7.46 (0.296)	$3.45\ 10^{-4}$ ($2.53\ 10^{-5}$)
	c	11	6.01 (0.429)	$3.39\ 10^{-4}$ ($4.38\ 10^{-5}$)
Page & Hubbard (1987)	b	14.8	9.07 (0.043)	$5.26\ 10^{-3}$ ($5.45\ 10^{-5}$)
Bayne & Worral (1980)	a	10‡	10.8 (2.61)	$3.74\ 10^{-4}$ ($1.30\ 10^{-4}$)
Seed (1969)	c		3.46 (0.282)	$2.56\ 10^{-4}$ ($3.61\ 10^{-5}$)
	c		4.70 (0.360)	$2.24\ 10^{-4}$ ($2.80\ 10^{-5}$)
	c		3.97 (0.461)	$4.14\ 10^{-4}$ ($7.96\ 10^{-5}$)
	c		7.48 (0.313)	$2.48\ 10^{-4}$ ($1.81\ 10^{-5}$)
	c		6.19 (0.485)	$3.52\ 10^{-4}$ ($4.56\ 10^{-5}$)
	c		12.2 (1.74)	$2.05\ 10^{-4}$ ($3.89\ 10^{-5}$)
	c		7.68 (0.245)	$5.44\ 10^{-4}$ ($3.87\ 10^{-5}$)

‡ estimated mean temperature at site of sampling
† a: size frequency; b: measured age; c: shell rings

tissues, where the gonads are locate, increases steadily after spawning. Total lipid accounts for up to 30% of the egg dry weight (Pieters *et al.*, 1980).

Bayne *et al.* (1975) carried out experiments with labeled ^{14}C to measure carbon incorporation in mantle tissue of mussels fed a low and high ration (non-growing and growing mussels respectively). Their results show that more ^{14}C was transferred to the eggs at low than at high rations. Bayne *et al.* (1982) suggested that development of the gametes stops when the carbohydrate content in the mantle tissue is high and gametogenesis is at an early stage. The carbohydrates are then used as energy sources for the mussels when food conditions are poor. This means that energy is mostly allocated to the gametes. Only during early development and under poor feeding conditions allocation of energy to gonads may be stopped. This is consistent with (8).

The ration level of adults is apparently important for the condition of their offspring. Bayne *et al.* (1975) observed that larvae developed from the gametes of adults fed a low ration had a lower growth rate than larvae from well fed adults. This is qualitatively consistent with the DEB model (Kooijman, 1986c)

Somatic production has an optimum at an intermediate age of the mussel while gonadic production increases with increasing age (Bayne & Worrall, 1980; Thompson, 1981; Rodhouse *et al.*, 1986). The DEB model implies that, at constant food density, the maximum body growth occurs at $W_\infty 8/27$ (Kooijman, 1986a). Fig. 16 shows the data and the curves fitted on the basis of the DEB model for three populations, in Stony Brook Harbour, New York (USA) (Rodhouse *et al.*, 1986), and in the Lynher and Cattewater estuaries, Morecombe Bay (U.K.) (Bayne & Worrall, 1980). The fitted curves represent the shell length and yearly somatic and gonadic production which are fitted simultaneously with four free parameters. The trends in the data are well described by the DEB model.

The fraction κ shows marked regional differences. The value of κ in the British populations are 0.94 (SD 0.0067) and 0.99 (SD 0.0095) respectively, while the population in Stony Brook Harbour has a value of 0.71 (SD 0.050). These differences might be explained by a genetic control of fecundity as demonstrated by Rodhouse *et al.* (1986), Hilbish & Zimmerman (1988) and Gardner & Skibinsky (1990). There is no concensus in literature about which external or internal factor induces spawning (Bayne, 1976 p19). In the next section, we assume that spawning occurs at the first of May. For the Dutch

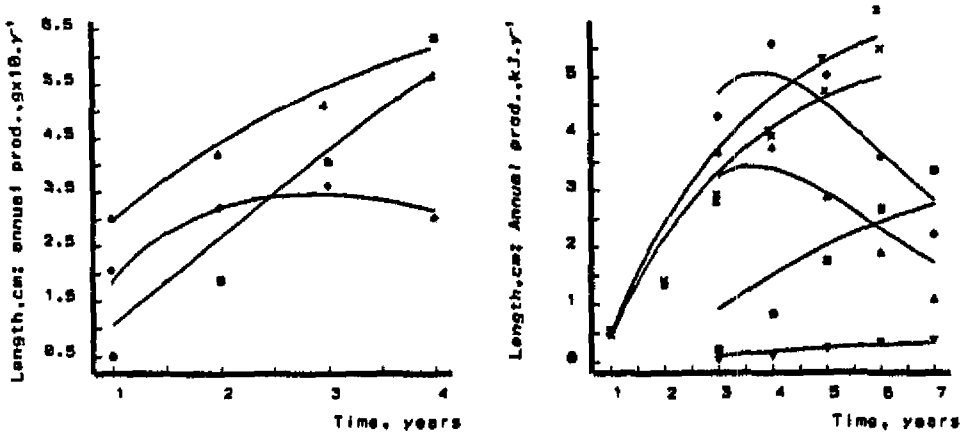

Figure 16: Somatic and gonadic yearly production in three populations. Data from Rodhouse *et al.* (1986), left, and Bayne & Worrall (1980), right. The estimated parameters in the left figure at an roughly estimated temperature of 15°C are $a = 1.01$ (SD 0.19), $ma = 4.2$ (SD 0.7) 10^{-3} d^{-1} and $\kappa = 0.71$ (0.074), given $v_{15} = 0.23$ mm.d^{-1} and $f = 0.49$, a dry weight–wet weight conversion of 0.12, with $e(0) = 0.46$, $W(0) = 1$ cm^3 at 12°C. For the right figure: $a = 1.05$ (SD 0.073), $ma = 5.0$ (SD 0.1) 10^{-3} d^{-1} and $\kappa_1 = 0.94$ (SD 0.01) and $\kappa_2 = 0.99$ (SD 0.01) with $e_{0,1} = 0.4, W_{0,1} = 6.16$ mm^3, $f_1 = 0.59$, $e_{0,2} = 0.3, W_{0,2} = 4.36$ mm^3, $f_2 = 0.51$ and $v_{15} = 0.19$ mm.d^{-1}.

Delta area, which we will discuss, this is a realistic assumption.

Discussion

The DEB model provides a framework to describe a wide variety of physiological processes. Many data from the literature could not be used to test the theory and estimate the parameters, because essential information for their interpretation had not been provided. Differences in parameter values obtained from data taken from the literature are due to differences in experimental methods, temperature, salinities, water depths and food conditions and, to some extent, genetic variation. The following parameter estimates summarize the results for the tests against experimental data: $a = 1.03$, $m = 0.00517$ d^{-1}, and $v = 0.23$ mm.d^{-1} at 15°C. This gives a maximal length of 13.3 cm and a maximal starvation time of 67.7 days for a 3 cm mussel. It is not known to which extend populations differ genetically in their parameter values or how the parameter values depend on environmental variables like salinity.

The early budget studies simply describe growth as proportional to the

difference between assimilated and respirated energy (Winberg, 1956). The SFG concept conceives growth as the sum of somatic and gonadic production. These approaches do not allow for variations in internal states such as storage, which makes it impossible to accomodate results like those presented in Fig.13. When SFG is expressed on a dry weight basis, changes in the energy buffer do result in a positive or negative SFG which give a false impression of actual growth in transient situations such as recovery from starvation.

The models developed for mussel or filterfeeder growth are usually based on allometric scaling relations and SFG calculations. Ross & Nisbet (1991) modified the DEB model in order to predict spawning of *M. edulis*. They altered the von Bertalanffy size–based growth equation into the sigmoid Gompertz age–based one and dropped the proportionality of assimilation rate to surface area. The data here tested against the DEB model gave no reason to alter the underlying assumptions. Sigmoid growth curves are expected on the basis of the DEB model when food densities and temperatures vary through the seasons. It would be hard to explain non–sigmoid growth curves, which are also frquently observed, on the basis of the Gompertz curve. The second one is the basic measure for body size. No other concept seems so simple at first glance and proved to be so difficult afterwards. The DEB model is based on volume, in which case the custom of standardization to fixed dry weights gives misleading results.

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ANIMAL ENERGY BUDGETS AFFECT THE KINETICS OF XENOBIOTICS

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ABSTRACT

On the basis of a model for energy budgets, which includes the dynamics of stored energy, a model has been proposed for the kinetics of non-metabolized xenobiotic compounds, which may be lipophilic. The surface area coupled uptake is via food and/or water through the aqueous fraction of the animal. The partitioning to non-aqueous structural body mass and to stored materials (i.e. lipids, carbohydrates and proteins) is taken instantaneously. The result is a simple first order kinetics with variable coefficients. The bioconcentration factor has been evaluated. Model predictions have been tested against data from the literature.

INTRODUCTION

The kinetics of xenobiotics is of importance in connection with environmental monitor programs, as preamble for understanding effects of toxic compounds and, as a special case, for medical purposes when the xenobiotic concerns a pharmaceutic. One compartment models do not always give a satisfactory fit with experimental data. For this reason more compartment models has been proposed (see e.g. Curtis *at al* (1977), Ružić (1972)). Because of their larger number of parameters, the fit is better, but an acceptable physical identification of the compartments is usually not possible. These models therefore contribute little to our understanding of the kinetics as a process. The purpose of this paper is to incorporate elementary knowledge about chemical exchange that is not compound-specific and about animal physiology that is not species-specific into a model for the kinetics of non-metabolised compounds.

For terrestrial animals, the usual uptake of xenobiotics from the environment is via food. Sometimes, uptake is via the lung or directly through the surface. In the aquatic environment uptake directly from water is especially

important for hydrophilic organic compounds (Bruggeman *et al.*, 1981) and metal (Borchardt, 1981, Riisgard *et al.*, 1987). In aquatic animals that are chemically isolated from their environment, like aquatic insects, birds and mammals, the usual uptake is through food only. See e.g. Walker (1990) for a discussion of uptake routes. Excretion is through the surface directly, via excretion products and via gametes. Accumulation of lipophilic compounds and partitioning between different organs can be explained by the occurrence of stored lipids. Schneider (1982) found large differences of PCB concentrations in different organs of the cod, but they did not differ when based on the phospholipid-free fraction of extractable lipids. Models for the feeding conditions dependent kinetics have been proposed by e.g. Lassiter & Hallam(1988), Hallam & de Luna(1984), Hallam *et al.*(1989). The models presented in these papers have a large number of parameters. The present paper aims at modelling the kinetics of xenobiotics in a parameter sparse way, assuming instantaneous partitioning of the compound in the organism, as proposed by Barber *et al.*(1988). It differs from their model by the coupling to a model for the uptake and allocation of energy, which has been extensively tested, Evers & Kooijman(1989), Kooijman(1986a, b, c, 1988), Zonneveld & Kooijman(1989). One of the key features of this model is that food uptake, and so excretion, is proportional to surface area, resulting in relatively simple kinetics of xenobiotics allowing several uptake and excretion routes. Other features are a cyclic change in lipid rich compounds, due to the reproductive behaviour and predictions for concentration-body size relations.

MODEL SPECIFICATION

The tissue is divided into four compartments: the aqueous fraction of volume V_a, the non-aqueous fraction of the structural component of the body of volume V_w, the non- aqueous fraction of the stored energy reserves available for utilization of volume V_s, and the non-aqueous fraction of the energy reserves set apart with the destination of reproduction of volume V_r. Energy rich compounds like glycogen, proteins and lipids are assumed to be replaced by water when food conditions grow poor. This has been found for mussels by Pieters *et al.*(1979) and for snails by Zonneveld & Kooijman(1989). We assume that the animal remains isomorphic during its development, from which follows that each organ occupies a fixed fraction of the structural body mass. Moreover we assume homeostasis, i.e. the chemical composition of the

non-aqueous fraction of the structural body mass and the energy reserves remain constant. However, we allow for chemical differences between these two compartments. The aqueous body volume is therefore a fixed fraction of the structural component of the body plus the part of the energy reserves that is not filled with energy rich components. So $V_a = (1-\alpha_w)W + \alpha_e(1-e)W$ for W denoting the structural body mass, e the energy reserves as a fraction of the maximum energy reserves, α_w the non-aqueous fraction of the body size and α_e the maximum volume of energy reserves as a fraction of body size. The volume occupied by non-aqueous biomass, energy reserves and reproduction reserves are taken to be $V_w = \alpha_w W$, $V_e = \alpha_e e W$ and $V_r = \alpha_e r W$, where r denotes the cumulative energy investment into reproduction since the last reproductive output as a fraction of the maximum energy reserves. At reproduction it is reset to zero. Wet weight, W_w, of an individual is taken to be

$$W_w = d_s(V_a + V_w + V_e + V_r) = d_s(1 + \alpha_e(1+r))W \tag{1}$$

where d_s is the specific density, which is close to 1 g/cm^3. The redistribution of the xenobiotic over the four compartments is assumed to be fast with respect to the exchange with the environment (see the section on time scales). This assumption is supported by the study of the elimination rate of 4,4'-dichlorobiphenyl (PCB15) in the pond snail *Lymnaea stagnalis* by Wilbrink *et al.*(1989), who found the elimination rates to be equal for different organs. The fact that structural biomass consists of organs differing in partition coefficients for the xenobiotic, is covered naturally through the assumptions of isomorphism and homeostasis together with instantaneous partitioning. We can therefore relate the total number of moles of xenobiotic inside the animal, C_+, to its concentration in the aqueous fraction, c_a, which is assumed to be the only compartment which communicates directly with the environment. We have

$$\begin{aligned} C_+ &= C_a + C_w + C_e + C_r = V_a c_a + V_w c_w + V_e c_e + V_r c_r \\ &= (1 + \alpha_e + \alpha_w(P_{wa} - 1) + \alpha_e e(P_{ea} - 1) + \alpha_e r P_{ea}) W c_a \\ &= \alpha_e h W c_a \end{aligned} \tag{2}$$

where the C's denote the amount of xenobiotic compound in moles and the c's the concentrations in mol/volume; $P_{wa} = c_w/c_a$ is the partition coefficient of xenobiotic between the non-aqueous structural biomass and the aqueous

phase; $P_{ea} = c_e/c_a$ that of the energy reserves and the aqueous phase. The partition coefficients are assumed to be fixed values. $\gamma = 1 + \alpha_e^{-1} + (P_{wa} - 1)\alpha_w/\alpha_e$ and

$$h = \gamma + (P_{ea} - 1)e + P_{ea}r \tag{3}$$

are introduced to shorten the notation. See table 1 for a list of the parameters and main variables.

The uptake as well as elimination are assumed to be proportional to the surface area of the isomorphic animal, thus proportional to $W^{2/3}$. See e.g. Evers & Kooijman (1989) for a discussion on the proportionality of ingestion with surface area. Uptake via water is proportional to surface area, because isomorphism ties surface area of e.g. gills to total surface area. We assume that water is locally well mixed, such that the animal will not deplete its immediate surroundings from xenobiotic. So we do not follow e.g. Norstrom *et al.*(1976) by relating uptake to oxygen consumption. The absence of the connection between oxygen uptake and accumulation of PCB in guppies has been experimentally supported by Opperhuizen & Schrap (1987). When a simple diffusion type of kinetics applies, we arrive at

$$C'_+ = W^{2/3}\left(r^*_{da}c_d + r^*_{pa}f c_p - r^*_{ad}c_a\right) \tag{4}$$

where the r^*'s denote the transport rates from the compartment indicated in the first index to the second one and f denotes the scaled functional response $f = X/(K+X)$, for K being the saturation constant and X the food density. From (2) we obtain

$$C'_+ = \alpha_e(hW)c'_a + \alpha_e(h'W + hW')c_a \tag{5}$$

Substitution into (4) results in

$$c'_a = \frac{r_{da}c_d + r_{pa}f c_p}{hW^{1/3}} - c_a\left(\frac{r_{ad}}{hW^{1/3}} + \frac{W'}{W} + \frac{h'}{h}\right) \tag{6}$$

where $r_{da} = r^*_{da}/\alpha_e$, $r_{pa} = r^*_{pa}/\alpha_e$ and $r_{ad} = r^*_{ad}/\alpha_e$. Although this equation defines, together with an initial condition, the dynamics of the xenobiotic in the animal, it will be difficult, if not impossible to measure the concentration in the aqueous fraction. More relevant seems the concentration in the wet weight $c_{ww} = C_+/W_w$. Substitution of (1) and (2) gives

Table 1: The parameters and main variables of the xenobiotic and the energy budget model.

Par.	Var.	Dimension	Interpretation
	c_d	mol.length^{-3}	conc. in the water
	c_p	mol.length^{-3}	conc. in the food (as volume)
	c_{ww}	mol.weight^{-1}	conc. on the basis of wet weight
r_{pa}		length.time^{-1}	uptake rate from food
r_{da}		length.time^{-1}	uptake rate from water
r_{ad}		length.time^{-1}	elimination rate
P_{ea}		-	partition coeff. en.reserves/aqueous fraction
γ		-	compound parameter
	f	-	food density/saturation const. plus food density
	W	length^3	body size
	e	-	energy reserves/max.energy reserves
	r	-	cum.energy to reprod./max.energy density
α_e		-	max.vol.reserves/vol.body
d_a		weight.length^{-3}	specific density of the body
v		length.time^{-1}	energy conductance
κ		-	fraction utilized energy to growth + maint.
a		-	costs of growth/κ max.energy density
b		time^{-1}	maintenance costs/κ max.energy density
W_b		length^3	body size at hatching
W_j		length^3	body size at first maturation
t_s		time	time at spawning or reproduction, $s = 1, 2, ..$

$$c_{ww} = \frac{c_a h}{d_a(1 + \alpha_e^{-1} + r)} \tag{7}$$

After substitution into (6) and application of the chain rule for differentiation again, we arrive at

$$c'_{ww} = \frac{r_{da}c_d + r_{pa}fc_p}{d_a(1 + \alpha_e^{-1} + r)W^{1/3}} - c_{ww}\left(\frac{r_{ad}}{hW^{1/3}} + \frac{W'}{W} + \frac{r'}{1 + \alpha_e^{-1} + r}\right) \tag{8}$$

This description of the kinetics of a xenobiotic has thus 6 free parameters: r_{da}, r_{pa} and r_{ad} of dimension length per time and the dimensionless parameters α_e, γ and P_{ea}. See table 1 for a list of primary parameters and variables.

To complete the model, it is necessary to specify the processes of feeding, storage, growth and reproduction. Following Kooijman(1986), food intake is taken to be a hyperbolic function of food density and proportional to surface area. Assimilation energy stocks the energy storage. Expressed as a density, so a ratio of stored energy and body volume, energy storage follows a simple first order dynamics, with a rate inversely proportional to body length. A fixed fraction of the energy utilized from storage, is spent on growth plus maintenance. The latter is taken proportional to body volume. The rest of the utilized energy is spent on development plus reproduction. The latter drain is first collected in a buffer, which is emptied at spawnings, triggered by environmental factors. Development stops and reproduction starts as soon as a certain cumulated amount of energy is spent on increasing the state of maturity, which here occurs upon reaching a certain body size. The energetic costs of maintaining a certain degree of maturation is taken proportional to the minimum of the actual body volume and that at first maturation, at the expense of the energy flow to development and reproduction (see Zonneveld & Kooijman, 1989). Here, we will express,the stored energy density and energy allocated to reproduction as fractions of the maximum stored energy density, which thus become dimensionless quantities. These model elements result in the following dynamics for body volume, scaled energy density and scaled energy allocation to reproduction:

$$W' = \frac{(evW^{2/3} - bW)_+}{e + a} \tag{9}$$

$$e' = vW^{-1/3}(f - e) \tag{10}$$

$$R' = \frac{(1 - \kappa)e}{e + a}(vaW^{2/3} + bW) - (1 - \kappa)bW_j \tag{11}$$

$$R' = \begin{cases} evW^{2/3} - \kappa bW - (1-\kappa)bW_j & \text{for } e \geq W^{1/3}b/v \text{ and } W > W_j \\ evW^{2/3} - \kappa bW & \text{for } e < W^{1/3}b/v \text{ and } W > W_j \end{cases} \quad (12)$$

Now, $\tau = R/W$ and $R = \int_{t_\tau}^{t} R'dt$, where t_τ denotes the time of latest reproduction, which should not be earlier than the time at first maturation, i.e. when $W = W_j$. The change in reproduction energy density, r', is found through its definition $r' = R'/W - RW'/W^2$

For spawning occurring at t_s, we still have to define the behaviour of c_{ww} around this time point. Kooijman(1986c) argued that a freshly laid egg can be realistically regarded as materials representing an amount of stored energy, with a negligible size of structural biomass. Little chemical transformation is required to transform energy set apart for reproduction into that of eggs. Therefore it seems straightforward, at least for females, to let transduce the xenobiotic that rests in these reserves to eggs. We can relate the wet weight concentration just after spawning, i.e. at t_s^+, to that just before spawning, i.e. at t_s^-, arriving at

$$c_{ww}(t_s^+) = c_{ww}(t_s^-)\frac{1+\alpha_e^{-1}+r}{1+\alpha_e^{-1}}\frac{h(t_s^+)}{h(t_s^-)} \quad (13)$$

For $P_{es} < 1 + (P_{ws} - 1)\alpha_w/(1 + \alpha_e(1-e))$ this means a decrease in c_{ww}. So, for a well fed animal for which $e = 1$, $P_{es} < 1 + (P_{ws} - 1)\alpha_w$ means a decrease in c_{ww} at spawning. Independent from a change in c_{ww} at t_s, the production of eggs makes up an elimination route which can be substantial.

When reproduction occurs as soon as enough energy has been accumulated for a single egg and the energy investment in an egg is small, thus r is negligibly small, we can not simply put $r = 0$ in (8), despite the fact that according to (13) c_{ww} does not change at t_s. The reason is that the time between subsequent spawnings can in this case reduce as well. This means that the elimination rate of size $P_{es}\alpha_e R' c_s$, which should then be introduced into (4), need not be negligibly small. As a consequence, h'/h in the second term of (6) and $\frac{r'}{r+1+\alpha_e^{-1}}$ in the second term of (8) should be replaced by $P_{es}r'/h$. After these substitutions, we can safely put $r = 0$ and still obeying the preservation law for the xenobiotic. Species differ widely in the timing of the reproduction process. Small animals, like those in plankton usually reproduce more or less continuously, while the larger ones in temperate climates usually reproduce once a year only.

It is also possibile is that no xenobiotic is transduced through the reproduction process, as has been found by Wilbrink *et al.*(1989) for 4,4'-DCB in *Lymnaea*. In that case the last factor in (13) should be omitted, resulting in an increase of c_{ww} due to the reduction in wet weight.

Figures 1 & 2 illustrate the performance of the model to describe the accumulation / elimination behaviour of the compounds hexachlorobenzene ($\log K_{ow} = 5.45$, Russel & Gobas, 1989) and 2- monochloronaphthalene ($\log K_{ow} = 3.90$, Opperhuizen, 1986). The mussel and fish, respectively, were not fed during the experiment, which implies that their energy reserves decreased during the experiment. As a consequence the small fish kept at a bit higher temperature than the larger mussel, depleted its energy reserves relatively faster, so that it starts to eliminate during the accumulation phase of the experiment. (See Kooijman, 1986b for a theory on the relation between body size and energy reserves.) The model succesfully describes this phenomenon. The experiments have been short enough to assume that the size of the test animals did not change and that the energy allocation to reproduction has been negligibly small during the experiment. The concentration in water changed during accumulation. We therefore fitted a cubic spline to these concentrations and used this spline in (8) to obtain the concentrations in the wet weight. The free parameters have been estimated according to the least squares criterion.

INITIAL CONDITIONS

Although the concentration in the hatchling contributes little to that later on because of the factor $W^{-1/3}$ in (8), consistency requires its evaluation. If the xenobiotic is transferred from mother to hatchling, the initial value of c_{ww} depends on the contents of xenobiotic in the mother and her feeding condition. Experience with chronic toxicity tests learns that most effects occur at hatching, meaning that an egg must be considered as chemically rather isolated from its environment, apart from gas exchange of course. Neglecting the contribution via sperm, the c_{ww} of the hatchling therefore equals the ratio of content of xenobiotic of the egg at formation in the mother and its wet weight $d_s(1 + \alpha_e)W_b$. The energy content of an egg as a fraction of maximum energy reserve of the hatchling is according to Kooijman(1986c)

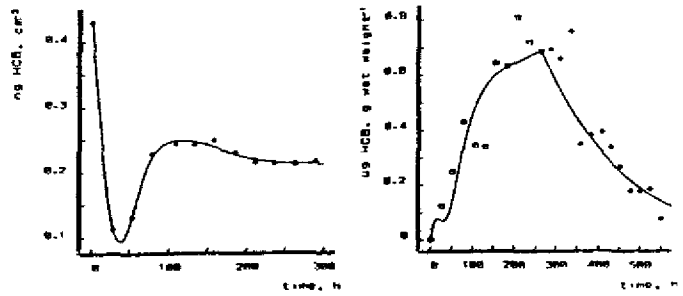


Figure 1: The measured concentration of hexachlorobenzene in the water and in the 6.03 cm^3 freshwater mussel *Elliptio complanata* at 20°C during an accumulation / elimination experiment. Data from Russel & Gobas (1989). The least squares fitted curves are the cubic spline function for concentrations in the water and the model based expectation for that in the wet weight. The parameter values with s.d. were $r_{da}/(1+\alpha_e^{-1}+r) = 43.38$ (2.43) cm.h^{-1}, $P_{ea}/\delta = 0.3$ (0.89), $r_{ad}/\delta v = 1.16$ (0.46) for $v = 0.01$ cm.h^{-1} with $\delta = \gamma + P_{ea}r$.

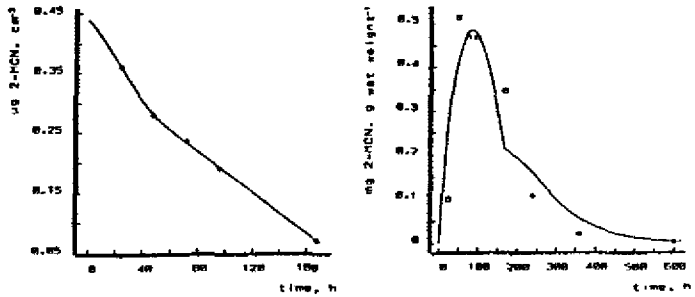


Figure 2: The measured concentration of 2-monochloronaphthalene in the water and in the 0.22 cm^3 female guppy *Poecilia reticulata* at 22°C during an accumulation / elimination experiment. Data from Opperhuizen (1986). The least squares fitted curves are the cubic spline function for the concentrations in the water and the model based expectation for that in the wet weight. The parameter values with s.d. were $r_{da}/(1+\alpha_e^{-1}+r) = 20.47$ (5.20) cm.h^{-1}, $P_{ea}/\delta = 3.33$ (17.95), $r_{ad}/\delta v = 0.44$ (0.56) for $v = 0.014$ cm.h^{-1} with $\delta = \gamma + P_{ea}r$.

$$e_0 = 1.1a + e_b\left(1 - \frac{1}{4e_b}\left(\frac{W_b}{W_m}\right)^{1/3}\right)^{-3} \tag{14}$$

where the scaled reserve energy density of the hatchling, e_b, equals that of the mother at egg formation and the maximum body size $W_m = (v/b)^3$. The initial content in the egg is in accordance with (2): $c_e\alpha_e P_{ea} c_0 W_b$, where c_e is the concentration in the aqueous phase of the mother at egg formation. Substitution of (7) results in

$$c_{ww}(0) = c_{ww}\frac{P_{ea}c_0(1 + r/(1+\alpha_e^{-1}))}{\gamma + (P_{ea}-1)e + P_{ea}r} \tag{15}$$

where c_{ww}, e and r refer to the values of the mother at the moment of egg formation.

TIME SCALES

From (8), we observe that the relaxation time of c_{ww} equals

$$\left(\frac{r_{ad}}{hW^{1/3}} + \frac{W'}{W} + \frac{r'}{1+\alpha_e^{-1}+r}\right)^{-1}$$

Its maximum value is obtained for $W' = 0$, $r' = 0$, $W = W_m$, $e = 1$ just before spawning, where $r = r_m = \int_0^{t_*} r'dt$. The maximum relaxation time is then $W_m^{1/3}(\gamma - 1 + P_{ea}(1+r_m))r_{ad}^{-1}$. Its *minimum* value is obtained for $W = W_b$, which implies, $r' = r = 0$. The relaxation time reduces to $\frac{l_b}{b}(\frac{\alpha}{1+\beta e} + \frac{e-l_b}{e+\alpha})$, for $l_b = W_b^{1/3}b/v$, $\alpha = \frac{r_{ad}}{\gamma r}$ and $\beta = \frac{P_{ea}-1}{\gamma}$. Its minimum value is obtained for

$$e = \min\{1, \max\{l_b, \frac{l_b + a - \alpha a \pm (1-\beta a)\sqrt{(l_b+a)\alpha/\beta}}{\alpha - \beta(l_b+a)}\}\}$$

For increasing lipophilicity, so P_{ea} and thus β increase, the relaxation time increases. The minimum value tends to $\frac{l_b}{b}\frac{1+a}{1-l_b}$, which completely depends on the energy budget. This minimum relaxation time sets the time frame for the present model. All processes with much smaller relaxation times, like the kinetics of the xenobiotic and storage materials in the blood compartment (c.f. Bruggeman *et al.*(1981)) can be regarded as being in pseudo equilibrium. So, the assumption of instantaneous partitioning of the xenobiotic compound

can be relaxed to the condition that the relaxation time of the redistribution process is small in comparison with this minimal value.

When the rate $r_{ad}/hW^{1/3}$ is large with respect to $W'/W+r'/(1+\alpha^{-1}+r)$, the model reduces to a simple first order kinetics, but the parameters still depend on the size of the organism.

BIOCONCENTRATION FACTOR

The bioconcentration factor, BF, is an important concept in the kinetics of xenobiotics. It is usually defined as the ratio of the concentration in the organism and the concentration in the environment, which both are taken constant. This implies that food density is taken constant as well. In the strict sense, the present model does not have such a factor, because the energy set apart for reproduction shows a cyclic behaviour, so does the BF. We can approach the concept BF for animals that ceased growth, so $W' = 0$. At constant food density this occurs when they reach their ultimate size $W_\infty = (fv/b)^3$. The energy density then becomes $e = f$. The energy density set apart for reproduction is $r = tr'$, where t represents the time since last spawning. For this particular values for W and e we have from (11) $r' = (1-\kappa)b(1-W_j/W_\infty)_+$. Therefore we have

$$h(t) = \gamma + (P_{ea}-1)f + P_{ea}r't$$

which is linear in t. This simplifies (8) to an extent that it can be solved explicitly, giving

$$\begin{aligned} c_{ww}(t) &= v(t)\left(\int_0^t \frac{u(x)}{v(x)}dx + c_{ww}(0)\right) \text{ where} \\ u(x) &= W_\infty^{-1/3}\frac{r_{da}c_d + r_{pa}fc_p}{d_s(1+\alpha_e^{-1}+xr')} \text{ and} \\ v(x) &= \exp\{-\int_0^x \left(\frac{r_{ad}}{h(y)W_\infty^{1/3}} + \frac{r'}{1+\alpha_e^{-1}+r'y}\right)dy\} \\ &= \frac{1+\alpha_e^{-1}}{1+\alpha_e^{-1}+xr'}\left(\frac{h(0)}{h(x)}\right)^{r_{ad}/W_\infty^{1/3}r'P_{ea}} \end{aligned}$$

When t_i is the period between subsequent broods or spawnings and t_s is time at spawning, in equilibrium we must have that $c_{ww}(t_s^+ + t_i) = c_{ww}(t_s^-)$. Using

(13), which we rewrite as $c_{ww}(t_s^-) = c_{ww}(t_s^+)g(t_i)$ with $r = tr'$, we can solve $c_{ww}(t_s^+)$ and obtain

$$\begin{aligned} c_{ww}(t_s^+) &= \frac{\int_0^{t_i} u(x)/v(x)\,dx}{g(t_i)/v(t_i) - 1} \\ &= \frac{r_{da}c_d + r_{pa}fc_p}{d_s(1+\alpha_e^{-1})}\,\frac{\gamma + f(P_{ea}-1)}{r_{ad} + W_\infty^{1/3}P_{ea}r'} \end{aligned} \tag{16}$$

In order to arrive at the BF, we have to divide by the concentration in the environment. Sometimes, the water concentration is taken for aquatic organisms, but it seems more lucid to include the xenobiotic in the food in the environment as well. In that case, the BF just after spawning is given by $c_{ww}(t_s^+)(c_d + Xc_p)^{-1}$, while that just before spawning is $g(t_i)$ times as large. In any case, the BF still depends on the concentration in the environment as long as uptake via food contributes significantly. This greatly reduces the usefulness of this concept.

CONSTANT ENVIRONMENTS

When food density, as well as the concentration of xenobiotic in the water and in the food do not change since long, the concentration in the food will be proportional to that in the water, let us say $c_p = P_{pd}c_d$. The energy density will be constant at $e = f$. When we choose the maximum length, $W_m^{1/3} = v/b$ as our unit for length l, b^{-1} as unit for time t°, and c_d as unit for concentration in the wet weight c, we effectively remove all dimensions of the problem and obtain a maximum reduction of the number of parameters. Scaled length as function of scaled age is found from (9):

$$l(t^\circ) = f - (f-l_b)\exp\{\frac{-t^\circ}{3(f+a)}\} \tag{17}$$

The energy drain to reproduction rate as a fraction of the maximum stored energy reduces for small amounts of accumulated energy for reproduction to

$$r'(t^\circ) = (1-\kappa)\left(\frac{f+af/l(t^\circ)}{f+a} - \frac{l_j^3}{l^3(t^\circ)}\right) \tag{18}$$

The dynamics of the scaled concentration in the wet weight now reduces for $l < l_j$ from (8) to

$$c'(t^\circ) = \frac{r^\circ_{da} + f r^\circ_{pa}}{l(t^\circ)} - c(t^\circ)\left(\frac{r^\circ_{ad}/l(t^\circ)}{\gamma + (P_{ea}-1)f} + \frac{f/l(t^\circ) - 1}{a+f}\right) \qquad (19)$$

where the new dimensionless compound parameters are $r^\circ_{da} = \frac{r_{da}}{bW_m^{1/3}} \frac{1}{d_v(1+\alpha_e^{-1})}$, $r^\circ_{pa} = \frac{r_{pa}}{bW_m^{1/3}} \frac{P_{pd}}{d_v(1+\alpha_e^{-1})}$ and $r^\circ_{ad} = \frac{r_{ad}}{bW_m^{1/3}}$. For $l > l_j$, thus after an scaled age of $3(a+f)\ln\frac{f-l_b}{f-l_j}$, the dynamics depends on the times of spawning. For short periods between subsequent broods and small amounts of energy accumulated for reproduction we have:

$$c'(t^\circ) = \frac{r^\circ_{da} + f r^\circ_{pa}}{l(t^\circ)} - c(t^\circ)\left(\frac{r^\circ_{ad}/l(t^\circ) + P_{ea} r'(t^\circ)}{\gamma + (P_{ea}-1)f} + \frac{f/l(t^\circ) - 1}{a+f}\right) \qquad (20)$$

The initial scaled concentration depends on the size of the mother. When we consider a young born from a fully grown mother, which thus has a scaled length of $l = f$, a scaled energy drain to reproduction of $r' = (1-\kappa)(1-l_j^3/f^3)$, and a concentration of

$$c(\infty) = \frac{(\gamma + f(P_{ea}-1))(r^\circ_{da} + f r^\circ_{pa})}{r^\circ_{ad} + f P_{ea}(1-\kappa)(1-l_j^3/f^3)} \qquad (21)$$

The scaled initial concentration becomes from(15):

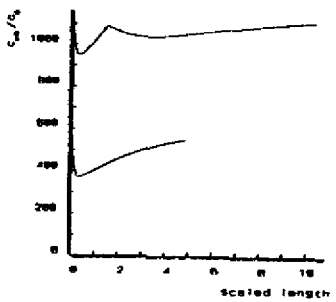
$$c(0) = \frac{e_0 P_{ea}(r^\circ_{da} + f r^\circ_{pa})}{r^\circ_{ad} + f P_{ea}(1-\kappa)(1-l_j^3/f^3)} \qquad (22)$$

The concentration in the wet weight will increase during the lifetime of an individual when

$$\frac{c(\infty)}{c(0)} = \frac{\gamma + f(P_{ea}-1)}{e_0 P_{ea}} > 1 \qquad (23)$$

Depending on the exchange rates relative to the growth rate, the concentration will first drop after hatching because of the dilution through growth. At maturation, the accumulation in females can decrease due to elimination through reproduction. As an example, c is given as a function of t° Fig.3. An important conclusion from this figure is that the fact that a xenobiotic slowly accumulates into an animal not only depends on the properties of the xenobiotic, but also on the changing physiology of the animal.

Figure 3: The concentration of xenobiotic on the basis of wet weight as a fraction of that in the water, as a function of scaled age in a constant environment. The xenobiotic parameters are $r^\circ_{da} = 20$, $r^\circ_{pa} = 1000$, $r^\circ_{ad} = 50$, $\gamma = 30$ and $P_{ea} = 100$. The energetic parameters are $l_b = 0.1$, $l_j = 0.4$, $a = 0.2$, $\kappa = 0.3$ for $f = 1$ (upper curve) and $f = 0.4$ (lower curve).



BODY SIZE RELATIONS

Since energy budgets depend on body size, we can expect that the BF based on (16) as well depends on the ultimate body size a species can reach.. The theory behind this reasoning is presented in Kooijman (1986b). For studying the BF-body size relation, we assume that reproduction takes place once a year for all species. Since r_{pa} is proportional to the surface area-specific ingestion rate, the theory states that it is proportional to the cubic root of the body size. This also holds for the maximum storage density (Kooijman, 1988), thus for b^{-1}, which makes $W_\infty^{1/3} r'$ independent from body size. Although the maximum storage density scales with the cubic root of body size, it does not imply that the volume of the reserves as a fraction of that of the body scales in this way. Large animals seem to utilize storage compounds with a higher energy capacity more frequently. Nonetheless, α_e will increase, thus γ will decrease with body size, but we expect that this is of minor influence on the BF. The other parameters, r_{da}, r_{ad}, P_{ea}, P_{wa}, α_w, κ, W_j/W_∞, d_v do not depend on body size. Therefore we expect that the BF at high food densities is linear in the cubic root of body size, with a slope depending on the uptake via food, em i.e. $BF \propto r_{da} + r_{pa} P_{pd}$. Note that we did not assume any interference of uptake and elimination (or transformation) with the metabolism of the animal. Figure 4 illustrates that the BF for the highly lipophyllic compound 2,4,5,2',4',5' hexachlorobiphenyl (PCB153) for aquatic animals depends on body size indeed, and that this can be explained on the basis of the present reasoning.

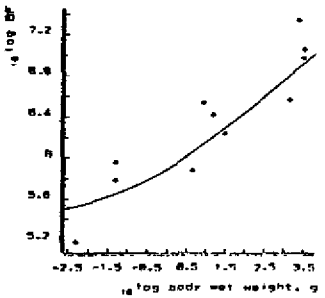


Figure 4: The bioconcentration factor for PCB153 in aquatic organisms in the field, as given in Oliver & Niimi(1988), Niimi & Oliver (1989) and from the Dutch Ministry of Public Works and Transport. The curve represents the least squares fit of the linear relationship between the BF and the cubic root of the body size. $\frac{r_{da}}{r_{pa}P_{pd}}(\frac{d_e}{W_w})^{1/3} = 2.18\ cm^{-1}$.

DISCUSSION

The results presented in this paper support the already widely accepted view that the kinetics of at least some compounds depend on the lipid content, thus on the feeding condition of the animal. The understandig of the kinetics therefore requires a notion of the energy uptake, use and allocation by the animal. With a well tested and relatively simple model for the latter at hand, we are able to cope with a rich variety of kinetics on the basis of very simple uptake and elimination behaviour of the compound. It does not seem feasible to use data on the kinetics of xenobiotics to obtain parameter values related to the energy budget of the animals under the test conditions. This should be done more directly. Since little attention hase been given in the literature to the physiology of the experimental animals, this model for the kinetics, as well as competing ones, can not be tested rigorously at the moment. The large standard deviations of the parameter estimates is a result of this problem. We think that the present exercise does make clear that it is really hard to test models assuming complex uptake mechanisms as long as obvious physiological changes related to the nutrition are not considered.

The usual effect of metabolism on xenobiotic organic compounds is a reduction of the lipophilicity. It is not difficult to incorporate e.g. Michaelis-Menten kinetics for this transformation. The result will be a decrease in the overall level. The logic behind this mechanism can be seen when toxic effects occur upon accumulation beyond some threshold value. Some LC50-time curves could well be described this way (Kooijman, 1981, 1983). Because

of the instantaneous partitioning, crossing a threshold value in the aqueous phase corresponds with crossing some other threshold value in another phase. It therefore does not matter where we place the threshold, as long as it is a free parameter, to be estimated from observed effects. This is obviously a pleasant property of a model that is not compound specific. When the metabolites are more toxic than the original compound and reach significant levels, the whole process is of course much more complex.

In Kooijman & Metz(1983), a toxic compound is assumed to affect parameter values of the energy budget model. Although this implies a highly time varying effect for dynamical populations, it is basically a static approach. The present formulation allows a dynamical approach. Since the concentration of a wide class of chemicals is predicted to increase with size, so usually with age, the model offers one possible explanation for lifetime reducing effects of chemicals.

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Energetics affect xenobiotic kinetics in Mytilus edulis.

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Abstract

Data from the literature are used to estimate the parameters of a model for the dynamics of xenobiotics, which includes the dynamics of stored energy. The model has been proposed for the kinetics of a non-metabolized xenobiotic compound, which may be lipophilic (Kooijman & van Haren 1990 [9]). The surface area coupled uptake is via food and water through the aqueous fraction of the animal. The partitioning to non-aqueous structural body mass and to stored materials (i.e. lipids, carbohydrates and proteins) is taken instantaneously. The result is a simple first order kinetics with variable coefficients.

1 Introduction

The interpretation of environmental monitoring programs for xenobiotics, like the Mussel Watch, is hampered by locally fluctuating conditions of food density, temperature and xenobiotic load. These are known to affect the accumulation and elimination kinetics. Feeding history and body size also influence the uptake and elimination of xenobiotics by organisms (Kooijman & van Haren 1990 [9]. This is important in the interpretation of long lasting experiments which may span several seasons.

A physiologically based xenobiotics model was derived in Kooijman & van Haren (1990) [9], which builds on a pure physiological model that was applied to *Daphnia* by Evers and Kooijman (1989) [4], and *Lymnea* , by Zonneveld and Kooijman (1989) [15]. The model was then applied to data concerning the physiology of the mussel *Mytilus edulis*, in van Haren and Kooijman (1991) [13]. Now that the main parameters for physiological processes (including growth, energy dynamics and reproduction) are known, the

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aim of this paper is to apply data from several uptake - elimination experiments to the xenobiotics model, using the parameter values estimated in van Haren and Kooijman (1991) [13], and estimate the new compound-specific parameters. A comparison of the model and a one compartment model (with constant coefficients) is given in the Discussion.
Although the xenobiotic compounds may have effects on the physiology of the organism, in the present model it is assumed that this is not the case. In the model structural biomass and energy density are the two core variables, reproduction is a derived variable from those two, and the dynamics of the xenobiotic compound depend on those three physiological variables. Furthermore, all parameters are considered to be independent of the xenobiotic concentration. For a particular compound and animal, it should be evaluated if this assumption holds.

2 Model description

A dynamic energy budget (DEB) model for the description of growth and energy dynamics was derived in Kooijman (1986a) for *Daphnia magna* [5]. The model predicts scaling relations between body size and physiological parameters over a wide variety of organisms (Kooijman 1986b, 1988 [7, 8]). The study of scaling of physiological characteristics with body size [7] and the successful description of of growth in animals [8] and of egg development in birds and fish (Kooijman 1986c [6]) suggest that this model might have wide applicability. We only give some key assumptions and relevant formulae here.

Uptake of food is proportional to the surface area of the organism. Maintenance is assumeed to be proportional to volume. At constant food density growth and respiration are then proportional to a weighted sum of surface area and volume (von Bertelanffy growth). It is assumed that the organism does not change in shape during growth (isomorphic growth).

Energy from assimilated food is first stored in the storage compartment. Mobilizes energy is allocated with a fixed fraction to growth and maintenance, while the remainder is spent on reproduction, see figure 1 (left) for a schematic representation of the energy flows. When the energy reserves run low, growth ceases.

These assumptions boil down to the following system of differential equa-

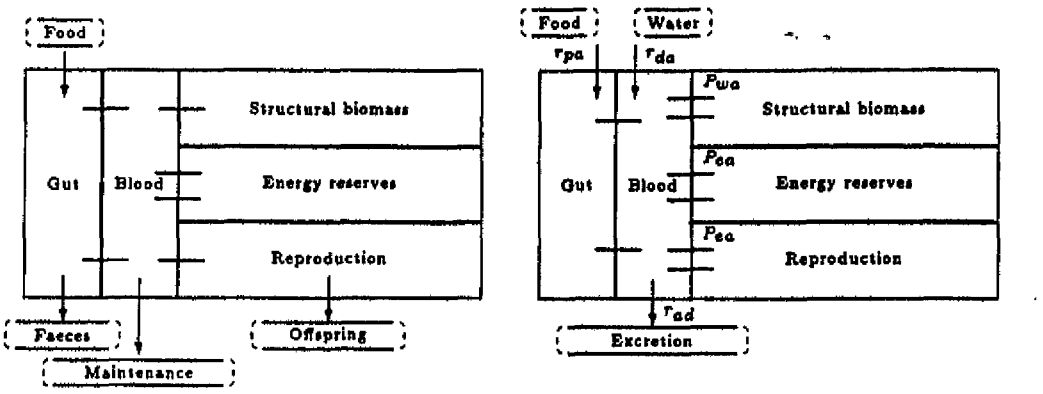

Figure 1:
Schematic representation of the compartments through which energy flows. (left) Body compartments to wich the xenobiotics are partitioned (right).

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tions for body size expressed as the volume of the structural biomass, energy reserves expressed as a fraction of the maximum energy reserves, and scaled reproduction, which is the cumulative energy allocation per maximum energy density and is thus a volume:

$$W' = \frac{(e\dot{v}W^{2/3} - a\dot{m}W)_+}{e+a} \quad (1)$$

$$e' = \dot{v}W^{-1/3}(f-e) \quad (2)$$

$$R' = \frac{(1-\kappa)e}{e+a}(\dot{v}aW^{2/3} + a\dot{m}W) - (1-\kappa)a\dot{m}W_j \quad (3)$$
$$\text{for } e \geq W^{1/3}a\dot{m}/\dot{v} \text{ and } W > W_j$$

$$R' = e\dot{v}W^{2/3} - \kappa a\dot{m}W - (1-\kappa)a\dot{m}W_j \quad (4)$$
$$\text{for } e < W^{1/3}a\dot{m}/\dot{v} \text{ and } W > W_j$$

To include the dynamics of the xenobiotics, four seperate body fractions are distinguished, *i.e.* the watery fraction (blood), the structural component

of biomass, stored energy reserves and energy stored in the gonads, see fig. 1 (right). The xenobiotic compounds are, once take up, instantenuously partitioned over these body fractions. The resulting differential equation for the concentration on basis of wet weight is:

$$c'_{ww} = \frac{\dot{r_{da}} c_d + \dot{r_{pa}} f c_p}{\dot{d_s}(1 + \alpha_e^{-1} + r) W^{1/3}} - c_{ww} \left(\frac{\dot{r_{ad}}}{h W^{1/3}} + \frac{W'}{W} + \frac{r'}{1 + \alpha_e^{-1} + r} \right) \quad (5)$$

where $h = \gamma + (P_{ea} - 1)e + P_{ea} r$ and $\gamma = 1 + \alpha_e^{-1} + (P_{wa} - 1)\alpha_w / \alpha_e$. See table 1 for a list of the frequently used parameters and variables and Kooijman & van Haren 1990 [9].

In equation 5 $r = R/W$ which is the reproduction energy density (dimensionless), where $R = \int_{t_r}^{t} R' dt$, t_r denoting the time of latest reproduction, which should not be earlier than the time at first maturation, i.e. when $W = W_j$. The change in reproduction energy density, r', is found through its definition $r' = \frac{R'W - RW'}{W^2}$.

3 Parameter estimation

3.1 Estimation procedures

The data were obtained from tables in the literature, or by means of a x,y tablet from figures. We used a fourth order Adams Predictor-Corrector method (Burden and Faires 1985 [2]) to obtain a numerical solution of equations 1—5. To calculate the total sum of squares (TSS) we interpolated between the mesh points of the integration procedure with a cubic Hermite spline. The derivatives of TSS with respect to the parameters (*i.e.* the normal equations) were approximated by the forward difference method. The roots of the normal equations were solved with the Gaus-Newton method for systems of nonlinear equations (Richter and Söndgerath 1990 [12]) Standard deviations of the parameters were estimated according to the large sample theory of maximum likelihood estimators (Cox and Hinkley 1974 [3]), where we assumed a normal distribution for the scatter around the deterministic model. When data were available for more than one set of external conditions (xenobiotic concentration, food density, temperature etc.), a simultaneous fitting procedure was used.

The number of parameters of the model will be reduced by one if it is assumed that $P_{ea} >> 1$ in eq. 5. Because P_{ea} can be interpreted in terms of the n-octanol-water partition coefficient for the xenobiotic (which are of many orders of magnitude larger than 1, especially for lipophilic compounds) this assumption seems to be valid. By dividing $\dot{r_{ad}}$ and the compound parameter h by γ, two new compound parameters are formed ($\dot{r_{ad}}/\gamma$ and P_{ea}/γ) in stead of three. The new equation then becomes:

$$c'_{ww} = \frac{\dot{r_{da}} c_d + \dot{r_{pa}} f c_p}{d_s(1+\alpha_e^{-1}+r)W^{1/3}} - c_{ww}\left(\frac{\dot{r_{ad}}/\gamma}{(1+\frac{P_{ea}}{\gamma}(e+r))W^{1/3}} + \frac{W'}{W} + \frac{r'}{1+\alpha_e^{-1}+r}\right) \quad (6)$$

This procedure introduces a large dependency between the two new compound parameters. But it remains necessary as long as few data are available that describe the uptake / elimination dynamics for animals under different food conditions that are necessary to estimate these parameters.

The parameters of equations 1–4 were estimated seperately from data concerning physiology only, in van Haren and Kooijman (1991) [13] and were set at fixed values when fitting the parameters of the toxicant kinetics.

3.2 Temperature correction

All rate constants are denoted with a dot, for example $\dot{v}$. These parameters depend on the temperature and are continuously adjusted by an Arrhenius type correction with an Arrhenius temperature of $T_A = 10000$ K, which would be approximately the same as an correction with a Q_{10} of 3. The estimates are given for a reference temperature of 15°C. The parameter, $\dot{p}$, is adjusted for a temperature, T, (in K) as follows:

$$\dot{p}(T) = \dot{p_{ref}} \exp\{T_A(\frac{1}{T_{ref}} - \frac{1}{T})\}$$

The rate constants $\dot{v}$ and $\dot{b}$ in the fysiological equations, and $\dot{r_{da}}$, $\dot{r_{pa}}$ and $\dot{r_{ad}}$ in the accumulation equation are thus corrected for fluctuating temperatures.

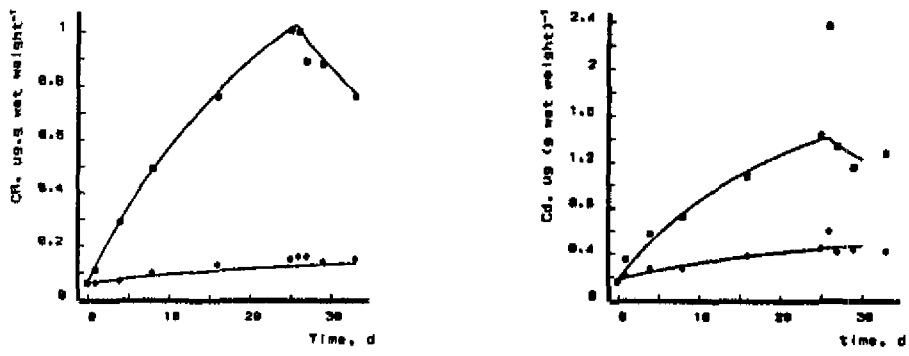

Figure 2:

Simultaneous fit for two regimes of concentration for chromium (left) and cadmium (right). Physiological parameters: $\dot{v} = 0.1$, $a = 1.03$, $a\dot{m} = 0.00517$, $\kappa = 0.96$, $W_j = 0.067$, $a_e = 0.95$. Initial conditions for state variable e and R: 0.3 and 0.5 respectively. Data from Adema (1981) [1]

3.3 Results

Fig 2 data from Adema (1981) [1] for Chromium and Cadmium together with simultaneous fits for the model. There were two external concentrations during the accumulation fase. From day 25 on, no additional metal was added to the water and only the background concentration remained.

In the plots on the left of fig 3 the simultaneous fits for the model are given for data from Adema (1983) [1] with three concentrations during the accumulation fase.

In the upper two plots of fig 4 data from Pruell (1986) [11] were analyzed for the organic micropollutants Fluoranthene and Benzo(a)pyrene. The data on two PCB's are from NOSPEC (1989) [10], which are field data from 2, 10 and 60 kilometers from the western coast of Holland in the North Sea (lowest plots). See table 2 for the estimates of the compound-specific parameters.

4 Discussion

Zinc and copper are trace metals *i.e.* most organisms maintain a basal concentration of them, since they are necessary for some key enzymes, thus there are no xenobiotics. When it is assumed that above a certain necessary con-

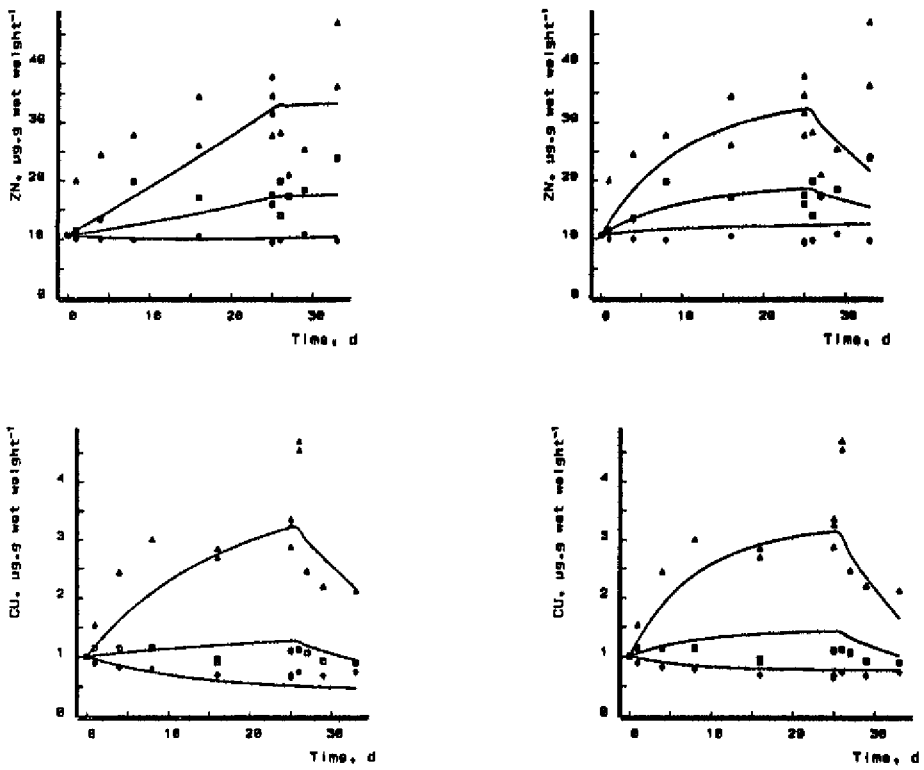

Figure 3:

Simultaneous fits for three external concentrations of zinc (upper two) and copper (lower two). The mussels were starved, adter day 25 the concentrations were dropped to the lowest possible concentration. The plots on the right are obtained when the model is extended with a basal need (for Zinc: 11.1 μg.(g wet weight)$^{-1}$, for Copper: 0.256 μg.(g wet weight)$^{-1}$). (data from Adema 1983 [1]). For physiological parameters see legend of figure 2

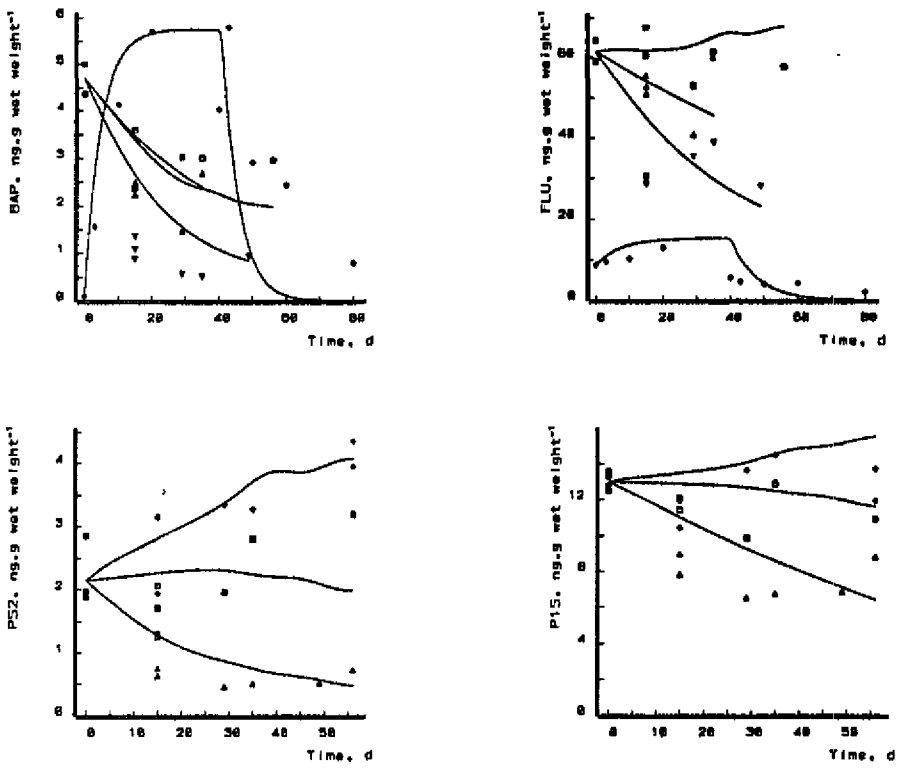

Figure 4:
B(a)P (upper left) and FLU (upper right) ,data from Pruell (1986) [11] for the accumulation / elimination curve, the three other data sets from NOSPEC 1989 [10]), PCB52 (lower left) and PCB153 (lower right) (data from NOSPEC 1989 [10]). The NOSPEC set consists of three sites in the North Sea at 2 (upper curve), 10 (middle curve) and 60 (lower curve) km from the western coast. Because of missing points in the data set of NOSPEC, the dataset of 10 km and 60 km are shorter). For physiological parameters, see legend of figure 2

centration the metals are toxic, the present model can be adjusted easily. This minimal necessary concentration is estimated from the data, together with the uptake / elimination parameters, and the resulting fit is substantially improved. This is shown in the plots on the right of figure 3. Especially for zinc the difference is remarkable, since the elimination constant $r_{ad}^{\cdot}/\gamma$ is now estimated at a realistic value, which can be seen in the curvature of the model function.

Fluoranthene and Benzo(a)pyrene are substances that are metabolized. This bio-transformation is apparent from the data in fig 4 (upper right, lowest curve, data from Pruell (1986) [11]). Fluoranthene is degraded after some time, but clearly before the mussel is put in a clean water environment (at day 40). This effect is not accounted for in the model, unless the biotransformation is a pure first-order process, which would result in a higher value of $r_{ad}^{\cdot}$. In the experiment of Pruell, the biotransformation is clearly an effect that is not a first order process from the onset of the experiment onwards, it is only apparent after some days, probably due to the time necessary to make the appropiate degrading enzymes.

A very elegant aspect of the model for the concentration dynamics (eq. 5) is that it is exactly of the form of a one compartment model:

$$C' = \dot{p} - \dot{q}C \tag{7}$$

From equation 6 it is clear in which way the coefficients of the one compartment model depend on the size of the animal and on the energetic variables. Fig 5 (left) shows the elimination rate ($\dot{q}$ in eq. 7, second half of equation 6) as a function of P_{ea} and $r_{ad}^{\cdot}$. When $r_{ad}^{\cdot}$ is zero the elimination rate is not zero, since the second term of the elimination rate in equation 6 ($\frac{W'}{W}$) is the dilution of the toxic compound over the body of the organism due to growth. Fig 5 (right) shows the elimination rate as a function of body length and (constant) food density. The elimination rate was set to zero for those combinations of length and food density where it is impossible for the animal to survive, *i.e.* when $e < \frac{W^{1/3}a\dot{m}}{\dot{v}}$. The plus-sign in both plots represents the common point (the intersection point of the two planes in 5-D hyperspace).

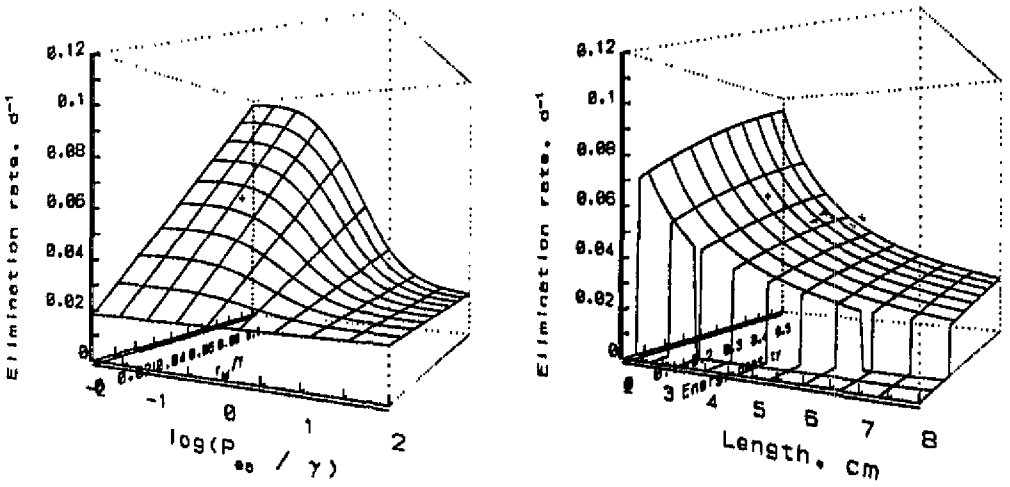

Figure 5:

Elimination rate as a function of basic parameters of the main model. Left: Elimination rate ($\dot{q}$ in eq. 7) as a function of P_{ea}/γ and r'_{ad}/γ for a 3 cm mussel. Constant food condition assumed so that $e = f = 0.3$. The plus-sign in (right) corresponds to this parameter combination.
Right: Elimination rate as a function of length and constant energy density with eq. 6. $P_{ea}/\gamma = 0.1$, $r'_{ad}/\gamma = 0.05$. The plus-sign in (left) corresponds to this parameter combination.
Physiological parameters: $\dot{v} = 0.1$, $a\dot{m} = 0.00517$. $a = 1.05$, $r = 0.5$, $r' = 0$, $a_e = 0.95$

The physiology of the animal is of great importance only when body size and energy reserves change considerably during an experiment. In an experiment that, for instance, lasts for several seasons, all the physiological variables (length, wet weight, glycogen or fat weight and dry weight) should be measured together with the concentrations of the toxicants of course. Such an experiment would probably cost a lot of animal lives, but a sound comparison between the two models requires all this.

More important than the quantitative comparison ('the goodness of fit' test) is that for animals with different shape, size, food conditions, fat content, reproductive activity, it is directly apparent what the uptake and elimination rates ($\dot{p}$ and $\dot{q}$ in eq. 7) will be. With eq. 7 only, the parameters are to be estimated again each time the animal enters a new state of any physiological variable. Experiments that are done under different conditions or with different size animals can be compared directly. The different routes for uptake of the toxicants are distingishable in the model (r'_{pa} and r'_{da}), so that uptake via food en via water can be seperated, which is not possible in the one-compartment model (eq. 7). The use of multi-compartment models

in stead of the simple one-compartment model only increases the number of parameters, without knowing their dependence on other physiological conditions. Also, it is possible to predict some of the effects of the lipophility of a xenobiotic compound on the uptake / elimination kinetics (via P_{ea}, P_{wa} and γ).

In figure 7 data are presented from van Haren (1990) [14] together with model functions from the one compartment model for copper and cadmium. The input functions are shown in figure 6. Temperature data are fitted for interpolation by a sinusoidal function quite easily, an exponential decay was chosen for the concentration of the metals in the environment. It is remarkable that the concentrations of cadmium and copper are very closely correlated (see connected data points in the figure). However, in the data the order of the concentrations for the different length classes is reversed (see legend). Parameter estimation on these data with the one compartment model is impossible, because the deviations of the model solution from the data points is not a known stochastic variable, but are caused by systematic differences between the data points (the mussels of the points of a length class do not belong to the same cohort and have thus different histories). Only when the 'noise' on the model solution is assumed to be a normal distribution with homogeneous variance, a simple least squares estimation procedure can be performed.

In van Haren (1990) [14] it was tried to solve this problem, by taking different age classes as seperate variables, and shifting the mussels between them, but this approach was not very satisfactory.

In figure 8 data are presented from van Haren (1990) [14] together with model functions from the present model. Spawnings were set in the model to take place in the first week of may. The concentration jump due to the clearance of the reproduction compartment in the animal is given by the formula (see Kooijman 1990 [9]):

$$c_{ww}(t_s^+) = c_{ww}(t_s^-)\frac{1+\alpha_e^{-1}+r}{1+\alpha_e^{-1}}\frac{h(t_s^+)}{h(t_s^-)} \tag{8}$$

For $P_{ea} < 1 + (P_{wa}-1)\alpha_w/(1+\alpha_e(1-e))$ this means a decrease in c_{ww}. The cumulative allocation to the reproduction compartment R is set to zero

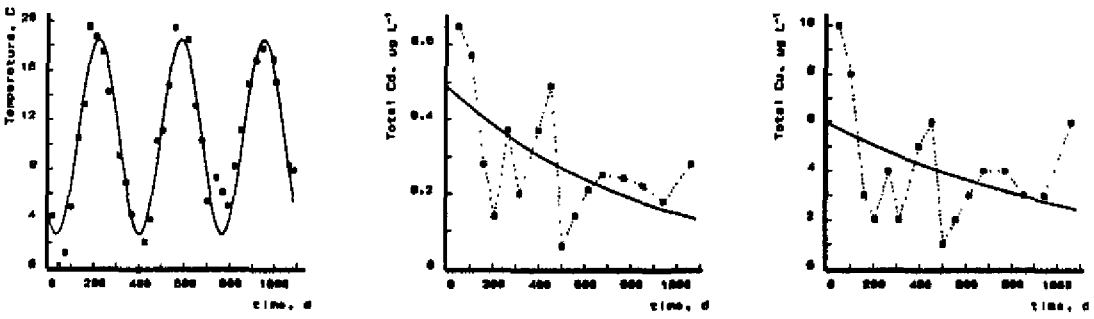

Figure 6:

Forcing functions over the years 1986, 1987 and 1988 for data set of van Haren (1990) [14], time in days since January 1^{st}, 1986.
Left: Temperature with sinusoidal interpolation function:

$$(T(t) = 10.6 + 7.9\sin(2\pi\tfrac{t+236}{365}))$$

Middle: Total Cd with exponential interpolation function:

$$(Cd(t) = 0.49e^{-0.0012t} \text{ in } \mu\text{g L}^{-1})$$

Right: Total Cu with exponential interpolation function:

$$(Cu(t) = 5.97e^{-0.00082t} \text{ in } \mu\text{g L}^{-1})$$

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at the same time. Because the mussels that were collected each year were put in length classes, some severe problems arise when trying to estimate the parameters. For instance, the mussels in length class 5 (56–66mm) in 1988 are not to be compared with the ones in that class in 1986. In some way, a model solution should be fitted to the small mussels in 1986 and the larger ones later on. Furthermore, the small mussels in 1988 did not exist in 1986 yet! The best a model can do, is reconstructing with a given set of parameters what the history of each point might have looked like. In order to show what the model predicts for the past of each of the mussels of the data points, 10 simulation for animals of lengths 0.5 – 6.8 cm were done in an environment obtained from the input functions (see figure 6). The solutions of the metal concentrations in the mussels were plotted in figure 8. Of course, it is not possible to test the two model against each other, because in neither case parameters can be estimated to obtain the best performance of the models, because any influence of the most important trend (growth)

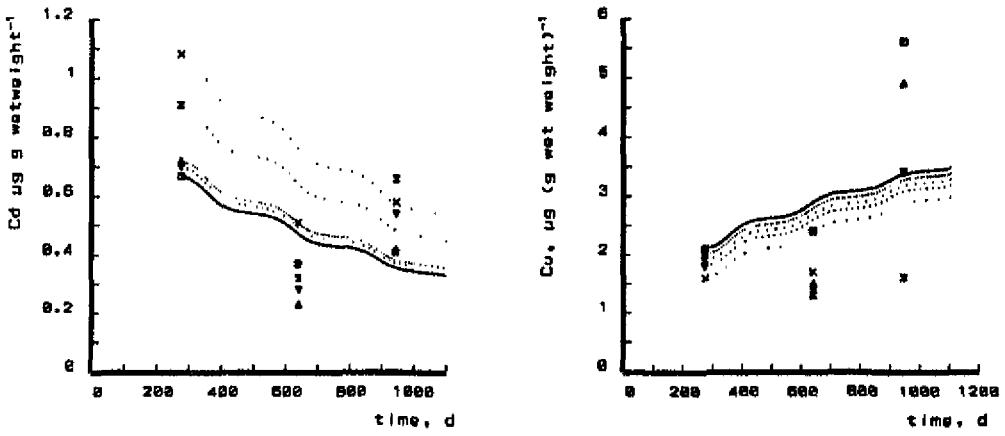

Figure 7:
The one compartment model together with data from SAWES project also published in van Haren (1990) [14]. On the x-axis time in days since January 1^{st}, 1986.
The data were collected according to length classes of the animals. The length classes are: 25-30 mm, 31–37 mm, 38–46 mm, 47–56 mm and 57–66 mm. The following Markers: $\square, \triangle, \triangledown, \boxtimes, \times$ denote the length classes respectively. Model solutions for the different classes are shown (solid line: smallest group, most widely spaced dots on line: largest group), for the 1986 group, with these initial concentrations. Both $\dot{p}$ and $\dot{q}$ are corrected for temperature, and the total metal concentrations in the water were taken as the input functions (see figure 6).
Left: Cadmium, parameters: $\dot{p} = 0.635$, $\dot{q} = 0.0$
Right: Copper, parameters: $\dot{p} = 0.65$, $\dot{q} = 0.0$

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was eliminated by collecting mussels once a year in fixed length classes.

5 Acknowledgements

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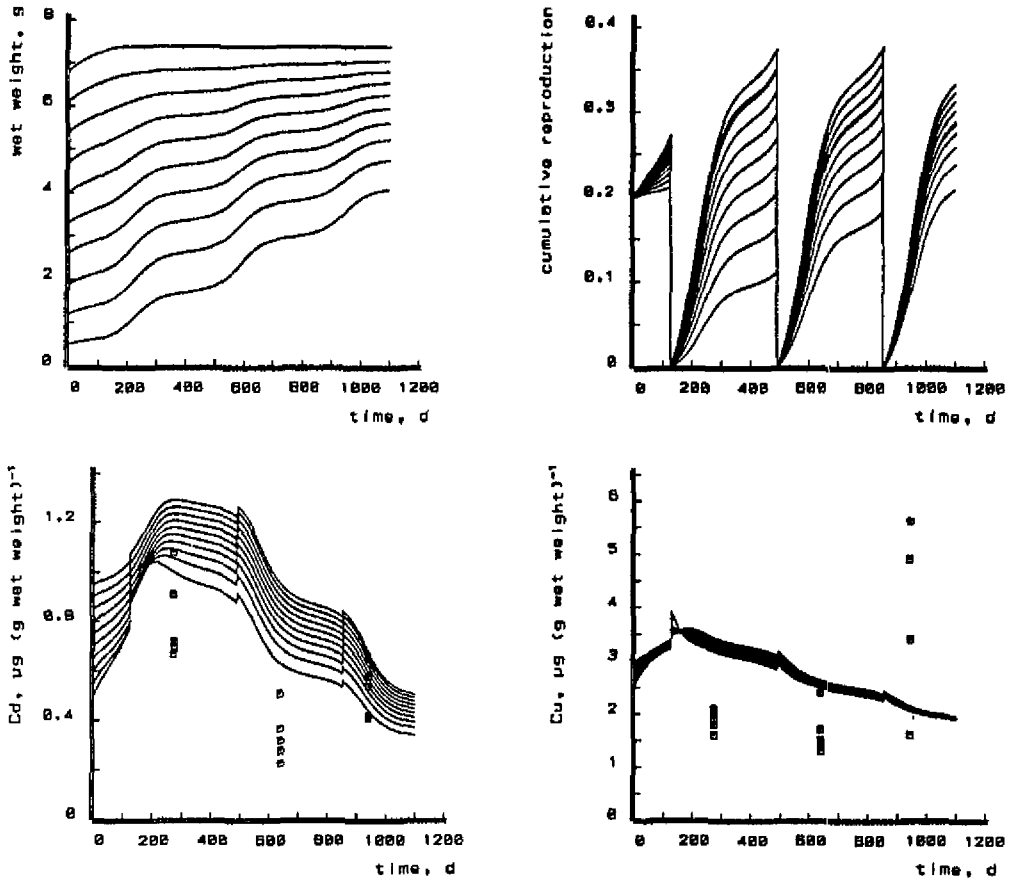

Figure 8:

Simulations of a group of mussels of different size, starting on the first of January 1986, according to the present model together with the same data as in figure 7. Input functions for dissolved and particulate metal concentrations from the original data set. (not shown in figure 6).

Upper Left: Growth of wet weight in time, for animals of weight .5 (lowest curve) to 6.8 (upper curve) gram on day 0.

Upper Right: Cumulative allocation of energy to reproduction, reset every year in the beginning of May.

Lower Left: Cadmium

Lower Right: Copper

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Table 1: The parameters and main variables of the xenobiotic and the energy budget model.
# denotes the number of molecules, see for further details Kooijman (1990) [9]

Par.	Var.	Dimension	Interpretation
	c_d	#.length^{-3}	conc. in the water
	c_p	#.length^{-3}	conc. in the food (as volume)
	c_{ww}	#.mass^{-1}	conc. on the basis of wet weight
$\dot{r}_{da}$		length.time^{-1}	uptake rate from water
$\dot{r}_{pa}$		length.time^{-1}	uptake rate from food
$\dot{r}_{ad}$		length.time^{-1}	elimination rate constant
P_{ea}		-	partition coeff. energy reserves/aqueous fraction
γ		-	compound parameter
	f	-	functional response: $f = \frac{X}{K+X}$
	X	mass.length^{-3}	food density
	W	length^3	body size
	e	-	energy reserves/max.energy reserves
	R	-	cum.energy to reprod./max.energy density
	r	-	fraction of the energy (volume) / body volume: $r = \frac{R}{W}$
K		mass.length^{-3}	saturation constant
$\dot{v}$		length.time^{-1}	energy conductance
α		-	costs of growth/κ max.energy density
$\dot{m}$		time^{-1}	maintenance rate constant
κ		-	fraction utilized energy to growth + maintenance
α_e		-	max.vol.reserves/vol.body
d_s		mass.length^{-3}	specific density of the body
W_b		length^3	body size at hatching
W_j		length^3	body size at first maturation
t_s		time	time at spawning or reproduction, $s = 1, 2, ..$

Table 2: The parameter estimates

compound	r_{da} (cv) $cm.d^{-1}$	r_{pa} (cv) $cm.d^{-1}$	r_{ad}/γ (cv) $cm.d^{-1}$	P_{ea}/γ (cv) -	reference
Metals					
Cadmium	93.0(14)	0.00309	0.0834(23)	0.25	Adema (1981) [1]
Chromium	22.8(3.4)	[2]	0.07(6.1)	0.25	Adema (1981) [1]
Zinc	23.0(18)	[2]	0.00865(128)	0.25	Adema (1981) [1]
Zinc [1]	85.7(21)	[2]	0.271(23)	0.25	Adema (1981) [1]
Copper	137.5(13)	[2]	0.16(14)	0.25	Adema (1981) [1]
Copper [1]	149(13)	[2]	0.20(15)	0.25	Adema (1981) [1]
Omico's					
PCB52	1000	0.20(33)	0.621(38)	2	NOSPEC (1989) [10]
PCB153	1000	0.12(17)	0.164(17)	2	NOSPEC (1989) [10]
B(a)P	7100(24)	0.0025(65)	0.58(25)	2	Pruell (1986) [11]
FluA	910(70)	0.013(20)	0.368(23)	2	Pruell (1986) [11]

[1] Parameter estimates when it is assumed that only above a concentration trace metals are toxic (see Discussion). This concentration level was estimated from the data at 10.56 $\mu g.(g\ wet\ weight)^{-1}$, for Zinc, and for Copper at 0.256 $\mu g.(g\ wet\ weight)^{-1}$

[2] No data from experiments with contaminated food were available on chromium, zinc and copper.

De parameters voor de wadpier Arenicola marina

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In het artikel (Kooijman, S.A.L.M. (1986). Energy budgets can explain body size relations. Journal of Theoretical Biology 121: 269-282.) wordt het DEB model opgezet met de parameters κ, ζ, η, K, $\{I_m\}$, $\{A_m\}$, $[S_m]$, L_b, en L_j, waaraan de vormconctante α nog kan worden toegevoegd.
De maximale lengte L_m hangt als volgt af van deze parameters: $L_m = \kappa \{A_m\} / \zeta$. Omdat κ en ζ procesparameters zijn die niet afhangen van de grootte van het individu, komt een verschil in uiteindelijke lengte van verschillende diersoorten voor rekening van de parameter $\{A_m\}$. Zo zal $\{A_m\}$ dus lineair mee varieren met L_m. Voor $\{I_m\}$, $[S_m]$ en K kunnen soortgelijke redeneringen worden opgezet, zie het genoemde artikel. De parameters van het DEB model zo als die in de bioaccumulatie artikelen worden gebruikt, zijn functies van deze oorspronkelijke parameters ($a = \eta / \kappa [S_m]$, $m = \zeta / \eta$, $v = \{A_m\}/[S_m]$), en hoe zij afhangen van L_m volgt uit hun defenities, zie de onderstaande tabel.

parameter:	κ	ζ	η	K	$\{I_m\}$	$\{A_m\}$	$[S_m]$	L_b	L_j	m	a	v
par $\propto L_m^i$ i:	0	0	0	1	1	1	1	1	1	0	-1	0

Omdat alle parameters waarin lengten voorkomen zijn uitgedrukt op basis van derde machts wortels van volumes, moet gekeken worden of het volume horend bij de maximale lengte verschillend is voor beide dieren. Als uitgegaan wordt van een vormconstante van de mossel van 0.33 met maximale lengte van 9 cm, van de wadpier 0.1 (uitgaande van een cilinder van 30 cm lang en 1 cm diameter) en een maximale lengte van 30 cm, dan zijn die volumina ($W = (\alpha L)^3$) voor beide dieren hetzelfde, en dus is er helemaal geen correctie nodig voor de parameters tussen de mossel en de wadpier.

De shape coefficient α van een bepaalde vorm legt de relatie vast tussen een bepaalde lengtemaat L en het volume W:

$$W = (\alpha L)^3$$

De α voor de mossel is bijvoorbeeld 0.33, voor de langste lengte. Om de α van de wadpier te berekenen, moet van een bepaalde vorm (hier bijvoorbeeld een cilinder van L cm lang en D cm in doorsnede, de inhoud (W) berekend worden, en dan kan de α voor een bepaalde lengtemaat – lengte van het dier of doorsnede – α berekend worden.
De inhoud van een cilinder is $L.(\pi(D/2))^2$. De shape coefficient van de cilinder berekend voor de lengte van de cilinder is dan:

$$\alpha = \frac{W^{1/3}}{L} = \frac{(L.\pi(D/2)^2)^{1/3}}{L}$$

waarmee je met een lengte van 30 cm en een doorsnede van 1 cm uitkomt op een α voor de wadpier van 0.1.

Effects of feeding conditions on toxicity for the purpose of extrapolation

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ABSTRACT

1 Mathematical models can be most helpful in attempts to understand the way effects of toxic substances show up under various conditions. They are essential for extrapolation and prediction, especially when effects have to be quantified.
2 In some cases, there is a tight relation between effects and toxicokinetics, i.e. uptake / elimination behaviour of compounds.
3 It can be shown that, at least for some compounds, the toxicokinetics depends on feeding conditions. This alone makes it necessary to account for energetics in the use of laboratory observations for predictions and interpretation concerning field data.
4 It can also be shown that, given certain effects on individuals, the consequences for populations depend sensitively on energetics. This leads to an even tighter link between ecotoxicology and energetics.
5 A basic problem is that realistic models involve a relatively large number of parameters, even under the most simple assumptions about kinetics and effects. This constraints possibilities for extrapolation and prediction.
6 All in all, a close link between experimental and modelling programs is necessary.

INTRODUCTION

The aim of this paper is to present some general ideas underlying a joint technical research program of our Theoretical Biology group, and experimentally oriented groups at the Free University and MT-TNO. For technical details, one should consult articles in the reference list, which provide ample discussion of the relevant literature. In this paper, I will focus on animals although the concepts used are applicable to other organisms as well.

Although ecotoxicology is basically a quantitative science which calls for a modelling approach, the investment in model based research is small in comparison with that in purely experimental research. For this reason, it might be helpful to make a few remarks on the usefulness of models in an ecotoxicological context.

Mathematics as a language is very useful in the formulation of quantitative relationships and in the development of concepts. One should real-

ize that syntactically (mathematically) correct formulations need not make sense. The indiscriminate use of P and r^2 values to underpin quantitative statements in many papers on ecology reveals a worrying lack of interest in the statistical backgrounds. Such a costume confuses rather than contributes to the reasoning.

The first useful application of mathematics is directly connected with experiments. Within a proper modelling framework, it is much easier to
- set priorities in experimental programs (Kooijman *et al.*, 1987a; Kooijman, 1988)
- design experiments like the choice of the exposure period in relation with the properties of the chemical and the size of the test animals, the choice of concentrations and number of test animals to be applied etc. (Kooijman, 1981, 1983; Kooijman *et al.*, 1987a)
- interprete data like the relation between no-effect levels (NEL) and LC50 values (Kooijman, 1981)
- quantify like the estimation of the NEL as affected by the experimental set-up.

The second type of application relates to the comparison of data obtained under different circumstances (Kooijman and Van Haren, 1990). Usually a lot of factors contribute to uptake and elimination rates, concentration factors etc. Without models it is hard to evaluate the data involved and to obtain useful conclusions. The interpretation of data from biomonitoring programs frequently suffers from this problem.

The third field of applications is in relating different levels of biological organization (Kooijman and Metz, 1983; Kooijman, 1985; Kooijman *et al.*, 1987b; Hallam *et al.*, 1989). For example, effects on individuals have consequences for populations (see Van der Hoeven, 1991) and ecosystems. It is seldom easy to evaluate these consequences. Without models it is impossible.

A basic problem in ecotoxicology is that ecosystem responses to stress from pollution are perhaps the most relevant (Kooijman *et al.*, 1987a; Kooijman, 1988; see the Discussion), but also the most difficult to quantify and interpret. It is easy to understand that people involved in legislation are pressing for research programs on this topic. It is not always easy to convince them that lack of knowledge on fundamental issues in physiology and ecology strongly limits the feasability of the short-term programs. Since mathematical models need to implement such knowledge, they can not be used to generate it without adequate experimental back-up. When one is

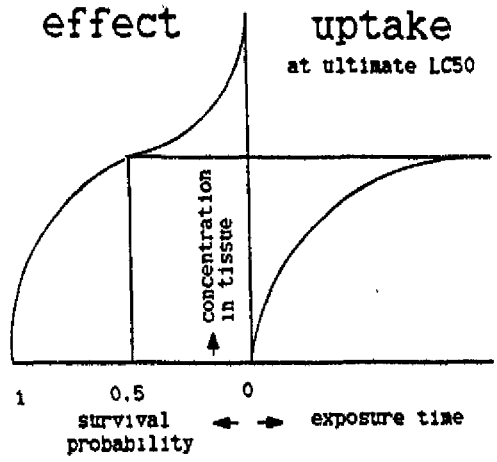

Figure 1: The relation between uptake and survival.

serious in the aim to predict ecosystem responses to pollution, one has to accept that it is a long term aim which only comes into perspective when one is willing to support long-term research programs in this field. The practical problems of today and tomorrow have to be solved in another way (Kooijman, 1987), which can only be unsatisfying. In the end, when we have finally generated sufficient insight into ecosystem dynamics we still might arrive at the obvious message: don't pollute.

UPTAKE *vs* EFFECTS

An important link between toxicology and ecotoxicology concerns the relation between toxicokinetics and effects. Toxicology, which has its roots in human health problems and pharmacokinetics, has a rather strong focus on metabolic transformations and suborganismal compartmentation. However, a compound is of interest to ecotoxicology only through its effects on the ecological behaviour of organisms.

As a first approximation effects seem to show up as soon as the concentration in the organism exceeds some threshold value, which might scatter among individuals (see e.g. Tas and Opperhuizen, 1991; McCarty, 1990; and Fig. 1). When all individuals in a cohort follow the same uptake kinetics of a toxicant from the environment, the fraction of individuals showing no effects at a certain exposure period corresponds to the fraction of individuals whose threshold concentration in the tissue is below the acquired concentration. The log logistic and log normal distribution are popular choices to describe the scatter of threshold values among individuals (Kooijman, 1981). Since their motivation is purely empirical, it is a weakness in theory based on this description. It is perhaps surprising that when we assume a simple first order linear kinetics for the uptake and elimination, the observed survival

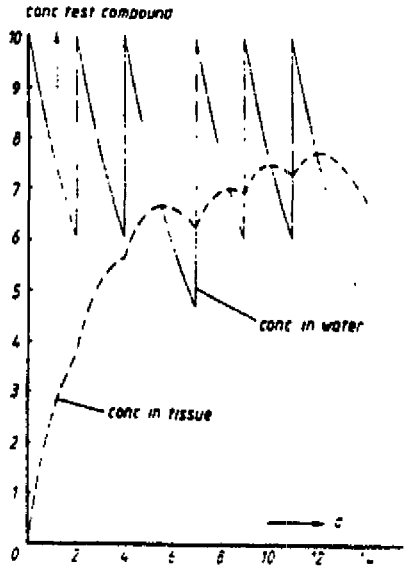

Figure 2: The expected concentration of xenobiotic in tissue, when the concentration in the water decreases exponentially and the uptake-elimination behaviour follows a first order kinetics.

pattern for simple compounds can be described very well (see Kooijman, 1983; McCarty, 1990).

This even works in the slightly more complex situation where the concentration of the compound is not constant (Kooijman, 1981). In a chronic toxicity test with daphnids, where the media are refreshed every 2, 2 and 3 days, compounds like cadmium absorb to the algae, which settle down. Cadmium is thus growing less available after refreshment of the medium. This process approximately follows a linear first order kinetics. So, we expect a concentration in the water and in the tissue as shown in Fig. 2. The survival pattern of the daphnids is well described, see Fig. 3. The point is now that the disappearance rate of cadmium can be estimated from the survival data. It corresponds very well with the one measured in the media, see Fig. 4. This provides a strong support for the assumption that toxicokinetics and effects are coupled.

Besides effects on survival, those on reproduction are of relevance to ecotoxicology. It can be affected directly, or indirectly via e.g. a change in growth, maintenance or feeding behaviour. Animal energetics provides a useful framework to evaluate this indirect effect to reproduction quantitatively (see e.g. Kooijman *et al.*, 1987a; Widdows and Donkin, 1991). The size of the effect can again be related to the concentration in the tissue.

UPTAKE *vs* PHYSIOLOGY

Under controlled conditions, many compounds seem to follow a simple first order kinetics in their uptake and elimination behaviour. The rates frequently

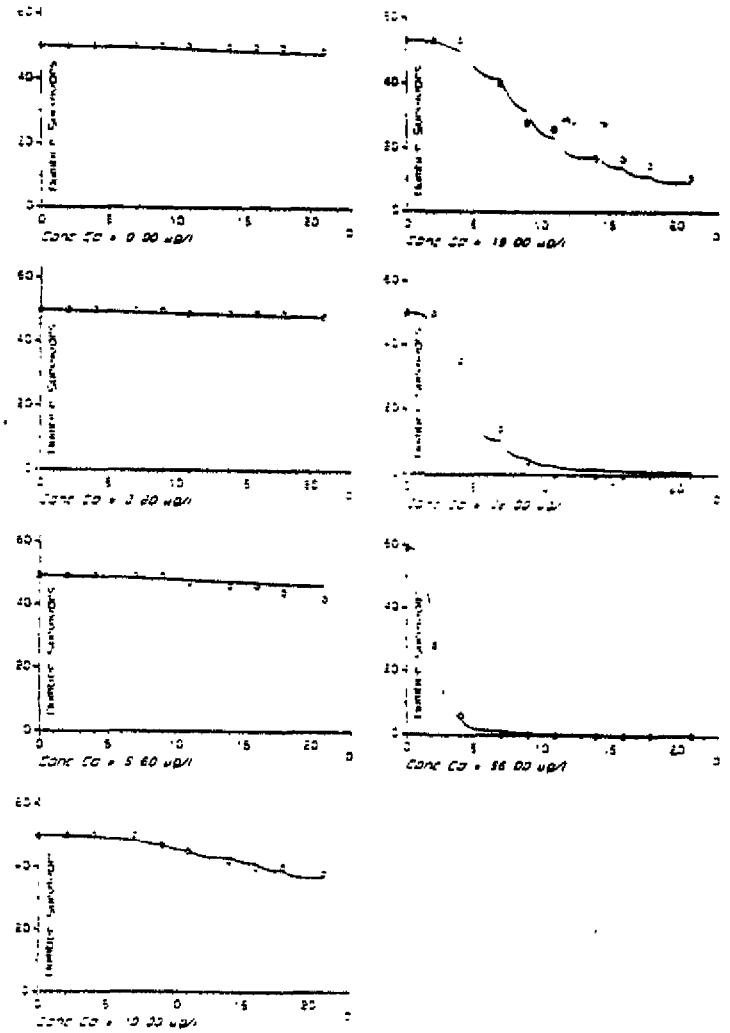

Figure 3: The observed and expected number of surviving *Daphnia* exposed to different exponentially decreasing concentrations cadmium chloride, as described by a first order kinetics for the uptake-elimination behaviour.

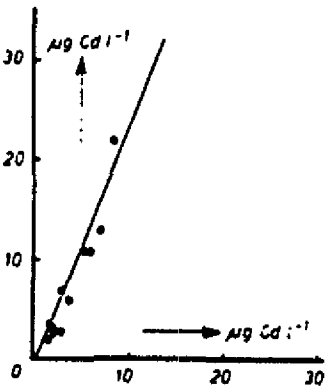

Figure 4: The measured concentration of cadmium in the water after refreshment of test media plotted against that just before refreshment. The line is not based on the points shown, but on the survival data presented in Fig.3.

depend on body size (see e.g. Hickie *et al.*, 1990) and on environmental conditions such as food availability. To explain connections between these factors, I will discuss the process in more detail (Kooijman, 1981). The assumption that food availability is a major factor modulating effects is based on three arguments. Firstly, uptake via food can be an important uptake root (see e.g. Schrap, 1991). Secondly, it is tightly linked to lipid content in the animal (see e.g. Van den Heuvel *et al.*, 1990; Van de Guchte *et al.*, 1990 for its importance). There exists a voluminous literature on the relation between bio-accumulation factors and K_{ow} values of compound (see e.g. Gobas, 1991). Thirdly, the consequences of effects on individuals for the behaviour of populations can sensitively depend on food availability (Kooijman *et al.*, 1983; Kooijman, 1985; Hallam *et al.*, 1989).

The general idea is presented in Fig. 5. Assume that an animal can be decomposed into structural biomass (i.e. a certain combination of carbohydrates, proteins and lipids) and in reserve materials (i.e. another combination of carbohydrates, proteins and lipids), which primarily function as energy reserves. Suppose that it has control over its chemical composition, such that structural biomass and reserves do not change in composition, a property known as homeostasis. We assume further that the partitioning of the xenobiotic over the watery fraction, carbohydrates, proteins and lipids, is fast compared to the exchange of the xenobiotic in the watery fraction and the environment. The uptake via food and the exchange with the environment is taken to be a linear first order process, with a rate proportional to the surface area. Since the feeding rate is also taken proportional to surface area and the animal is assumed to be isomorphic (i.e. it does not change shape during development), this set of assumptions leads to a rather simple kinetics for the xenobiotic.

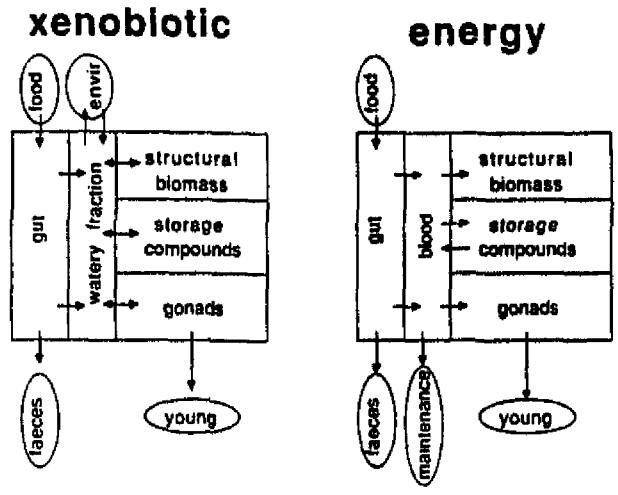

Figure 5: The toxicokinetics and energetics of an individual. The two-sided arrows refer to rapid exchanges.

These assumptions have to be supplemented with additional ones concerning energetics. The following assumptions seem to apply at least approximately for a wide variety of species: there are three size-defined life stages, embryos which do not feed, juveniles which do not reproduce, and adults; food uptake depends hyperbolically on food density; the reserve density, i.e. the ratio of the amount of reserves and body volume, follows a linear first order process with a relaxation time proportional to body length; a fixed fraction of the utilized energy is spent on growth plus maintenance, the rest on reproduction plus development; the maintenance costs are proportional to body volume; the initial size of an embryo is negligibly small and the reserve density at hatching equals that of the mother at egg production.

The kinetics can be classified as a linear first order kinetics with variable coefficients. The variation in the coefficients depends on changes in size, reserves, feeding rate and reproduction. When the exposure period is short enough, we are back at our familiar first order kinetics with constant coefficients. So the model represents an extension of simple first order kinetics, which is an alternative for the frequently applied more-compartment models (see e.g. Timmermans *et al.*, 1990). Since these models have more parameters than the one-compartment model, they usually give a better fit, but it is hard to identify the different compartments physically. Therefore their value for understanding the process is limited.

The combination of isomorphism, homeostasis and instantaneous partitioning is a strong one, which makes modelling workable. An important consequence is that when the concentration in one organ exceeds some threshold value specific for that organ, the concentration in another organ will exceed some other threshold value. So we do not have to bother about details of the cause of the effects. We even might relate effects to the concentration in a non-target organ or to that in the whole body.

The derivation of the model is a bit complicated due to the fact that exchange rates depend on concentration differences, i.e. on intensive quantities, while the mass preservation law involves absolute amounts, i.e. on extensive quantities. When volumes are changing, this leads to minor complications, especially with respect to the process of accumulation of reserves and the way they contribute to measurements of quantities such as wet weight and dry weight.

The application of the model is illustrated in Fig. 6. The fit is satisfying, but for the moment it is not possible to use this as a critical test for the model because too little is known about the energetics during the experiments. This gives too much freedom in the choice of parameter values. This is a major problem with existing data in the literature: we were not able to locate sources giving adequate information on both toxi okinetics and energetics.

DISCUSSION

A model like the one presented has to be supplemented with models for the transport and the fate of compounds in the environment and with population dynamics and foodweb considerations, to make it useful in a wider ecotoxicological perspective (Kooijman *et al.* 1987a, 1987b). It can perhaps help to understand why concentration-effect curves based on animals from laboratory cultures tend to be much steeper compared with curves based animals collected from the field. The significance of this phenomenon lies in the interpretation of no-effect levels based on laboratory animals.

The variety of compound-specific kinetics and effects, and of species-specific energetics, that have been described is huge. This calls for simplifying outlines of the main processes that are a common denominator. For many purposes it is essential to keep the picture as simple as possible. The risk of loosing the finer details in particular applications will have to be taken for

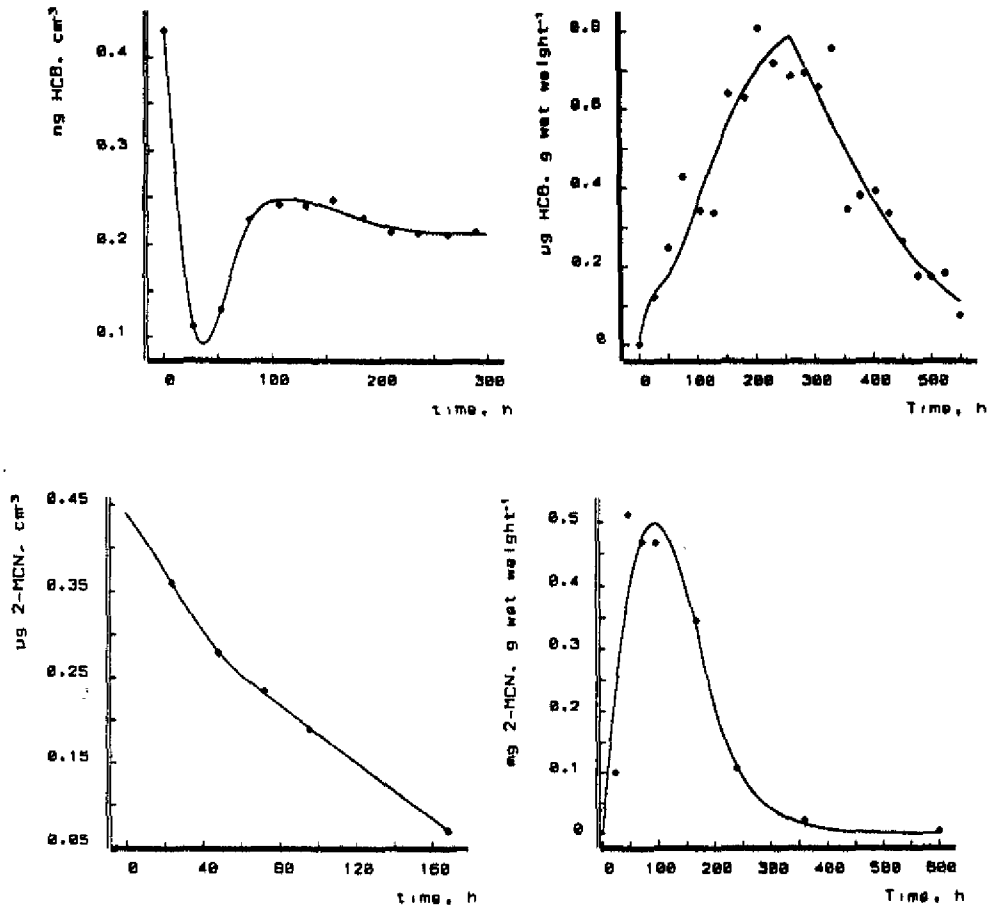

Figure 6: The uptake-elimination of hexachlorobenzene (log K_{ow}=5.45) in *Elliptio* (above) and of 2- monochloronaphtalene (log K_{ow}=3.9) in *Poecilia* (below). Left: concentration in the water with cubic spline functions used for interpolation. Right: concentration in the tissue with model based descriptions. Data from Russel and Gobas (1989) and Opperhuizen (1986), respectively.

granted.

Some processes are too poorly understood at the moment to allow a quantitative description which is not highly species and compound specific. The process of metabolic transformation is an example (see Sijm *et al.*, 1991; Keizer *et al.* 1990), who point out that the transformation is highly species-specific). At the moment, it is only implicitly incorporated into the present model-formulation. When it follows a first order kinetics, it only affects the value of the elimination rate. When it follows a different kinetics, it has to be incorporated in an explicit way. Another example is that of physiological adaptation, which may involve a wide variety of mechanisms (see Calow, 1991). Although is not too difficult to do some wild guesses for model formulations, the result is inevitably that the number of parameters is increased, which make it more difficult to test it critically.

When a response to a compound is species-specific and when one wants to evaluate its implications for integrated systems like communities, one has to realize that models with many parameters have not contributed to our understanding of the behaviour of such systems so far. I believe that it is possible to formulate useful and parameter sparse models for integrated systems on the basis of input/output behaviour. Such models can only be used to study global problems. The fate of a particular species is not one of them unless it has a major impact on the dynamics of the integrated system. The classification of questions into specific ones or global ones is obviously simplistic. A continuum would be more realistic. It is not yet clear to what extent ecosystem models can in the end be used to study less global questions.

When an integrated system breaks down due to pollution, one can reasonably infer that most species cannot survive. On the other hand, when an integrated system is hardly affected in its global performance by a given stress, it is surely possible that many species will disappear altogether. Depending on the scale in time and space, this is highly undesirable. Problems of ecotoxicological concern are at a variety of levels of integration (see De Kruijf, 1991). I hope that problems raised in ecotoxicology stimulate physiological and ecological research to provide a useful framework to interconnect these levels. Although some progress has been made, much remains to be done.

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