



Integrating sediment biogeochemistry into 3D oceanic models: A study of benthic–pelagic coupling in the Black Sea



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ABSTRACT

Three-dimensional (3D) ecosystem models of shelf environments should properly account for the biogeochemical cycling within the sea floor. However, a full and explicit representation of sediment biogeochemistry into 3D ocean models is computationally demanding. Here, we describe a simplified approach to include benthic processes in 3D ocean models, which includes a parameterization of the different pathways for organic matter mineralization and allows for organic matter remobilization by bottom currents and waves. This efficient approach enables decadal simulations that resolve the inertial contribution of the sea floor to the biogeochemical cycling in shelf environments. The model was implemented to analyze the benthic–pelagic coupling in the northwestern shelf of the Black Sea. Three distinct biogeochemical provinces were identified on the basis of fluxes and rates associated with benthic–pelagic coupling. Our model simulations suitably capture the seasonal variability of in situ flux data as well as their regional variation, which stresses the importance of incorporating temporally varying sediment biogeochemistry and resuspension/redeposition cycles in shelf ecosystem models.

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1. Introduction

Marine sediments play a key role in the global oceanic biogeochemical cycles (e.g., [Hedges, 1992](#); [Arndt et al., 2011](#); [Huettel et al., 2014](#)) and are particularly important in the biogeochemical functioning of shelf ecosystems ([Middelburg and Soetaert, 2004](#); [Soetaert and Middelburg, 2009](#)). The coupling between pelagic and benthic compartments is particularly tight in shallow coastal and shelf areas ([Heip et al., 1995](#)), where a significant part of the primary production escapes degradation in the water column, and is mineralized within the upper layer (5–20 cm) of sea floor ([Middelburg and Meysman, 2007](#)). For example, [Dunne et al. \(2007\)](#) estimate that 30% of the local primary production is respired in the sediment of near shore environments (<50 m depth) and 18% in shelf areas (50–200 m). In addition, part of the marine primary production depends on the transfer of nutrients and organic matter across the land–ocean continuum to the ocean, and the magnitude of this transfer depends on the capacity of the shelf ecosystems to “filter” the inputs from the land

([Regnier et al., 2013](#)). As a significant part of this filtering is mediated within shelf sediments, a proper and quantitative understanding of the benthic–pelagic coupling in shelf environments is necessary to accurately describe the biogeochemical cycling at basin scales ([Fennel et al., 2006](#)).

In the coming decades and centuries, both open ocean as well as shelf ecosystems will become increasingly stressed by rising temperatures, acidification and deoxygenation, which will affect biogeochemical cycles and ecosystems in ways that we are only beginning to understand ([Gruber, 2011](#)). Changes in the magnitude and seasonality of the pelagic production directly affect the quantity and quality of the organic matter that arrives at the sediment surface ([Townsend and Cammen, 1988](#)). The resulting impacts on net diagenetic rates ([Nixon et al., 2009](#)), the time lags associated with benthic–pelagic coupling ([Rudnick and Oviatt, 1986](#); [Soetaert and Middelburg, 2009](#)) and the composition of benthic communities ([Kirby et al., 2007](#)) are complicating factors that compromise our ability to predict the response of shelf ecosystems to changing external forcings.

Biogeochemical cycling within shelf sediments is affected by local environmental conditions such as the amount of pelagic primary production that reaches the bottom ([Soetaert et al., 1996b](#);

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Dollar et al., 1991), the bottom water temperature (Van Cappellen et al., 2002), as well as bottom oxygen and nutrient concentrations (Wijsman et al., 1999; Soetaert et al., 2000; Fulweiler et al., 2008; Dale et al., 2011). Consequently, biogeochemical transformations within the sediment and, by extension, the exchange between sediment and overlying water, can exhibit important spatial, seasonal and interannual variability (e.g., Friedrich et al., 2002; Fulweiler et al., 2010). This variability can have important implications for carbon sequestration (e.g., Hedges and Keil, 1995), eutrophication (Cercio and Cole, 1993; Gypens et al., 2008; Fulweiler et al., 2010; Bohlen et al., 2012) and coastal hypoxia (Turner et al., 2008; Peña et al., 2010; Capet et al., 2013). The measurement of benthic–pelagic fluxes is logistically challenging, and consequently few datasets are available, relative to the intrinsic spatial and temporal variability of benthic–pelagic coupling (Cardoso et al., 2010). Detailed three-dimensional (3D) model simulation are therefore required to better resolve the variability of benthic pelagic coupling and to assess its implications for large scale biogeochemical budgets.

In recent decades, 3D biogeochemical ocean models have become indispensable tools to explore the mid- and long-term evolution of marine ecosystems under various aspects of global change (e.g., climate change, eutrophication, acidification). Increasingly complex descriptions of pelagic biogeochemistry are coupled to 3D hydrodynamic models (Doney, 1999; Arhonditsis and Brett, 2004; Follows and Dutkiewicz, 2011), extending the range of resolved scales and the accuracy of shelf-ocean exchanges (Greenberg et al., 2007). Meanwhile, detailed regional models have been developed which specifically target the simulation of the biogeochemistry of shelf environments (Cercio and Cole, 1993; Moll and Radach, 2003; Proctor et al., 2003; Fennel et al., 2006; Smits et al., 2013). In a similar fashion, sophisticated stand-alone models of benthic biogeochemistry have been developed, which can resolve multiple elemental cycles and reproduce the vertical distribution of solids and solute fractions within the surface sediment (e.g., Soetaert et al. (1996a); Dale et al. (2008); Holstein and Wirtz (2009); Krumins et al. (2013), see also reviews by Arndt et al. (2013); Paraska et al. (2014)). These studies depict a complex and variable sediment biogeochemistry, whose representation in 3D ocean model remains challenging (Arndt et al., 2013).

However, models of pelagic and benthic biogeochemistry are typically not coupled or connected. Too often, the choice of a lower boundary condition in water column models is a matter of convenience, rather than an accurate and mechanistic representation of sediment–water exchange (Soetaert et al., 2000). Reflective bottom boundary conditions (see the classification of Soetaert et al. (2000)) consider instantaneous mineralization and diagenetic rates that are either fixed, or assumed to directly respond to one environmental factor (e.g., oxygen concentration in Fennel et al., 2006). While providing a satisfying first order variability of benthic pelagic coupling (Soetaert et al., 2000), the reflective boundary approach neglects the environmental controls on diagenetic rates and the time lag that separates organic matter accumulation and mineralization in marine sediments. Such approaches can therefore not account for benthic feedbacks on changing biogeochemical regimes. On the other hand, coupling 3D ocean models to dynamic, vertically resolved, sediment models is demanding in terms of implementation (e.g., model initialization, parameterization and validation in a 3D space, data needs, different scale ranges of benthic and pelagic biogeochemistry) and computational resources, especially for long-term simulations (e.g., climatic scenarios), ensemble simulations (e.g., model error assessment, sensitivity analysis), or high resolution implementations (e.g., for detailed study of estuarine/cross-shelf circulation). When a sediment model is coupled to a 3D ocean model, the simulations typically have a restricted character: they consider a limited number of el-

ements (e.g., Heinze et al., 1999; Palastanga et al., 2011), compute the benthic–pelagic coupling off-line (Gehlen et al., 2006), perform short-term simulations (e.g., Luff and Moll, 2004) or restrain the complexity of the benthic model component to allow analytical solutions (e.g., Holt et al., 2012; Butenschön et al., 2015). Finally, 3D biogeochemical modelling studies rarely account for the physical impact of bottom currents on sediments, although it has been shown that this can affect the variability of benthic–pelagic coupling, notably by inducing the resuspension of settled materials and reducing the net deposition (Hopkinson Jr, 1985; 1987; Wainright and Hopkinson Jr, 1997; Stanev and Kandilarov, 2012). A noteworthy exception to this rule is to be found in the ERSEM model (Butenschön et al., 2015).

By comparing 1D benthic–pelagic coupling setups with different levels of complexity, (Soetaert et al., 2000) suggested to rely on meta-modelling to reduce the complexity of benthic components, as an ideal balance between computing demand and attained accuracy.

The main objective of this paper is to present an efficient and accurate approach for the coupling of the benthic and pelagic compartments in 3D ocean models that enables long term simulations, while including a reliable representation of benthic–pelagic interactions. To meet these objectives, the approach proposed here combines two main features: (1) it implements a simplified and semi-empirical modelling of sediment biogeochemistry (i.e., early diagenesis), which represents the main pathways of organic matter mineralization and their variability, and (2) it explicitly accounts for the impact of bottom physical stress on particulate matter deposition and resuspension.

In order to highlight the skill and relevance of this approach, the model was used to simulate the benthic–pelagic coupling in the northwestern shelf of the Black Sea, an area characterized by strong environmental gradients and important variability of the benthic–pelagic coupling processes. Model results are compared to available field data and are used to analyze the variability of diagenetic processes under the influence of changing bottom water conditions. We evaluate the implications of benthic–pelagic coupling for the Black Sea biogeochemical cycling at basin scale and the sensitivity of this coupling to the calibration of resuspension parameters. Finally, we discuss the benefits and limitations of the proposed approach to include benthic–pelagic coupling in 3D ocean models as well as the potential for future enhancements.

2. Materials and methods

2.1. Study area: The Black Sea Northwestern shelf

The Black Sea region is located on the transition between the sub-tropical latitudes and the temperate climate zones, and is influenced by the atmospheric teleconnection patterns over both Europe and Asia (North Atlantic Oscillation, and East Asia/West Russia oscillation, Cherneva et al. (2008); Capet et al. (2012)). These combined influences result in an important variability of atmospheric conditions at both seasonal and interannual scales. Particularly in the northwestern part of the Black Sea, cold air penetrates from the north, facilitated by flat lands, which trigger strong northern and northeastern wind events. The river drainage area of the Black Sea is 5.2 times larger than the Black Sea surface, which is high in comparison to other parts of the Mediterranean Sea, where this ratio typically ranges from 0.4 to 2 (Ludwig et al., 2009). The resulting high riverine discharge relative to the basin volume influences the hydrodynamical structure of the Black Sea through freshwater inputs, and also impacts the biogeochemical structure through nutrient and sediment loads.

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