Ecological Informatics
January 2012, Volume 7, Issue 1, Pages 71–80
http://dx.doi.org/10.1016/j.ecoinf.2011.11.007

A physical–biogeochemical coupling scheme for modeling marine coastal ecosystems

Ramón Filgueira[a, b, *], Jon Grant[b], Cédric Bacher[c], Michel Carreau[d]

[a] Consejo Superior de Investigaciones Científicas (CSIC), Instituto de Investigaciones Marinas, c/Eduardo Cabello 6, 36208 Vigo, Spain
[b] Department of Oceanography, Dalhousie University, Halifax, Canada NS B3H 4J1
[c] French Institute for Sea Research (IFREMER), BP70, 29280 Plouzané, France
[d] Hatch Ltd, 5 Place Ville Marie Suite 200, Montréal, Québec, Canada H3B 2G2

[*]Corresponding author : Ramón Filgueira, email address : ramonf@iim.csic.es

Abstract:

Ecological modeling of dynamic systems such as marine environments may require detailed spatial resolution when the modeled area is greatly influenced by complex physical circulation. Therefore, the simulation of a marine ecosystem must be underlain by a physical model. However, coupling hydrodynamic and biogeochemical models is not straightforward. This paper presents a modeling technique that can be used to build generic and flexible fully-spatial physical–biogeochemical models to study coastal marine ecosystems using a visual modeling environment (VME). The model core is constructed in Simile, a VME that has the capacity to create multiple instances of submodels that can be interconnected, producing a fully-spatial simulation. The core is designed to assimilate a choice of different hydrodynamic models by means of matrices, enhancing its compatibility with different software. The biogeochemical model can be modified by means of a graphical interface, which facilitates sharing within the scientific community. This paper demonstrates the application of the coupling scheme to mussel aquaculture in Tracadie Bay (PEI, Eastern Canada). The model was run for two different years, 1998 and 1999, and indicated that mussel biomass exerts a top-down control of phytoplankton populations, causing a maximum chlorophyll depletion of 61.0% and 80.3% for 1998 and 1999 respectively. The difference between both years highlights the importance of inter-annual variability, which is significant from an ecosystem-level perspective because it reveals the relevance of applying a precautionary policy in the management of aquaculture activity. Therefore, the proposed core developed in Simile is a generic and flexible tool for modeling long-term processes in coastal waters, which is able to assimilate a choice of hydrodynamic models, constituting a novel approach for generating fully-spatial models using visual modeling environments.

Highlights

► An offline physical–biogeochemical coupling scheme for marine systems is presented. ► The scheme can be used as a generic core to create fully-spatial models. ► The biogeochemical model can be easily modified using the Simile's GUI. ► Its application is demonstrated in an aquaculture site in PEI (Eastern Canada).

Keywords: Physical–biogeochemical coupling; Marine spatial planning; Aquaculture; Simile

1. Introduction

Dynamic ecosystem models provide a powerful approach to predict the consequences of natural or anthropogenic changes related to pollution, climate change, land-use patterns and other impacts. Models of marine ecosystems contain many examples of successful application of this approach, including nutrients cycles, contaminant dispersion, eutrophication and aquaculture-ecosystem interactions (e.g., Sarmiento et al., 1993; Chapelle et al., 1994; Baretta et al., 1995; Allen et al., 2010; Filgueira and Grant, 2009; Grant and Filgueira, in press). Ecosystem models have been used in the field of shellfish aquaculture to evaluate how the energy flow toward cultured biomass may potentially alter the food supply for other trophic levels such as natural benthos (Cloern, 1982; Dowd, 2003). In addition, ecological modelling is valuable in the study of bivalve growth and/or culture carrying capacity (Bacher et al., 1998; Dowd, 1997; Duarte et al., 2003; Ferreira et al., 1998; Grant et al., 2007a; Pastres et al., 2001; Raillard and Menesguen, 1994) and the effects of aquaculture on the ecosystem (Chapelle et al., 2000; Dowd, 2005). Carrying capacity models have been applied to manage cultivation areas (Bacher et al., 1998; Duarte et al., 2003; Ferreira et al., 1998) or increase profit in new areas (Heral, 1993). Given that coastal ecosystems are influenced largely by hydrodynamics, dynamic fully-spatial models must be underlain by a hydrodynamic model including the influence of diffusion–advection forced by tides, winds, and density gradients.

Circulation is the spatial manifestation of these processes and division of the environment into grid cells (e.g. finite element grid) allows these flows to be spatially resolved. The grid cells are not only connected, but they are conservative with respect to water flux, requiring a

hydrodynamic model based on equations of water motion. Although the models can be simplified, as in tidal prism calculations, spatial resolution is also sacrificed. There are many examples in which a hydrodynamic model is integrated with ecosystem fluxes to create spatial simulations (e.g. Ferreira et al., 2008; North et al., 2010), but this integration is not straightforward. For example, visual modelling environment (VME) software such as Stella (http://www.iseesystems.com) allows users to create models without writing code (Muetzelfeldt and Massheder, 2003). This has many advantages such as increased availability of simulation tools to non-specialists (i.e. researchers without in-depth knowledge of informatics/code programming), sharing of models between users, and efficient re-use of submodels (Silvert, 1993). Despite the sophistication of some VMEs, the ability to incorporate spatial realism as well as hydrodynamics has been limited and according to our knowledge there are no studies in the literature in which VMEs were used to generate detailed spatial resolution models of dynamic systems such as marine environments. VMEs have been more successfully applied to terrestrial environments (e.g. Elshorbagy et al., 2006; Randhir and Tsvetkova, 2011) in which physical processes such as groundwater flow can be simplified relatively easily compared to coastal hydrodynamics. For marine environments, improved ability to easily construct coupled physical-biogeochemical fully-spatial models based on VME would be beneficial, because it is a natural extension of the spatial context fostered by GIS, marine spatial planning and ecosystem-based management.

In addition, although the examples cited above are well-developed marine ecosystem models, the methodology is not easily adapted to other locations. Our focus in this paper is to provide insight about the integration of biogeochemical and ecological data with circulation models using object-oriented software, and to deliver a generic and flexible coupling environment

where the effort to export the model to other locations is reduced. The coupling scheme is developed in Simile (Appendix A), which is well suited to spatial models because it allows 'multiple instances' of a given submodel that can be interconnected, creating spatial connections (Muetzelfeldt and Massheder, 2003). In this study we demonstrate the application of the coupling scheme with an example from an aquaculture site in Prince Edward Island (Eastern Canada). In this example we used AquaDyn to create the hydrodynamic model and Matlab to calculate and deliver water exchange coefficients into Simile. We emphasize that AquaDyn and Matlab are not specific requirements of the coupling scheme, they are the tools used in this specific example. Other hydrodynamic models such as open source FVCOM (http://fvcom.smast.umassd.edu/) can also be used, as well as the open source Octave (http://www.gnu.org/software/octave/), R (http://www.r-project.org/) or Scilab (http://www.scilab.org/) instead of Matlab (http://www.mathworks.com/).

2. Material and Methods

2.1. Description of the physical-biogeochemical coupling scheme

In detailed spatial resolution models software must keep track of spatial locations and be suited to mapping, which is not generally a feature of VME applications. Fully-spatial models require more spatial complexity than the few boxes that can easily be set up in commercially-available VMEs. However, Simile is highly adaptable to handling spatial information, but there may be similar capacity in other software. Simile allows 'multiple instances' of a submodel that can represent the topology of the finite element grid created by the hydrodynamic model. These finite element grids are commonly composed by triangles or

squares called elements, which are defined by nodes and links (Figure 1a). The hydrodynamic model reports water velocity and direction for each node, allowing a calculation of water exchange between elements, which accounts for the hydrodynamics of the spatial connections. The crux of the coupling scheme is as follows (Figure 2):

- The hydrodynamic model generates a finite element grid and corresponding hydrodynamic regime.
- Simile reads the spatial topology of the finite element grid and hydrodynamics, which allow the coupling with the biogeochemical model.
- The biogeochemical results from Simile track the spatial topology, which can then be exported to GIS.

2.2. Adapting hydrodynamic results to Simile

The steps described in this section are common to all hydrodynamic models that can deliver results organized in matrices such as AquaDyn (Appendix A) or FVCOM. The following procedures (See Appendix B for a detailed description) were automated through a Matlab script:

- Velocity vectors are combined as root mean square velocities across grid boundaries to calculate the water flux in each element link for each time step. It is recommended the smallest time step possible be combined with the available computational power in order to provide the best resolution to the time series.
- Water fluxes of each time step are combined to generate average volumetric water exchange for each link.
- An optimization algorithm is applied to minimize the potential residual water imbalance caused by the averaging procedure.

- A matrix is generated with the averaged volumetric water exchange for each link.

We present an example using averaged hydrodynamics rather than time-dependent flows in order to simplify the coupling scheme. The volumetric water exchange between elements is calculated simultaneously in the whole grid following a first order upwind scheme. The water exchange between two adjacent elements is not calculated as a net flow but as a dispersion flow. This is a generalization of the tidal prism method at the scale of each element such that for each link between two adjacent elements, two averaged flows are calculated, one going from element *i* to *j* and one going from *j* to *i*. These exchange coefficients are divided by the volume of the elements where the flow enters in order to provide rates expressed as percentage day^{-1}.

2.3. Simile structure to read spatial information

Simile establishes relationships between the different submodels, which represent the elements of the grid, using its 'Condition' function, which specifies whether a connection between submodel instances exists. The use of 'Condition' requires a specific submodel that is described in Appendix C. This submodel allows reading the topology and the hydrodynamics of the hydrodynamic model by means of matrices. Therefore, this submodel provides a template that can be used as a core to develop any physical-biogeochemical model in Simile without further altering the coupling scheme itself.

In order to verify that water exchange parameterized within Simile is consistent with the physics predicted by the hydrodynamic model, a simple verification process is suggested. Both Simile and the hydrodynamic model are set up in the same way to run a model in which

a conservative tracer is the only component. Assuming a constant concentration of the tracer at the boundary and a lower and homogeneous distribution inside the bay at time 0, the model is run until equilibrium is reached. By comparing the tracer distribution in the bay after a period of time, we determine if Simile is correctly assimilating the hydrodynamics. It is very important to compare the general pattern and not the high frequency events, because the hydrodynamic model is using a continuous time series of water exchange and depth, including tidal variation, while Simile is using averaged values. This verification procedure is an internal control of the coupling process and does not exempt the researcher from validation of the physical and biogeochemical model.

2.4. Exporting the results to GIS

Simile outputs provide a single value for each triangular element, but these triangles are differently sized. Therefore, if these data were plotted in GIS, the weighting represented by the area of the triangle would not be preserved. This can be corrected by calculating the position of geometric reference points (Figure 1) within each triangle (Script available on request) based on its geometry:

- Centroid: the point of intersection of triangle medians (the lines joining each vertex with the midpoint of the opposite side). The centroid is the center of mass of an element and therefore the single value output by Simile.
- Nodes: the triangle's vertices calculated as the average of the centroids sharing the same vertex.
- Midpoints between the centroid and each node: calculated as the average between the centroid and the corresponding vertex.

These geometric points provide a grid that accounts for the differential area of grid cells. The maps we show below (Figure 4 and 10) were created with this method and plotted using AquaDyn capabilities. In addition, the Cartesian coordinates used in the hydrodynamic model may be normalized to UTM and used in any GIS.

2.5. Tracadie Bay Example

2.5.1. Study Site and objective

An example of the coupling approach is presented for Tracadie Bay, Prince Edward Island, Canada (Figure 3). The bay is a small (16.4 km^2 at mean tide and 13.8 km^2 at low tide), shallow (maximum depth 6 m) barrier beach inlet with semidiurnal tides (range of 0.6 m). It is open to the Gulf of Saint Lawrence through a single narrow channel. Exchange of the bay with the offshore is up to 500 $m^3 s^{-1}$ (Dowd, 2003), which results in a turnover of the entire volume of the Bay every 4-10 days (Dowd, 2005). Winter Harbour empties into the southeast of Tracadie Bay where Winter River drains a large watershed, but the input of freshwater is low for much of the year (~1 $m^3 s^{-1}$; see also Cranford et al., 2007). Mussel culture in the bay is located as shown in Figure 3 and the biomass calculated according to Dowd (2003, 2005), who estimated a standing stock of between 1 and 2 x 10^6 kg wet weight mussels. The standing stock of 1.5 x 10^6 kg wet weight of mussels is considered the actual scenario in Tracadie Bay and it is homogeneously distributed in culture areas (Figure 3). Tissue weight was calculated assuming a condition index of 30%. Dry weight was calculated assuming water content of 80% and a carbon content of 40% mussel dry weight.

The goal of this example is to analyze phytoplankton depletion due to suspension feeding contrasting two consecutive years, 1998 and 1999, with different far-field conditions, and to

205 demonstrate the potential of the model for studying the implications of inter-annual variations
206 in carrying capacity estimations. The main purpose of this example is to show how to apply
207 the coupling scheme. Implications of the model for aquaculture environment interactions
208 have been explored in the references cited below.
209
210 ***2.5.2. Hydrodynamic Model***
211 The boundaries and depths of the bay were digitized from a hydrographic chart. The finite
212 element mesh was generated within AquaDyn, tuning mesh size and density. The 2D
213 hydrodynamics was forced by a time series of sea level, and friction was applied via a
214 Manning coefficient. The resulting triangular mesh contained 544 elements, and 1454
215 connections across links. Application of an AquaDyn model to Tracadie Bay was validated
216 using sea level data (Grant et al., 2005). In the present study, the hydrodynamic model was
217 further ground-truthed by comparing the modulus of velocity vector in Node # 236 with
218 current meter time series available for the same location (46º23'56''N, 62º59'56''W) and
219 period between 15 June and 15 September 2002.
220
221 ***2.5.3. Biogeochemical model***
222 The biogeochemical model used in Simile is based on a classical PNZ model (phytoplankton
223 (P) – Nutrients (N) – Zooplankton (Z)) with the addition of mussel (M) and detritus (D)
224 submodels. Given the minimal effect of Zooplankton in the results, this submodel was turned
225 off in subsequent scenarios. All the submodels are characterized in terms of carbon per cubic
226 meter (mg C m^{-3}), with the exception of dissolved nutrients, which are expressed as
227 milligrams of nitrogen per cubic meter (mg N m^{-3}). The equations of the model are based on
228 Kremer and Nixon (1978), a brief description of the different terms is given in Table 1 and a

detailed description as well as the exact values of the parameters are given in Grant et al. (1993, 2007a, 2008), Dowd (1997, 2005) and Filgueira and Grant (2009). The differential equations are as follows:

$$\frac{dP}{dt} = +P_{growth} - P_{mortality} - M_{grazing} \pm P_{mixing} \quad \text{Eq. 1}$$

$$\frac{dN}{dt} = +N_{river} + M_{excretion} - P_{uptake} \pm N_{mixing} \quad \text{Eq. 2}$$

$$\frac{dD}{dt} = +D_{resuspension} + M_{feces} + P_{mortality} - D_{sinking} - M_{grazing} \pm D_{mixing} \quad \text{Eq. 3}$$

$$\frac{dM}{dt} = +M_{net\ growth} + M_{seeding} - M_{mortality} - M_{harvesting} = 0 \quad \text{Eq. 4}$$

The mussel compartment biomass is assumed to be constant over time, so that the mussel biomass interacts with the ecosystem model as a forcing function rather than a response variable (Dowd, 2005). By manipulating forcing by mussel biomass, some of the more uncertain steps related to aquaculture activity are not required (for example, farming processes like harvesting and seeding, or bivalve size distribution). In addition, bivalve mortality rate is not explicit in the model. In essence, this assumption means that the growth of the bivalves and seeding activity is compensated by mortality rate and harvesting, providing the constant biomass.

The model was run between 15 June and 15 September for two years, 1998 and 1999. The main differences between both years are related to suspended detritus content and wind speed. Average organic detritus content of 857±250 mg C m^{-3} and 565±193 mg C m^{-3} was observed in 1998 and 1999, respectively. In addition, the percentage of days with wind speeds higher than 5 m s^{-1}, the threshold for bottom resuspension (Filgueira and Grant, 2009; Walker and Grant, 2009), was 8.89 % and 2.22 % in 1998 and 1999, respectively. Waite et al.

(2005) and Filgueira and Grant (2009) provide further details of the model as well as the boundary conditions.

Ground-truthing was carried out by comparing the modelled chlorophyll values in Element # 182 (See Figure 3 for location) with observations in both years, 1998 and 1999. The time series were analyzed with major axis regression method (RMA) following Duarte et al. (2003). The significance of the regression was tested using ANOVA and comparison of the slope and intercept with 1 and 0, respectively, carried out following Zar (1984).

3. Results

3.1. Ground-truthing

The average measured water speed values and standard deviation were higher than the modelled values (Table 2), because current meter dataset contains extreme values, caused by strong local winds, which exert a bias in the time series comparison. A better indicator of central tendency for skewed distributions is the median, which minimizes the contribution of extreme values and outliers. Median values of the model, 4.18 cm s^{-1}, were in good agreement with the current meter values, 4.48 cm s^{-1}, suggesting that the circulation model realistically reproduced the hydrodynamics.

The calculation of the first order upwind scheme error (Appendix B) in the chlorophyll compartment resulted in an averaged value over the elements and time of 0.029% (maximum 1.005%) and 0.097% (maximum 1.738%) respectively, which is an excellent indication that cell size and daily averaging time step are small enough. In addition, the verification test

described (Section 2.3) was performed in order to verify that Simile is correctly assimilating the hydrodynamics from AquaDyn. Both models were set up with a constant tracer concentration in the boundary of 2 units m^{-3} and an initial tracer concentration in the domain of 1 unit m^{-3}. The distribution of the tracer after 10 days (Figure 4) shows a similar pattern in both AquaDyn and Simile. The largest discrepancies between both approaches are located in the northeastern part of the bay. Two elements (See Figure 3 for location) were analyzed in detail for a longer period of time, one located in the northeastern part of the bay (element 385) and another located in the southern section (element 182). Original AquaDyn time series were transformed by applying a moving average regression in order to smooth high frequency events with a period lower than one day (e.g. wind and tides), in order to provide an average value for each day (Figure 5). This analysis highlights the better agreement in the southern section, element 182. However, the discrepancies between AquaDyn and Simile in the northern section, element 385, become smaller with time. Although the tracer is slightly different in this element after 30 days, this convergence pattern and the similar spatial distribution indicate that Simile is properly assimilating the AquaDyn output of the hydrodynamics.

Ground-truthing of the coupled physical-biogeochemical model was carried out by comparing modelled and observed values of chorophyll. The ANOVAs indicated that the regressions (1998: *Modelled* = 1.13±0.14 *Observed* +11.95±17.14, $r^2 = 0.47$, $p<0.05$; 1999: *Modelled* = 0.85±0.09 *Observed* +36.34±25.78, $r^2 = 0.52$, $p<0.05$) are statistically significant. Analysis of the slopes showed that in 1998 the model follows the same pattern as the observations ($p=0.356$). However, in 1999 the slope was less than 1 ($p<0.05$), indicating that

298 the results of the model are offset from the observations. The intercepts are greater than 0
299 indicating that the model is slightly enriched in chlorophyll compared to the observed values.
300
301 ***3.2. Model results***
302 The physical-biogeochemical model was run between 15 June and 15 September in two
303 scenarios for each year (1998 and 1999): without mussels and with a mussel standing stock of
304 1 x 10^6 kg wet weight, the minimum biomass in Tracadie Bay according to previous studies
305 (Dowd, 2003, 2005). Model outputs are shown as the percentage of chlorophyll depletion in
306 the mussel scenarios compared to the non-mussel scenario. The bay-averaged chlorophyll
307 depletion over the studied period ranged from 4.8% to 44.4% and 10.3% to 58.6% in 1998
308 and 1999, respectively (Figure 6). The maximum daily depletion observed in an element in
309 the bay was 61.0% and 80.3% for 1998 and 1999, respectively. The time-averaged
310 chlorophyll depletion for the whole bay was 26.6±8.1% and 30.0±8.8% for 1998 and 1999,
311 respectively. These differences are caused by the variation in boundary forcing conditions
312 between years. The time-averaged chlorophyll depletion (Figure 7) is related to the culture
313 area displaying decreases in depletion in the direction of nutrient sources, i.e. toward Winter
314 River and the inlet (Gulf Saint Lawrence), where culture density is negligible. In addition, the
315 effect of different boundary conditions between years can be observed, showing more intense
316 and extended chlorophyll depletion in 1999 compared to 1998.
317
318
319 **4. Discussion**
320 The ability to couple physical and biogeochemical models is fundamental to simulating
321 marine ecosystems. These coupling schemes can be classified as ‘integration’, ‘online

coupling' and 'offline coupling'. Integration refers to utilizing physical exchange in a reduced spatial resolution, e.g. rates averaged across space for a box model. At the other end of the linkage spectrum between physics and biogeochemistry, online coupling indicates that both physical and biogeochemical models run simultaneously. In between are offline coupling techniques, where the physics is run first and the biogeochemical model is run subsequently using physical outputs at different time steps but the same spatial scale. Fully spatial models constructed in VMEs require offline coupling given the limited connectivity with physical simulation software. Our motivation in the present study is to provide insight into the integration of physical and ecological data using a visual modelling environment (VME), which, to our knowledge, is the first example in the literature in which a VME is used to generate a fully spatial model.

There are other approaches in the literature (Table 3) that usually require expertise in language programming and/or specific sophisticated software to create/modify modules, and in some cases the structure of these modules is rigid and non-modifiable. The coupling scheme described in this paper represents a novel approach to create fully-spatial models using a Visual Modelling Environments (VME). VMEs such as Stella or Simile have commonly been used in scientific literature given their smooth learning curve. VMEs are based in objects that represent stocks, flows, variables and their interactions. The connections of these objects symbolize ecological processes, and the fact that they can be visualized facilitates access to non-programmers. These visual symbols make it easier to spread and share models in the scientific community, a cornerstone for improving the conceptual design of any model.

346 The general scheme described in this paper constitutes a generic and flexible core for
347 coupling physical-biogeochemical models in coastal areas. The specifics of the ecosystem
348 model are initially developed in Simile and the submodels described in this paper allow the
349 coupling of hydrodynamics constructed in a different modelling environment, which can be
350 2D or 3D. In fact, the described scheme is quite flexible and can be used with only a few cells
351 to construct a box model. When the coupling scheme is applied to a new site, the
352 biogeochemical model can be re-used and the principal effort is focused on the hydrodynamic
353 model. Once the model is developed, the results can be exported to GIS for mapping,
354 increasing the connectivity of the model with other applications. Another advantage of the
355 coupling scheme developed in Simile is that the optimization tool PEST (Model-Independent
356 Parameter ESTimation, Watermark Numerical Computing) is integrated into Simile. PEST
357 can be used with two objectives in mind: (1) tune parameters in order to calibrate the model,
358 avoiding "eyeball" calibrations, or with the appropriate dataset estimates unknown or
359 uncertain parameters, and (2) optimize management strategies according to a variety of
360 criteria (e.g. Filgueira et al., 2010).
361
362 The coupling technique used in Simile follows an offline unidirectional scheme, that is, the
363 hydrodynamic model is run first and the results are delivered to the biogeochemical model
364 that is run subsequently, without providing feedback to the hydrodynamic model. This is not
365 a problem in this particular case given that the feedback of the biogeochemical model is not
366 relevant for the hydrodynamics of the bay. In fact, in shallow waters, tides, winds and
367 freshwater, runoff drives components of the circulation (Kjerfve and Magill, 1989). The
368 hydrodynamics are averaged following a first-order upwind scheme before being delivered to
369 the biogeochemical model. Since this averaging process dilutes the effect of high frequency

events, the application of the model scheme is limited to the study of long-term processes. These aspects of offline coupling must be taken into account when the general goals are set.

The described coupling scheme was applied to Tracadie Bay, a shallow bay with extensive aquaculture activity. This application is presented as an example of the coupling scheme and not as a research exercise itself. The bay is an excellent test bed because we have conducted a variety of field and modellling studies there. Grant et al. (2008) employed a model of seston depletion in Tracadie Bay in which AquaDyn results were coupled with a Matlab ecosystem model. Although specific to average seasonal nutrient, temperature, and boundary conditions, maps of seston depletion (Figure 4B in Grant et al., 2008) show near-identical patterns to those depicted in Figure 7. In addition, the chlorophyll depletion values of 61.0% and 80.3% for 1998 and 1999, respectively, are in good agreement with the values observed by Grant et al. (2007b, 2008) in the same bay during a short-term experiment. These authors predicted a 67% reduction in chlorophyll in the north-south transect of Tracadie bay, the main axis of the bay where mussel culture is located.

The approaches to shellfish aquaculture models can be divided into box models and fully-spatial physical-biogeochemical models (Grant and Filgueira, in press). Although it is possible to simplify hydrodynamics and include them in a box model, the spatial detail provided by a fully-spatial physical-biogeochemical model is desirable for two reasons. (1) high spatial resolution allows us to simulate the effects of farm location on the ecosystem and the interaction between farms (e.g. Figure 7). Therefore, management policies related to spatial arrangement of farms can be pursued as well as a prediction of bivalve growth rate as a function of culture biomass in each location. (2) The results can be mapped, an obvious

advantage for representing trends and gradients in marine systems. Spatial resolution can also affect the results of the model, especially when processes are dependent on concentration (Fennel and Neumann, 2004).

In conclusion, we have focused on Simile, which incorporates a graphical user interface, is an object-oriented software, and offers the capability of topology recognition using matrices, an ideal modelling platform from which to pursue physical-biogeochemical simulation. The coupling scheme has satisfied tests of internal and external consistency and conservative behavior, and shown results compatible with previous field and modelling studies of the test location. The Simile coupling scheme has the following positive characteristics: (1) the biogeochemical model can be modified by way of a user-friendly graphical interface; (2) knowledge of programming language is minimized; (3) results can be exported to GIS, and (4) an optimization tool (PEST) is integrated. Therefore, the proposed core developed in Simile is a generic and flexible tool for modelling long-term processes in coastal waters, which is able to assimilate a choice of hydrodynamic models, constituting a novel approach for generating fully-spatial models using visual modelling environments.

Acknowledgements

This research was funded by a Strategic Project Grant and Discovery Grant from the Natural Sciences and Engineering Research Council of Canada (NSERC) to JG. RF salary was supported by an Angeles Alvariño (Xunta de Galicia) contract and a Xunta de Galicia fellowship co-funded by the European Social Fund (Operative Program Galicia 2007-2013).

Appendix A. Software description

Simile is a graphical system-dynamics modelling tool that incorporates object-oriented concepts. The software is available from Simulistics Ltd. Visit http://www.simulistics.com or email info@simulistics.com for details. Simile is available for Windows (95 onwards), Linux (all) and MacOS (OSX 10.3 onwards). It takes between 20 and 50 MB of disk space depending on the platform. Simile has a proprietary license but its data formats are open. Models can be freely distributed, and those built with Simile Enterprise can be run on a free version of the software.

AquaDyn is a two dimensional free surface water hydrodynamic and dispersion software that uses a finite element technique to solve the St-Venant equations. AquaDyn takes into account bathymetry, bed friction, wind stress, turbulent dissipation and complex coastlines. The software can be obtained from Hatch Ltd. Email or call Michel Carreau (mcarreau@hatch.ca; +1 514-864-5500 (ext. 6108)) for further details. The entire package once installed takes less then 10 megabytes of space. Each model within AquaDyn is stored within one project file which contains all inputs and outputs; the file size is typically smaller then 3 megabytes. The software executable has been available since 1995 (the source code is not available for distribution) and can be run on any Windows 32 bits operating system.

In addition to the validation performed by the developers, AquaDyn has been used and validated in several studies carried out by our research group (Grant and Bacher, 2001; Grant et al., 2005, 2008), various engineering consulting firms and schools (Belanger et al., 2000; Ministère des resources naturelles – Québec, 2002).

Appendix B. Volumetric flow calculation (Matlab script available on request).

Every node (shared vertex) within AquaDyn is represented with an X and Y Cartesian value in the grid. For each node AquaDyn provides values for three quantities: water speed in x-direction, water speed in y-direction and water depth at each time step. AquaDyn stores the results in matrices that can be programmatically retrieved and manipulated. In an AquaDyn model each element (grid cell) can be surrounded by a maximum of 3 elements and a minimum of 1 element. Boundary elements always have less than 3 surrounding elements. The exchange of water for a given element is defined in relation to each of the surrounding elements in the mesh in terms of volumetric exchange. The volumetric flow through a link from one element to another is calculated by multiplying the net velocity by the cross-sectional area through the side:

Volumetric Flow = (net velocity) x cross-sectional area

= (net velocity) x (average depth at the two nodes of the link) x (length of link)

The net velocity (nx.u+ny.v) is defined as the projection of the velocity vector (u, v) at the centre of each side (link) into the unit perpendicular vector of the link (nx, ny). The units of the velocity vector (u, v), where u is the average velocity in the x-direction at the two ends of the link and v is similarly defined for the y direction, are adjusted to meters per day, which are compatible with Simile time steps. The unit perpendicular vector (nx, ny) is defined to point towards the centre of the element (Figure B.1a). Therefore a positive/negative net velocity indicates that flow is into/out of the element.

Taking into account the node coordinates, (xA, yA) and (xB, yB), the (nx, ny) vector is calculated as follows (Figure B.1a):

$nx = -(yA-yB)/[(xA-xB)^2+(yA-yB)^2]^{0.5}$

$ny = (xA-xB)/[(xA-xB)^2+(yA-yB)^2]^{0.5}$

or

$nx = (yA-yB)/[(xA-xB)^2+(yA-yB)^2]^{0.5}$

$ny = -(xA-xB)/[((xA-xB)^2+(yA-yB)^2]^{0.5}$

In order to compute which of the vectors is directed into the element, the (nx, ny) vector must be compared with the direction of the vector (px, py), whose origin is the middle of the link and terminus is the opposite node (Figure B.1b). If the quantity nx.px+ny.py is positive, (nx, ny) and (px, py) follow the same direction into the element, and vice versa for negative values.

AquaDyn provides a time series for water velocity and depth at each node, and the protocol described above can be applied to each time step. However, in Simile the coupling is simplified and the Matlab script delivers to AquaDyn the volumetric water exchange as a daily average for each link following a first order upwind scheme. The error of this scheme is kept to a minimum if the spatial and temporal variation of the concentration of a conservative tracer remains small for each element and time step:

$$Error_{spatial}\ (\%) = \left(\frac{|\Delta Conc.|}{\overline{Conc.}}\right)^2_{spatial} x100 \qquad \text{Eq. B. 1}$$

$$Error_{time}\ (\%) = \left(\frac{|\Delta Conc.|}{\overline{Conc.}}\right)^2_{time} x100 \qquad \text{Eq. B. 1}$$

where $|\Delta Conc.|$ is the absolute difference in concentration between two connected elements at a given time (Eq. B.1), or between two time steps for the same cell (Eq. B.2). $\overline{Conc.}$ is the mean concentration of both values for each case. The calculation of this error is crucial in evaluating the general error of the coupling scheme.

The numerical procedure carried out to calculate the exchange and the averaging process can cause a residual water imbalance within the bay. Therefore, a minimization algorithm under constraint (pinv function in Matlab) was applied to the averaged exchange in order to minimize the water imbalance (to make the net flows zero) while keeping the correction factors as small as possible (script available on request). After this process, two CSV files are created, one with the averaged volume (m^3) of each element, the other with the averaged volumetric exchange rates (d^{-1}), *Exchange-Entry* and *Exchange-Exit*, as well as the identification numbers of *Entry-Box* and *Exit-Box*, i.e. which elements are linked. This CSV file contains one row for each link, i.e between every adjacent element pair and therefore defines the spatial connections between them in a way interpretable by Simile.

503 **Appendix C. Simile structure to read spatial information (Files available on request).**

504 The use of 'Condition' requires variables to identify multiple instances saved in arrays inside
505 Simile or in external CSV files. These index variables, *Entry-Box* and *Exit-Box*, are used to
506 identify associations between elements in the grid and the calculated water volumetric
507 exchange rates, *Exchange-Entry* and *Exchange-Exit*, to incorporate the hydrodynamics.
508
509 The following example, considering the dynamics of total suspended particulate matter
510 (TPM, turbidity) in a bay (Figure C.1) provides a template that can be used as a core to
511 develop any application of the coupling scheme in Simile. The 'number of instances' (an
512 innate property of all submodels in Simile) of the *Bay* submodel was modified to create *n*
513 copies that represent the *n* elements of the spatial grid. Two submodels were created to
514 manage the *Inflow* and *Outflow* of TPM and another one, *Connections*, that allows loading of
515 external data from CSV files by using 'Fixed Parameter' variables. The *Connections*
516 submodel has a 'number of instances' equal to the number of connections between elements,
517 i.e. the number of rows of the external CSV file. *Inflow* and *Outflow* submodels were related
518 with 'Exclusive Role' to the *Connections* submodel and 'Normal Role' to the *Bay* submodel.
519 The *Inflow* and *Outflow* submodels establish if there is a connection between any two
520 elements by means of the 'Condition' functions (*Cond1* and *Cond2* in Figure C.1). For
521 example, the *Inflow* submodel checks if the *Box_Number* variable from the *Bay* submodel
522 matches the *Entry-Box* variable value (which depends on the rows of the external CSV file).
523 If there is a match, the corresponding *Exit-Box* (the same row as the *Entry-Box* value) is
524 matched with the appropriate *Box_Number* in the *Bay* submodel. Given these prescribed
525 connections, the flow exchange is taken from the same row of the CSV file as the data input
526 (*Exchange-Entry* and *Exchange-Exit*). Once these exchanges are established, the physical-

material coupling is completed. Therefore if an element exports TPM, the appropriate mass flux of TPM (concentration * exchange) will be removed from the TPM compartment and the same amount of TPM will be added to the element that receives the TPM. All the rows of the CSV file, exchange between elements, are processed by Simile at the same time, therefore the hydrodynamic of the whole bay is coupled simultaneously, preserving continuity in the system.

Although hydrodynamics are coupled with the biogeochemical model as described above, a fully-spatial model requires that individual variables also be initialized in space, e.g. the initial concentration of TPM in each element. Figure C.2 shows the same model with the addition of two new submodels to introduce the initial TPM value in each element. This is accomplished using an external CSV file which contains two columns, the element index variable and the initial TPM value in that element (*Box* and *Initial TPM Value*, respectively). The submodel called *Initial TPM* reads these variables from an external CSV file using 'Fixed Parameter' variables. The submodel called *Initial Condition* checks if the *Box_Number* variable from the *Bay* submodel matches the *Box* variable value from the *Initial TPM* submodel (which depends on the rows of the external CSV file). If there is a match the *Initial TPM Value* will be introduced into the *Bay* submodel as the initial value of TPM for the *Box_Number* element. The same procedure can be applied to other variables, such as the presence/absence of aquaculture, providing a very fine spatial resolution of the initial conditions.

548 **References**

549 Allen, J.I., Aiken, J., Anderson, T.R., Buitenhuis, E., Cornell, S., Geider, R.J., Haines, K.,
550 Hirata, T., Holt, J., Le Quere, C., Hardman-Mountford, N., Ross, O.N., Sinha, B., While, J.,
551 2010. Marine ecosystem models for earth system applications: The MarQUEST experience.
552 J. Marine. Syst. 81, 19-33.
553
554 Bacher, C., Duarte, P., Ferreira, J.G., Héral, M., Raillard, O., 1998. Assessment and
555 comparison of the Marennes-Oléron Bay (France) and Carlingford Lough (Ireland) Carrying
556 Capacity with ecosystem models. Aquat. Ecol. 31, 379-394.
557
558 Bacher, C., Grant, J., Hawkins, A., Fang, J., Zhu, P., Duarte, P., 2003. Modelling the effect of
559 food depletion on scallop growth in Sungo Bay (China). Aquat. Living. Resour. 16, 10-24.
560
561 Baretta, J.W., Ebenhoh, H., Ruardij, P., 1995. The European-regional-seas-ecosystem-model,
562 a complex marine ecosystem model. Neth. J. Sea. Res. 33, 233-246.
563
564 Behm, P., Boumans, R.M.J., Short, F.T., 2004. Spatial modeling of eelgrass distribution in
565 Great Bay, New Hampshire, in: Constanza, R., Voinov, A. (Eds.), Landscape simulation
566 modelling. A spatially explicit, dynamic approach. Springer-Verlag, New York, pp. 173-196.
567
568 Belanger, M., Carreau, M., Vincent, A. 2000. A test field calibration to validate shallow-
569 water codes: the case of the Ste- Marguerite River with AquaDyn. Centre de Recherche en
570 Calcul Applique (CERCA) Technical Report TR-2006-01, University of Montreal.
571

572 Chapelle, A., Lazure, P., Menesguen, A., 1994. Modeling eutrophication events in a coastal
573 ecosystem – sensitivity analysis. Estuarine Coast. Shelf Sci. 39, 529-548.
574
575 Chapelle, A., Menesguen, A., Deslous-Paoli, J.M., Souchu, P., Mazouni, N., Vaquer, A.,
576 Millet, B., 2000. Modelling nitrogen, primary production and oxygen in a Mediterranean
577 lagoon. Impact of oysters farming and inputs from the watershed. Ecol. Model. 127, 161-181.
578
579 Cloern, J.E., 1982. Does the benthos control phytoplankton bio- mass in southern San
580 Francisco Bay? Mar. Ecol. Prog. Ser. 9, 191–202.
581
582 Cranford, P.J., Strain, P.M., Dowd, M., Hargrave, B.T., Grant, J., Archambault, M.C., 2007.
583 Influence of mussel aquaculture on nitrogen dynamics in a nutrient enriched coastal
584 embayment. Mar. Ecol. Prog. Ser. 347, 61-78.
585
586 Dowd, M., 1997. On predicting the growth of cultured bivalves. Ecol. Model. 104, 113-131.
587
588 Dowd, M., 2003. Seston dynamics in a tidal inlet with shellfish aquaculture: a model study
589 using tracer equations. Estuarine Coast. Shelf Sci. 57, 523-537.
590
591 Dowd, M., 2005. A bio-physical coastal ecosystem model for assessing environmental effects
592 of marine bivalve aquaculture. Ecol. Model. 183, 323-346.
593

Duarte, P., Meneses, R., Hawkins, A.J.S., Zhu, M., Fang, J., Grant, J., 2003. Mathematical modelling to assess the carrying capacity for multi-species culture within coastal waters. Ecol. Model. 168, 109-143.

Elshorbagy, A., Teegavarapu, R.S.V., Ormsbee, L., 2006. Assessment of pathogen pollution in watersheds using object-oriented modeling and probabilistic analysis. J. Hydroinform. 8, 51-63.

Fennel, W., Neumann, T., 2004. Introduction to the modelling of marine ecosystems. Elsevier Oceanography Series, 72. Elsevier, Amsterdam.

Fennel, K., Wilkin, J., Levin, J., Moisan, J., O'Reilly, J., Haidvogel, D., 2006. Nitrogen cycling in the Middle Atlantic Bight: Results from a three-dimensional model and implications for the North Atlantic nitrogen budget. Glob. Biogeochem. Cycles 20, GB3007, doi:10.1029/2005GB002456.

Ferreira, J., Duarte, P., Ball, B., 1998. Trophic capacity of Carlingford Lough for aquaculture - analysis by ecological modelling. Aquat. Ecol. 31, 361-379.

Ferreira, J.G., Hawkins, A.J.S., Monteiro, P., Moore, H., Service, M., Pascoe, P.L., Ramos, L., Sequeira, A., 2008. Integrated assessment of ecosystem-scale carrying capacity in shelfish growing areas. Aquaculture 275, 138-151.

617 Filgueira, R., Grant, J., 2009. A box model for ecosystem-level management of mussel
618 culture carrying capacity in a coastal bay. Ecosystems 12, 1222-1233.
619
620 Filgueira, R., Grant, J., Strand, Ø., Asplin, L., Aure, J., 2010. A simulation model of carrying
621 capacity for mussel culture in a Norwegian fjord: role of forced upwelling. Aquaculture 308,
622 20-27.
623
624 Grant, J., Bacher, C., Cranford, P.J., Guyondet, T., Carreau, M., 2008. A spatially explicit
625 ecosystem model of seston depletion in dense mussel culture. J. Mar. Syst. 73, 1555-168.
626
627 Grant, J., Bugden, G., Horne, E., Archambault, M.-C., Carreau, M., 2007b. Remote sensing
628 of particle depletion by coastal suspension-feeders. Can. J. Fish. Aquat. Sci. 64, 387-390.
629
630 Grant, J., Cranford, P., Hargrave, B., Carreau, M., Schofield, B., Armsworthy, S., Buerdett-
631 Coutts, V., Ibarra, D., 2005. A model of aquaculture biodeposition for multiple estuaries and
632 field validation at blue mussel (*Mytilus edulis*) culture sites in eastern Canada. Can. J. Fish.
633 Aquat. Sci. 62, 1271-1285.
634
635 Grant, J., Curran, K.J., Guyondet, T.L., Tita, G., Bacher, C., Koutitonsky, V., Dowd, M.,
636 2007a. A box model of carrying capacity for suspended mussel aquaculture in Lagune de la
637 Grande-Entrée, iles-de-la-Madeleine, Québec. Ecol. Model. 200, 193-206.
638

639 Grant, J., Dowd, M., Thompson, K., Emerson, C., Hatcher, A., 1993. Perspectives on field
640 studies and related biological models of bivalve growth, in: Dame, R. (Ed.), Bivalve filter
641 feeders and marine ecosystem processes. Springer, New York, pp. 371-420.
642
643 Grant, J., Filgueira, R., (in press). The application of dynamic modelling to prediction of
644 production carrying capacity in shellfish farming, in: Shumway, S (Ed.), Shellfish
645 aquaculture and the environment. John Wiley & Sons, New York.
646
647 Héral, M., 1993. Why carrying capacity models are useful tools for management of bivalve
648 molluscs culture, in: Dame, R. (Ed.), Bivalve filter-feeders in estuarine and coastal
649 ecosystems. NATO ASI Series, pp. 455-477.
650
651 Kjerfve, B., Magill, K.E., 1989. Geographic and hydrodynamic characteristics of shallow
652 coastal lagoons. Mar. Geol. 88, 187-199.
653
654 Kremer, J., Nixon, S.W., 1978. A Coastal Marine Ecosystem: Simulation and Analysis.
655 Springer-Verlag, New York.
656
657 Maxwell, T., Constanza, R., 1994. Spatial ecosystem modelling in a distributed
658 computational environment, in: van den Bergh, J., van der Straaten, J. (Eds.), Towards
659 Sustainable Development: Concepts, Methods, and Policy. Island Press, Washington DC.
660
661 Maxwell, T., Constanza, R., 1995. Distributed modular spatial ecosystem modelling.
662 International Journal of Computer Simulation 5, 247-262.

663

664 Maxwell, T., Constanza, R., 1997a. An open geographic modelling environment. Simulation
665 Journal 68, 175-185.
666
667 Maxwell, T., Constanza, R., 1997b. A language for modular spatio-temporal simulation.
668 Ecol. Model. 103, 105-113.
669
670 Ministère des resources naturelles – Québec, 2002. Régularisation des crues du bassin versant
671 du lac Kénogami. Saguenay-Lac-Saint-Jean 621 1-01-005
672
673 Muetzelfeldt, R., Massheder, J., 2003. The Simile visual modelling environment. Eur. J.
674 Agron. 18, 345-358.
675
676 North, E.W., King, D.M., Xu, J., Hood, R.R., Newell, R.I.E., Paynter, K., Kellogg, M.L.,
677 Liddel, M.K., Boesch, D.F., 2010. Linking optimization and ecological models in a decision
678 support tool for oyster restoration and management. Ecol. Appl. 20, 851-866.
679
680 Pastres, R., Solidoro, C., Cossarini, G., Canu, D.M., Dejak, C., 2001. Managing the rearing of
681 *Tapes philippinarum* in the lagoon of Venice: a decision support system. Ecol. Model. 138,
682 231-245.
683
684 Pereira, A., Duarte, P., 2005. EcoDynamo: Ecological Dynamics Model Application. DITTY
685 Report. Available at http://www.dittyproject.org/Reports.asp
686

687 Pereira, A., Duarte, P., Norro, A., 2006. Different modelling tools of aquatic ecosystems: A
688 proposal for a unified approach. Ecol. Inform. 1, 407-421.
689
690 Raillard, O., Ménesguen, A., 1994. An ecosystem model for the estimating the carrying
691 capacity of a macrotidal shellfish system. Mar. Ecol. Prog. Ser. 115, 117-130.
692
693 Randhir, T.O., Tsvetkova, O., 2011. Spatiotemporal dynamics of landscape pattern and
694 hydrologic process in watershed systems. J. Hydrol. 404, 1-12.
695
696 Sarmiento, J.L., Slater, R.D., Fashman, M.J.R., Ducklow, H.W., Toggweiler, J.R., Evans,
697 G.T., 1993. A seasonal 3-dimensional ecosystem model of nitrogen cycling in the North-
698 Atlantic euphotic zone. Global Biochem. Cy. 7, 417-450.
699
700 Shchepetkin, A.F., McWilliams, J.C., 2005. The Regional Ocean Modelling SystemL A split-
701 explicit, free-surface, topography following coordinates ocean model. Ocean Model. 9, 347-
702 404.
703
704 Silvert, W., 1993. Object-oriented ecosystem modeling. Ecol. Model. 68, 91-118.
705
706 Spillman, C.M., Hamilton, D.P., Hipsey, M.R., Imberger, J., 2008. A spatially resolved
707 model of seasonal variations in phytoplankton and clam (*Tapes philippinarum*) biomass in
708 Barbamarco Lagoon, Italy. Estuarine Coast. Shelf Sci. 79, 187-203.
709

Umgiesser, G., Canu, D.M., Solidoro, C., Ambrose, R., 2003. A finite element ecological model: a first application to the Venice Lagoon. Environ. Modell. Softw. 18, 131-145.

Waite, L., Grant, J., Davidson, J., 2005. Bay-scale spatial growth variation of mussels *Mytilus edulis* in suspended culture, Prince Edward Island, Canada. Mar. Ecol. Prog. Ser. 297, 157-167.

Walker, T.R., Grant, J., 2009. Quatifying erosion rates and stability of bottom sediments at mussel aquaculture sites in Prince Edward Island. J. Marine. Syst. 75, 46-55.

Zar, J.H., 1984. Biostatistical Analysis. New Jersey: Prentice-Hall.

Figure Legends

Figure 1. Triangular unstructured finite grid example. A. Structure and nomenclature of the components of the grip. B. Additional points calculated to plot Simile results in GIS software.

Figure 2. Coupling scheme developed for Tracadie Bay: triangular finite grid created in AquaDyn, example of water exchange file delivered by Matlab and description of the structure developed in Simile, which combines the biogeochemical model and the submodel that reads the spatial topology and executes the hydrodynamics.

Figure 3. Study area. A. Tracadie Bay (Prince Edward Island, Canada). B. Triangular unstructured grid of Tracadie Bay created in AquaDyn. The circle represents Node # 236, where the current-meter was deployed, and the two coloured elements are Element # 182 (South) and # 385 (North), where the conservative tracer verifications were performed.

Figure 4. Conservative tracer concentration (units m^{-3}) in Tracadie Bay after 10 days in AquaDyn and Simile.

Figure 5. Time series of conservative tracer concentration (units m^{-3}) in Element # 182 and # 385 in AquaDyn and Simile.

Figure 6. Bay averaged time series of chlorophyll depletion (%) in both 1998 and 1999. Continuous line represents the average value and dotted lines the standard deviation.

Figure 7. Time averaged percentage of chlorophyll depletion (%) in both 1998 and 1999.

Figure B.1. Structure of the element defined by the nodes A (xA,yA), B (xB,yB) and C (xC,yC) and vectors used to calculate the flow through the link A-B. A. Perpendicular vector (nx, ny) to the link A-B. B. Vector (px,py) which origin in the middle of the link A-B, D (xD,yD), and directed to the opposite node of A-B, C (xC,yC).

Figure C.1. Simile model of a bay in which only the TPM is considered. *Inflow*, *Outflow* and *Connections* submodels provide the information to couple AquaDyn to Simile. The submodel called *Submodel – Legend* describes the different symbols used in the model according to the nomenclature used in Simile (Muetzelfeldt and Massheder 2003).

Figure C.2. Simile model with a submodel to establish initial values at the beginning of the simulation.

Figure 1

Click here to download high resolution image

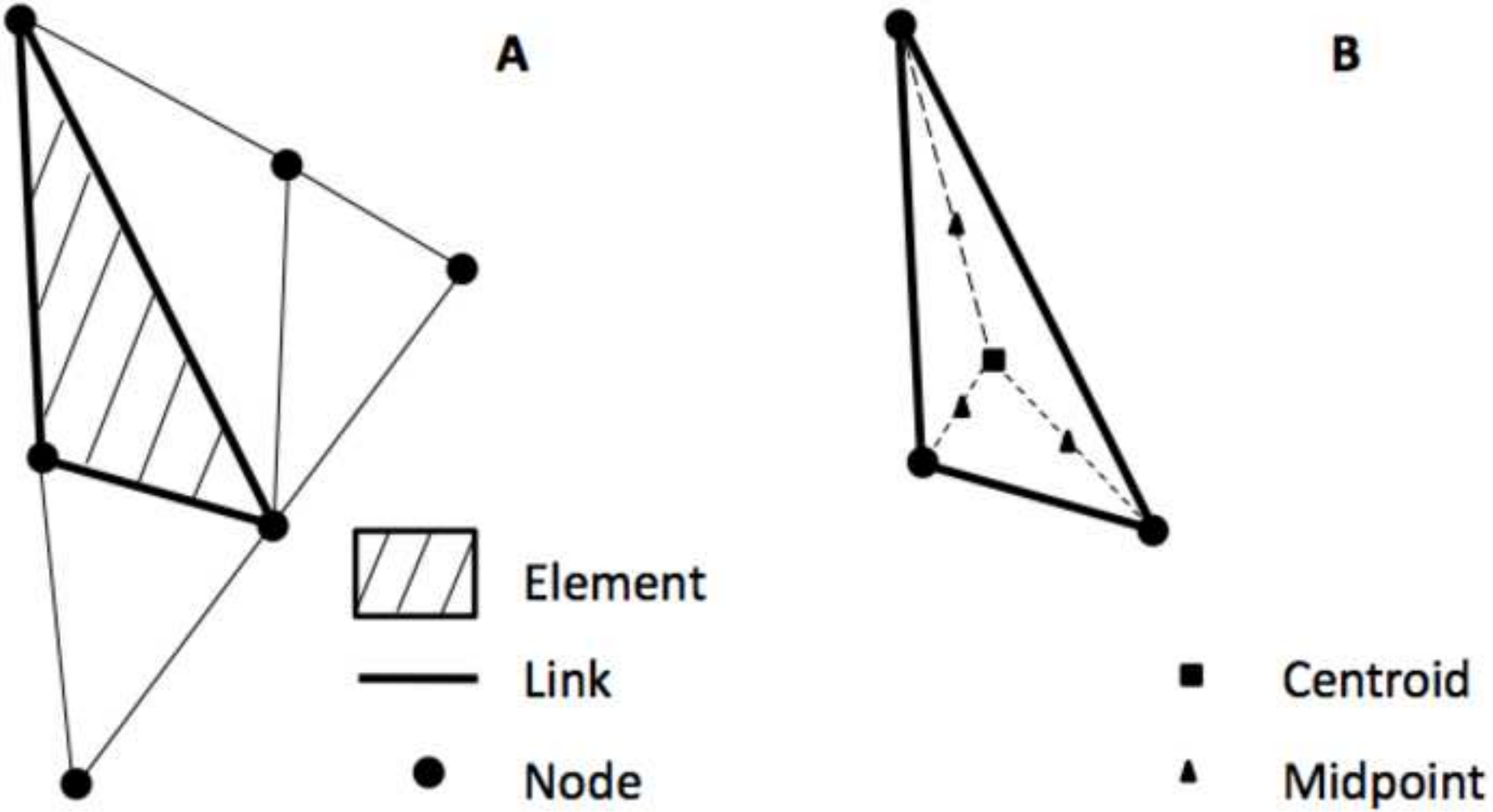
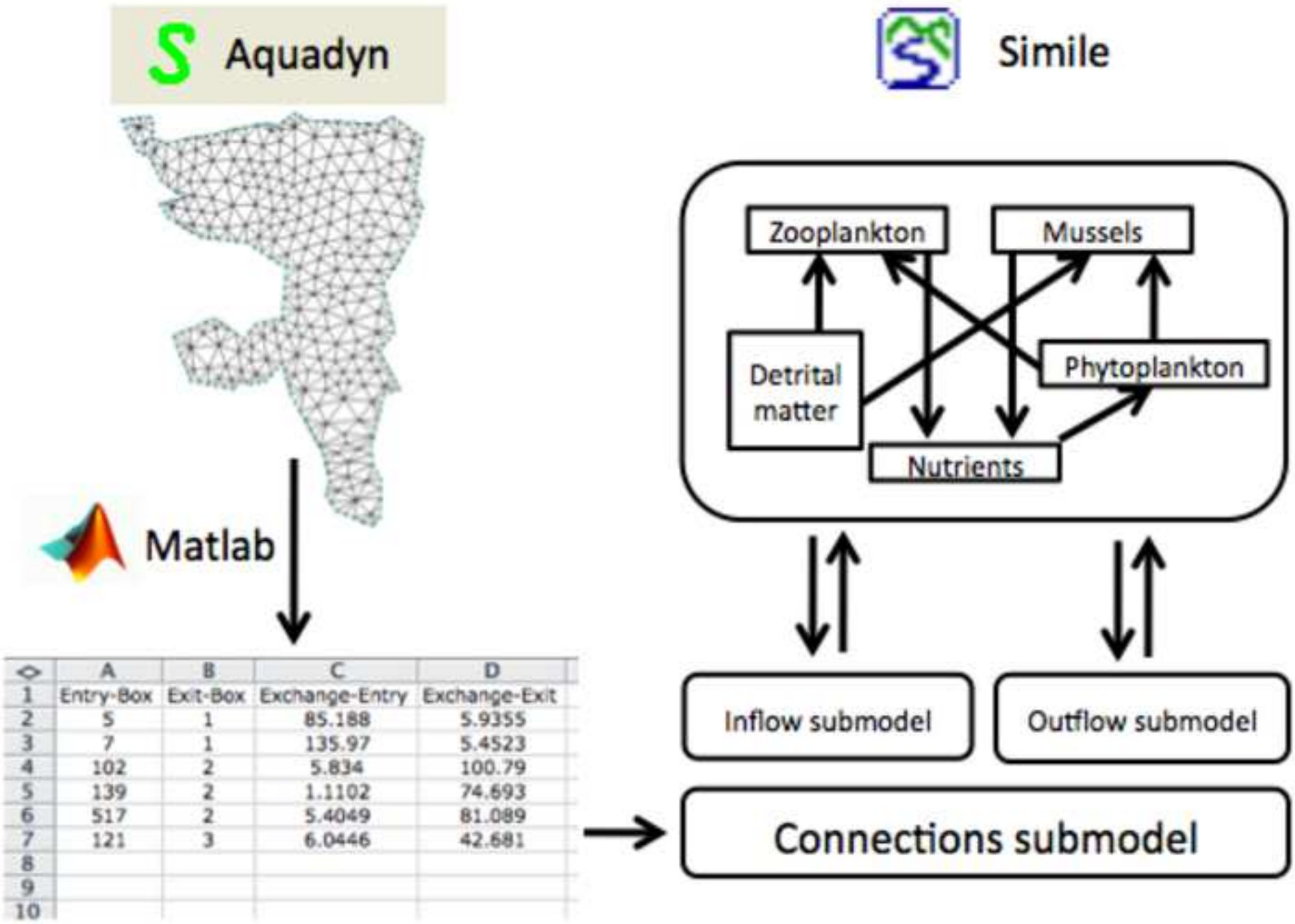


Figure 2

Click here to download high resolution image



	A	B	C	D
1	Entry-Box	Exit-Box	Exchange-Entry	Exchange-Exit
2	5	1	85.188	5.9355
3	7	1	135.97	5.4523
4	102	2	5.834	100.79
5	139	2	1.1102	74.693
6	517	2	5.4049	81.089
7	121	3	6.0446	42.681
8				
9				
10				

Figure 3

Click here to download high resolution image

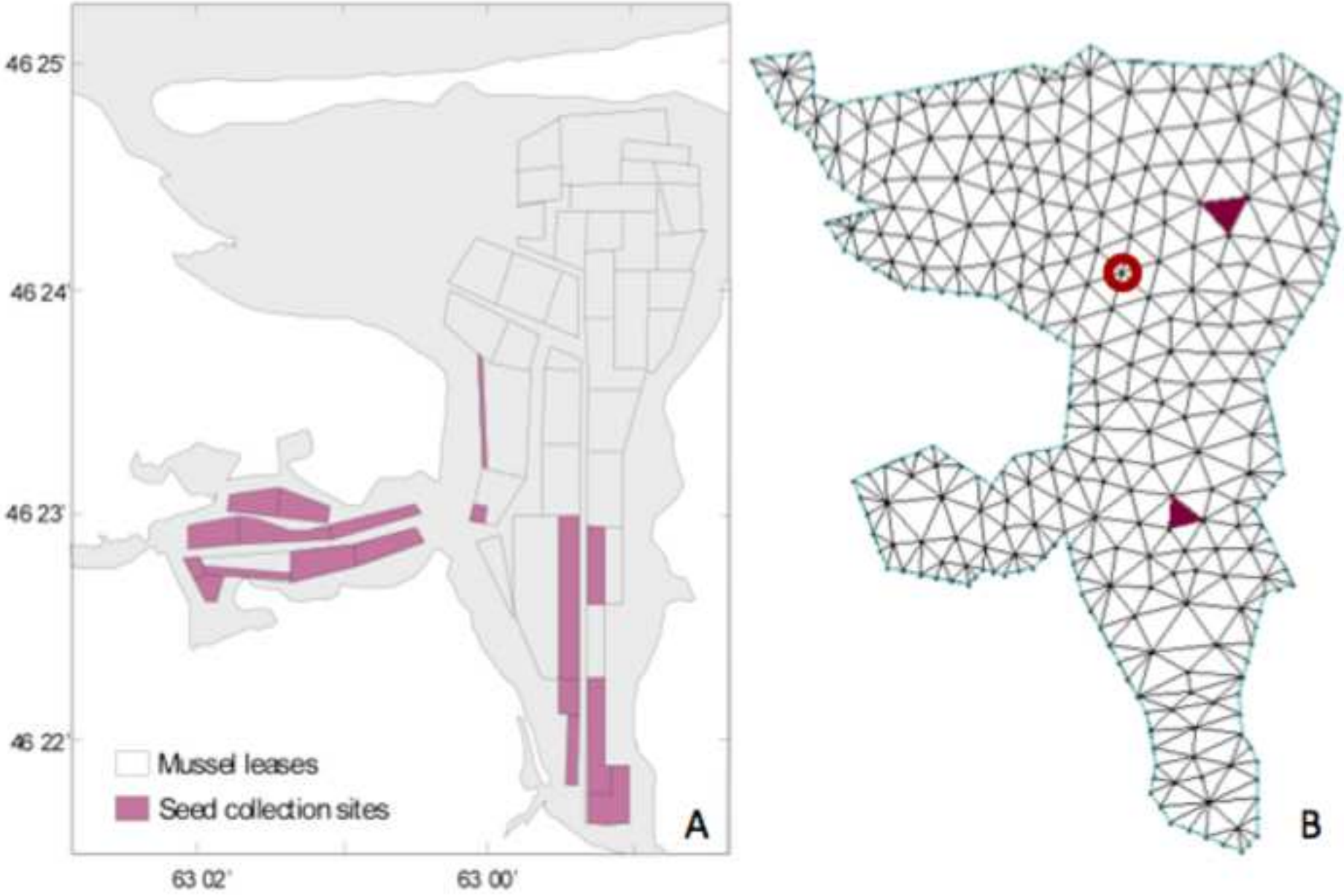


Figure 4

Click here to download high resolution image

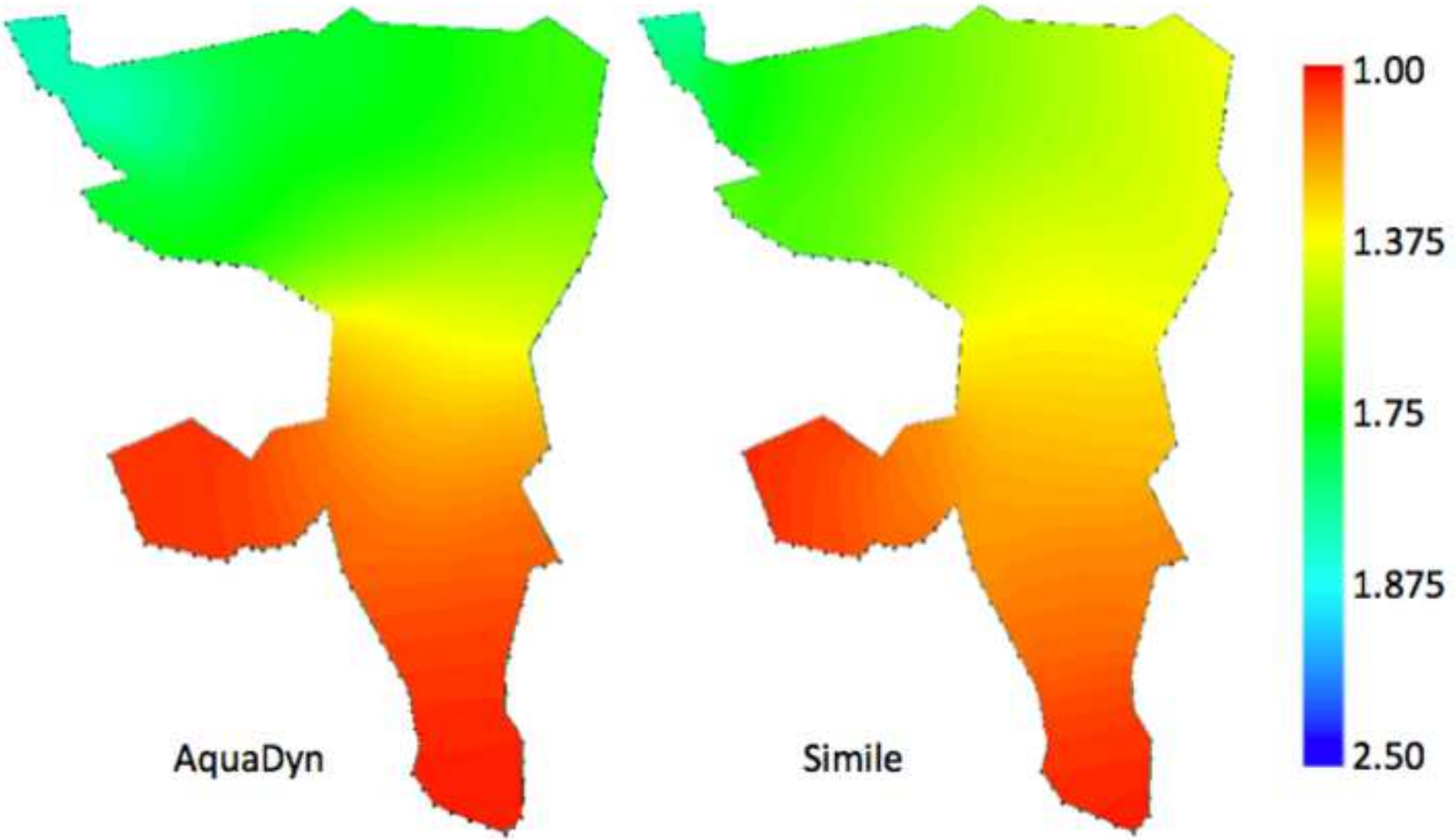


Figure 5

Click here to download high resolution image

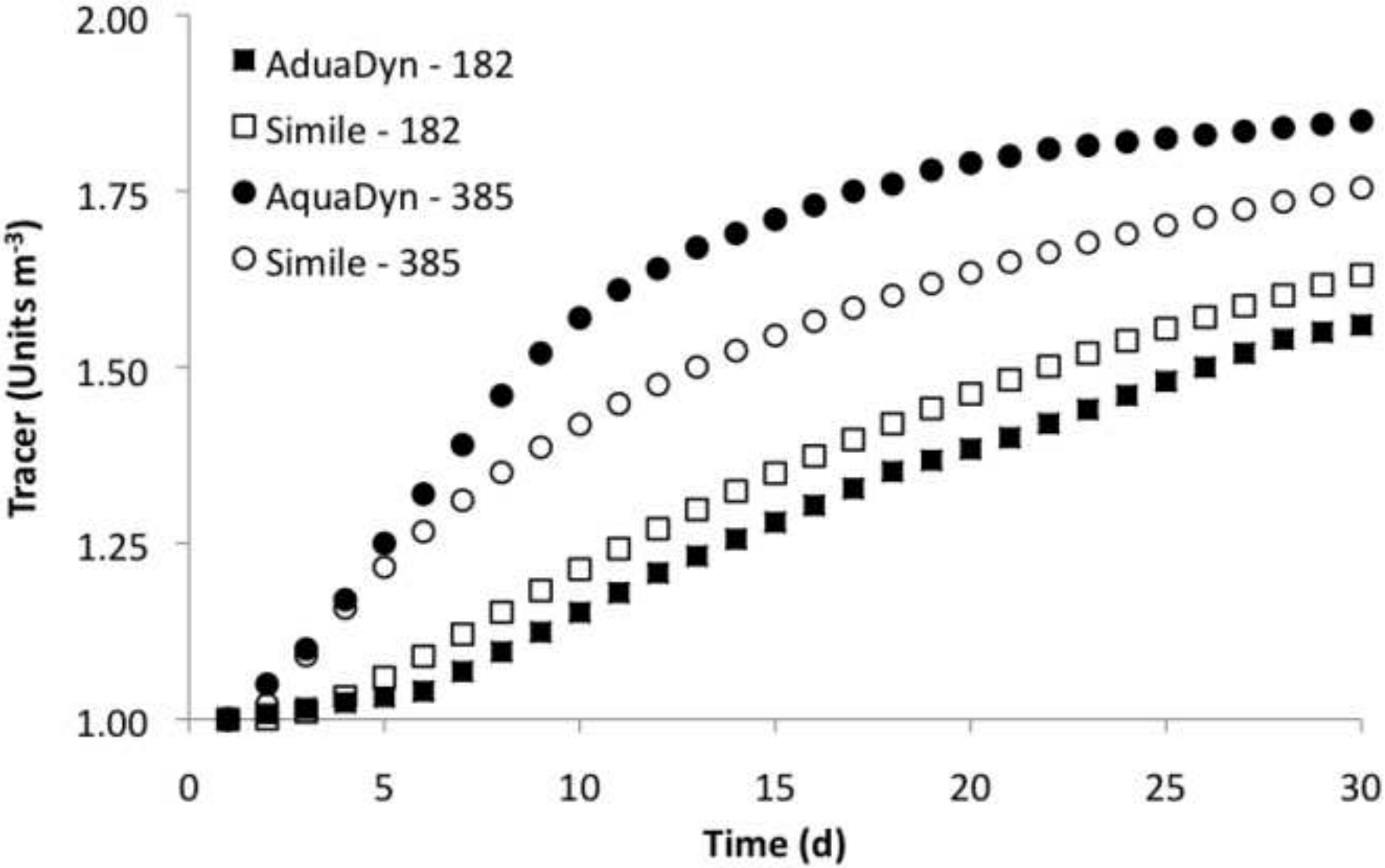


Figure 6

Click here to download high resolution image

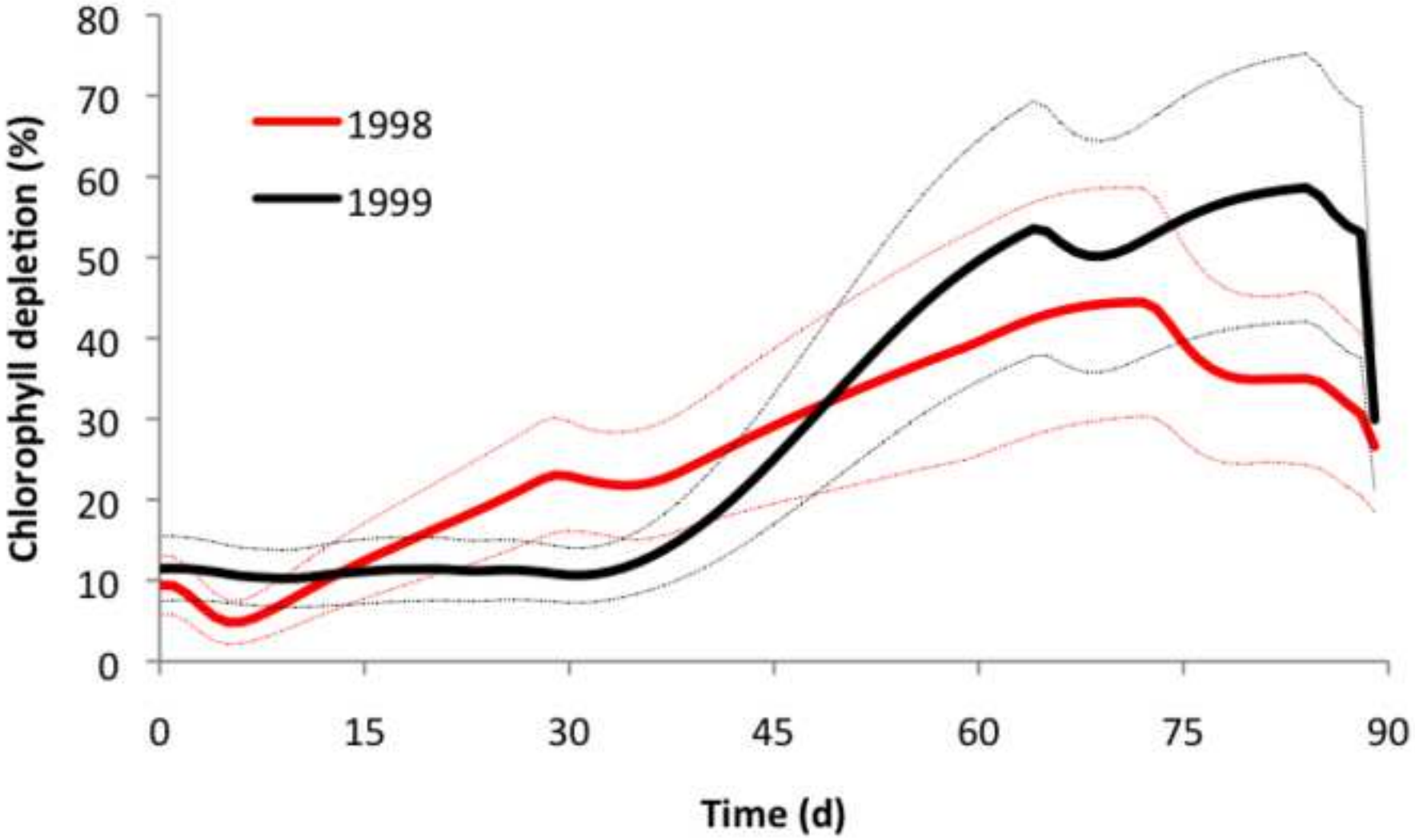


Figure 7

Click here to download high resolution image

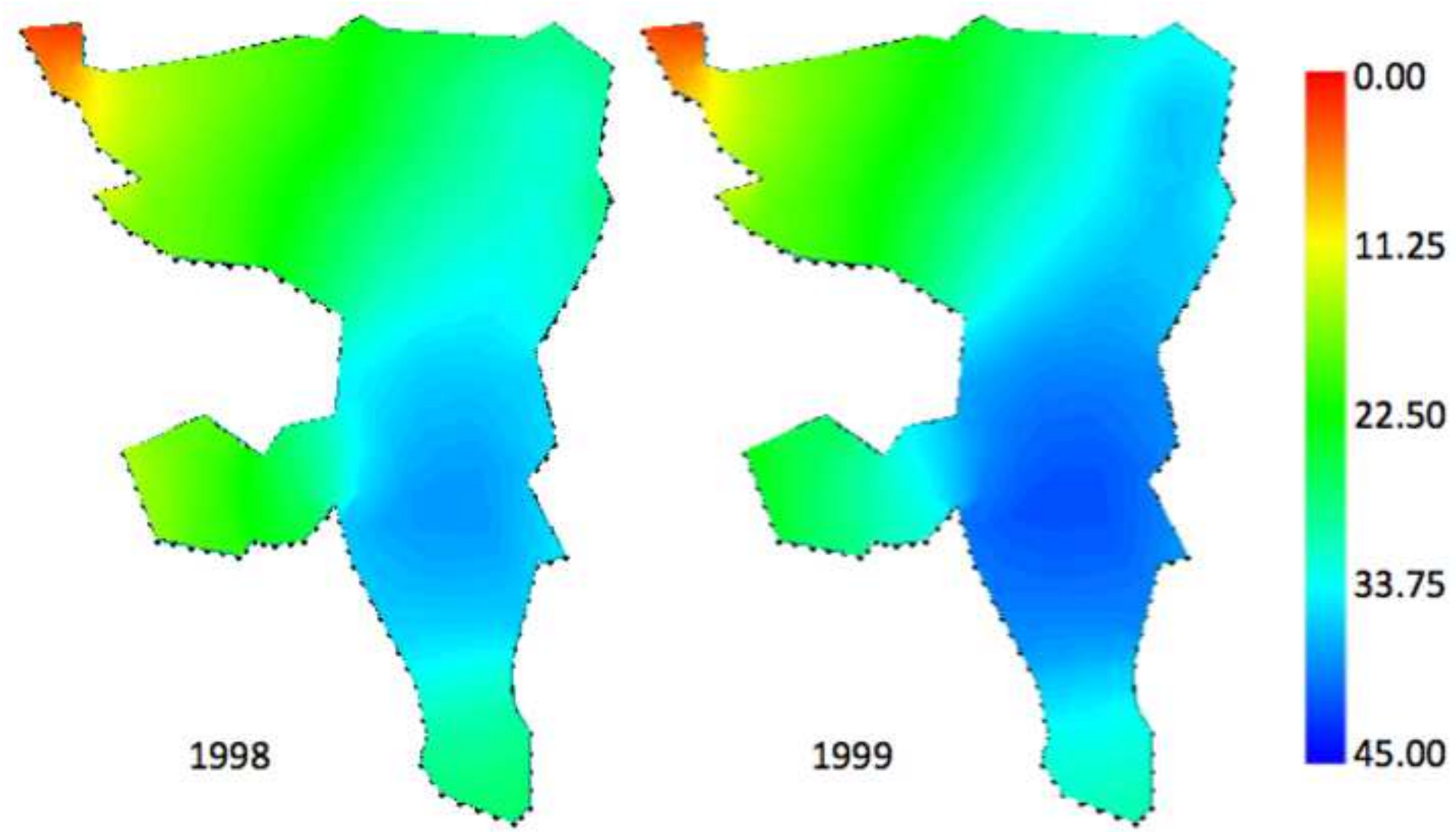


Figure B-1
Click here to download high resolution image

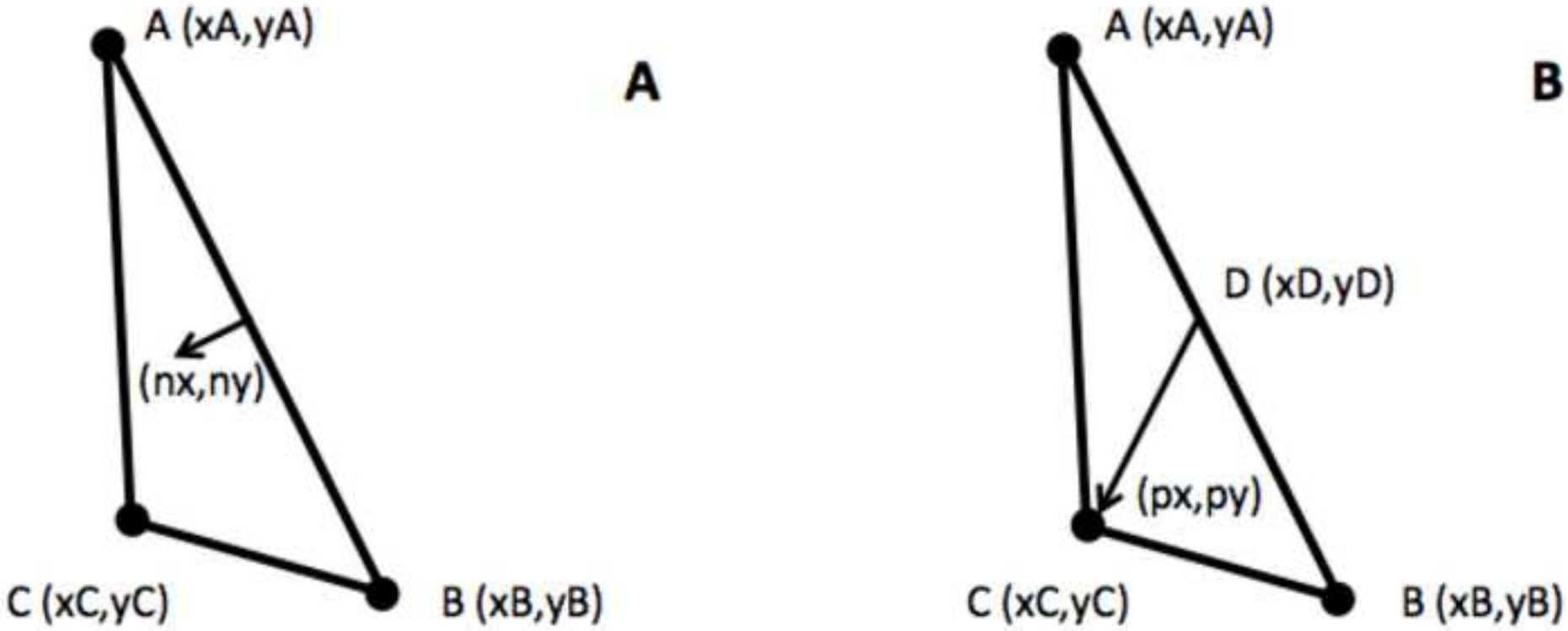


Figure C-1

Click here to download high resolution image

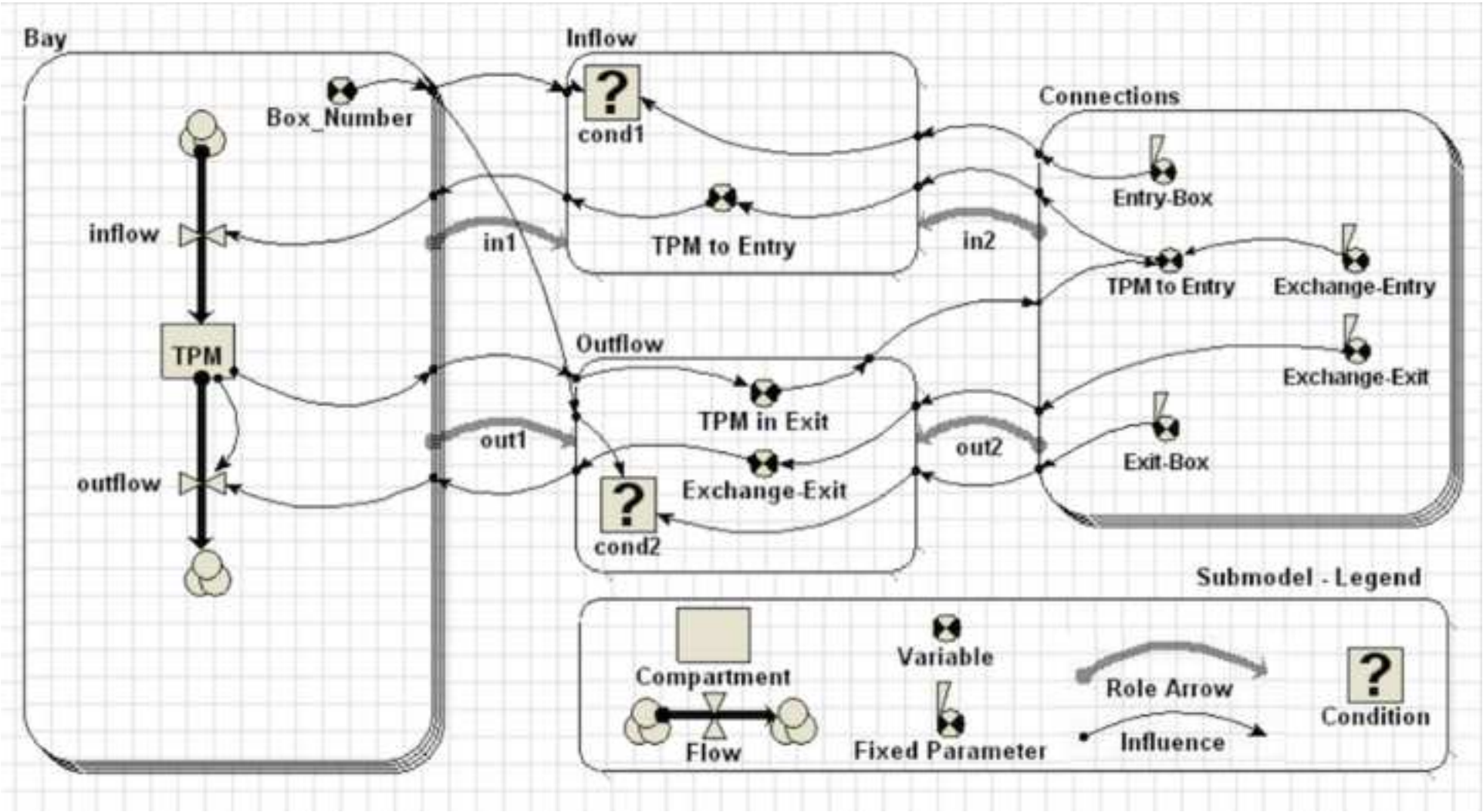


Figure C-2
Click here to download high resolution image

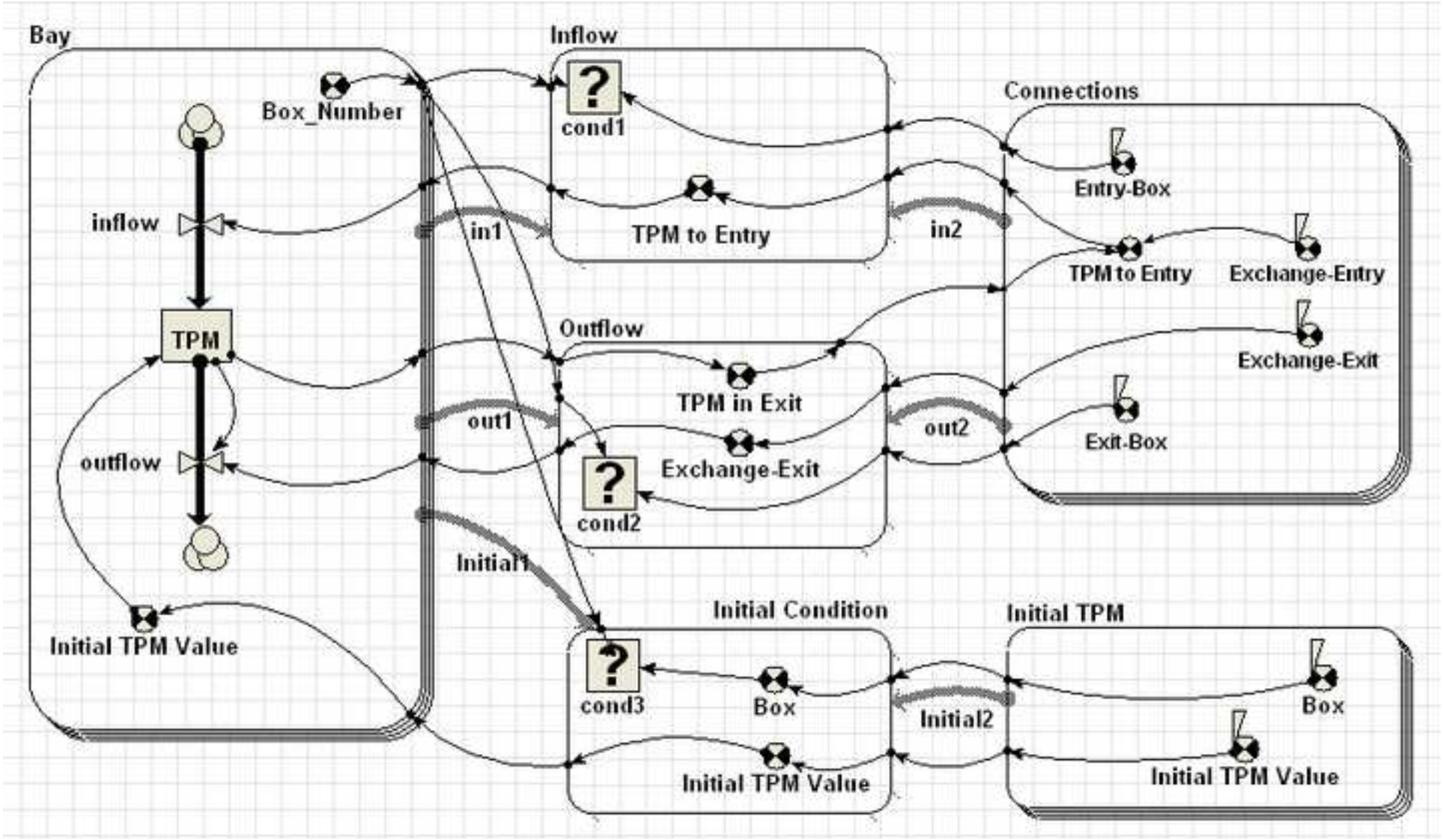


Table 1. General model equations and description.

Term	Definition	Reference
dP/dt	Phytoplantkton change rate (mgC m^{-3} d^{-1})	
P_{growth}	Phytoplankton growth	
$P_{mortality}$	Phytoplankton mortality	
$M_{grazing}$	Mussel grazing on phytoplankton	Eq. 7 in Grant et al. (2007)
P_{mixing}	Exchange of phytoplankton with adjacent elements and far field	
dN/dt	Nitrogen change rate (mgN m^{-3} d^{-1})	
N_{river}	Nitrogen river discharge	River discharge x River Nitrogen concentration
$M_{excretion}$	Mussel nitrogen excretion	Eq. 17 in Grant et al. (2007)
P_{uptake}	Phytoplankton nitrogen uptake	
N_{mixing}	Exchange of nitrogen with adjacent elements and far field	Eq. 15 in Grant et al. (2007)
dD/dt	Detritus change rate (mgC m^{-3} d^{-1})	
$D_{resuspension}$	Detritus resuspension forced by wind	See Filgueira and Grant (2009)
M_{feces}	Mussel feces production	Eq. 5 in Grant et al. (2007)
$P_{mortality}$	Phytoplankton mortality	See above
$D_{sinking}$	Detritus removal by sinking	
$M_{grazing}$	Mussel grazing on detrital matter	Eq. 5 in Grant et al. (2007)
D_{mixing}	Exchange of detritus with adjacent elements and far field	
dM/dt	Mussel change rate (mgC m^{-3} d^{-1})	
$M_{net\ growth}$	Mussel net growth	Eq. 1 in Grant et al. (2007)
$M_{seeding}$	Income of mussel biomass by seeding	These rates are not calculated, their sum is assumed to compensate $M_{net\ growth}$
$M_{mortality}$	Mussel natural mortality	
$M_{harvesting}$	Mussel mortality by harvesting	

Table 2. Analysis of velocity modulus measured with the current meter (46º23’56’’N, 62º59’56’’W) and the closest node in AquaDyn model, Node # 236. Values are in cm s^{-1}.

	Current Meter	**AquaDyn**
Maximum	21.57	7.66
Minimum	0.18	0.09
Mean	5.09	3.67
Standard Dev.	2.93	1.35
Median	4.48	4.18

Table 3. Summary of different modelling environments, most relevant characteristics, classification of coupling and references.

Modelling environment	Characteristics	Coupling	References / Examples
General modelling environments			
Spatial Modelling Environment	Object oriented simulation environment Specific programming language Possibility to be coupled to other software	Integration / Offline	Maxwell and Constanza, 1994, 1995, 1997a, 1997b
Matlab / Fortran	Programming language High flexibility and mathematical power Possibility to be coupled to other software	Integration / Offline / Online	Fennel and Neumann, 2004 Umgiesser et al., 2003
GEMSS / ROMS	Physical modelling environment Possibility to use pre-generated, but usually non-modifiable biological models	Online	Fennel et al., 2006
Aquaculture examples			
Not specified	Improve economic yield of *Tapes phillipinarum* culture (Venice Lagoon)	Not specified	Pastres et al., 2001
EcoDynamo	Simulate physical, biogeochemical and anthropogenic processes in aquatic ecosystems Possibility to be coupled to other software	Offline	Pereira et al. 2006
EcoWin2000 /Delft3D-Flow / ShellSIM	EcoWin2000 is a platform for integration of different submodels or software Evaluate carrying capacity for aquaculture (Northern Irleand)	Offline	Ferreira et al., 2008
Matlab - AquaDyn	Evaluate bivalve grazing activity (Tracadie Bay)	Offline	Grant et al., 2008
ELCOM / CAEDYM	Elucidate temporal and spatial variability of food supply to clams (Barbamarco Lagoon)	Offline	Spillman et al., 2008

GEMMS (Generalized Environmental Modelling System for Surfacewaters), ROMS (Regional Ocean Modelling System), ELCOM (Estuary and Lake Computer Model), CAEDYM (Computational Aquatic Ecosystem Dynamic Model), EcoDynamo (Ecological Dynamic Model).