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Module Bivalve Manual

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July 18, 2019

1 Overview

This document describes the main processes, equations and general structure of the bivalve's activity included in the MOHID Water Modelling System, as well as a brief description on how to use it.

Bivalve's metabolic processes are described using the Dynamic Energy Budget (DEB) theory, developed at the VU University Amsterdam (Kooijman, 1986, 2000, 2010). DEB theory is a metabolic theory that aims to describe the physiological response of an organism to changes in its environment. The theory uses a set of assumptions and principles to translate functional description of the organisms metabolic processes into differential equations. It assumes that the various energetic processes, such as assimilation and maintenance, are dependent either on surface area or on body volume (Kooijman, 2010). Because a DEB model is based on a generic theory, the same model structure can be applied to different species, where only parameter values differ. Variability in growth and reproduction between individuals of the same species are assumed to be mainly caused by differences in environmental conditions (temperature, food).

Besides the individual, this module simulates an individual based population model, meaning that the population dynamics is represented by several cohorts' trajectories. Each cohort consists of identical individuals born at the same time and showing identical properties (e.g. size, biomass) throughout their life, if lived in the same environmental conditions. The population model is thus responsible for the book-keeping of the information generated by the individual model over time, one for each cohort with some additional, population specific processes.

2 Integration philosophy and general considerations

The coupling philosophy assumes that the biogeochemical processes only depend on the environmental and physiological conditions of the individuals in a particular place and time. In MOHID, which is based on a computational grid to solve the transport equations, the methodology consists in building a biogeochemical module, organized in such form that the *sinks and sources* term is independent of the grid and of the grid cell location. This term is solved separately, but consistently, from the advection and diffusion terms. This independence allows for the biogeochemical module to be implemented in any type of grid (1D, 2D, 3D) and thus can be seen as a zero-dimensional model, where external forcing conditions are provided (ex: light, temperature, salinity) and mass fluxes between state variables (e.g. phytoplankton, ammonia, bivalve) are computed for each control volume using only the *sinks and sources* term of equations. This is also an efficient way to guarantee a high level of robustness in the code and to maintain it. The present study followed this methodology by building a Module Bivalve that computes the time evolution of bivalve properties (e.g. size, biomass, development) for each cohort in each grid cell, as well as the correspondent effect on other water properties concentrations (e.g. phytoplankton, ammonia) due to their activity. MOHID structure also enables that almost any process can be switched on/off. As a result, the model is flexible and easy to use in different systems, conditions, scenarios and most of all, enables the study of particular processes within the system. The bivalves' state variables make use of this structure. For

example, bivalve larvae transport can be switched on/off depending on the individual length. During the larvae phase the individual is subject to transport by currents and turbulence, and once it reaches a certain size, the individuals settle, and the transport is switched off.

2.1 From the environment to the individual

The activity of an individual bivalve depends on its physiological condition and also on environmental factors. Environmental factors are usually not constant over time or space. Individuals react to those changes, and they may do this in different ways. The individual model built in this study describes the reaction of an 'average individual' to changes in the environmental conditions, assuming that the number of individuals is big enough to minimize the effect of individuality. So, in the present model individuals only change through grow and development. Besides, the possibility that individuals may change either through phenotypic flexibility or genetic adaptations is not considered.

DEB theory was used to build a model to simulate metabolic processes in a bivalve individual, in relation to environmental conditions. The basic principles and formulations are valid for all different stages of the individual, meaning that the same set of equations can be used to simulate their complete life cycle. The set of equations and the principles behind them are not simple and not easy to understand, but they are for sure simpler than reality. So far, models based on DEB theory have been able to simulate a wide range of processes in a wide range of species, see <http://www.bio.vu.nl/thb/deb/>. The standard DEB model does include the main features of an individual, but specific processes can and should be added to simulate particular features of the target species, considered important for the aim of a particular study. A spawning event, which is dependent on temperature and gonad-somatic mass ratio (GSR), empties the reproduction buffer. Each spawning event gives origin to a new cohort in the system. To avoid the possible exponential increase in cohorts, a minimum time between spawning events can be imposed. Different types of particles, food and/or inorganic material, can be retained by bivalves through filtration, if needed.

2.2 From the individual to the population

The population of bivalves is represented by several cohorts. Each cohort consists of a number of identical individuals born at the same time and with the same properties (e.g. size, biomass, state of development), which growth and activity is described by a new instance of the individual model. The population model is thus responsible for the book-keeping of the information generated by the individual model over time, one for each cohort. Each cohort is simulated as an independent entity which can interact with other cohorts through food competition. Other population processes included are initial egg mortality, background mortality, and predation (including cannibalism).

2.3 From the population to the ecosystem

Populations directly affect the trophic levels below and above them. But indirectly they will also affect the food of their food, or the predators of their predators. Hence, the first step when upgrading from a population model to the ecosystem is to establish the main actors (properties, species, or groups of species), where a balance must be found between what it is known and what can reasonably be simulated. In its simpler setup the main actors of the presented model are: one algae species (phytoplankton), one bivalve species and bacteria (implicitly simulated by including the mineralization of organic matter). More algae and bivalve species can however be simulated, as long as data and parameters are available.

All the actors live in the changing environment that can have strong tidal effects and some dependence on fresh water discharges. The simulation of these processes is made through the use of the other MOHID capabilities. In this way, the feedback of each bivalve cohort activity in the ecosystem, including food depletion, is naturally simulated in each time step and the effect of tide on the food supply is simulated by the advection-diffusion processes between grid cells.

Cannibalism is included in the model, if the complex feeding option is switched on, as the filtration of larvae by adult mussels.

2.4 From the theory to numerical modelling

The incorporation of the individual based population model complied with MOHID rules and benefited from some of its advanced programming features. For example, the bivalves model is programmed using an object oriented approach, which allows the definition of several different bivalve species, each one with the same functional organization but with a different set of parameters. Each species is defined by one or more cohorts and each cohort is simulated independently with its own set of processes. All cohorts share the same set of equations. The development of the population model posed some challenges, namely the dynamic allocation of newborn cohorts and deallocation of dead cohorts. Typically in a sequential code, there is a construction phase (memory allocation), a computing phase (solving the algorithms) and a deconstruction phase (memory release). Because of this particular model, a run time dynamic allocation/deallocation of memory was implemented. This is triggered by the population processes and not known a priori. MOHID uses a property list, which includes all the constituents that are simulated (e.g. phytoplankton, ammonia, sediments, mussel reserves, number of mussels, etc). This list is created at the beginning of a new simulation based on a configuration file. Now, new properties can be added or removed from the list with no limitations during run time. For example when a new cohort from a certain species is created by a spawning event simulated by the model, 6 new properties are added to the list, namely number of individuals, length, reserves, structure, maturity and reproduction buffers. These properties are then ready to enter the computational cycle with no need for additional modifications.

Cohort properties are simulated in an Eulerian approach, using a computational grid. In each grid cell, a transport equation is solved for each property, simulating advection and turbulent mixing (when at a larvae stage) and physiological processes. During most of their life cycle, bivalves' have a fixed position, thus the advection and

diffusion term is null. Individuals from the same cohort located in the different locations can develop differently (e.g. grow faster or slower) if environmental conditions are unequal at these locations. During the larvae stage, advection and turbulent mixing are important as they are responsible for the actual transport of individuals. The activation of these processes in run time is also new, as well as its deactivation once the individuals reach the juvenile stage and settle. Larvae from the same cohort are subject to different environmental conditions during their initial period of life, and they will grow differently. When they are mixed due to transport, the model takes their concentrations and mass fluxes into account to perform a weighted average of the cohort properties. This is especially important to assure a correct methodology of the highly interdependent cohort properties. Thus, the Eulerian approach introduces some limitations due to 'numerical diffusion' generated in the case of larvae transport when solving the advection term of the transport equation. This is mostly caused by high gradients between larvae concentrations (from a specific cohort) with the ambient water and it can be minimized by the use of fine computational grids and small integration time steps. Different approaches could be followed, namely using a Lagrangian scheme that allows the elimination of the advection term. However, this would create other difficulties regarding information exchange between the Lagrangian and Eulerian model properties, and possibly increase the computational efforts. The computational time is actually one of the main challenges in the current model. It can increase significantly depending on how many cohorts are generated and how much time they remain as larvae. For that reason, the model is able to aggregate spawning events by including a minimum time between them, which is set as a parameter. The detail with which the exact birth date of a new cohort is simulated depends on the aim of the study. In addition, the model is able to be coupled with the simplest (Module Water Quality) or the more complex (Module Life) model options to compute the pelagic biogeochemical processes, thus allowing control over the computational efforts necessary to simulate them. One final important note is that although the model is very complex, and computationally demanding, it was built in a very flexible way, meaning that almost all the processes and options can be switched on or off. Thus, the complexity of the model is entirely defined by the user, which will have to make decisions depending on the aim and time of the study. The model is written in FORTRAN 95 using object oriented programming (OOP) paradigms. Although FORTRAN 95 is not an object oriented programming language (OOL), FORTRAN modules can act as classes of common OOL (Decyk et al., 1997; Akin, 1999; Miller and Pinder, 2004). The model uses several object oriented features such as encapsulation, polymorphism, function overloading and inheritance. Such features allow for the versatility of the model for complex ecosystem simulations through maintaining a simple and organized code, especially when dealing with multiple species, large number of cohorts, species interaction (e.g., predation and competition) as well as multiple types of food.

2.5 From the model to the environment

The time scale of estuarine ecology depends on the time scales of ecological processes and on the time scale of the forcing functions. For that reason, the ecological model must run for time periods much longer than those involved on hydrodynamics, nevertheless requiring similar resolutions for explicitly simulating the transport processes. Fine grid resolution should imply better results and model boundaries should be set far from the study

area, but these options do have some costs in terms of increased computational time. There is thus a compromise between the model resolution, the overall simulated area and time, besides with what detail should processes be simulated and the number of state variables necessary to do so. In addition, boundaries require data which should be more detailed and precise as they are closer from the study area.

3 Processes Description

Figure 1 represents a scheme of the individual model and the main formulations and necessary parameters used in the model are presented in the tables presented in the following sections.

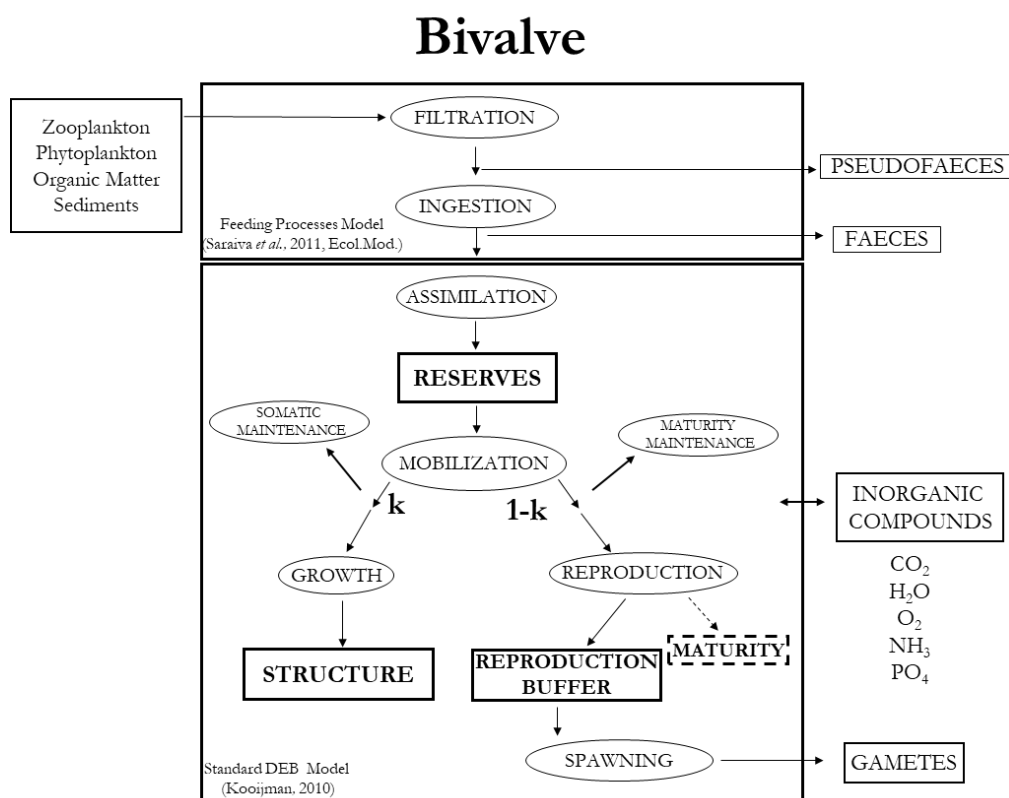


Figure 1. Global Scheme for the DEB Model for bivalve. Ellipses represent the main processes involved in the organism metabolism and mass fluxes are indicated as \dot{J}_x . Boxes with solid lines represent the organism mass compartments and solid arrows the associated flux; dotted box represents energy investment and dotted arrow its inflow; dashed line box represents a mass compartment outside the organism and the dashed arrow represents the respective outflow from the organism Saraiva et al. (2012).

Table 1. All possible model state variables and forcing functions. i represents the number of the cohort (Saraiva et al., 2014).

level	symbol	description	units	formulation
Environment	T	temperature	K	
	X_0	inorganic particles	mg l^{-1}	
	X_1	algae	mol Cl^{-1}	
	$n_{X_1}^N$	algae N/C ratio	$\text{mol N mol}^{-1} \text{C}$	
	$n_{X_1}^P$	algae P/C ratio	$\text{mol P mol}^{-1} \text{C}$	
	P^S	shrimp abundance	$\# \text{m}^{-2}$	
	P^C	crab abundance	$\# \text{m}^{-2}$	
	P^B	bird abundance	$\# \text{m}^{-2}$	
Individual	M_{Vi}	structure	mol C^V	Saraiva et al. (2012)
	M_{Ei}	reserve	mol C^E	Saraiva et al. (2012)
	M_{Hi}	maturity	mol C^E	Saraiva et al. (2012)
	M_{Ri}	reproduction buffer	mol C^E	Saraiva et al. (2012)
	Ai	age	y	
Population	Ni	individuals in cohort i	#	$\frac{dN_i}{dt} = -m_i^S P^S - m_i^C P^C - m_i^B P^B - m^N N_i - m^F N_i$
	nC	number of cohorts	#	$\Delta nC = B - D$

3.1 Individual Model

The standard DEB model assumes that the body mass of the organism is partitioned into the abstract quantities of 'structure' and 'reserve', which act as state variables. All assimilated energy is first stored as reserve; subsequently the reserve is utilized to fuel the other metabolic processes, following the so-called k-rule: a fixed fraction of mobilized reserve is used for somatic maintenance and growth (increase in structure), the rest is used for maturity maintenance and maturation (embryos and juveniles) or reproduction (adults). Maturity is also a key concept in the theory and represents the total energy invested in the development of the organism. During the juvenile stage, the fraction of energy allocated to reproduction is used to develop reproductive organs and regulation systems, increasing the maturation level of the organism. After reaching a particular threshold, no more development is needed, and the organism becomes an adult. Hereafter, it allocates this flux to the reproduction buffer, for further gametes production and release into the water. Based on the principle of mass conservation of each element in the system (e.g. C, H, O, N, P), and the computed organic fluxes, the mineral fluxes to (and from) the water column are the result of a mass balance. The feedback of the individual processes on the system can thus be straightforwardly followed. A detailed description of the individual model can also be found in Saraiva et al. (2012) where the model performance was tested for different locations in the North Sea.

In recent years, important improvements have been made around the DEB theory. The theory itself still uses the same core principles, although new or particular topics have been developed to explain, verify or test the model against specific features that turn up in the observations. The clarification of the concepts and variables, and their relation and translation into real measurable quantities (Sousa et al., 2008, e.g.), as well as the developments on the parameter estimation (Lika et al., 2011a,b; Marques et al., 2019, e.g.), facilitates the theory implementation and promotes its use.

In summary, the basic main assumptions of the standard DEB model Kooijman (2010) are:

1. an organism is characterized by a structural body (individual structure biomass), reserve (biomass available for direct use), maturity level (amount of energy spent in the organism development) and a reproduction

Table 2. Model formulations for feeding processes. Simple feeding is adapted from Kooijman (2006) and complex feeding is adapted from Saraiva et al. (2012). X_1 represents algae and X_0 inorganic material concentration.

option	process	symbol	description	units	formulation
1-Impose filtration	Filtration	$\dot{J}_{X_i F}$	filtration rate	$\text{molC d}^{-1} \text{ g d}^{-1}$	$\dot{J}_X = f \frac{\{\dot{p}_{X_m}\}}{\mu_E} V^{2/3}$
	Ingestion	$\dot{J}_{X_i I}$	ingestion rate	$\text{molC d}^{-1} \text{ g d}^{-1}$	$\dot{J}_{X_i I} = \dot{J}_{X_i F}$
		$\dot{J}_{P_i F}$	pseudofaeces production rate	$\text{molC d}^{-1} \text{ g d}^{-1}$	$\dot{J}_{P_i F} = 0$
	Assimilation	\dot{J}_{EA}	assimilation rate	$\text{molC}^E \text{ d}^{-1}$	$\dot{J}_{EA} = y_{EXV} * \dot{J}_{X_i I}$
		$\dot{J}_{P_i I}$	faeces production rate	molC d^{-1}	$\dot{J}_{P_i I} = \dot{J}_{X_i I} - \dot{J}_{EA}$
2-Simple filtration	Filtration	f	scaled functional response	adim	$f = \frac{X_1}{X_1 + K'(X_0)}$
		$K'(Y)$	apparent half-saturation coefficient	adim	$K'(Y) = K_X (1 + \frac{X_0}{K_Y})$
		$\dot{J}_{X_i F}$	filtration rate	$\text{molC d}^{-1} \text{ g d}^{-1}$	$\dot{J}_X = f \frac{\{\dot{p}_{X_m}\}}{\mu_E} V^{2/3}$
	Ingestion	$\dot{J}_{X_i I}$	ingestion rate	$\text{molC d}^{-1} \text{ g d}^{-1}$	$\dot{J}_{X_i I} = \dot{J}_{X_i F}$
		$\dot{J}_{P_i F}$	pseudofaeces production rate	$\text{molC d}^{-1} \text{ g d}^{-1}$	$\dot{J}_{P_i F} = 0$
	Assimilation	\dot{J}_{EA}	assimilation rate	$\text{molC}^E \text{ d}^{-1}$	$\dot{J}_{EA} = y_{EXV} * \dot{J}_{X_i I}$
		$\dot{J}_{P_i I}$	faeces production rate	molC d^{-1}	$\dot{J}_{P_i I} = \dot{J}_{X_i I} - \dot{J}_{EA}$
3-Complex filtration	Filtration	\dot{C}_R	clearance rate	$\text{m}^3 \text{ d}^{-1}$	$\dot{C}_R = \frac{\{\dot{C}_{Rm}\}}{1 + \sum_{i=0}^1 \frac{X_i \{\dot{C}_{Rm}\}}{\{\dot{J}_{X_i Fm}\}}} V^{2/3}$
		$\dot{J}_{X_i F}$	filtration rate	$\text{molC d}^{-1} \text{ g d}^{-1}$	$\dot{J}_{X_i F} = \dot{C}_R X_i$
	Ingestion	$\dot{J}_{X_i I}$	ingestion rate	$\text{molC d}^{-1} \text{ g d}^{-1}$	$\dot{J}_{X_i I} = \frac{\rho_{X_i I} \dot{J}_{X_i F}}{1 + \sum_{i=1}^n \frac{\rho_{X_i I} \dot{J}_{X_i F}}{\{\dot{J}_{X_i Im}\}}}$
		$\dot{J}_{P_i F}$	pseudofaeces production rate	$\text{molC d}^{-1} \text{ g d}^{-1}$	$\dot{J}_{P_i F} = \dot{J}_{X_i F} - \dot{J}_{X_i I}$
	1-Simple Assimilation	\dot{J}_{EA}	assimilation rate	$\text{molC}^E \text{ d}^{-1}$	$\dot{J}_{EA} = y_{EXV} * \dot{J}_{X_i I}$
		$\dot{J}_{P_i I}$	faeces production rate	molC d^{-1}	$\dot{J}_{P_i I} = \dot{J}_{X_i I} - \dot{J}_{EA}$
		\dot{J}_{EA}	assimilation rate	$\text{molC}^E \text{ d}^{-1}$	$\dot{J}_{EA} = \dot{J}_{EAE} + \dot{J}_{EAV}$
		\dot{J}_{EAV}	algae structure assimilation rate	$\text{molC}^E \text{ d}^{-1}$	$\dot{J}_{EAV} = y_{EXV} \dot{J}_{X_i I} (1 - f_E)$
	2-Complex Assimilation	\dot{r}_C	-	$\text{molC}^E \text{ d}^{-1}$	$\dot{r}_C = \dot{J}_{X_i I} f_E$
		\dot{r}_N	-	$\text{molC}^E \text{ d}^{-1}$	$\dot{r}_N = \dot{J}_{X_i I} f_E \frac{n_{X_1}}{n_P}$
		\dot{r}_P	-	$\text{molC}^E \text{ d}^{-1}$	$\dot{r}_P = \dot{J}_{X_i I} f_E \frac{n_{X_1}}{n_E}$
		\dot{J}_{EAE}	algae reserves assimilation rate	$\text{molC}^E \text{ d}^{-1}$	
		$\dot{J}_{EAE} = \left(\frac{1}{\dot{r}_C} + \frac{1}{\dot{r}_N} + \frac{1}{\dot{r}_P} - \frac{1}{\dot{r}_C + \dot{r}_N} - \frac{1}{\dot{r}_C + \dot{r}_P} - \frac{1}{\dot{r}_N + \dot{r}_P} + \frac{1}{\dot{r}_C + \dot{r}_N + \dot{r}_P} \right)^{-1}$			
		$\dot{J}_{P_i I}$	faeces production rate	molC d^{-1}	$\dot{J}_{P_i I} = \dot{J}_{X_i I} - \dot{J}_{EA}$

buffer (biomass allocated to future gametes production);

- the chemical composition (C, H, O, N, and P assumed as the main elements) of reserve and structure are constant (strong homeostasis);
- if food density is constant then the ratio between reserve and structure (reserve density) tends to a constant value (weak homeostasis);
- the life cycle of the individual has three different life-stages: embryonic (no feeding, the embryo relies on stored energy supplies), juvenile (feeding starts but resources are not yet allocated to the reproduction buffer), and adult (organism is mature and able to reproduce);
- the metabolic switching (from embryo to juvenile and juvenile to adult) is linked to maturity level;
- κ -rule: a fixed fraction of mobilized reserve is used for somatic maintenance and growth (increase of structural mass), the rest for maturity maintenance and maturation (increase of maturity in embryos and juveniles) or reproduction (adults);
- the reserve density at constant food density does not depend on the amount of structure (weak homeostasis);

Table 3. Model formulations, continuation: standard DEB model adapted from Kooijman (2010). X_1 represents algae and X_0 inorganic material concentration.

process	symbol	description	units	formulation
Mobilization	\dot{J}_{EC}	mobilization flux	$\text{molC}^E \text{d}^{-1}$	$\dot{J}_{EC} = \frac{[E]}{\frac{[EG]}{\mu_E} + \kappa[E]} \left(\frac{[EG]}{\mu_E} \dot{v} V^{2/3} + \dot{J}_{ES} \right)$
Somatic Maintenance	\dot{J}_{ES}	somatic maintenance	$\text{molC}^E \text{d}^{-1}$	$\dot{J}_{ES} = \frac{[\dot{p}_M]}{\mu_E} V$
Growth	\dot{J}_{EG}	flux allocated to growth	$\text{molC}^E \text{d}^{-1}$	$\dot{J}_{EG} = \kappa \dot{J}_{EC} - \dot{J}_{ES}$
	\dot{J}_{VG}	growth	$\text{molC}^V \text{d}^{-1}$	$\dot{J}_{VG} = y_{VE} \dot{J}_{EG}$
Maturity	\dot{J}_{EJ}	maturity maintenance	$\text{molC}^E \text{d}^{-1}$	$\dot{J}_{EJ} = k_J M_H$
Reproduction	\dot{J}_{ER}	flux allocated to reproduction/maturity	$\text{molC}^E \text{d}^{-1}$	$\dot{J}_{ER} = (1 - \kappa) \dot{J}_{EC} - \dot{J}_{EJ}$
	\dot{J}_{ER}^M	flux to maturity	$\text{molC}^E \text{d}^{-1}$	$\dot{J}_{ER}^M = \begin{cases} \dot{J}_{ER}, & \text{if } M_H < M_H^p \\ 0, & \text{otherwise} \end{cases}$
	\dot{J}_{ER}^R	flux to reproduction buffer	$\text{molC}^E \text{d}^{-1}$	$\dot{J}_{ER}^R = \begin{cases} 0, & \text{if } M_H < M_H^p \\ \dot{J}_{ER}, & \text{otherwise} \end{cases}$
Spawning	\dot{J}_{ER}^{spawn}	spawning	$\text{molC}^E \text{d}^{-1}$	$\dot{J}_{ER}^{spawn} = \begin{cases} k_R M_R / R^{spawn}, & \text{if } GSR \geq GSR^{spawn} \wedge T \geq T^{spawn} \\ 0, & \text{otherwise} \end{cases}$
	N^{spawn}	number of gametes released	$\# \text{d}^{-1}$	$N^{spawn} = \dot{J}_{ER}^{spawn} / M_E^0$
Inorganic Fluxes	\dot{J}_{NH_3}	ammonia flux	molNd^{-1}	
	\dot{J}_{NH_3}			$\dot{J}_{NH_3} = -(-\dot{J}_{X_i F} n_{X_1}^N + \dot{J}_{P_i F} n_{X_1}^N + \dot{J}_{P_i I} n_{X_1}^N + \dot{J}_{VG} n_V^N + \dot{J}_E n_E^N + \dot{J}_{ER}^R n_E^N)$
	\dot{J}_{PO_4}	phosphate flux	molPd^{-1}	
	\dot{J}_{PO_4}			$\dot{J}_{PO_4} = -(-\dot{J}_{X_i F} n_{X_1}^P + \dot{J}_{P_i F} n_{X_1}^P + \dot{J}_{P_i I} n_{X_1}^P + \dot{J}_{VG} n_V^P + \dot{J}_E n_E^P + \dot{J}_{ER}^R n_E^P)$
	\dot{J}_{H_2O}	water flux	molHd^{-1}	
	\dot{J}_{H_2O}			$\dot{J}_{H_2O} = -(-\dot{J}_{X_i F} n_{X_1}^H + \dot{J}_{P_i F} n_{X_1}^H + \dot{J}_{P_i I} n_{X_1}^H + 3 \dot{J}_{NH_3} + \dot{J}_{VG} n_V^H + \dot{J}_E n_E^H + \dot{J}_{ER}^R n_E^H)$
	\dot{J}_{CO_2}	carbon dioxide flux	molCd^{-1}	
	\dot{J}_{CO_2}			$\dot{J}_{CO_2} = -(-\dot{J}_{X_i F} + \dot{J}_{P_i F} + \dot{J}_{P_i I} + \dot{J}_{NH_3} + \dot{J}_{VG} + \dot{J}_E + \dot{J}_{ER}^R)$
	\dot{J}_{O_2}	dioxygen flux	$\text{molO}_2 \text{d}^{-1}$	
	\dot{J}_{O_2}			$\dot{J}_{O_2} = -\frac{1}{2}(-\dot{J}_{X_i F} n_{X_1}^O + 4 \dot{J}_{PO_4} + 2 \dot{J}_{H_2O} + 2 \dot{J}_{CO_2} + \dot{J}_{P_i F} n_{X_1}^O + \dot{J}_{P_i I} n_{X_1}^O + \dot{J}_{VG} n_V^O + \dot{J}_E n_E^O + \dot{J}_{ER}^R n_E^O)$

8. somatic maintenance is proportional to the amount of structure and maturity maintenance proportional to the level of maturity.

In addition, the presented model also assumes:

1. the bivalve is an isomorph organism (its shape does not change during growth);
2. the conversion between the real and the structural length is made by a fixed dimensionless shape coefficient (δ_M);
3. the organism is able to use the reproduction buffer to cope with somatic maintenance costs (re-absorption of gametes) during starvation periods and if that is not enough, structure will be used;
4. the bivalve is able to reduce its maturity level in order to cope with maturity maintenance.

Table 4. Model auxiliar compound parameters and other quantities.

symbol	description	units	formulation
$V^{1/3}$	volumetric length	cm	$V^{1/3} = \left(\frac{M_V}{[M_V]} \right)^{1/3}$
$[M_V]$	volume specific structural mass	$\text{molC}^V \text{cm}^{-3}$	$[M_V] = \frac{dV}{w_V}$
$[E]$	reserves density	$\text{molC}^E \text{cm}^{-3}$	$[E] = \frac{M_E}{V_E}$
M_H^b	cumulative maturity spent until birth	molC^E	$M_H^b = \frac{E_{Hb}}{\mu_E}$
M_H^p	cumulative maturity spent until puberty	molC^E	$M_H^p = \frac{E_{Hp}}{\mu_E}$
Y_{VE}	yield coefficient of structures on reserves	$\text{molC}^V \text{molC}^{E-1}$	$Y_{VE} = \frac{[M_V] \mu_E}{[E_G]}$
\dot{k}_M	somatic maintenance rate coefficient	d^{-1}	$\dot{k}_M = \frac{[p_M]}{[E_G]}$
\dot{k}_J	volume specific maturity maintenance	d^{-1}	$\dot{k}_J = \dot{k}_M$
GSR	gonado-somatic ratio	$\text{molC}^R \text{molC}^{-1}$	$GSR = \frac{M_R}{M_V + M_E + M_R}$
L	organism length	cm	$L = \frac{V^{1/3}}{\delta_M}$
D	organism total weight	$\text{g}(ww)$	$WW = \frac{M_V w_V + (M_E + M_R) w_E}{\psi_{af} dw / dw \cdot \psi_{dw} / ww}$

3.1.1 State variables and forcing functions

Four state variables characterize the organism, i.e. the individual structure biomass, M_V (molC^V); reserve, M_E (molC^E); maturity level, M_H (molC^E) and reproduction buffer, M_R (molC^E) (Table 1). The forcing functions of the model are ambient temperature and the concentration of particles in the water, either inorganic (non food material, expressed in mg/l) or algae (food, expressed in molC/l for C,N, and P).

3.1.2 Feeding

The feeding processes can be simulated assuming three different complexity levels: (1) Impose filtration, (2) Simple filtration, and (3) Complex filtration. Formulation details are given in Table 2.

1. Impose filtration

Impose filtration assumes that feeding is constant. Filtration rate is computed to ensure that the functional response equals the value set by the user in the `<begin_species>` block of Bivalve input file (`F_FIX`). This option is meant to be used in tests and theoretical scenarios and for that reason there is **no feedback** of bivalves activity in the water column properties and mass balance is not fulfilled. Also it assumes that phytoplankton is the only source of bivalve food in the system.

2. Simple filtration

Simple filtration assumes that the functional response (f value) follows a Holling type *II* equation assuming a fixed, species dependent half-saturation constant. The interference of inorganic particles follows the (Kooijman, 2006) formulation, assuming an apparent half saturation constant that depends, on the silt concentration in the water column. This interference is activated by including 'cohesive sediment' property in the `<<begin_particle>>` block, in the `<begin_species>` block in the Bivalve input file. The

simple filtration option in combination with the activation of keyword `FEEDBACK_ON_WATER` means that there will be a feedback of the filtration process in the food and silt concentration in the water but only if the food concentration is not given as a time series in the water properties file (because the food concentration is ultimately controlled by the water properties module). The aim of this keyword is to be able to use the model for testing and theoretical scenarios where food should be kept constant, neglecting the feedback in the water quality. By default the keyword is not active.

3. Complex filtration

Filtration, ingestion and assimilation are assumed to be separate processes following (Saraiva et al., 2011a). The Synthesizing Units concept (SU), introduced in the DEB theory by Kooijman (1998, 2000, 2010), is used to describe those processes. For each particle type i in the water column, with density X_i , a flux of particles is retained through filtration (the product of clearance rate by the particles concentration, $X_i \dot{C}_R$). In the model, clearance rate is regulated by substitutable and sequential SU's where any substrate can be separately filtered and the handling of one food type by the filtration apparatus interferes with the possible handling of other food types. Once retained in the gills, particles are then lead to the palps, where the selection is made between particles transported to the mouth to be ingested and particles which are rejected and transported back to the water as pseudofaeces ($\dot{J}_{P_i F}$). The same type of mechanism (substitutable and sequential SU's) is used to explain and describe both filtration and ingestion. The formulation derived is then similar to Holling type II functional response, although extended to the situation with **several types of food**. Filtration and ingestion are assumed as two SU systems connected by open handshaking protocol, i.e. the first SU releases its products irrespective of the state of the next SU, with the consequent production of pseudofaeces (filtered material that the ingestion process is not able to handle). The selection of particles in the ingestion process is made by assuming a different binding probability for each type of food ($\rho_{X_i I}$), representing a different affinity of the ingestion apparatus(palps) for each particle.

The third and last feeding step is assimilation, defined as the process where the particles are absorbed and converted into the organism's reserve. The efficiency in the conversion of food into the reserves depends on how the organism is able to absorb food particles, which ultimately depends on the similarity of the chemical composition of food and reserves. Conversion efficiency, therefore, depends on the type of food. The adopted assimilation formulation for algal reserves assumes a parallel and complementary substrate for the synthesis of bivalve reserve tissue. Differences in the chemical composition between bivalve reserve tissue and ingested food, determines the production of faeces ($\dot{J}_{P_i A}$). More details on the model assumptions, formulations and parameter estimation can be found in Saraiva et al. (2011a).

3.1.3 Mobilization

The mobilization rate, \dot{J}_{EC} , is the rate at which energy is used from the reserve. As a consequence of the homeostasis assumption, the mobilization of the reserve occurs at a rate proportional to the reserve density, which is

the ratio between reserves (mass, molC) and structure (volume, m³), and thus inversely proportional to structure (Kooijman, 2010).

3.1.4 Somatic Maintenance

Somatic maintenance, \dot{J}_{ES} , stands for all processes necessary to 'stay alive', or to maintain the integrity of the animal's body and this maintenance term can generally be decomposed in contributions that are proportional to structural body volume (structure maintenance costs) and to surface area (e.g. osmotic work in brackish waters, endotherms) (Kooijman, 2010). This second type of contribution to maintenance (proportional to the organism surface area) is considered to be null because we assume that the bivalve is not affected by the possible changes in salinity at the study locations and also because bivalves are ectotherms, not spending energy on temperature regulation.

3.1.5 Growth

Growth, \dot{J}_{VG} , represents the increase of structural body mass of the organism. The flux of reserve available for growth, \dot{J}_{EG} , is computed as the difference between the amount of energy allocated to growth/maintenance, following the κ - rule, and the somatic maintenance. The increase in structural body mass, i.e. the growth, is computed by assuming a yield coefficient (y_{VE}) resulting from the stoichiometric balance of mass transformations (Kooijman, 2010).

3.1.6 Maturity and Reproduction

During the juvenile stage, the fraction of energy allocated to reproduction is used to develop reproductive organs and regulation systems, increasing the maturation level of the organism. Maturity represents the mass, or energy, investment in the development of the organism. When the organism reaches a particular maturity level (M_H^p), no more development is needed and it becomes an adult. Hereafter, it allocates this flux, \dot{J}_{ER} , to the reproduction buffer for further gametes production and release into the water. Thus, this maturity threshold controls stage transitions. Maturity requires maintenance, proportional to the maturity level, which can be thought to relate to the maintenance of regulating mechanisms and concentration gradients (Kooijman, 2010). The present model assumes, for simplicity, that the maturity maintenance rate coefficient is equal to the somatic maintenance rate coefficient, $k_M = k_J$, implying that the stage transitions occur at fixed amount of structure.

3.1.7 Spawning

The allocation of energy to reproduction is accumulated in a reproduction buffer. This leads to an increasing of the gonad-somatic mass ratio (GSR, gonadal tissue fraction of the total biomass) over time. Spawning events occur if the GSR and the temperature are above the respective thresholds (GSR^{spawn} and T^{spawn}). The model considers that the gametes production, i.e. the conversion of the reproduction buffer content into embryo reserve has overhead costs. The dimensionless factor, k_R , represents the fraction that is fixed in eggs and $1 - k_R$ the dissipation fraction. In line as field observations from (Cardoso et al., 2007), the model assumes that one spawning

event does not empty the reproduction buffer content completely but that a minimum value of GSR is maintained inside the organism. For simplicity, the model considers that each gamete (sperm cell or egg) produced will have a constant value of reserve density that equals the reserve density of the mother when in optimal condition and that the spawning events are instantaneous.

3.1.8 Inorganic Compounds

Mineral fluxes are represented by the amount of CO_2 , H_2O , O_2 , NH_3 and PO_4 used or released by the individual in the processes described above. They can be computed on basis of the principle of mass conservation for each element in the system (C,H,O, N, P) using the organic fluxes computed before.

3.1.9 Temperature effect

All physiological rates depend on the body temperature and the model assumes that all physiological rates are affected in the same way (Pouvreau et al., 2006). The dependency is usually well-described by the Arrhenius relation, within a species-specific tolerance range of temperatures (option 1). However, we can also assume a more complex description (option 0), where each rate is controlled by SUs having an inactive configuration at low and high temperatures as presented in Kooijman (2010). Formulations are presented in Table 5.

Table 5. Temperature dependency formulations, adapted from Kooijman (2000).

option	symbol	formulation
0-Complex temperature correction	$\dot{k}(T)$	$\dot{k}(T) = \dot{k}_1 e^{\left(\frac{T_A}{T_1} - \frac{T_A}{T}\right) \frac{s(T)}{s(T_1)}}$ $s(T) = \left(1 + e^{\left(\frac{T_{AL}}{T} - \frac{T_{AL}}{T_L}\right)} + e^{\left(\frac{T_{AH}}{T} - \frac{T_{AH}}{T_H}\right)}\right)^{-1}$
1-Simple temperature correction	$\dot{k}(T)$	$\dot{k}(T) = \dot{k}_1 \exp\left(\frac{T_A}{T_1} - \frac{T_A}{T}\right)$

3.1.10 Model parameters

https://www.bio.vu.nl/thb/deb/deblab/add_my_pet/ is a database of DEB model parameters available for use. The collection includes estimations of parameters for about 1000 species of organisms. Most of the values results from the application of the covariation method described in Lika et al. (2011a). This method is based on the minimization of the weight sum of squares deviation between data and model results. The data include a collection of observations (single data points and/or time series) and a set of pseudo-data (average of parameters obtained from a large collection of organisms, used to restrict the possible parameter combinations). The general idea behind the covariation method is to let all available information compete, or interact, to produce the end result, implying the estimation of all parameters from all data sets simultaneously. More information on the method, the estimation procedure can be found at the referred website as well as the code to implement the estimation procedure. In the present document, a parameter list for mussels (*Mytilus edulis* and for the pacific oyster (*Crassostrea gigas*) is presented. The parameter values mostly follow the estimations made by Saraiva

et al. (2011b) and (Bernard et al., 2011), used respectively in Saraiva et al. (2011b) and Saraiva et al. (tted).

3.2 Population

In the model, the population consists of several cohorts, and each cohort represents a group of identical individuals born at the same time. The underlying idea is that organisms of the same species, born at the same time and place and moving together, will experience the same environmental conditions and will consequently follow the same growth and development trajectory over time. The population dynamics will be represented by the cohort trajectories, characterized by their individual properties (e.g. size, biomass, state of development), and also by its number of individuals. The population model is, in fact, responsible for the book-keeping of the information generated by the individual model over time (one for each cohort), with all the state variables representing every cohort. It also includes the effect of processes at the population level, namely mortality by predation (including cannibalism) or by natural causes. While the individual model is responsible for the computation of the changes in the individual variables, i.e., size, biomass, and state of development, the population model is responsible for the changes in the number of individuals in each cohort (by mortality) and the change in the number of cohorts (by managing births and deaths of cohorts).

As population specific processes, the model includes: initial egg mortality, background mortality, food competition, cannibalism, and imposed predation by shrimps, crabs and birds. Predator abundance and intake are considered a forcing function in the model, meaning that there is no feedback from the bivalve population on the predators. Each predator has a prey size range preference, and the predation impact in each cohort is proportional to the fraction of the number of individuals in the cohort and the total number of prey available.

The coupling with the ecosystem model enabled the inclusion of two additional mortality effects in the population: (i) mortality by velocity above 0.5 m/s, assuming that bivalves are flushed away and eventually die, and (ii) mortality by wrong settlement, meaning that a settlement probability is imposed on each location, based on the fact that mussels have a preference to settle on substrates with coarse shell debris (wa Kangeri et al., 2014). The underlying assumption is that non-settled bivalves will eventually die, due to the effect of currents or burying. The settlement occurs instantaneously when, and where, the individual length is higher than 0.026 cm (de Vooy, 1999).

Food competition is simulated by assuming that when an individual consumes a food item, that item cannot be consumed again by other individuals. Total food intake of the population (summing over all individuals) has a major impact on the resource density, which in turn affects the individual food intake. Thus, this feedback is crucial for the population dynamics and is included in the present model.

The main formulations concerning specifically the population model are listed in Tables 8. A more detailed description of the processes included in the model and its specific assumptions can be found in the following sections and in Saraiva et al. (2014).

3.2.1 Birth of a new cohort

The birth of a new cohort (B) occurs if there is a spawning event. Spawning events occur instantaneously if the GSR and the temperature are above respective thresholds, in agreement with field and laboratory observations performed by different authors (e.g. Chipperfield, 1953; Wilson and Seed, 1974; Podniesinski and McAlice, 1986; Hummel et al., 1989; Thorarinsdóttir, 1996). For simplicity, the model assumes that all the individuals will have maximum reserve density at hatching. This assumption implies a constant egg size, which is thus independent of the condition of the mother. Also, the new cohort will start with the (juvenile) stage immediately following hatching, thus neglecting the short embryonic stage. From the reproduction buffer content of the parents and knowing the newborn properties, a number of gametes are expected N_t^{spawn} . From these, only a part will succeed and become a newborn individual (N^0), as an effect of the initial egg mortality.

3.2.2 Initial egg mortality

Initial egg mortality parameter (m^{egg}) pretends to include all the mortality processes during the egg and larvae phase: e.g., dispersion, egg viability, fertilization probabilities, settlement failure, and possible predation by other predators besides shrimps, crabs and birds. These processes are grouped in the model as a single constant parameter.

3.2.3 Background mortality

The concept of background mortality is commonly used in fish population dynamics, where it includes all possible causes of death except fishing (Pauly, 1980). We assume in this study that the background mortality (m^N) is constant and accounts for e.g., mortality due to diseases and storms.

3.2.4 Food competition and extra starvation mortality

Food competition is one of the main density dependent processes happening within the population. Food is limited and the model assumes that it is shared by all the individuals in the population depending on their filtration skills and abundance. For each cohort a potential filtration is computed based on the environmental conditions, their individual size and the number of individuals. From these values, a whole population potential filtration is computed, summing all the filtration of all the cohorts. If the amount of food in the environment is not enough to fulfil the mussel needs, the food will be redistributed to all the cohorts based on their relative potential filtration, i.e., the more demanding cohorts will benefit from more food items. This assumption is consistent with the assumption made before, that the individuals in each cohort will always remain identical, suffering from starvation exactly in the same way. As described before, the intense starvation can lead to the use of structure to cope with the somatic maintenance (shrinking) and to the reduction of its maturity level (rejuvenation). The model assumes that these processes are reversible if the maturity and structure amounts are higher than the assumed birth values,

meaning that the organisms can increase again their maturity and reach adult stage without any physiological consequences. If the state variables reach irreversible values (lower than the values reached at birth), the individuals will die. However, to simulate possible differences between individuals (e.g. position and extreme local food depletion), an extra starvation mortality suggested by Maar et al. (2009) is considered when the condition of the individuals is low and the scaled reserves density is lower than 0.1. This assumption pretends to simulate the death of individuals in the cohort due to local food depletion preventing the sudden death of the whole cohort.

3.2.5 Predation

Currently, the model assumes three possible predators for bivalves that are based on the Wadden Sea ecosystem: shrimps, crabs and birds. Predator abundance and intake are considered a forcing function in the model, meaning that there is no feedback from the bivalve population on the predator variables. It is assumed that each predator has a prey size range preference, and the impact of their predation on the number of individuals in each cohort is proportional to the fraction of total prey available in the system that the cohort represents.

3.2.6 Cannibalism

Cannibalism is included in the model by the allowing the adults mussels to feed on their on larvae. Filtration and ingestion are assumed to be equal to any other particle. Assimilation is considered 100% efficient since both individuals (predator and prey) have the same biomass composition.

3.2.7 Cohort death

The whole cohort dies when: (1) reaches an age limit, (2) by intense starvation (described before) or (3) a insignificant number of individuals remain. The first two causes are biological and the last one is basically imposed for technical reasons, to avoid following a constantly increasing number of cohorts, being some of them not significantly important for the population state due to their low number of individuals.

Table 6. DEB parameters (and respective keywords) and other parameters and conversion factors. (dw) represents dry weight, ($AFDW$) ash-free dry weight, (ww) wet weight, max: maximum, s.a.: surface area, *this study* is indicated for the parameters that were computed based in field data obtained in this study and *assumed* is indicated for the parameters that are result from *wise* guesses within this study.

keyword	symbol	description	units
V_COND	\dot{v}	energy conductance	cmd^{-1}
KAPPA	κ	allocation fraction to growth and somatic maintenance	-
pM	$[\dot{p}_M]$	volume specific somatic maintenance	$\text{Jd}^{-1}\text{cm}^{-3}$
EG	$[E_G]$	specific cost for structure	Jcm^{-3}
DELTA_M	δ_M	shape coefficient	-
ME_0	M_E^0	initial reserve mass at optimal food conditions	molC^E
EH_B	E_{Hb}	maturity at birth	J
EH_P	E_{Hp}	maturity at puberty	J
KAP_R	κ_R	reproduction efficiency	-
GSR_MIN	GSR^{min}	minimum gonado-somatic ratio in the organism	$\text{molC}^R\text{molC}^{-1}$
GSR_SPAWN	GSR^{spawn}	gonado-somatic ratio to spawn	$\text{molC}^R\text{molC}^{-1}$
T_SPAWN	T^{spawn}	minimum temperature for spawning	$^{\circ}\text{C}$
F_FIX	f	constant food density parameter	-
PXM_FIX	$\{\dot{p}_{X_m}\}$	maximum surface area-specific ingestion rate	$\text{Jd}^{-1}\text{cm}^{-2}$
K_FOOD	K_X	Food half saturation coefficient	mgCL^{-1}
K_SED	K_Y	Inorganic material half saturation coefficient	mgL^{-1}
YEX	y_{EXV}	yield coefficient of reserves in algae structure	$\text{molC}^E\text{molC}^V$
CRM	$\{\dot{C}_{Rm}\}$	Maximum surface area specific clearance rate	$\text{m}^3\text{d}^{-1}\text{cm}^{-2}$
JX1FM	$\{\dot{J}_{X_1Fm}\}$	Algae maximum surface area-specific filtration rate	$\text{molC d}^{-1}\text{cm}^{-2}$
JX0FM	$\{\dot{J}_{X_0Fm}\}$	Inorganic material maximum surface area-specific filtration rate	$\text{g d}^{-1}\text{cm}^{-2}$
RO_X1	ρ_{X_1I}	Algae binding probability	-
RO_X0	ρ_{X_0I}	Inorganic material binding probability	-
JX1IM	\dot{J}_{X_1Im}	Algae maximum ingestion rate	molC d^{-1}
JX0IM	\dot{J}_{X_0Im}	Inorganic material maximum ingestion rate	g d^{-1}
DV	$d_V = d_E$	bivalve structure and reserves specific density	$\text{g}_{(dw)}\text{cm}^{-3}$
MU_E	μ_E	bivalve reserves chemical potential	Jmol^{-1}
Tref	T_{ref}	reference temperature	K
TA	T_A	Arrhenius temperature	K
TL	T_L	Lower boundary tolerance range	K
TH	T_H	Upper boundary tolerance range	K
TAL	T_{AL}	Arrhenius temperature for lower boundary	K
TAH	T_{AH}	arrhenius temperature for upper boundary	K
ME_B	ME_B	New born individual reserves, at optimal food conditions	molC
MV_B	MV_B	New born individual structure, at optimal food conditions	molC
MH_B	MH_B	New born individual structure, at optimal food conditions	molC
L_B	L_B	New born individual length, at optimal food conditions	molC
LIFE_SPAN	a^{\dagger}	life span	y
E_M	E_M	Maximum reserve capacity	Jcm^{-3}
RESERVES_nH	n_E^H	chemical composition of bivalve reserve	molH/molC
RESERVES_nO	n_E^O	chemical composition of bivalve reserve	molO/molC
RESERVES_nN	n_E^N	chemical composition of bivalve reserve	molN/molC
RESERVES_nP	n_E^P	chemical composition of bivalve reserve	molP/molC
STRUCTURE_nH	n_E^H	chemical composition of bivalve structure	molH/molC
STRUCTURE_nO	n_E^O	chemical composition of bivalve structure	molO/molC
STRUCTURE_nN	n_E^N	chemical composition of bivalve structure	molN/molC
STRUCTURE_nP	n_E^P	chemical composition of bivalve structure	molP/molC
	$\psi_{afdw/dw}$	bivalve ash-free dry weight to dry weight conversion factor	$\text{g}_{(afdw)}\text{g}_{(dw)}^{-1}$
	$\psi_{dw/ww}$	bivalve ash-free dry weight to dry weight conversion factor	$\text{g}_{(dw)}\text{g}_{(ww)}^{-1}$
	w_E/w_V	bivalve reserves/structure relative molecular mass	$\text{g}_{(afdw)}\text{molC}^{-1}$

Table 7. Food specific parameters (and respective keywords) and other parameters and conversion factors.

keyword	symbol	description	units
RATIOHC	m_X^H	H fraction in algae biomass	mgH/mgC
RATIOOC	m_X^O	O fraction in algae biomass	mgO/mgC
RATIONC	m_X^N	N fraction in algae biomass	mgN/mgC
RATIOPC	m_X^P	P fraction in algae biomass	mgP/mgC
RATIOSiC	m_X^H	Si fraction in algae biomass	mgSi/mgC
RATIOCHLC	m_X^H	CHL fraction in algae biomass	mgCHL/mgC
SIZE	L_{food}	size of food particle	cm
F_E	f_E	reserves fraction in algae biomass	-

Table 8. Population model main formulations. * represents the predator (S for shrimp, C for crab or B for bird).

process	symbol	description	units	formulation
Cohort Birth	B	new cohort	#	$B = \begin{cases} 1, & \text{if } \sum_{i=1}^{nC} N_i^{spawn} > 0 \\ 0, & \text{otherwise} \end{cases}$
	N_i^{spawn}	gametes released individuals in the new cohort	# d ⁻¹	Saraiva et al. (2012) $N^0 = N_i^{spawn} (1 - m^{egg})$
Starvation	m_i^F	starvation extra mortality	d ⁻¹	$m_i^F = \frac{1}{100 \exp(-70 e_i)} (-1), \text{ if } e_i \leq -1$ Maar et al. (2009)
Predation	m_i^S	shrimp predation	# d ⁻¹	$m_i^S = \rho^S \{j_{Xm}^S\} \frac{N_i}{N_t^S} \frac{1}{w_i} A_{Ci}^S$
	m_i^C	crab predation	# d ⁻¹	$m_i^C = \rho^C m_t^C \frac{N_i}{N_t^C} A_{Ci}^C$
	m_i^B	bird predation	# d ⁻¹	$m_i^B = \rho^B j_X^B \frac{N_i}{N_t^B} \frac{1}{AFDW_i} A_{Ci}^B$
	$\{j_{Xm}^S\}$	shrimp max ingestion rate	molC d ⁻¹ cm ⁻²	$\{j_{Xm}^S\} = \frac{\{\dot{p}_{Xm}^S\}}{\mu_E} L_S^2$
	N_t^*	prey available for predator *	#	$N_t^* = \sum_{i=1}^{nC} N_i A_{Ci}^*$
	A_{Ci}^*	cohort availability for predator *	adim	$A_{Ci}^* = \begin{cases} 1, & \text{if } L_{mP}^* \leq L_i \leq L_{MP}^* \\ 0, & \text{otherwise} \end{cases}$
Cohort Death	D	number of cohorts to die	#	$D = \sum_{i=1}^{nC} D_i$
	D_i	cohort i state	adim	$D_i = \begin{cases} 1, & \text{if dead } \begin{cases} N_i < \text{MinValue, or} \\ M_{Hi} < M_H^b \wedge M_{Vi} < M_{Vb}, \text{ or} \\ M_{Vi} < M_V^b \wedge L_i < L_b, \text{ or} \\ A_i > a^\dagger \end{cases} \\ 0, & \text{if alive} \end{cases}$

Table 9. Population model specific parameters (and respective keywords).

keyword	symbol	description	units
M_NATURAL	m^N	background mortality	d ⁻¹
M_SPAT	m^{egg}	initial egg mortality	d ⁻¹
DENSITY_MAXVALUE		maximum density	#m ⁻²
MAX_VELOCITY	V_{max}	maximum velocity	ms ⁻¹
FEEDING_RATE	$\{p_{Xm}^S\}$	predator max ingestion rate	J d ⁻¹ cm ⁻²
SIZE	L_S	predator average size	cm
MINPREYSIZE	L_{mprey}^S	predator minimum prey size	cm
MAXPREYSIZE	L_{Mprey}^S	predator maximum prey size	cm
DIET_FRACTION	ρ^S	fraction of mussels in predator diet	adim

4 Module Bivalve User Manual

4.1 Practical notes

- Module bivalve is coupled with either Water Quality and Life pelagic models although it has only been tested with the first option.
- The model units are individuals m^{-2} because the model is intent to be 2D. The 3D configuration can be easily implemented by testing in which cell the bivalve is
- The model requires a Bivalve input file and some additional properties in the WaterProperties file
- The model creates 5 additional variables for each cohort created in the system (Structure, Reserves, Maturity, Reproduction and Number of individuals in the cohort)
- the model requires initial conditions of each of these 5 properties, given in the WaterProperties file
- the bivalve can filtered different types of particles taht should be listed inside the species block of the Bivalve input file
- for each of those particles the user should verify that the BIVALVE keyword in the water properties file is switched on (value 1) inside the species block of the Bivalve input file
- For each type of particle the user must also indicate if the particles is to be considered as food or not
- The inorganic properties dependence is required, the property cohesive sediments should be added to the list of particles inside the species block of the Bivalve input file and ORGANIC option selected as false (0)
- switching the population model on is done in the Bivalve input file and it is specific for each species
- each cohort created will be tagged by its date of born
- cohorts start always has larvae, meaning that they will have advection-difusion processes
- Settlement probability is also given in the WaterProperties file, as shown in the example, and it can be constant in the complete domain, or it can be given by an hdf file
- The keywords suggesting the testing of parameters only work in the stand alone configuration that is not part of MOHID last version code, meaning that they will not work under this configuration.
- Although built to be used with Life pelagic model, the model was not fully tested with this option
- Parameters default values are based on *Mytilus edulis* and are based on Saraiva et al. (2014)

4.2 Bivalve input file

To use Module Bivalve the model requires an addition input file called *Bivalve.dat*. In this file all the keyword related to the bivalve individual and population characteristics should be defined, e.g. main options for model use (Table 10), individual parameters species-specific (Table 11 and Table 12), food items or particles able to be filtered (Table 13) and species specific predators (Table 14).

Table 10. Main keywords to use in bivalve input file.

keyword	symbol	description	units	default value/option	reference/option
DT		model time step	s		
DENSITY_UNITS		choose bivalve units	-	0	m^2
BIVALVE_OUTPUT_TIME		output time	-	1	m^3
PELAGIC_MODEL		coupled pelagic model	-	0. 86400.	
			-	WaterQuality	
			-	Life	
NITROGEN		Nitrogen?	-	0/1	
PHOSPHOR		Phosphorus?	-	0/1	
		feeding model	-	1	Impose filtration
FEEDING_MODEL			-	2	Simple filtration
			-	3	Complex filtration
CORRECT_FILTRATION		filtration depends on cohorts needs	-	0/1	
INDEX_OUTPUTS		cell index with output	-		
MASS_BALANCE		output the mass balance	-	0/1	
MIN_NUMBER		minimum number in a cohort	#	0.0001	
TESTING_PARAMETERS		testing parameters?	-	0/1	
MIN_SPAWN_TIME		minimum time between spawning events	s	86400	
OLD		continuous run?	-	0	
<begin_species>					
«begin_particle»					
«end_particle»					
«begin_predator»					
«end_predator»					
<end_species>					

4.3 WaterProperties file changes

Water properties input file to MOHID also has to include some changes if the Module Bivalve is to be coupled. The first change is to select the properties that will be changed due to the bivalve activity. In a standard application the list of properties that should be used by MOdule Bivalve includes: oxygen, ammonia, phosphorus concentration, particulate organic nitrogen, particulate organic phosphorus, carbon dioxide, phytoplankton and cohesive sediment (if included in the list of properties in Bivalve input file).

```
<beginproperty>
...
BIVALVE                : 1
...
5 <endproperty>
```

Listing 1. WaterProperties File: add a property to the Bivalve model.

In addition, each bivalve species has to be defined WaterProperties file and for each species the user has to define the settlement probability matrix (which can be an hdf file or a scalar) and the list of cohorts of this species with the values of the respective initial conditions of the associated properties (structure, reserves, reproduction buffer content and number of individuals in the cohort) and some necessary additions properties (length and age). The options for the initialization method follow the same rules as the other properties defined in the file and liked with the Module Fillmatrix in MOHID.

```

<beginproperty>
...
BIVALVE                : 1
...
5 <endproperty>

<begin_species>
NAME                    : bivalve1
UNITS                    : /m2
10 OLD                    : 0
WARN_ON_NEGATIVE_VALUES : 1

LARVAE_TRANSPORT        : 0

15 COHORT_OUTPUT_HDF      : 1
COHORT_BOX_TIME_SERIE   : 0

POPULATION_OUTPUT_HDF    : 0
POPULATION_BOX_TIME_SERIE : 0
20

BYSIZE_OUTPUT_HDF        : 0
BYSIZE_BOX_TIME_SERIE    : 0

NUMBER_SIZE_CLASSES      : 18
25 SIZE_CLASSES           : 0. 0.026 0.1 0.5 1.2 4. 8. 10. 12. 14. 16.

<<begin_settlement>>
INITIALIZATION_METHOD    : CONSTANT
DEFAULTVALUE             : 1.0
30 <<end_settlement>>

<<begin_cohort>>
STRUCTURE                 : 1.17E-03
RESERVES                  : 4.89E-04
35 MATURITY               : 3.75E-06
REPRODUCTION              : 0.0000E+00
LENGTH                   : 3.91E+00
NUMBER                    : 400
AGE                       : 0
40 INITIALIZATION_METHOD  : CONSTANT
<<end_cohort>>
<end_species>

```

Listing 2. WaterProperties File: species properties definition.

4.4 Output

- There are at least 3 time series output files (need to be switched on by the user and the location is given by the index number) and refer to: (1) individual properties for each cohort; (2) population properties; (3) size distribution of the population
- index selection is not ideal but could be changed in the future
- time series are switched on in the Bivalve input file
- Results are also written in HDF files: by cohort, by population and by size class, that are switch on in the water properties file
- By choosing mass conservation option there will be an addition file that shows the mass balance of the bivalve model. The test will show a mass balance constant over time only if there are no predators, considering the same NC ratios in the food and in bivalve or if the model is running with Life pelagic model and complex filtration. This is because of the way the mass balance is computed rather than the limitations. As far as checked the model conserves mass under all the options.

Table 11. Keywords to be used in bivalve input file, in the `<begin_species>` block. The default value corresponds to the parameter values assumed for *Mytilus edulis* in Saraiva et al. (2014). Continuation on Table 12.

keyword	symbol	description	units	default value/option
<begin_species>				
NAME				
DESCRIPTION				
TESTING_FILENAME		name of the file to test parameters		not in use
POPULATION		population?	-	0/1
FEED_ON_LARVAE		cohorts feed on larvae?	-	0/1
LARVAE_MAXSIZE		maximum size of a larvae	cm	0.26
NUMBER_OF_COHORTS		initial number of cohorts	#	
COHORT_OUTPUT		output by cohorts?	-	0/1
BYSIZE_OUTPUT		output by size?	-	0/1
SIZE_STEP		step to generate the size classes	cm	
MAX_SIZECLASS		maximum size for size classes	cm	
«begin_size_classes»				
«end_size_classes»				
V_COND	\dot{v}	energy conductance	cmd^{-1}	0.183
KAPPA	κ	allocation fraction to growth and somatic maintenance	-	0.45
pM	$[\dot{p}_M]$	volume specific somatic maintenance	$\text{Jd}^{-1}\text{cm}^{-3}$	44
EG	$[E_G]$	specific cost for structure	Jcm^{-3}	3900
DELTA_M	δ_M	shape coefficient	-	0.175
ME_0	M_E^0	initial reserve mass at optimal food conditions	molC^E	1.33×10^{-9}
EH_B	E_{Hb}	maturity at birth	J	1.79×10^{-4}
EH_P	E_{Hp}	maturity at puberty	J	1.78
KAP_R	κ_R	reproduction efficiency	-	0.75
GSR_MIN	GSR^{min}	minimum gonado-somatic ratio in the organism	$\text{molC}^R\text{molC}^{-1}$	0
GSR_SPAWN	GSR^{spawn}	gonado-somatic ratio to spawn	$\text{molC}^R\text{molC}^{-1}$	0.47
T_SPAWN	T^{spawn}	minimum temperature for spawning	$^{\circ}\text{C}$	18.7
F_FIX	f	constant food density parameter	-	only with option 1
PXM_FIX	$\{\dot{p}_{X_m}\}$	maximum surface area-specific ingestion rate	$\text{Jd}^{-1}\text{cm}^{-2}$	1027
K_FOOD	K_X	Food half saturation coefficient	mgCL^{-1}	0.4
K_SED	K_Y	Inorganic material half saturation coefficient	mgL^{-1}	40.4
YEX	y_{EXV}	yield coefficient of reserves in algae structure	$\text{molC}^E\text{molC}^V$	0.75
CRM	$\{\dot{C}_{Rm}\}$	Maximum surface area specific clearance rate	$\text{m}^3\text{d}^{-1}\text{cm}^{-2}$	0.096
JX1FM	$\{\dot{J}_{X_1Fm}\}$	Algae maximum surface area-specific filtration rate	$\text{molCd}^{-1}\text{cm}^{-2}$	4.8×10^{-4}
JX0FM	$\{\dot{J}_{X_0Fm}\}$	Silt maximum surface area-specific filtration rate	$\text{gd}^{-1}\text{cm}^{-2}$	3.5
RO_X1	ρ_{X_1I}	Algae binding probability	-	0.4
RO_X0	ρ_{X_0I}	Inorganic material binding probability	-	0.4
JX1IM	\dot{J}_{X_1Im}	Algae maximum ingestion rate	molCd^{-1}	1.3×10^4
JX0IM	\dot{J}_{X_0Im}	Inorganic material maximum ingestion rate	gd^{-1}	0.11
DV	$d_V = d_E$	bivalve structure and reserves specific density	$\text{g}_{(dw)}\text{cm}^{-3}$	0.09
MU_E	μ_E	bivalve reserves chemical potential	Jmol^{-1}	4.74×10^5

Table 12. Continuation: Keywords to be used in bivalve input file, in the `<begin_species>` block. The default value corresponds to the parameter values assumed for *Mytilus edulis* in Saraiva et al. (2014). Continuation on Table 12.

keyword	symbol	description	units	default value/option
Tref	T_{ref}	reference temperature	K	293
TA	T_A	Arrhenius temperature	K	5800
TL	T_L	Lower boundary tolerance range	K	281
TH	T_H	Upper boundary tolerance range	K	298
TAL	T_{AL}	Arrhenius temperature for lower boundary	K	75000
TAH	T_{AH}	Arrhenius temperature for upper boundary	K	30000
ME_B	ME_B	New born individual reserves	molC	1.28E-10
MV_B	MV_B	New born individual structure	molC	8.97E-13
MH_B	MH_B	New born individual structure	molC	3.76E-10
L_B	L_B	New born individual length	molC	0.003
LIFE_SPAN	a^\dagger	life span	y	
E_M	E_M	Maximum reserve capacity	Jcm ⁻³	
RESERVES_nH	n_E^H	chemical composition of bivalve reserve	molH/molC	1.8
RESERVES_nO	n_E^O	chemical composition of bivalve reserve	molO/molC	0.53
RESERVES_nN	n_E^N	chemical composition of bivalve reserve	molN/molC	0.15
RESERVES_nP	n_E^P	chemical composition of bivalve reserve	molP/molC	0.006
STRUCTURE_nH	n_E^H	chemical composition of bivalve structure	molH/molC	1.8
STRUCTURE_nO	n_E^O	chemical composition of bivalve structure	molO/molC	0.53
STRUCTURE_nN	n_E^N	chemical composition of bivalve structure	molN/molC	0.15
STRUCTURE_nP	n_E^P	chemical composition of bivalve structure	molP/molC	0.006
M_VELOCITY	m^V	fraction of individuals died due to high velocity	/d	0
MAX_VELOCITY	V_{max}	maximum velocity tolerable for the species	/d	0
M_NATURAL	m^N	natural/background mortality	d ⁻¹	[0,1[
M_SPAT	m^{egg}	initial egg mortality	d ⁻¹	[0,1[
M_STARVATION		Starvation?	-	0/1
DENSITYLIMIT		Density limit?	-	0/1
DENSITY_MAXVALUE		maximum density in each cell	# ⁻³	
SIMPLE_ASSI		simple assimilation?	-	0/1
SIMPLE_TEMP		simple Arrhenius function?	-	0/1
«begin_particle»				
«end_particle»				
<end_species>				

Table 13. Keywords to use in bivalve input file, in the `<<begin_particle>>` block. The default value corresponds to the parameter values assumed for *Mytilus edulis* in Saraiva et al. (2014).

keyword	symbol	description	units	default value/option
<begin_species>				
<<begin_particle>>				
NAME				
DESCRIPTION		the food		
ORGANIC		is this an organic particle?	-	0/1
SILICA_USE		silica?	-	0/1
RATIO_VARIABLE		N and P ratios variable?	-	0/1
RATIOHC	m_X^H	H fraction in algae biomass	mgH/mgC	0.18
RATIOOC	m_X^O	O fraction in algae biomass	mgO/mgC	1.18
RATIONC	m_X^N	N fraction in algae biomass	mgN/mgC	0.15
RATIOPC	m_X^P	P fraction in algae biomass	mgP/mgC	0.02
RATIOSiC	m_X^H	Si fraction in algae biomass	mgSi/mgC	0.024
RATIOCHLC	m_X^H	CHL fraction in algae biomass	mgCHL/mgC	0.017
SIZE	L_{food}	size of food particle	cm	0.2
F_E	f_E	reserves fraction in algae biomass	-	0.5
<<end_particle>>				
<end_species>				

Table 14. Keywords to use in bivalve input file, in the `<<begin_predator>>` block. The default value corresponds to the parameter values assumed for *Mytilus edulis* in Saraiva et al. (2014).

keyword	symbol	description	units	default value/option
<begin_species>				
<<begin_predator>>				
NAME				
DESCRIPTION				
SIZE	L_*	predator average size	cm	1.0
MINPREYSIZE	L_{mprey}^*	predator minimum prey size	cm	0.026
MAXPREYSIZE	L_{Mprey}^*	predator maximum prey size	cm	0.1
FEEDING_RATE	$\{\dot{p}_{Xm}^*\}$	predator max ingestion rate	$J d^{-1} cm^{-2}$	48.35
FEEDING_UNITS		units selection		1 $\#d^{-1} ind^{-1}$ 2 AFDWd $^{-1} ind^{-1}$ 3 $J d^{-1} cm^{-2}$
FEEDING_TIME		time options		1 Always 2 LowTide 3 HighTide
DIET_FRACTION	ρ^*	fraction of mussels in predator diet	adim	
AFDW_DW		conversion of afdw in dw	adim	
DW_C		conversion of dw in gCarbon	adim	
CORRECT_TEMP		temperature correction?	adim	1
SIMPLE_TEMP		simple temperature correction?	adim	1
P_Tref		Temperature reference for predator	K	
P_TA		Arrhenius temperature for predator	K	
P_TL		Lower Boundary tolerance rang	K	
P_TH		Upper Boundary tolerance range	K	
P_TAL		Arrhenius temperature for lower boundary	K	
P_TAH		Arrhenius temperature for upper boundary	K	
<<end_predator>>				
<end_species>				

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