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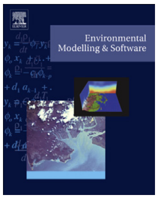

Sediment diagenesis models: Review of approaches, challenges and opportunities☆

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ABSTRACT

A range of sediment diagenesis modelling approaches have been developed over the last two decades, however, the diversity makes it difficult to identify the best approach for a particular aquatic system. This study summarised and categorised the variables, parameterisations and applications of 83 models published since 1996. The choice of variables and processes used was found to be largely arbitrary. Models have been applied to a range of environments, however, there was no corresponding difference in approach or complexity. The major challenges and opportunities for the development of the models include: aligning conceptual models of organic matter transformations with measurable parameters; gathering accurate data for model input and validation, including datasets that capture a range of timescales; coupling sediment models with ecological and spatially-resolved hydrodynamic models; and making the models more accessible for water quality and biogeochemical modelling studies by developing a consistent notation through community modelling initiatives.

1. Introduction

Chemical interactions between the sediment and the water column are a key component of aquatic biogeochemistry and ecology. The upper layer of the sediment can have more chemical processes than the entire overlying water column (Boudreau, 2000) and it is a hotspot for biogeochemical function. An exploration of the physical, chemical and biological dynamics in this near-surface sediment, termed early diagenesis, gives us a better understanding of the natural processes that shape elemental pathways, and allows us to assess the effects of human activity, which include the disruption of nutrient, oxygen and carbon cycles associated with eutrophication and contamination of aquatic ecosystems.

Sediment models are part of the greater group of increasingly sophisticated models that parameterise and combine transport processes and reaction pathways, in order to explore the system responses of complex aquatic environments (see, for example, Steefel et al., 2005; Soetaert and Herman, 2008, for general works). The models of this field are able to estimate chemical concentrations and reaction rates at a temporal and vertical resolution that is difficult to reproduce with in situ or laboratory experimentation (Luff and Moll, 2004). Reactive transport models have also been developed to examine specifically a range of systems and processes, including marine organic matter degradation (Arndt et al., 2013), carbon cycles (Mackenzie et al., 2004), hypoxic waters (Peña et al., 2010), aquatic ecology (Arhonditsis and Brett, 2004; Jørgensen, 2010; Mooij et al., 2010), groundwater (Hunt and Zheng, 2012), and heavy metal transport (Boudreau, 1999). In recent years, increasing attention has been given to analysing the development of the features and applications of reactive transport models (see, for example, Jakeman et al., 2006; Robson et al., 2008) and developing standards for assessing their performance and suitability (Bennett et al., 2013). With this context, it is therefore timely to analyse the development and performance of a large body of literature that has emerged on sediment reactive transport models.

The basis of numerical sediment diagenesis models was laid out by Berner (1980) and further developed by authors such as Van Cappellen et al. (1993), Van Cappellen and Wang (1995), and Boudreau (1997, 2000); readers wishing to understand the theory of diagenesis models should begin with these publications. The fundamentals were taken into early numerical models by authors

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such as Rabouille and Gaillard (1991a, b), Tromp et al. (1995), Furrer and Wehrli (1996), Dhakar and Burdige (1996) and Park and Jaffé (1996). Of the models that were developed in this period, the studies by Boudreau (1996), Van Cappellen and Wang (1996) and Soetaert et al. (1996a) have emerged as the basis for most of the numerical models developed by other authors since then (these three are cited 155, 294 and 201 times, respectively, in ISI Web of Knowledge, as of December 2013). The studies that developed from these three papers share some common process descriptions and general conceptual bases (Fig. 1), however, many variations in the implementation and the increasing complexity of the biogeochemical processes in subsequent applications have made it difficult to absorb the terminology, compare the models and identify the best approaches for a given application that an aquatic ecosystem modeller entering the field may be interested in. Further, while many of the original models were intended for the coastal or open ocean, they have since been applied widely across the spectrum of aquatic environments, including from oligotrophic to eutrophic inland and coastal waters. The connection between models purpose, structure and performance (as has been done recently for more general models of P dynamics by Robson, 2014) remains unexplored.

It is the aim of this article to conduct a review and meta-analysis of sediment diagenesis model publications that have emerged since the theoretical texts and the key 1996 model applications. By doing so we aimed *a)* to identify commonality between the studies and define a practical classification of commonly used approaches, *b)* to compare the model studies in the context of the questions they address and study environments, *c)* based on the above analysis, to identify challenges for the development and improvement of sediment diagenesis models and opportunities for advancing model accuracy and performance, and *d)* ultimately to assist and encourage the uptake and application of these models by the wider ecological modelling community.

2. Analysis approach and scope

We gathered 83 sediment diagenesis modelling studies from the peer reviewed literature in the period between 1996 and 2013, which are listed after the main reference list at the end of the paper. We considered vertically multi-layered, rather than one- or two-layer models, process-based rather than empirical models and numerical rather than analytical models. The focus of this analysis is not on the software codes themselves, which have been examined by Meysman et al. (2003a), nor the numerical solution methods.

This analysis is primarily focussed on the multi-G models that were developed from the G model of Berner (1980). ‘Continuous-G’ models have also been developed, in which the properties of the complex mixture are considered to be a function of depth, which in turn has reflected organic matter age (originally by Middelburg, 1989 then Boudreau and Ruddick, 1991, followed up recently by authors such as Wallmann et al., 2008; Arndt et al., 2009; Vähätalo et al., 2010; Rodriguez-Murillo et al., 2011; Gelda et al., 2013). The advantages of these empirical models are that they can be adjusted to fit depth profiles closely, they require few input parameters and they recognise the importance of the changing reactivity of organic matter over time, which is a factor that many other models do not take into account (Van Cappellen et al., 1993). However, the continuous-G model studies generally neglect the reactions of the oxidants and other secondary and mineral reactions that are important in determining other environmental geochemical processes, such as the fluxes of nutrients, oxygen and contaminants, and so this analysis is solely focused on multi-G models. Rather than organic matter reactivity being assigned as proportional to depth or age, multi-G models have a few distinct pools each with different reactivity. The origins of most of the recent multi-G models can be traced back to one of three sources that had developed Berner's model, based on either the CANDI model (Boudreau, 1996), the STEADYSED model (Van Cappellen and Wang, 1996), or the OMEXDIA model (Soetaert et al., 1996a). As will be explained in

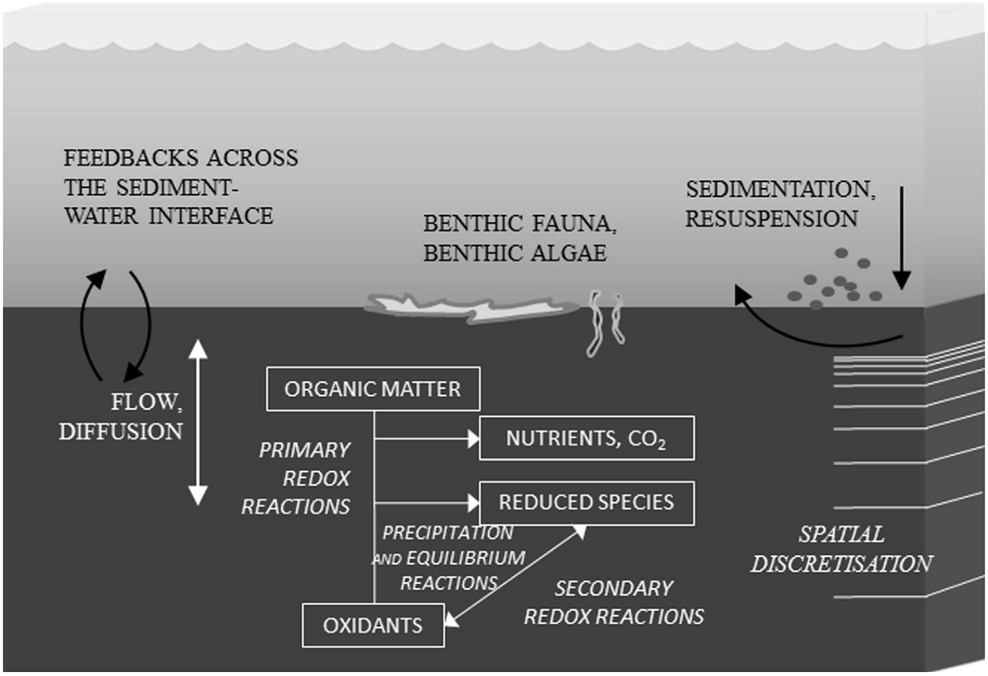

Fig. 1. Schematic of the main physical and chemical processes that cause chemical concentration and flux change in the sediment and across the sediment–water interface, and therefore are included in most sediment diagenesis models. The chemicals and reaction processes included in different studies vary widely and are shown in the following tables.