ECASA - Model description template

1	**Name of model**	*Reporter/Institute (email address) Daniele Brigolin & Roberto Pastres, DCF-Unive. (brigo@unive.it)*
1.a	**EDMA: an Early Diagenesis Model for Aquaculture**	
1.b	*21/12/2007*	

2	**Short DESCRIPTION of model**	
2.a	*Main state variables:*	OC (Organic Carbon) in sediment; NO_3^-, DIP (Dissolved Inorganic Phosporus), NH_4^+, SO_4^{2-}, TS (H_2S + HS^-), DO concentrations in interstitial water.
2.b	*Scale to which applicable:*	Local, A.
2.c	*General description.* *NB: if the model is complicated, or has easily distinguishable components (such as a physical and a biological sub-models) that can be, or have been, used separately, it may be easier to complete one form for each of the main components.*	EDMA (Brigolin, 2007) was developed under the BRNS (Biogeochemical Reaction Network Simulator) [Regnier et al., 2002], a simulation environment in which biogeochemical reactions are coupled with transport processes. This Reaction Transport Model can be used to simulate: – the main pathways of degradation of the organic matter; – the most important processes of oxidation of the degradation product as well as the main transport mechanisms, i.e. diffusion (including bioturbation) and advection, which take place in a sediment core. On this basis, the nutrient fluxes at the sediment water interface, e.g. NH_4^+, DIP, can be estimated. The general equation reads as: $$\frac{\partial(1-\varphi)C_s}{\partial t} = -\frac{\partial(1-\varphi)\omega C_s}{\partial z} + \frac{\partial}{\partial z}\left[\frac{\partial(1-\varphi)D_B C_s}{\partial z}\right] + R((1-\varphi)C_s, \beta, t) \quad (1)$$ $$\frac{\partial \varphi C_w}{\partial t} = -\frac{\partial \varphi \omega C_w}{\partial z} + \frac{\partial}{\partial z}\left[\frac{\partial \varphi D_B C_w}{\partial z} + \frac{\partial \varphi D_m / (1 - \ln \varphi^2) C_w}{\partial z}\right] + R(\varphi C_w, \beta, t) \quad (2)$$ where Eq. (1) and (2) describe, respectively, the reaction-advection-diffusion processes in the solid and in the interstitial water. C is the state vector, t is the time, z is the depth, φ is the porosity of the sediment, ω is the infiltration velocity, D_m is the molecular diffusion, D_b is the bioturbation term and R is the reaction rate term which depends on β , the vector of parameters. The reaction network, which is a modification of the one reported by Wang and Van Cappellen (1996), was specifically designed for the study aquaculture impacts in coastal marine sites.
2.d	*Key semi-universal*	The model parameters can be divided in two categories, site-specific parameters and reaction

	parameters and example values (which should apply at least regionally or for at least one type of water body); summarize any restrictions or reservations about these parameters	specific-parameters, although the distinction between the two types of parameters is somewhat arbitrary. The first category comprises the parameters characterizing the depositional environment: the transport parameters, which include the bioturbation coefficient, and other physical properties of the sediment such as the porosity and density. The second category includes reaction rate coefficients, apparent equilibrium constants, and limiting concentrations of electron acceptors. Bioturbation coefficient and the organic matter degradation rate are highly variable and should be estimated at each site.
2.e	*Main forcing data needed - initial values of state variables; boundary conditions; inputs; imposed environmental conditions; generalized loss terms. State whether single values or time-series needed.*	Forcing data: time series of water temperature at the bottom and/or in the sediment. Boundary conditions: OC flux from the water column to the sediment; Fe(III) and Mn (IV) fluxes from the water column to the sediment; concentration of O_2, NO_3^-, NH_4^+, SO_4^{2-}, Mn^{2+}, Fe^{2+}, DIP in bottom waters. Initial conditions: -
2.f	*Restrictions to use of model*	

3	**possibly relevant INDICATORS and example EcoQOs**	
3.a	***D**river*	
3.b	***P**ressure*	
3.c	***S**tate*	
3.d	***I**mpact*	In deposition models, such as DEPOMOD (Cromey et al., 2002) the degradation of the organic matter is simulated using a simple decay model, e.g. the G-model (Berner, 1980). The application of an early diagenesis model, such as EDMA, could simulate the dynamic of biochemical parameters which can be considered environmental impact indicators (Porrello et al., 2005; Chamberlain et al., 2001). In this way one could estimate other effects of the OM enrichement in surficial sediment, such as the decrease in the DO concentration and the related increase in the concentration of sulphides, ammonia and reactive P in the interstitial water.
3.e	***R**esponse*	

4	**STATUS of model** *NB: refers to scientific theory and equation set; distinguish from implementation*	
4.a	*Origin(ator) of model concept and initial formulation:*	Reactive Transport Modelling group of the University of Utrecht (NL)

		(http://www.geo.uu.nl/~rtm/index.php?page=proje)
4.b	*Present status of model, including scientific basis of claimed robustness and key matters still needing study:*	
4.c	*Present use:*	
4.d	*Potential use and development in ECASA :*	EDMA can be usefully coupled with a deposition model, e.g. DEPOMOD (Brigolin et al., submitted)

5	**IMPLEMENTATION of model**	
5.a	*State of implementation :* *(This refers to realization of model theory in numerical algorithms, spreadsheets, computer programs, etc. to provide solutions of the model equations when supplied with appropriate forcing data.*	EDMA was developed by means of BRNS. The BRNS is a modeling environment in which Reaction Transport Models can be constructed in a fully automated way. The set of equations, which represent the relevant biogeochemical processes included in a reaction network, are defined within the MAPLE symbolic programming environment (Regnier et al., 2002; Regnier et al., 1997). Within MAPLE, conservation equations for all the chemical constituents pertaining to the reaction network are constructed, and the information necessary for their numerical solution is assembled and processed symbolically. The results, along with additional user-specific information (e.g. parameter values, boundary and initial conditions) are then translated into fully structured FORTRAN code, combined with general transport routines, and linked to standard linear-algebra solvers. The FORTRAN code could then be included as a routine in other programming environment.
5.b	*State of documentation (which describes how to use an implementation as well as giving model theory)*	The PhD thesis from Brigolin (2007), provides a description of EDMA application in combination with DEPOMOD and MERAMOD, respectively in Loch Creran and the Northern Adriatic Sea. The website of the RTM group (http://www.geo.uu.nl/~rtm/index.php?page=proje) provides a general description of the BRNS environment.
5.c	*Intellectual property concerns - if none stated here, model and implementation will be deemed to freely available on request*	Available to ECASA participants

6.	TESTING of model	
6.a	*Summary of conditions and measurements needed:* *Refer back to 2.e if necessary. Highlight observations needed for model testing.*	Fundamental are OC profiles in the sediment, since Organic Carbon is the fuel of all diagenetic processes. In order to calibrate the model, useful measures are the profiles of TS, DIP, NH_4^+, Fe^{2+}, Mn^{2+}, DO, SO_4^{2-} and pH in the interstitial water.
6.b	*Criteria for model rejection*	

7	OTHER models	
7.a	*Used explicitly or implicitly with this model*	DEPOMOD, MERAMOD.
7.b	*Similar models (which might serve roughly the same purpose in relation to mariculture)*	The G-model, Berner (1980) used in DEPOMOD.

8. REFERENCES cited *show in bold the most important paper describing the model*

Berner RA (1980) Early Diagenesis: A Theoretical Approach. Princeton Univ. Press.

Brigolin, D., Pastres, R., Nickell, T.D., Cromey, C.J., Aguilera, D.R. and Regnier, P. submitted to Marine Ecology Progress Series. Modelling the impact of intensive aquaculture on early diagenetic processes in sea loch sediments.

Brigolin (2007). Development of Integrated Numerical Models for the Sustainable Management of Marine Aquaculture. PhD thesis University of Venice, 152 pp.

Chamberlain, J., T.F. Fernandes, P. Read, T.D. Nickell and I.M. Davies. 2001. Impactsof deposits from suspended mussel (Mytilus edulis L.) culture on the surrounding surficial sediments. ICES J. Mar. Sci. 58: 411-416.

Cromey, C.J., Nickell, T.D. & Black, K.D. (2002). DEPOMOD - modelling the deposition and biological effects of waste solids from marine cage farms. Aquaculture, 214, 211-239.

Porrello, S., Tomassetti, P., Manzueto, L., Finoia, M.G., Persia, E., Mercatali, I., and Stipa, P., 2005. The influence of marine cages on the sediment chemistry in the Western Mediterranean Sea. Aquaculture, 249: 145-158.

Regnier, P., O'Kane, J.P., Steefel, C.I., Vanderborght, J.P., 2002. Modeling complex multi-component reactive-transport systems: towards a simulation environment based on the concept of a Knowledge Base. Applied Mathematical Modelling, 26: 913-927.

Regnier, P., Wollast, R., and Steefel, C.I. (1997) Long-term fluxes of reactive species in macrotidal estuaries: Estimates from a fully transient, multicomponent reaction-transport model. Marine Chemistry 58, 127-145.

Wang, Y. and Van Cappellen, P., (1996) A multicomponent reactive transport model of early diagenesis: Application to redox cycling in coastal marine sediments. Geochimica et Cosmochimica Acta. Vol 60, No 16: 2993-3014.