Progress in Oceanography 133 (2015) 55–65

Contents lists available at ScienceDirect

Progress in Oceanography

journal homepage: www.elsevier.com/locate/pocean

Simulating aggregate dynamics in ocean biogeochemical models

George A. Jackson [a,*], Adrian B. Burd [b]

[a] Department of Oceanography, Texas A&M University, College Station, TX 77843-3146, USA
[b] Department of Marine Sciences, University of Georgia, Athens, GA 30602, USA

ARTICLE INFO

Article history:
Available online 6 September 2014

ABSTRACT

The dynamics of elements in the water column is complex, depending on multiple biological and physical processes operating at very different physical scales. Coagulation of particulate material is important for transforming particles and moving them in the water column. Mechanistic models of coagulation processes provide a means to predict these processes, help interpret observations, and provide insight into the processes occurring. However, most model applications have focused on describing simple marine systems and mechanisms. We argue that further model development, in close collaboration with field and experimental scientists, is required in order to extend the models to describe the large-scale elemental distributions and interactions being studied as part of GEOTRACES. Models that provide a fundamental description of trace element–particle interactions are required as are experimental tests of the mechanisms involved and the predictions arising from models. However, a comparison between simple and complicated models of aggregation and trace metal provides a means for understanding the implications of simplifying assumptions and providing guidance as to which simplifications are needed.

Introduction

Marine particles affect, even control, major oceanic biogeochemical properties studied by GEOTRACES (Fig. 1). These include material fluxes, elemental depth profiles, and trace-metal partitioning (e.g., Fowler and Knauer, 1986; Lee et al., 2004). However, marine particles come in a wide range of types and sizes from submicrometer colloids to large macro-scale objects, both living and dead. Rates of relevant chemical, physical and biological processes involving particles (coagulation, transport from solution, absorption, consumption etc.) depend on particle size, abundance, and composition (e.g., Leal, 1992; Burd et al., 2007). To understand and accurately model particulate processes in the oceans requires, at a minimum, a description of particle concentration as a function of particle size.

At its most basic, a particle is a solid thing, possibly an organism, possibly a non-living organic or inorganic residue, possibly a mixture of all of these. It could be a fish, a copepod, an algal cell, a fecal pellet produced by a copepod eating an alga, a fragment of dead krill, a silica shell, TEP, or an amalgam of all these. Such an amalgam, or aggregate, may be known as “marine snow”. A particle is a transient object, as small particles collide or are eaten and combine and change to disappear in their old forms and morph into new, larger particles and as large particles break up into smaller ones. Their compositions change as they collect and release material from solution. They fall at speeds that depend on their sizes, shapes, densities, and compositions, moving mass with them. The rates of all these processes depend on the sizes of the individual particles as well as the size distribution of all particles. To sample them accurately, as well as to understand what they are doing, requires an appreciation and an understanding of the particles size distributions, as well as the processes that change their properties.

It has long been recognized that dynamics of living and non-living particles play a significant role in ocean geochemistry. The importance of particle scavenging in determining trace metal distributions has been recognized since the mid-1950s (Goldberg, 1954; Turekian, 1977). Bacon and Anderson (1982) compared different models of thorium adsorption onto multiple classes of particulate material (sinking and non-sinking), concluding that there was a continuous exchange of thorium between particulate and dissolved pools. Since then, two different but complementary approaches have been used to examine the role of particles. The more theoretical approach has used elements of coagulation theory to understand how the combination of aggregation and size-dependent adsorption affect observed thorium size-fractionation and partition coefficients onto aggregates (Honeyman and Santschi, 1989; Burd et al., 2000, 2007). The other approach uses a few (usually two) operationally defined particle size classes to represent the distribution of trace metals between the dissolved pool and particles of different sizes (e.g., Clegg and Whitfield,

---

* Corresponding author. Tel.: +1 979 845 0405.
E-mail addresses: gjackson@tamu.edu (G.A. Jackson), adrianb@uga.edu (A.B. Burd).

http://dx.doi.org/10.1016/j.pocean.2014.08.014
0079-6611/

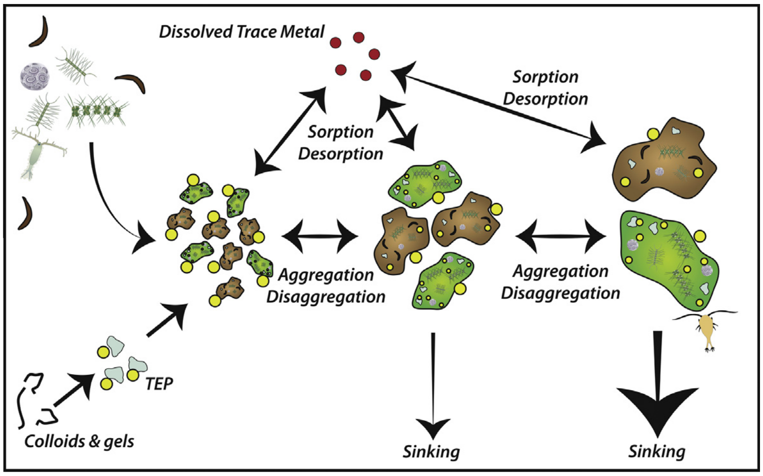

Fig. 1. Conceptual diagram of the role of particles in GEOTRACES research. Trace metals (signified by the yellow circles) sorb preferentially onto smaller particles (e.g., colloids), which are subsequently incorporated into aggregates. Processes of aggregation and disaggregation move these trace metals between different particle size classes. Biological processes (e.g., zooplankton consumption of aggregates) incorporate trace metals into fecal material that can sink and can be incorporated into aggregates. (Phytoplankton and zooplankton symbols courtesy of the Integration and Application Network, University of Maryland Center for Environmental Science (ian.umces.edu/symbols)). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

1990, 1991; Clegg et al., 1991). Although the latter has been preferred, the more detailed, theoretical approach, albeit more challenging, has much to offer in understanding trace metal distributions in the oceans and in the interpretation of relevant data.

In this article, we briefly review coagulation theory, outlining where the theory has made useful and successful predictions, and discuss the status of aggregate models relevant to the GEOTRACES program. We also discuss the advantages that more detailed coagulation models have over simpler ones, particularly in relation to ocean geochemistry, and discuss directions for future research. While most such models are inspired by descriptions of interactions of individual constituents, the simplifications required in a community model result in their use to describe average, community properties.

Particle structure

Not only do marine particles vary in size but they also vary in the shapes, structures, and compositions that affect their properties and behaviors. Particles such as fecal pellets are relatively solid and, for a given species, have discernable relationships between their sizes and various characteristics (e.g., settling speed). Aggregates, on the other hand, are porous particles and show more variability in their relationships between size and other characteristics. The structure of particles also affects how one interprets various observations. For example, for solid particles, the ratio of a surface-active trace metal (e.g., thorium) to a bulk characteristic such as organic carbon would be expected to vary according to the ratio of surface area to volume of the particles, or as $1/d$ (where d is a measure of the particle length). However, for a fractal particle, this ratio will be constant (Burd et al., 2000; Buesseler et al., 2006).

Possible measures of particle size include mass, volume, and any one of several types of diameter (Jackson et al., 1997). Using particle mass as the descriptor has advantages for theories and models because mass is conserved in particle interactions and is easy to track, although knowing the diameter for any particle is also crucial for calculating rates of particle transformations.

Most experimental methods for measuring particles determine some form of particle length. Because aggregated particles are composed of both smaller particles and included water, the lengths reported by different techniques can vary as a function of how these measures are affected by the aggregate porosity.

When people compare aggregate mass to diameter, they usually find that it follows a relationship of the form $m \sim d^f$, where m is the particle mass and f is the fractal dimension. If particles had a constant density, f would equal 3. In fact, values obtained for oceanic particles range from 1.5 to 2.3 (e.g., Logan and Wilkinson, 1990; Burd and Jackson, 2009), indicating that particle mass rises more slowly than volume as a result of the increasing porosity of larger particles. The fractal relationship can be used to create a length-based particle property that is conserved separately from mass conservation when particles collide and transform into a larger, more massive particle (Jackson, 1998).

Describing particle concentrations as function of size

All particle models start with the need to describe the concentrations of particles as a function of some size measure. Some particles, such as individual biological organisms, exist as distinct objects encompassing a relatively small range of sizes. However, most suspended and sinking particles in the ocean are collections composed of a combination of smaller particles accumulated from different sources. This is true for fecal pellets, collected by animal feeding, and marine snow. The first problem for developing an understanding of oceanic particles is to choose ways to describe particles that provide the maximum useful information about them. Knowing how best to characterize the particles themselves leads to an understanding of how best to describe their concentrations.

An aggregate composed of unit sub-particles, all of the same size, can be described in terms of the number of those units. This approach to describing particles allows one to track easily the concentrations of particles of different sizes. While simple in theory, this approach is not very practical, particularly for large particles. For example, distinguishing between the concentrations of particles with 1000 and those with 1001 algal cells is neither experimentally practical nor particularly useful; furthermore, this method does not work when there is more than one source of particle components. Particle size spectra overcome these issues by representing the concentration of particles per particle size, where size could be diameter or mass, and, as a result, have become the preferred way to describe the size dependence of particle concentrations (e.g., McCave, 1984).

Measurements of particle concentrations in different size ranges can be used to calculate particle size spectra. For example,