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Sediment unmixing using detrital geochronology

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ABSTRACT

Sediment mixing within sediment routing systems can exert a strong influence on the preservation of provenance signals that yield insight into the effect of environmental forcing (e.g., tectonism, climate) on the Earth's surface. Here, we discuss two approaches to unmixing detrital geochronologic data in an effort to characterize complex changes in the sedimentary record. First, we summarize 'top-down' mixing, which has been successfully employed in the past to characterize the different fractions of prescribed source distributions ('parents') that characterize a derived sample or set of samples ('daughters'). Second, we propose the use of 'bottom-up' methods, previously used primarily for grain size distributions, to model parent distributions and the abundances of these parents within a set of daughters. We demonstrate the utility of both top-down and bottom-up approaches to unmixing detrital geochronologic data within a well-constrained sediment routing system in central California. Use of a variety of goodness-of-fit metrics in top-down modeling reveals the importance of considering the range of allowable that is well mixed over any single best-fit mixture calculation. Bottom-up modeling of 12 daughter samples from beaches and submarine canyons yields modeled parent distributions that are remarkably similar to those expected from the geologic context of the sediment-routing system. In general, mixture modeling has the potential to supplement more widely applied approaches in comparing detrital geochronologic data by casting differences between samples as differing proportions of geologically meaningful end-member provenance categories.

1. Introduction

The sedimentary record is an archive of global change over geologic time. It records the influence of tectonism, climate, sea level, and anthropogenic effects on the evolution of the Earth's surface. Tracking variations in sediment provenance is an effective means of determining the influence of environmental change on sediment generation, transport, and deposition within sedimentary systems (Dickinson, 1974; Graham et al., 1986; Gehrels, 2014; Fildani et al., 2016; Mason et al., 2017). Temporal and spatial changes in sedimentary provenance may be signals of environmental change acting on the sediment routing system, including changing catchment drainage boundaries and/or differential erosion within existing drainage boundaries that reflect tectonic, climatic, and/or eustatic controls (Romans et al., 2016; and references within). In some cases, the presence of geologically distinctive materials in the sedimentary record makes interpreting changes in sedimentary provenance relatively straightforward. However, the complex process of sediment mixing that occurs during sediment transport can also obscure primary provenance signals, hampering efforts to decipher changes in sedimentary provenance (Fig. 1).

Geochronology of detrital minerals (hereafter, detrital geochronology) has emerged as a leading method to investigate the provenance of the sand- and silt-sized fraction of sediment (e.g., Fedo et al., 2003; Gehrels, 2014). To the extent that sediment source areas produce unique detrital age distributions, downstream sediment that is well mixed will reflect the relative sediment contributions from each of these sediment source areas (Fig. 1). More specifically, a given daughter detrital age distribution (D_o) can be modeled as a linear mixture of the n parent detrital age distributions that contributed to that daughter:

$$D_m = \sum_{i=1}^{n} \phi_i P_i \tag{1}$$

Where P_i is the ith parent distribution and ϕ_i is the relative contribution, or 'mixing coefficient' of the ith parent, and D_m is the modeled daughter distribution that best characterizes the actual, D_o. Here, the mixing coefficients must sum to 1 to honor the assumption that the daughter was sourced entirely and only from

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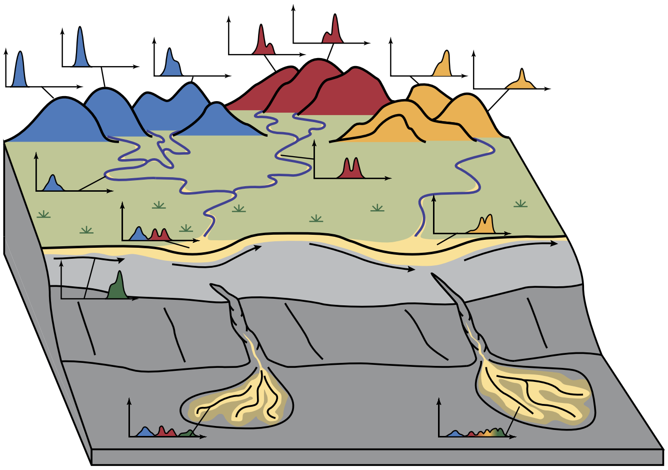

Fig. 1. Hypothetical sediment routing system characterized by four source areas (blue, red, yellow, and green; modified from Romans et al., 2016). Although not depicted, windblown sediment can also constitute an important source of sediment in some systems. The relative frequencies of a generic categorical variable (non-negative, sums to 1) are shown as probability density plots. Black arrows indicate longshore sediment transport. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

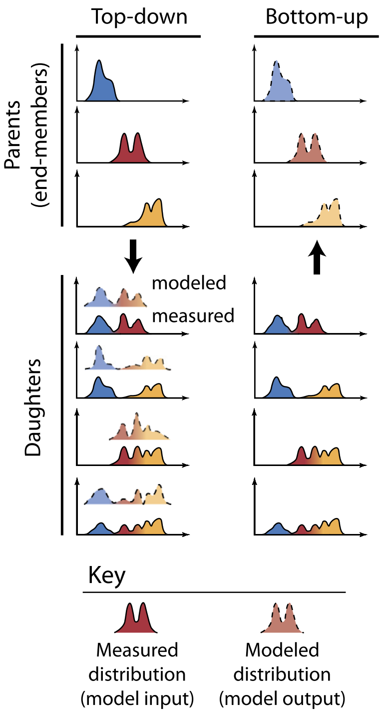

Fig. 2. Schematic depiction of two general approaches to numerical unmixing of sedimentary data. Model inputs (typically measured distributions) are shown with solid coloration, and model outputs (modeled distributions) are shown as partially transparent with a dashed outline. Top-down approaches use defined age distributions of parents, or mixing end-members, to model the best-fit combination to daughter mixtures (e.g., Amidon et al., 2005a, 2005b). Bottom-up approaches attempt to use a number of daughter distributions to model end-member, or parent, distributions (e.g., Dietze et al., 2012). (For interpretation of the colors in this figure, the reader is referred to the web version of this article.)

these parents. The distributions P and D describe the relative likelihood of a mineral grain of a particular age being found within a sample. Common practice is to estimate these distributions based on observed mineral ages in a geologic sample, often on the order of 60–300 individual observations. Detrital geochronologic distributions are commonly constructed by summing Gaussian distributions with a standard deviation that is defined by either the analytical uncertainty of the analysis (probability density plot, PDP) or a specified bandwidth (kernel density estimator, KDE) (Vermeesch, 2012).

A number of approaches have been developed to unmix sedimentary data, with a particular focus on grain size distributions (Weltje, 1997; Orpin and Woolfe, 1999; Weltje and Prins, 2003, 2007; Dietze et al., 2012; Paterson and Heslop, 2015; Yu et al., 2016). However, approaches to sediment unmixing using detrital geochronologic and/or thermochronologic data have not been widely developed or applied, with some notable exceptions (e.g., Amidon et al., 2005a, 2005b; Enkelmann and Ehlers, 2015; Kimbrough et al., 2015; Mason et al., 2017), despite these data types becoming increasingly used in sedimentary provenance studies that aim to reconstruct ancient source regions and paleocatchment boundaries (Gehrels, 2014; Lawton, 2014). Compared to grain size data, detrital age distributions may be better suited to tracing sediment mixing due to the specificity with which geochronology can identify particular source terrains. For these reasons, detrital geochronology may provide a particularly useful, but underutilized, data type for sediment unmixing calculations.

This study aims to review existing numerical approaches to sediment unmixing and provide recommendations for application of these techniques to detrital geochronologic datasets. In general, we find that unmixing calculations fall into two end-member categories: (1) 'top-down,' mixing models, and (2) 'bottom-up,' unmixing models (Fig. 2). To our knowledge, only top-down mixing models that forward model daughter populations by linear mixing of specified parent distributions have been applied to detrital geochronologic datasets (e.g., Amidon et al., 2005a, 2005b; Fletcher et al., 2007; Kimbrough et al., 2015; Mason et al., 2017). However, we contend that at least one bottom-up unmixing algorithm that was originally designed for grain size data (Paterson and Heslop, 2015) can also be effectively applied to detrital age distributions. This conclusion is supported by observations from Monte Carlo simulations of synthetic detrital age distributions. In the majority of synthetic cases, comparisons between actual and modeled parent age distributions yield at least as good of agreement as was observed in 95% of cases where a distribution was compared to a derivative of itself constructed from random sampling. Finally, we provide a case study that demonstrates the utility of both top-down and bottom-up mixture modeling in a well-constrained, modern fluvial-to-marine sediment routing system along the margin of central California (Sickmann et al., 2016).

2. Review of approaches to sediment unmixing

2.1. Top-down sediment mixing models

Top-down sediment mixing models use defined parent distributions to forward model daughter distributions. Mixing coefficients in this method are based on the best (or set of equally likely) values computed from an objective comparison between observed, D_o, and modeled, D_m, daughter distributions (e.g., a goodness-of-fit metric) (Equation (1), Fig. 2A). Many goodness-of-fit metrics have been defined for comparing detrital geochronologic data, including measures of the differences between cumulative distribution functions (e.g., $D_{\max}$ and $V_{\max}$) and the agreement between the shape of PDPs or KDEs (e.g., similarity, cross-correlation of PDPs) (see Saylor and Sundell, 2016, for a thorough review). In this approach, parent distributions must be known independently. In studies of modern sedimentary systems, parent distributions may be approximated by measurement of sediment within source area tributaries (e.g., Amidon et al., 2005a; Kimbrough et al., 2015; Mason et al., 2017) and/or measurement of bedrock distributions within the source area catchment (e.g., Amidon et al., 2005a; Saylor et al., 2013). In studies of ancient sedimentary systems, parent distributions cannot usually be measured directly and must