

NAME of model ShellSIM	reporter/institute (a): Tony Hawkins/PML Plymouth Marine Laboratory (PML), Prospect Place, Plymouth, PL1 3DH, UK AJSH@pml.ac.uk Tel. +44 1752 633 443
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Short DESCRIPTION of model (b)

ShellSIM (<http://www.shellsim.com/index.html>) is a dynamic model structure that simulates rapid and sensitive adjustments in feeding, biodeposition, metabolism, excretion, and growth among bivalve shellfish (oysters, mussels, clams, scallops), as occur in response to environmental changes in temperature, salinity, seston availability, seston composition and aerial exposure. Notably, whereas past models have been calibrated and optimized per species per site, ShellSIM is the first common model structure that simulates effectively upon calibration in separate species, and which can then be applied using the same calibration for each species reared in contrasting coastal and estuarine environments, thereby saving significant time and resources.

Novel elements whereby ShellSIM is both robust and adaptable across both species and environments include resolving the relative processing of living chlorophyll-rich phytoplankton organics, non-phytoplankton organics and the remaining inorganic matter during both differential retention on the gill and selective pre-ingestive rejection within pseudofaeces. In addition, the model predicts the separate energy contents of those phytoplankton and non-phytoplankton organics, the latter being highly variable; to predict rates of processing, organic compositions and energy contents for filtered, ingested and faecal matter. Based upon common principles of energy balance, dependent relations predict rates of energy absorption, energy expenditure, excretion and growth. These functional interdependencies have been established using standardized procedures over a broad range of species, and which now afford calibration for any given species of bivalve suspension-feeder, and which successfully replicate dynamic physiological adjustments across full natural ranges of temporal and spatial variability in different environments, ranging from relatively open water to more turbid estuaries. Significantly, the dynamic simulation of functional physiological interrelations allows integration with hydrodynamic and other models for temporal and spatial analyses of the complex feedbacks, both positive and negative, whereby suspension feeding shellfish interact with ecosystem processes under different culture scenarios.

Main state variables (c)

Main state variables and derivations include soft tissue energy, soft tissue weight, shell energy, shell weight, total dry weight, total wet weight and shell length. Functions predicted in the calculation of those state variables include separate calculations of the rates with which inorganic matter, phytoplankton organics and non-phytoplankton detrital organics are each filtered, rejected prior to ingestion as pseudofaeces, ingested and defecated as true faeces. Associated interrelations predict rates of energy absorption, excretion as ammonium, oxygen consumption, heat losses, reproductive losses and net energy balance.

Scale to which applicable

Individual shellfish, and populations thereof.

General description (d)

ShellSIM has been developed using STELLA™, an image-based modeling software produced by isee™ systems (<http://www.iseesystems.com>), as a dynamic model that uses differential equations to define functional dependencies and the resulting physiological responses to environmental change. Responses are integrated to describe time-varying rates of feeding and metabolism as component processes in the prediction of individual growth, the individual being treated as an input-output system with size and energy content

as state variables, with a minimum time step of one hour.

ShellSIM is available under license within the context of collaborative projects, and under license for a small fee outside of collaborative projects. Formats available under license include:

1. WinShell for Windows, an integrated development environment which will run ShellSIM either on a desktop or on Internet Explorer™; and
2. Dynamic link library (DLL), which may be called from any high-level language that can use dlls, such as FORTRAN, PASCAL, C or C++, for integration with other models.

When running ShellSIM as Winshell for Windows or dll versions, ShellSIM is upscaled to the population level, initialised with individual shellfish sizes expressed as total undissected live fresh weight (g), the required timestep (d), box volume (m^3) and the number of animals per box. The facility to determine box volume and the number of animals per box means that simulated rates of food consumption and nitrogen excretion can be and are expressed in terms of effects/fluxes per unit volume, and which are thus compatible with the modelling of concentrations at larger scales.

For example, when run as Winshell for Windows or dll versions, then upon each Julian Day, ShellSIM outputs include total fresh weight (g), shell length (cm) and growth (g dry soft tissue/individual/d), each per individual; as well as the total consumption of chlorophyll a ($\mu g/m^3/d$), consumption of detrital organics ($mg/m^3/d$), consumption of total particulate matter (TPM; $mg/m^3/d$), total faecal deposition of all matter ($mg/m^3/d$), total faecal deposition as organic matter alone ($mg/m^3/d$) and total excretion of ammonia ($\mu mol NH_4/m^3/d$), each as effected by all individuals entered per box.

Forcing data needed (e)

Forcing data are needed for water temperature and salinity, including seston availability determined as total particulate mass (TPM; $mg l^{-1}$), particulate organic mass (POM; $mg l^{-1}$), particulate inorganic mass (PIM; $mg l^{-1}$) and chlorophyll a (CHL; $\mu g l^{-1}$). An option for the additional input of particulate organic carbon (POC; $mg l^{-1}$) is not essential, but which enables prediction of the energy content of non-phytoplankton organics, as can vary between certain environments.

Possibly relevant INDICATORS (f)

Relevant indicators include (i) shellfish growth rates and shellfish condition (i.e. meat weight/shell wt or length), (ii) water quality measures such as of chlorophyll a and dissolved nitrogen, which are eaten and excreted by shellfish, respectively, and (iii) benthic measures of sediment organics, species composition and system processes, such as are influenced by the pseudofaeces and true faeces deposited by shellfish.

STATUS of model (g)

Origin(ator): ShellSIM has been developed by Tony Hawkins based upon research on feeding and metabolism in a variety of shellfish over the past 20 years, involving numerous projects throughout Europe and Asia.

Present development state (has been tested, under development, etc):

An earlier version of this model structure was developed, calibrated and validated for scallops cultured in China (Hawkins et al., 2002). Since then, that model structure has been substantially developed and branded as ShellSIM, based upon research at Plymouth Marine Laboratory and within the following projects:

1. **"ECASA"** - EU STREP "Ecosystem Approach for Sustainable Aquaculture"; 01/12/2004 to 30/10/2007; <http://www.ecasa.org.uk>
2. **"KEYZONES"** - EU CRAFT "To investigate sustainable biological carrying capacities of key European coastal zones"; 01/02/2005 to 01/02/2007; <http://www.keyzones.com>
3. **"SPEAR"** - EU INCO-DEV "Sustainable options for people, catchment and aquatic resources"; 01/12/2004 to 31/11/2007; <http://www.biaoqiang.org>
4. **"SMILE"** - DARDNI "Sustainable mariculture in Northern Irish lough ecosystems";

01/10/2004 to 31/01/2007; <http://www.ecowin.org/smile>

5. “**UISCE**” - Irish Sea Fisheries Board “Understanding Irish shellfish culture environments”; 22/02/2007 to 30/09/2008

Care has been taken to ensure ShellSIM is practicable and affordable, engaging the basic minimum of drivers required for reasonable accuracy. The need for measures such as include the relative abundances of different phytoplankton classes has been carefully assessed, and discounted on the basis of cost/benefit ratios.

Testing has established that the common dynamic structure within ShellSIM is both robust and adaptable, calibrated and validated to date against field measures of actual growth during normal culture in nine different species (Table 1).

Table 1. Summary of species and sites for which ShellSIM has been validated. Percentage errors are those observed between final predicted and final observed sizes after between 8 and 24 months of growth under normal culture practice at each site, the model having been initialised for sizes upon seeding at the beginning of each growth cycle.

Species	Type	Site	Error in predicted growth (%)	Culture	Context
Single standard set of parameters, optimised per species across sites					
<i>Mytilus edulis</i>	Mussel	Pertuis Breton, France	7	Pole	Literature
<i>Mytilus edulis</i>	Mussel	Oosterscheldt, Netherlands	6	Bottom	KEYZONES
<i>Mytilus edulis</i>	Mussel	Strangford Lough, N. Ireland	6	Rope	SMILE
<i>Mytilus edulis</i>	Mussel	Carlingford Lough, N Ireland	0	Rope	SMILE
<i>Mytilus edulis</i>	Mussel	Lough Foyle, N. Ireland	4	Rope	SMILE
<i>Mytilus edulis</i>	Mussel	Belfast Lough, N. Ireland	19	Bottom	SMILE
<i>Mytilus edulis</i>	Mussel	Clew Bay, Ireland	12	Rope	KEYZONES
<i>Crassostrea gigas</i>	Oyster	Sanggou Bay China	17	Rope	SPEAR
<i>Crassostrea gigas</i>	Oyster	Oosterscheldt, Netherlands	5	Bottom	KEYZONES
<i>Crassostrea gigas</i>	Oyster	Strangford Lough, N. Ireland	17	Trestle	SMILE
<i>Crassostrea gigas</i>	Oyster	Carlingford Lough, N Ireland	25	Trestle	SMILE
<i>Crassostrea gigas</i>	Oyster	Clew Bay, Ireland	10	Trestle	KEYZONES
<i>Crassostrea gigas</i>	Oyster	Loch Creran, Scotland	3	Trestle	KEYZONES
Calibrated and validated at single sites					
<i>Chlamys farreri</i>	Scallop	Sanggou Bay, China	<15	Lantern net	SPEAR
<i>M. galloprovincialis</i>	Mussel	Venice Lagoon, Italy	<15	Rope	ECASA
<i>Tapes philippinarum</i>	Clam	Venice Lagoon, Italy	<15	Bottom	ECASA
<i>Tegillarca granosa</i>	Cockle	Huangdun Bay, China	<15	Bottom	SPEAR
<i>Ostrea plicatula</i>	Oyster	Huangdun Bay, China	<15	Rope	SPEAR
<i>Sinonvacula constricta</i>	Clam	Huangdun Bay, China	<15	Bottom	SPEAR

Most importantly, when optimized per species in *Mytilus edulis* and *Crassostrea gigas* across a range of environments and culture practices, then applying a single standard set of parameters to simulate growth, ShellSIM simulates to < 25% error across that range of environments and culture practices.

Whereas past models have been calibrated and optimized per species per site, ShellSIM is the first common model structure that simulates effectively upon calibration in separate species, and which can then be applied using the same calibration for each species reared in contrasting coastal and estuarine environments, thereby saving significant time and resources.

Present use:

ShellSIM is currently being used for integrated ecosystem modelling of shellfish culture in Portugal, Scotland, Ireland, The Netherlands and China as part of the “ECASA”, “KEYZONES”, “SPEAR” and “UISCE” Projects detailed above.

Separate to those Projects, ShellSIM is also being integrated within the Farm Aquaculture Resource Management Model (FARMTM) (<http://www.farmscale.org/>) to assess culture

practise optimisation and environmental impacts including upon water quality at farm-scales as reported by Ferreira et al. (2007).

Claimed robustness and scientific basis of this:

The scientific basis whereby an earlier version of ShellSIM's model structure replicates dynamic adjustments in feeding and metabolism across full ranges of relevant natural variability, successfully simulating scallop growth from larvae or seed to harvestable size under different temporal and spatial scenarios of culture, has been reported by Hawkins et al. (2002) and Bacher et al. (2003). More recently, integration within FARM™ has been reported by Ferreira et al. (2007).

ShellSIM's robustness has more recently been established through successful calibration and validation of its common model structure in nine species to date, simulating to <25% error even when applying a single standard set of parameters to predict growth in the same species across contrasting environments and culture practices, as has been shown in *M. edulis* and *C. gigas* to date (Table 1).

To help further establish ShellSIM's credibility, we have undertaken analyses of goodness of fit based upon comparisons between simulated growth and observed growth using linear regression as described by Portilla and Tett (ECASA Internal Paper, 2007). Trans-site analysis of all measured and predicted data, using a single standard set of ShellSIM parameters, for *C. gigas* during normal culture in the Sanggou Bay (China), Oosterscheldt (Netherlands), Strangford Lough (Northern Ireland), Carlingford Lough (Northern Ireland), Clew Bay (Republic of Ireland) and Loch Creran (Scotland) indicated that the slope and intercept of fitted regression were both different from zero ($p < 0.05$), and that the slope is significantly different from 1 ($p < 0.05$). Similarly, trans-site analysis of all measured and predicted data, using a single standard set of ShellSIM parameters, for *M. edulis* during normal culture in the Pertuis Breton (France), Oosterscheldt (Netherlands), Strangford Lough (Northern Ireland), Carlingford Lough (Northern Ireland), Lough Foyle (Northern Ireland), Belfast Lough (Northern Ireland) and Clew Bay (Republic of Ireland) indicated that the slope and intercept of fitted regression were both different from zero ($p < 0.05$), and that the slope is significantly different from 1 ($p < 0.05$). On which basis, according to Oreskes et al. (1994), ShellSIM's generic performance when applying a single standard set of parameters to predict growth across a broad range of culture environments and practices throughout Europe and Asia is classified as "Fair" when tested for both *C. gigas* and *M. edulis*.

We consider this a significant step forward given the diversity of culture sites, additional variance conferred through the inclusion of different shellfish stocks and varying protocols employed in the measurement of environmental drivers.

IMPLEMENTATION OF MODEL

State of implementation (h)

Earlier and current versions versions, now branded as ShellSIM, have been used to:

- (i) simulate growth of individuals and populations (Hawkins et al. 2002);
- (ii) assess optimal densities for culture at different sites at the farm scale (Bacher et al., 2003);
- (iii) help optimise culture practise and predict environmental impacts including upon water quality at farm-scales (Ferreira et al., 2007c); and
- (iv) simulate interrelations between key ecosystem processes and shellfish cultured under different scenarios at bay scales (Duarte et al., 2003; Nunes et al., 2003; Zhang et al., 2004; Ferreira et al., 2005, 2006, 2007a, 2007b).

Within ECASA, ShellSIM is being integrated within EcoWin 2000 to simulate animal-environment interrelations including capacities for culture and associated impacts of that culture at system scales for *Crassostrea gigas* in Loch Creran, Scotland and *Tapes philippinarum* in the Ria Formosa, Portugal.

State of documentation

Journal papers and books (e.g. Hawkins et al., 2002; Bacher et al., 2003; Ferreira et al.,

2005, 2006, 2007a, 2007b, 2007c).

Intellectual property concerns

As described in (d) above, ShellSIM is available as executable code under license for no charge within the context of collaborative projects, including under license for a small fee outside of collaborative projects. Formats available include:

1. WinShell for Windows, an integrated development environment which will run ShellSIM either on a desktop or on Internet Explorer™; and
2. Dynamic link library (DLL), which may be called from any high-level language that can use dlls, such as FORTRAN, PASCAL, C or C++, for integration with other models.

TESTING

Summary of conditions and measurements needed - including critical forcing data (j)

Calibration of ShellSIM in any new species involves:

(i) Measuring short-term feeding responses to experimental changes in food availability and composition. These measures follow standardised procedures which can normally be undertaken in two species by three persons over one week. Plymouth Marine Laboratory travels with all associated equipment, requiring ready access to natural seawater.

(ii) Knowledge of the physiological effects of seawater temperature, salinity and aerial exposure. Often, this is in the literature, or which may in part be assumed from similar species.

(iii) Data describing relative relations between shell length, shell weight and tissue weight, including average C or energy contents of tissue and shell.

To initiate the model, we need to know shellfish size upon seeding/deployment, including when seeded and harvested.

To drive the model, measurements are needed for water temperature and salinity, including seston availability determined as total particulate mass (TPM; mg l⁻¹), particulate organic mass (POM; mg l⁻¹), particulate inorganic mass (PIM; mg l⁻¹) and chlorophyll a (CHL; µg l⁻¹). As stated above, particulate organic carbon (POC; mg l⁻¹) is optional, and which enables prediction of the energy content of non-phytoplankton organics, which can be important in certain environments.

To validate the model, data are required describing natural shellfish growth throughout the normal cycle of culture at each site, and which should ideally have been measured coincident in space and time with the above environmental drivers.

Criteria for model rejection

Criteria for model rejection include:

- (i) inadequate data describing environmental drivers and/or actual growth;
- (ii) > 20% error in simulated growth, as compared with measured growth; and/or
- (iii) variance (r^2) in observed growth explained by simulated growth is not significantly different from zero, according to Oreskes et al. (1994).

OTHER models

Used with this model (k)

FARM™: a web-based model for aquaculture resource management at the farm-scale.

EcoWin 2000 (E2K): an object-oriented programming (OOP) approach to implement ecological models for aquatic systems. The basic underlying structure is that of a spatial (1D, 2D and 3D) framework of boxes, within each of which the relevant biogeochemistry and population dynamics are resolved.

Delft3D: the Model System of the WL|Delft Hydraulics where hydrodynamical, ecological and

morphodynamical modules are integrated.

ASSETS™: for assessment of estuarine trophic status, building on the U.S. National Estuarine Eutrophication Assessment (NEEA) developed by NOAA.

Similar models (I)

Shellfish may selectively ingest and/or digest different particle types, whilst effecting compensatory adjustments that may help to maximize the utilization of particles rich in chlorophyll (Hawkins et al., 1999, 2001). To account for these capabilities, ShellSIM resolves separate processing of the organic matter within living phytoplankton, remaining non-phytoplankton organics (i.e. bacteria, protozoans, colloids and detritus) and inorganic matter. For each of these dietary components, a separate functional relation simulates filtration, pre-ingestive rejection and ingestion, affording prediction of absorption on the basis of the resulting organic content of ingested matter. By these means, ShellSIM is able to simulate feeding and growth over a broad range of environmental circumstances, whether in response to short-term tidal influences, seasonal effects or spatial differences.

In contrast, previous models of shellfish growth have not resolved any differential filtration of separate dietary components (e.g. van Haren and Kooijman, 1993; Ross and Nisbet, 1990; Brylinski and Sephton, 1991; Powell et al., 1992; Barillé et al., 1997; Scholten and Smaal, 1998; Solidoro et al., 2000). Others, although in some cases resolving the availability of living phytoplankton from remaining detrital organics, are without functional relations to simulate the highly responsive processes whereby living phytoplankton, remaining detrital organics and inorganic matter are differentially selected, rejected and/or absorbed (e.g. Raillard et al., 1993; Campbell and Newell, 1998; Grant and Bacher, 1998; Ren and Ross, 2001; Pouvreau et al., 2000, 2006).

Without such interrelations, one should not expect a model of shellfish physiology to account for the range of seston compositions such as occur between contrasting open water and estuarine environments. Nor would a simpler model simulate the dynamic consequences of those different seston compositions for energy absorption, excretion as ammonium, oxygen consumption, heat losses and reproductive. Nor would such a model be appropriate to undertake effective temporal and spatial analyses of the complex feedbacks, both positive and negative, whereby suspension feeding shellfish interact with ecosystem processes under different culture scenarios. More importantly, compared with less robust models that may only be "tuned" so as to perform well in a given environment, the main advance achieved by ShellSIM has been to simulate effectively upon calibration in separate species, and which can then be applied using the same calibration for each species reared in contrasting coastal and estuarine environments, thereby saving significant time and resources.

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