NEW DEVELOPMENTS IN THE MODELLING OF BIOTURBATION IN AQUATIC SEDIMENTS: RELATIONS BETWEEN LOCAL, NON-LOCAL, DISCRETE AND CONTINUOUS MODELS

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A general framework is proposed that classifies the existing bioturbation models according to two dividing lines: discrete/semi-discrete/continuous and local/non-local. Based on a common stochastic approach, which models biological reworking of particles as a position jump process, the relationships among the different model classes are exposed, and the assumptions underlying each model are explicitly derived. We find that discrete/semi-discrete/continuous formulations are principally equivalent, leaving two basic modelling formalisms: (1) the more inclusive non-local exchange formalism and (2) the local biodiffusion model, which is obtained as a special case of the former. An order of magnitude assessment reveals that under natural conditions, most modes of sediment reworking meet the condition for the non-local exchange formalism, but clearly violate the additional assumptions of the biodiffusion model, particularly for short-lived tracers. Nevertheless, in practice, the biodiffusion model has proven to be a valuable empirical model for sediment mixing. This apparent contradiction is referred to as the "biodiffusion paradox".

Introduction: a plethora of bioturbation models?

Burrowing, feeding and relocation of benthic organisms result in the displacement and mixing of sediment particles, a process commonly referred to as bioturbation (RICHTER, 1952; RHOADS, 1974; ALLER, 1982). A quantitative understanding of this phenomenon depends on models that provide a mathematical and preferably mechanistic description of biologically induced mixing processes (GOLDBERG & KOIDE, 1962). Such bioturbation models are a subcomponent of early diagenetic models, which employ a continuum description to the spatial and temporal distribution of certain tracers in the sediment environment (BOUDREAU, 1997).

In the past, a number of widely varying techniques have been used to arrive at a mechanistic mathematical description of bioturbation, such as random walks (BOUDREAU, 1989; WHEATCROFT et al., 1990), stochastic differential equations (BOUDREAU 1986a,b; MEYSMAN, 2001), finite difference mass balancing (BOUDREAU & IMBODEN, 1987; SOETAERT et al., 1996b; BOUDREAU, 1997; FRANCOIS et al., 1997), and Markov chain theory (FOSTER, 1985; TRAUTH, 1997; SHULL, 2001). Typically, these models were developed in a stand-alone fashion, focusing on particular bioturbation mechanisms with only marginal references to other modelling techniques. Consequently, the connection between the various types of models has only been given sparse attention, and a clear picture of their interrelation is lacking. The only link that is reasonably well studied is the transition from a discrete local bioturbation model to its fully continuous counterpart (BOUDREAU, 1989; WHEATCROFT et al., 1990). The latter equivalence comes down to the standard derivation of Fick's second law from an isotropic random walk (EINSTEIN, 1905; SMOLUCHOVSKI, 1916; Okubo, 1980).

In order to improve our ability to model and understand the complex phenomenon of bioturbation, it would be of great advantage to possess a broader, overall perspective of the various model approaches. In this light, we have carried out a critical re-examination of the theoretical foundations underlying the current theory of bioturbation. We examined the mechanistic foundations of the above-mentioned models and derived a general unifying framework. The existing models were obtained by implementing a common wandering particle approach. This exercise clearly establishes the relationships among the different model classes and exposes the assumptions underlying the various modelling approaches. Explicit criteria for the frequency, distance and symmetry of particle displacement in the associated mixing models were derived. The mathematical details of these derivations are given somewhere else (for details see MEYSMAN *et al.*, subm.), as here, we will only focus on the three important conclusions that can be drawn.

A unifying framework for bioturbation models

Basically, bioturbation models can be grouped into six categories using two classification principles (Fig. 1): (a) a mathematical criterion, i.e. discrete/semi-discrete/continuous models, and (b) a mechanistic criterion, i.e. local versus nonlocal. The existing bioturbation models thus can be grouped as: (1) local and discrete: 1D random walk models leading to Fickian diffusion (BOUDREAU, 1989; WHEATCROFT et al., 1990); (2) local and semi-discrete: the biodiffusor models of the socalled functional approach to sediment reworking (FRANCOIS et al., 1997, 2001); (3) local and continuous: averaging techniques for stochastic differential equations leading to Fickian diffusion (BOUDREAU, 1986a; MEYSMAN, 2001); (4) non-local and discrete: transition matrix models (FOSTER, 1985; TRAUTH, 1997; SHULL, 2001); (5) non-local and semidiscrete: the upward-conveyor, down-ward conveyor, regenerator and gallery-diffusor models of the functional approach (FRANCOIS et al., 1997, 2001) and (6) non-local and continuous: the non-local exchange function formalism (BOUDREAU & IMBODEN, 1987).

The first distinction is straightforward and unambiguous: discrete models are implemented *via* difference equations, semi-discrete (or equally semi-continuous) models employ ordinary differential equations, whereas full-continuum models are implemented via partial differential equations. In a second division, models can be labelled as local or non-local. This second criterion reflects the way particles are displaced as compared to the scale over which the tracer concentration changes. Non-local models use an arbitrary probability distribution to model particle displacement, which imposes no restriction on the direction and magnitude of the particle movements. The local or biodiffusion model forms a special case of the more general non-local model and requires particle displacement to be symmetric and small-scale (see below).

However, we could show that only the local/non-local trait provides a truly distinguishing factor. From a mechanistic point of view, the same assumptions and restrictions apply to the discrete, semi-discrete and continuous forms of a given model (whether local or non-local), and thus they provide the same description. This implies that only two archetypal models of bioturbation exist: the non-local exchange formalism and the local biodiffusion formalism.

The difference between local and non-local transport

Although the terms local and non-local transport have been used extensively in the bioturbation literature, until now, no quantitative basis has yet been provided to decide whether a process should be characterized as "local" or "non-local". WHEATCROFT *et al.* (1990) noted: "At some point diffusion is no longer an accurate descriptor of bioturbation and non-local models must be employed. The point at which a given step length shifts from being local to non-local is not clear-cut." Past distinctions between "local" and "non-local" transport were based on the "locality" concept, as introduced by BOUDREAU (1986b), who stated that sediment displacement should be (1) spatially random and (2) small-scale. Obviously, small-scale mixing constitutes a relative concept and hence, biological transport should be classified as either small-scale or large-scale as compared to some other length scale. Because no explicit expressions were provided for these length scales, locality remained a pure qualitative concept, and hence, past distinctions between "local" and "non-local" transport were intuitive and author-dependent.

Here we provide quantitative criteria to decide whether a given biological mixing process should be described via either a local or a non-local model. Most importantly, these criteria are not absolute (i. e. they are not inherent to the biological mixing process) but are truly relative features (the mixing process should be evaluated within a given geochemical context). The non-local exchange formalism is established as the more inclusive formalism, from which the local biodiffusion formalism can be obtained as a special case. Application of the non-local exchange formalism requires that the frequency criterion should be met. Bioturbation events must be sufficiently frequent as compared to the time of the tracer being studied. For a description via the local biodiffusion formalism, two additional assumptions are required. (1) The symmetry criterion ensures the directional randomness of the sediment mixing process and demands the symmetry of the exchange function. (2) The scale criterion quantifies whether sediment displacement is sufficiently small-scale and requires the mixing length δ^m to be smaller than the tracer length δ^{t} . This way, we have quantified the transition point between local and non-local transport (Fig. 2).

The validity of the biodiffusion model: The biodiffusion paradox

In a pioneering series of papers, BOUDREAU (1986a,b) and BOUDREAU & IMBODEN (1987) examined the theoretical constraints underpinning the biodiffusion model and as a result, some concerns were raised regarding the validity of Fickian diffusion as a general model for bioturbation. Our results here corroborate and even amplify these theoretical reservations against the biodiffusion model. The Fickian analogy is constrained by the stringent conditions of the symmetry criterion and the scale criterion. By evaluating these quantitative criteria for typical early-diagenetic environments (deep-sea, slope, coastal) we found that many commonly encountered sediment-reworking modes clearly violate the assumptions of the biodiffusion model, particularly for the short-lived tracers ²³⁴Th and ⁷Be, and for ²¹⁰Pb in high-deposition environments.

Nevertheless, the biodiffusion model has been applied in numerous radiotracer studies in both marine (e. g. NOZAKI *et al.*, 1977; COCHRAN, 1985; MULSOW *et al.*, 1998) and lacustrine environments (e. g. ROBBINS *et al.*, 1977; CHRISTENSEN, 1982; WALLING & HE, 1992). Furthermore, the biodiffusion model has been adopted as the standard description for bioturbation in so-called general diagenetic models, which provide an integrated reactive transport description of the geochemical cycles in surface sediments (e. g. VAN CAPPELLEN & WANG, 1996; SOETAERT *et al.*, 1996a). Moreover, down-core profiles of most radiotracers appear diffusive and thus, in practice, the biodiffusion model has proven to be a valuable empirical model for modelling sediment mixing. This quite astonishing contradiction is what we will term the "biodiffusion paradox".

One possible explanation for this "biodiffusion paradox" can be found in the alternative pseudo-advective-diffusive form of the non-local integro-differential conservation equation that we were able to derive. The latter hints at a clear link between the local biodiffusion model and non-local exchange model. Moreover, it results in an elegant procedure to calculate a formal biodiffusion coefficient from a non-local exchange distribution function. This constitutes an important step towards a direct derivation of the biodiffusion coefficient from biological data, i. e. an alternative for estimating the biodiffusion coefficient from the tracer profiles. However, to understand fully the biodiffusion paradox, we will need to build exchange functions, mechanistically based on realistic bioturbational behaviour of macro-organisms, solve the corresponding integro-differential equations, and compare these with solutions to its approximated form, the pseudoadvective-diffusion equation.

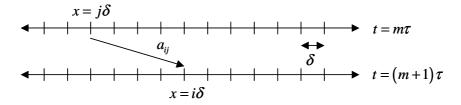
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	discrete	semi-continuous	continuous
local	I Isotropic Random walk	II Biodiffusor (functional approach)	III Biodiffusion
non-local	IV _{Transition} matrix	V Functional approach	VI Exchange function

Fig. 1. Classification of bioturbation models along two lines: process form (local/nonlocal) *versus* mathematical form (discrete/semidiscrete/continuous). Existing bioturbation models can be grouped as: (1) *local and discrete*: 1D random walk models leading to Fickian diffusion (BOUDREAU, 1989; Wheatcroft *et al.*, 1990); (2) *local and semi-discrete*: the biodiffusor models of the so-called functional approach to sediment reworking (FRANCOIS *et al.*, 1997, 2001); (3) *local and continuous*: averaging techniques for stochastic differential equations leading to Fickian diffusion (BOUDREAU, 1986a; MEYSMAN, 2001); (4) *non-local and discrete*: transition matrix models (FOSTER, 1985; TRAUTH, 1997; SHULL, 2001); (5) *non-local and semi-discrete*: the upward-conveyor, down-ward conveyor, regenerator and gallery-diffusor models of the functional approach (FRANCOIS *et al.*, 1997, 2001) and (6) *non-local and continuous*: the non-local exchange function formalism (BOUDREAU & IMBODEN, 1987).

(a) Non-local transport



(b) Local transport

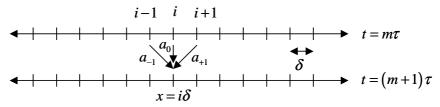


Fig.2. Bioturbation modelled as a jump process on a one-dimensional lattice. (a) Non-local transport: a particle can jump to any position on the lattice. (b) Local transport: a particle's jump is restricted to neighbouring positions.

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