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Organic-geochemical proxies of sea surface temperature in surface sediments of the tropical eastern Indian Ocean

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ABSTRACT

In this study we reconstruct sea surface temperatures (SSTs) using two lipid-based biomarker proxies (alkenone unsaturation index $U^{K'}_{37}$ and TEX_{86} index based on glycerol dibiphytanyl glycerol tetraethers) in 36 surface sediment samples from the Indonesian continental margin off west Sumatra and south of Java and the Lesser Sunda Islands. Comparison of measured temperatures (World Ocean Atlas 09) to reconstructed temperatures suggests that SST estimates based on $U^{K'}_{37}$ reflect the SE monsoon SST in the upwelling area south of Java and the Lesser Sunda Islands. Estimates based on TEX_{86} using the calibration for temperatures >20 °C (TEX^{H}_{86}) are up to 2 °C lower than $U^{K'}_{37}$-based SSTs. This offset is possibly related to either one or a combination of two factors: (i) the depth habitats of the source organisms and (ii) different seasonal production and/or seasonality of export associated with phytoplankton blooming triggered by primary productivity. In the non-upwelling area off west Sumatra, the alkenone-based SSTs are cooler than measured temperatures during the entire year, likely reflecting the limitations of the $U^{K'}_{37}$ proxy beyond 28 °C, while reconstructed temperatures based on TEX^{H}_{86} are consistent with mean annual SST.

1. Introduction

Accurate SST reconstructions are an important prerequisite for understanding the climate system. Two organic-geochemical proxies, namely $U^{K'}_{37}$ (alkenone unsaturation) and TEX_{86} (tetraether index of glycerol dibiphytanyl glycerol tetraether with 86 carbon atoms), are widely employed to reconstruct surface water temperatures in the oceans and in lakes.

Alkenones, di- and tri-unsaturated C_{37} methyl ketones, are synthesized by prymnesiophyte algae (Brassell et al., 1986). The coccolithophores *Emiliania huxleyi* and *Gephyrocapsa oceanica* are the two major source organisms of alkenones (Conte et al., 1998; Volkman et al., 1980). A range of alkenone studies in surface waters and cultures have demonstrated the close linkage between the alkenone unsaturation ratio and growth temperatures of the precursor organisms (Conte et al., 1992, 1994; Marlowe, 1984; Prahl et al., 1988; Volkman et al., 1995; Yamamoto et al., 2000).

For temperature estimation, the unsaturation is generally expressed as the $U^{K'}_{37}$ ratio (Prahl and Wakeham, 1987). Since its introduction in 1987, determination of alkenone unsaturation has become a widespread technique to reconstruct past SST from marine sediments. Previous calibration studies showed linear relationships between global marine core-top $U^{K'}_{37}$ and mean annual surface water temperature (Conte et al., 1998, 2006; Müller et al., 1998). The temperature range of the calibration spans from 2 to 28 °C. Sedimentary records of $U^{K'}_{37}$ correlate well with mean annual SST (ma SST) in the surface waters and have proven reliable and robust for reconstructing past SST changes (Herbert et al., 2003). However, occasionally observed deviations between global calibrations and sedimentary alkenone temperature are still contentious. Discrepancies between $U^{K'}_{37}$ and ma SST have been explained by physical factors such as, for instance, lateral redistribution of sediments (Benthien and Müller, 2000), ecological factors like export production originating from below the euphotic zone (Prahl et al., 1993, 2001; Ternois et al., 1997), influence of nutrients (Versteegh et al., 2001), and the thriving of alkenone-producers in specific seasons (Popp et al., 2006). In addition, species composition (Conte et al., 1998) and differential degradation of alkenones (Conte et al., 1992; Prahl et al., 1989) could also affect the temperature-estimates derived from $U^{K'}_{37}$.

Schouten et al. (2002) introduced another organic proxy, TEX_{86}, based on the relative distribution of glycerol dialkyl glycerol tetraethers (GDGT). These GDGTs are membrane lipids produced by marine Crenarchaeota, re-named Thaumarchaeota (Brochier-Armanet et al., 2008). The relative distribution of the GDGTs is suggested to vary with

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growth temperature, similar to the $U^{K'}_{37}$ (Schouten et al., 2013b and reference therein). In the last decade, several calibration studies using core-top sediments and archaeal cultures have been conducted, and linear as well as non-linear regressions with SST have been proposed (Liu et al., 2009; Schouten et al., 2002; Wuchter et al., 2006, Kim et al., 2008). More recently, the original proxy has been refined further into TEX^{H}_{86} and TEX^{L}_{86} by Kim et al. (2010) for temperatures higher and lower than 15 °C, respectively. The TEX_{86} proxy is expected to reflect the temperature in the upper parts of the water column (Schouten et al., 2002; Wuchter et al., 2006). Although the GDGT-based proxy has already been widely used, it remains uncertain as to how well it reflects ma SST. For example, some studies suggested that TEX_{86} does not reflect SST, but rather subsurface temperature due to additional production of GDGTs below the mixed layer (Huguet et al., 2007; Lee et al., 2008; Lopes dos Santos et al., 2010). Other studies have shown that the TEX_{86} may be biased due to seasonality in growth or export of Thaumarchaeota, e.g. towards summer temperature in the eastern Mediterranean (Leider et al., 2010) and the South China Sea (Jia et al., 2012), or towards winter temperature in the southern North Sea (Herfort et al., 2006). Additionally, it hast been suggested that the TEX_{86} signal reflects other temperatures than annual mean SST because Thaumarchaeota are outcompeted by phytoplankton including alkenone producers e.g., during upwelling events, and thus thrive during seasons or at depths less favorable for phytoplankton producers (Rommerskirchen et al., 2011; Wuchter et al., 2006, Lee et al., 2008; Turich et al., 2007). Another complication arises from input of terrestrially derived isoprenoid GDGTs (Weijers et al., 2006).

Hopmans et al. (2004) proposed the Branched and Isoprenoid Tetraether (BIT) index, a proxy for the relative abundance of terrestrial soil organic matter in the marine environment, which could bias the TEX_{86} (Herfort et al., 2006). The BIT index represents the ratio between crenarchaeol and three branched GDGT lipids in marine and lacustrine sediments, and is expected to be near 1 in soils and approach 0 in deep sea sediments with negligible contribution of soil-derived terrestrial organic matter (Hopmans et al., 2004). The proxy can potentially be used to assess whether a bias of the TEX_{86} index by input of soil-derived isoprenoid GDGTs is to be expected, and cut-off values of BIT <0.3 or <0.2 have been suggested (Weijers et al., 2006, Zhu et al., 2011). These values are not to be regarded globally reliable, as on the one hand potential impact of terrestrially derived isoprenoid GDGTs, depends not only on the relative contribution to total isoprenoid GDGTs in marine sediments but also on the relative abundance of those GDGTs that are relevant for TEX_{86} in the soils of the source area. The latter parameter in most cases is complicated to determine. On the other hand, BIT index determinations are not directly comparable between different laboratories (Schouten et al., 2013a), which is further complicating the use of BIT.

Generally, all temperature proxies have their uncertainties. To better understand the significance of each proxy, multiple proxies have been applied to the same sediment material. Comparison of $U^{K'}_{37}$ and TEX_{86} data for sediments and suspended particles has been reported in several publications (e.g., Huguet et al., 2006; Jia et al., 2012; Lee et al., 2008; Leider et al., 2010; Lopes dos Santos et al., 2010; Rommerskirchen et al., 2011). These studies attributed a significant potential source of uncertainty to different seasonal production and/or depth habitats of the source organisms.

In this study, we investigate the applicability of the $U^{K'}_{37}$ and TEX^{H}_{86} indices in the upwelling and non-upwelling areas of the eastern tropical Indian Ocean. We present alkenone and GDGT data from 36 surface sediment samples and compare the reconstructed temperatures to temperatures from the World Ocean Atlas 2009 in order to evaluate the factors influencing these proxies in the study area.

2. Study area

The eastern tropical Indian Ocean south of Java and the Lesser Sunda Islands (LSI) are strongly affected by the Australian–Indonesian Monsoon (AIM) system and the seasonal shifting of the Inter-Tropical Convergence Zone (ITCZ), which cause opposite seasonal characteristics at the sea surface (Tomczak and Godfrey, 1994; Webster et al., 1998). During the austral winter (Fig. 1b), the ITCZ is in the Northern Hemisphere and the southeast (SE) monsoon (July–September) winds are such that the southeast trades from Australia induce dry conditions off Java and the LSI. During the austral summer (January–March, Fig. 1a), the ITCZ migrates to northern Australia and the northwest (NW) monsoon is associated with the opposite wind direction from the Indonesian Seas and Asian continent carrying warm and moist air to the region. The precipitation rates over this region during NW monsoon are among the highest in the world resulting in maximum riverine discharge (Milliman et al., 1999). During this time, the predominant winds force the South Java Current (SJC) to flow from northwest to the southeast, before turning southward to eventually join the South Equatorial Current (SEC) (Fig. 1a). Advection of fresher Java Sea waters through the Sunda Strait and run-off from Sumatra and Java are responsible for the low-salinity "tongue" in the SJC (Qu and Meyers, 2005).

During the SE monsoon (Fig. 1b), the SJC and its prolongation, the SEC, flow westward along the southern coast of Java, when costal upwelling off Java and the LSI occurs (Tomczak and Godfrey, 1994). The upwelling is associated with higher chlorophyll-a concentration (Fig. 1f and g), higher salinities and SSTs that are 1–2 °C lower compared to the non-upwelling season (Gordon et al., 2005, Susanto et al., 2006). In contrast, the area off W and NW Sumatra does not show any significant seasonality in SST and precipitation and is considered a non-upwelling, ever-wet tropical region (Fig. 1a–c; Aldrian and Susanto, 2003).

The Indonesian Throughflow (ITF) connects the upper water masses of the Pacific and Indian Oceans and substantially influences the salinity and heat exchange between these oceans (Gordon and Fine, 1996). During the SE monsoon season (Fig. 1b), the sea level difference between the Western Pacific and the eastern Indian Ocean is largest, implying maximum strength in ITF (Tomczak and Godfrey, 1994). It is suggested that the Java upwelling system is counterbalanced by the ITF and, consequently, except for brief periods, fails to bring subsurface nutrients to the surface (Godfrey, 1996). In this case, the ITF branch through the Lombok Strait counteracts a significant SST depression off Java during the upwelling season.

3. Material and methods

3.1. Surface samples

In this study, we use the top 1 cm of multicore samples from 36 sites collected during PABESIA RV Sonne Cruise SO-184 in 2005 off west Sumatra and south Java and the LSI (Hebbeln et al., 2005) (Table 1, Fig. 1).

A set of $U^{K'}_{37}$ temperature estimates for the same samples has been published by Mohtadi et al. (2011). Most of the data reached the upper limit of this proxy, i.e. close or above 28 °C. Six of the samples analyzed here have been included in the global GDGT core-top calibration study of Kim et al. (2010), but for reasons of consistency have been re-analyzed in this study.

Modern surface sediment ages have been confirmed at nine selected stations by accelerator mass spectrometry (AMS) ^{14}C dates on planktic foraminifera (Mohtadi et al., 2011; Table 1). Two samples from off Sumatra show older ages implying that