Journal of Marine Systems 163 (2016) 12–22

Contents lists available at ScienceDirect

Journal of Marine Systems

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

Time series analysis of data for sea surface temperature and upwelling components from the southwest coast of Portugal

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ARTICLE INFO

Article history:
Received 4 February 2016
Received in revised form 1 June 2016
Accepted 3 June 2016
Available online 7 June 2016

Keywords:
Upwelling
Sea surface temperature
Structural breaks
Spectral analysis
Iberian Peninsula
Sagres

ABSTRACT

This study relates sea surface temperature (SST) to the upwelling conditions off the southwest coast of Portugal using statistical analyses of publically available data. Optimum Interpolation (OI) of daily SST data were extracted from the United States (US) National Oceanic and Atmospheric Administration (NOAA) and data for wind speed and direction were from the US National Climatic Data Center. Time series were extracted at a daily frequency for a time horizon of 26 years. Upwelling indices were estimated using westerly (Q_x) and southerly (Q_y) Ekman transport components.

In the first part of the study, time series were inspected for trend and seasonality over the whole period. The seasonally adjusted time series revealed an increasing slope for SST (0.15 °C per decade) and decreasing slopes for Q_x (-84.01 m^3 s^{-1} km^{-1} per decade) and Q_y (-25.20 m^3 s^{-1} km^{-1} per decade), over the time horizon. Structural breaks analysis applied to the time series showed that a statistically significant incremental increase in SST was more pronounced during the last decade.

Cross-correlation between upwelling indices and SST revealed a time delay of 5 and 2 days between Q_x and SST, and between Q_y and SST, respectively. A spectral analysis combined with the previous analysis enabled the identification of four oceanographic seasons. Those seasons were later recognised over a restricted time period of 4 years, between 2008 and 2012, when there was an extensive sampling programme for the validation of ocean colour remote sensing imagery. The seasons were defined as: summer, with intense and regular events of upwelling; autumn, indicating relaxation of upwelling conditions; and spring and winter, showing high inter-annual variability in terms of number and intensity of upwelling events.

1. Introduction

Upwelling occurs in several coastal regions of the world, affecting the biological productivity and dynamics of these regions (Schwing et al., 1996). An upwelling event occurs due to the interaction between the frictional stress of wind on the ocean surface and the rotation of the earth. As a consequence, transport occurs whereby the surface water mass moves to the right (in the Northern hemisphere), and is replaced by water from beneath the surface (Lluch-Cota, 2000; Price et al., 1987). This offshore movement of surface water masses is known as Ekman transport. The cold subsurface water that reaches the euphotic zone is generally rich in nutrients, stimulating primary production. For this reason, upwelling regions account for about 20% of the global fish catch despite comprising ~1% of the coastal regions of the world (Narayan et al., 2010; Pauly and Christensen, 1994). Due to the difficulty of measuring these events directly, as well as a scarcity of long time series (Schwing et al., 1996), the assessment of upwelling events is usually performed either by measuring the phenomenon inducing agents such as wind stress and Ekman transport, or by estimating the environmental changes resulting from upwelling, such as the increase in primary productivity and the marked decline in sea surface temperature (SST)[1] (Lluch-Cota, 2000).

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[1] Abbreviation List (alphabetical order): AVHRR — Advanced Very High Resolution Radiometer; BIC — Bayesian information criterion; NOAA — National Oceanic and Atmospheric Administration; OI — Optimum Interpolation; Q_x — Latitudinal component of Ekman transport, meaning upwelling conditions in the Western Coast; Q_y — Longitudinal component of Ekman transport, meaning upwelling conditions in the Southern Coast; RSS — Residual Sum of Squares; SST — Sea Surface Temperature.

http://dx.doi.org/10.1016/j.jmarsys.2016.06.002
0924-7963/

Over the last three decades, a SST data product has been made available from National Oceanic and Atmospheric Administration (NOAA) with the Optimum Interpolation (OI) 0.25 Degree Daily SST Analysis data (Reynolds et al., 2007), hereafter referred to as NOAA OI SST. This product enables a) the analysis of a large dataset, covering the recent period of global warming (Hansen et al., 2010; Lima and Wethey, 2012; Trenberth et al., 2007), and b) the possibility of comparing SST with upwelling indices based on wind stress, for a more complete characterisation of upwelling events.

The NOAA OI SST database is particularly robust, combining observations from satellite AVHRR sensors interpolated with observations from sensors on ships and buoys. Apart from global coverage at a daily resolution, it allows for the large-scale adjustments of remote sensors with respect to *in situ* data (Reynolds et al., 2007). Spurious variability has been further reduced by the continuous use of the same type of remote sensor type over the entire time series, operated from 9 different satellites (NOAA7 to NOAA19 and METOP-A) (Banzon et al., 2016). However, there are limitations due to the weakness of the bias correction in some areas, where there is limited availability of *in situ* data, especially in higher latitudes (Banzon et al., 2016). Furthermore, the SST is an aggregate of data collected over the entire day, and therefore there is no accounting for the diurnal variability (Banzon et al., 2016). Despite its limitations, the NOAA database has been one of the most used sources for global SST (e.g. Costoya et al., 2015; Girondot and Kaska, 2015; Khalil et al., 2016; Liu and Minnett, 2015; Marullo et al., 2014; Singh et al., 2013). SST is often analysed using statistical techniques for dependent data (time series).

The analysis of time series is an important and valuable approach adopted in several studies, for its ability to improve the spatial and temporal resolution of the major seasonal and inter-annual patterns in biological and oceanographic data (Vantrepotte and Mélin, 2010, 2011). These studies provide indicators about long-term changes in natural conditions, such as climate change, which is why such indicators are advised or even mandated for coastal water monitoring programmes (e.g. Water Framework Directive, 2000/60/EC) (Vantrepotte and Mélin, 2010).

1.1. Rationale

The Sagres region has had a significant water sampling programme for the validation of ocean colour remote sensing imagery between the end of 2008 and the beginning of 2012 (Cristina et al., 2009, 2014, 2015; Goela et al., 2013, 2014, 2015). Concurrent with satellite overpasses, the water column was sampled to use its bio-optical properties to validate satellite products in the Sagres region. Additionally, this comprehensive data set was used to derive and develop regional ocean colour algorithms. However, this development requires comprehensive knowledge of the seasonal patterns of the in-water constituents. In the case of Sagres, it has a narrow continental shelf with little influence from the coast, so that the seasons are probably better explained by changes in upwelling forcing, rather than the regular succession of calendar seasons and other underlying patterns (river discharges, winter runoffs, summer stratification, etc.) (Loureiro et al., 2005, 2011). There is a particular interest in identifying the oceanographic seasons off the Sagres region over the period of the water sampling programme related to the validation of remote sensing imagery. Indeed this time series study would provide a preliminary step in the overall characterisation of the seasonal pattern for bio-optical parameters in Sagres.

In such context, the intention was not to do a full characterisation of the upwelling process in Sagres, as this would require a robust *in situ* dataset. Instead, the study was conducted with practical and publically available databases, aiming to define oceanographic seasons by examining patterns and relationships in and between data sets for SST and upwelling indices, using statistical methodologies for dependent data. To fulfill this objective, the work was developed in three consecutive steps: 1) to conduct a preliminary analysis of the time series for SST and upwelling indices; 2) to verify the relationship between SST decreases (reflection of upwelling events) and favourable upwelling indices (forcing agents); and 3) to define the periodicity of upwelling events in the area, in order to delineate oceanographic seasons, especially during the sampling period for validation.

1.2. Sagres region

The study region is part of the Eastern North Atlantic Upwelling System (Wooster et al., 1976) and is located in a transition zone, where different upwelling fronts develop along the west and south of the study region.

Conditions favourable for upwelling are more intense and persistent along the west coast, induced by northerly winds, and are typically associated with summer (Fiúza et al., 1982; Loureiro et al., 2005; Relvas and Barton, 2002). Strong westerly winds can also induce occasional upwelling episodes against the typical warm counter current driven by a pressure gradient flowing along the south coast (Relvas and Barton, 2002). Upwelling filaments in the study region have been observed in satellite images for both SST and ocean colour (Fiúza, 1983; Haynes et al., 1993; Sousa and Bricaud, 1992; Sousa et al., 2008). Thus, the Sagres study site, located at 2 km from the coast (Site 1 in Fig. 1), can contain upwelled water collected from either the western or the southern coast, or a combination of both.

Time series studies on the persistence and intensity of winds and upwelling events on the Portuguese western coast describe several and sometimes contradictory scenarios. For example, Bakun (1990), Casabella et al. (2014), Lorenzo et al. (2005), and Ramos et al. (2013) reported an enhancement of favourable conditions for upwelling in recent years but, in contrast, other authors report a weakening in the number and intensity of upwelling events with climate alterations (Alvarez et al., 2008; Álvarez Salgado et al., 2008; Alves and Miranda, 2012; Lemos and Pires, 2004; Lemos and Sansó, 2006).

2. Methods

2.1. Time series sources

Data for wind speed and direction were obtained from the Blended Daily Averaged 0.25-degree Sea Surface Winds (at 10 m level) product, provided by the National Oceanic and Atmospheric Administration (NOAA) and National Climatic Data Centers (Zhang et al., 2006). The SST time series for the Portuguese coast was extracted from the NOAA OI daily SST with a 0.25-degree resolution model (Reynolds et al., 2007).

Ekman transport was calculated following Bakun (1973) and Cropper et al. (2014). Latitudinal (Q_x) and longitudinal (Q_y) components of Ekman transport were considered to be the upwelling indices whereby negative values of Q_x and Q_y, would indicate upwelling conditions along the western and southern coasts, respectively.

2.2. Time series analysis

A time series $\{Y_t\}_{t=1}^{N}$ is a collection of observations indexed by time t. In this study, time series were extracted for the period from 13th January 1988 to 31st December 2013, covering a time horizon of 26 years ($N =$ 9485 daily observations). Few missing observations were detected; in fact the longer interpolated lag was 5 days (0.97%). Where there were missing observations, estimation and imputation were performed with linear interpolation (R function na.interp() (Hyndman, 2015)). All the statistical analyses were performed using the R 3.2.2 software (R Core Team, 2015) and considered at a level of significance of 0.05.

2.2.1. Time series modelling

Classical decomposition methods have been widely identified in the marine sciences literature (e.g. Loisel et al., 2014; Mélin et al., 2011;