Ocean Data Assimilation in the Angola Basin

by

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Abstract

The predictability of the ocean currents and the Congo River plume within the Angola Basin was investigated using the Regional Ocean Modelling System (ROMS) with data assimilation (4D-Var).

Firstly, the impact of assimilating a novel remote-sensing data set, satellite-derived ocean currents (OSCAR) as compared to the more conventional satellite sea surface height (SSH) on ocean current predictability was assessed. In comparing 17 simulated and observed drifters throughout January-March 2013 using four different metrics, it was found that OSCAR assimilation only improves the Lagrangian predictability of ocean currents as much as altimetry assimilation.

The impact of combining the aforementioned remote-sensing observations (OSCAR or SSH) with drifters was then investigated throughout the same period to assess whether this combination could improve upon assimilating the drifters alone on ocean current predictability. It was found that the addition of drifters significantly improves the Lagrangian predictability of the ocean currents in comparison to either altimetry or OSCAR as expected. More surprisingly, the assimilation of either SSH or OSCAR with the drifter velocities does not significantly improve the Lagrangian predictability compared to the drifter assimilation alone, even degrading predictability in some cases.

Additionally, a new metric denoted the crossover time was formulated using the drifters, defined as the time it takes for a numerical model to equal the performance of persistence. In addition to ROMS, a global ocean model was also evaluated to demonstrate and quantify the metric fully.

Finally, the impact of assimilating a recently available advanced version of a satellite salinity product (SMOS), on the Congo River plume was investigated. With some metrics specifically focusing on validating the Congo River plume, it was found that the assimilation of SMOS improved the representation of the plume within the model as well as the modelled salinity fields.
Declaration of Originality

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Dedication

I dedicate my PhD thesis to my very supportive mum, my loving girlfriend, my grandparents, my sisters and finally my father, may he rest in peace.
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Chapter 1

Introduction

1.1 Motivation and Objectives

Data assimilation (DA) is often applied to improve an ocean model’s representation of the real circulation and scalar variables. DA has subsequently contributed to a significant rise in forecast skill (Rabier, 2006; Bauer et al., 2015). Its objective is to derive an optimal estimate of the current and future state of the system using observations together with information from the dynamical model (Lahoz et al., 2010a). Many major ocean modelling systems have implemented DA schemes (Dombrowsky et al., 2009), including the Regional Ocean Modeling System (Moore et al., 2011b), Nucleus for European Modeling of the Ocean (Mogensen et al., 2012), and Navy Coastal Ocean Model (Smith et al., 2015).

Despite advancements in the assimilation schemes themselves, ocean DA lags behind its atmospheric counterpart considerably regarding observations. The environment of the ocean means sampling is challenging, with satellite information only limited to the surface (Anderson et al., 1996). Buoys, profiling floats, remote sensing satellites, moorings, coastal radars, gliders and surface drifters make up the main observational data sets for the ocean.

Still, the often substantial improvement in forecasting is of great interest for many applications in the ocean, including producing accurate regional ocean currents that can be used
for responding to a major marine pollution event, or in perhaps more uniquely, river plume modelling.

The first results chapter (Phillipson and Toumi, 2017) explores the gap in the literature surrounding the assimilation of OSCAR, a novel upper ocean current analysis product produced via a combination of remote sensing instruments. Previously the impact of OSCAR assimilation on the modelled ocean currents has only been studied using a simplified DA technique known as nudging and without any comparison with the assimilation of other observations. Therefore, the objective of this chapter is to understand, for the current generation of advanced DA techniques, the impact of OSCAR assimilation as compared to say sea surface height (SSH), an observation shown to improve modelled ocean currents when assimilated that is also sampled from remote sensing instruments. This represents a first step to demonstrate the use of assimilating OSCAR within an advanced assimilation with implications in improving forecasts of ocean currents.

The second results chapter (Phillipson and Toumi, 2017) then focuses on a comprehensive multi-observational comparison of the additional benefits of the assimilation of surface drifters, floating GPS tracked buoys that sample the surface velocity of the ocean. Previous studies have typically focused on either the assimilation of solely drifters or together with SSH in less advanced DA schemes. Therefore, the objective of this chapter is to provide a quantification of the impact of assimilating drifter velocities both separately and together with the aforementioned remote sensing observations (OSCAR and SSH). This would have implications in modelling ocean currents for real time events such as oil spill applications. Additionally, to aid in the quantification of improvements in the modelled ocean currents, a new evaluation metric was formulated and is introduced in this second chapter (Phillipson and Toumi, 2018). Therefore, an additional objective was to utilise the persistence of ocean currents (derived from the surface drifters) in a unique way to determine the relative skill of the ocean model. This metric can then be easily implemented for any ocean model.

Finally, the last results chapter (submitted to Remote Sensing) investigates the feasibility of assimilating a recently revised satellite salinity product and the subsequent impact on modelling
a large river plume. This is the first time satellite salinity has been assimilated for coastal applications and therefore the objective of this chapter is to first, as a pilot study, showcase the successful assimilation of this data and second, explore any potential benefits on modelling river plumes. This would have implications on operational regional modelling as this represents a first step to showing the current generation of satellite salinity observations can be useful in an assimilation system.

The Angola basin was chosen as the region of interest for all applications. Its diverse ocean currents (Stramma and Schott, 1999), importance as a petroleum reservoir (Clifford, 1986), marine biodiversity (Boisrobert and Virdin, 2008) and significant river plume (Hopkins et al., 2013a) made for an attractive area of study. Furthermore, this thesis was the first application of data assimilation in the Angola Basin.

The thesis is structured as follows; the remainder of this chapter introduces the theory of data assimilation and the Angola Basin. Chapter 2 follows with a summary of the ocean model utilised and all the observational data that is assimilated. Chapter 3 is the first results chapter that focuses on satellite current assimilation. Chapter 4, the second results chapter concentrates on drifter assimilation combined with multiple observations, as well utilising drifter persistence forecasts in formulating the new evaluation metric. Chapter 5, the final results chapter focuses on satellite salinity assimilation for river plume modelling. Finally, Chapter 6 concludes the thesis with a retrospective highlighting applications and future work.

1.2 Data Assimilation

1.2.1 Background

Data assimilation’s primary objective is to use measured observations together with information from a dynamical model to derive an optimal estimate of the current and future state of the system, along with providing some knowledge of the uncertainty in this estimate (Lahoz et al., 2010b).
Chapter 1. Introduction

The data assimilation problem has to be stated in probabilistic terms since the errors in sampling the earth system (via uncertain measurements) and the errors in the dynamical model (via approximations of the model physics and parameterisations), are unknown. However useful estimates of the errors in the system can take the form of a probability density function (PDF) or quantities describing a PDF, i.e. first and second moments. Bayesian estimation provides a mathematical foundation and means to this probabilistic approach (Lorenc, 2014), relating probability distribution functions (PDF’s) representing different states of the system. Bayes’ theorem can be thought as a starting point whereby;

\[ P(A|B) = \alpha P(B|A)P(A) \]  

(1.1)

where \( P(A|B) \) is the posterior probability of event \( A \) given event \( B \) has occurred, \( \alpha \) is a normalization constant, \( P(A) \) is the prior probability of event \( A \), \( P(B|A) \) is the probability of event \( B \) given event \( A \) has occurred, and \( P(B) \) is the prior probability of event \( B \) (not shown).

Equation 1.1 can then be applied generally to the earth system where event \( A \) represents the state vector \( x = x_t \), a possible state of the true system, and event \( B \) represents the observations \( y_o \), thus Equation 1.1 becomes Equation 1.2.

\[ P(x_t|y_o) \propto P(y_o|x_t)P(x_t) \]  

(1.2)

The left-hand term is known as the posterior and is the PDF of every possible state \( x_t \) given the observations \( y_o \). The middle term is known as the likelihood, i.e. the PDF of the measurement given the state. The right-hand term is known as the prior and describes information about the state before any measurements.

A Gaussian assumption is crucial for the practical implementation of data assimilation in numerical weather prediction (NWP). In this application, the PDF’s in Equation 1.2 have very high dimensions, and thus one cannot calculate the full PDF. Instead under a Gaussian assump-
tion of errors, the PDF can be defined solely by the mean and covariance. This assumption is somewhat less justifiable in some cases, such as when the dynamical model has a systematic bias, thus containing errors that are no longer Gaussian.

Statistical linear estimation is the primary simplifying approach to the data assimilation problem that takes on board the Gaussian assumption (Lahoz and Schneider, 2014). Here Bayesian estimation is achieved when the system is linear, allowing the Best Linear Unbiased Estimate (BLUE) to be computed.

A ’best’ linear estimate of the solution to the non-linear DA problem can be derived through linearising the problem about the non-linear trajectory of the background. When the errors in the observations and model are assumed to be Gaussian, the data assimilation problem is equivalent to the maximum a posterior Bayesian estimate (Lahoz and Schneider, 2014).

The prior PDF will have a mean $x_f$ also known as $x_b$ denoting a short forecast estimating the background state and a covariance $B$, the background error covariance matrix. The likelihood PDF depends on the observation error and observation operator $H(x)$, which maps information in state $x$ space onto the observation $y_o$ space. Thus it will have a mean of $H(x)$ and covariance $R$, the observation error covariance matrix.

One can now write out explicitly each PDF in the form of an unbiased Gaussian (Lorenc, 2014), considering estimations of the possible state $x$ given deviations from $x_b$ and deviations from the observations $y_o$. The prior knowledge is then assumed to be that $x$ is near $x_b$, with a variance of the deviation from $x_b$ denoted $B$. Furthermore, the likelihood has observations near $H(x)$ ($x$ mapped to observation space) with a variance of the deviations $R$. $N(a, C)$ is denoted as the Gaussian probability distribution with expectation (mean) $a$ and covariance $C$.

$$P(x) = N(x; x_b, B)$$  \hspace{1cm} (1.3)
\[ P(x) \propto e^{\exp \left\{ -\frac{1}{2} (x - x_b)^T B^{-1} (x - x_b) \right\}} \]  
\[ \text{(1.4)} \]

\[ P(y) = N(H(x); y, R) \]  
\[ \text{(1.5)} \]

\[ P(y|x) \propto e^{\exp \left\{ -\frac{1}{2} (y - H(x))^T R^{-1} (y - H(x)) \right\}} \]  
\[ \text{(1.6)} \]

then using Bayes' theorem from Equation 1.2;

\[ P(x|y) = N(H(x); y, R) N(x; x_b, B) \]  
\[ \text{(1.7)} \]

\[ P(x|y) \propto e^{\exp \left\{ -\frac{1}{2} (y - H(x))^T R^{-1} (y - H(x)) + (x - x_b)^T B^{-1} (x - x_b) \right\}} \]  
\[ \text{-J[x]} \]  
\[ \text{(1.8)} \]

where \( J[x] \) is the known as the cost function.

From this formation, the state \( x_t \) can hence be estimated by finding the mode of \( P(x_t|y) \) via maximum a posterior probability (MAP) applied to the PDF or finding the mean of using notions of minimum variance. Equation 1.8 shows that the maximum probability and thus the mean of \( P(x_t|y) \) occurs when \( x \) minimises the cost function. Variational assimilation uses an iterative optimization method to minimize the cost function from Equation 1.8 (3D-Var and 4D-Var) while sequential assimilation involves solving an alternative formulation of \( P(x|y) \) that stems from the property of a Gaussian in the case of a linear \( H \) (Lorenc, 2014).
For the practical implementation of the above further assumptions are essential mainly due to the size of the problem (Lahoz and Schneider, 2014). Typical dimensions of current NWP models are of the order $\sim 10^9$ and with the number of observations typically of order $\sim 10^7-8$, the resulting covariance matrices become impossible to store. The most powerful supercomputers can store and process the model and observations vectors of billions of degrees of freedom, however, storing and performing matrix operations on full $n \times n$ matrices is both unaffordable and unfeasible. Thus modelling, representing and estimating both $B$ and $R$ matrices are of great importance for all data assimilation schemes (Lorenc, 2014).

In variational data assimilation, the method of control variable transforms (CVTs) is an essential step to model the background error covariance matrix $B$ and also to improve the conditioning of the problem (Lorenc, 2014). The basic procedure behind this method is to make a change of variable that simplifies the background term in Equation 1.8 and in doing so $B$ is substantially simplified (Bannister, 2008a,b). The improvement to the conditioning comes from the CVTs desired side effect to produce a more manageable approximation of the Hessian $(\frac{\partial^2 J(x_a)}{\partial x_a^2})$ (Lorenc, 2014), which needs to be computed for the minimisation of the cost function in a variational DA scheme. CVTs can be implemented and defined in a vast number of different ways and are often applied differently across NWP centres adding to the increasing complexity and differences between many DA systems. In sequential data assimilation, $B$ is typically estimated from an ensemble of short-range forecasts.

### 1.2.2 Variational Methods

As previously mentioned variational methods central principle is to minimise the cost function in Equation 1.8 to produce the most likely analysis $x_a$. The first term can represent the misfit between the model state and observations, denoted $J_o$ and the second term can represent the misfit between the model state and background state denoted $J_b$ (Lahoz and Schneider, 2014). This is the most general form of the cost function for variational methods which subsequently evolves and develops depending on the degree of complexity in the situation for which it is used (Talagrand, 2014).
The most straightforward situation, for example, occurs when the observations $y$ and background $x_b$ are available at the same time, say $k$. Thus this minimisation will produce an estimate of the state of the flow only at $k$ (Talagrand, 2010). This is known as three-dimensional variational analysis or abbreviated as 3D-Var, where the temporal dimension of the observations has been excluded.

A more complex situation occurs when one wants to assimilate observations over some period, i.e. the DA window, such that the evolution of the flow needs to be accounted for (Talagrand, 2014). Here the cost function changes to:

$$J[x_o] = \frac{1}{2}(x_o-x_o^b)^T B_k^{-1}(x_o-x_o^b) + \frac{1}{2} \sum_{k=0}^{K} (y_k-H_k(x_k))^T R_k^{-1} (y_k-H_k(x_k))$$  \hspace{1cm} (1.9)

where $x_o$ represents the initial condition at time $k = 0$.

The minimum of Equation 1.9 represents the initial condition model solution that will fit the evolution of the observations most closely, taking into account the misfit for the observations at their correct time. This variant was first termed by (Sasaki, 1970) as strong-constraint four-dimensional variational assimilation, abbreviated as strong-constraint 4D-Var. The term 'strong-constraint' represents the assumption of excluding the model error. When accounting for model error, this is then termed 'weak-constraint 4D-Var', and includes an additional term to the cost function in Equation 1.9, namely:

$$+ \frac{1}{2} \sum_{k=0}^{K-1} (x_{(k+1)} - M_k x_x)^T Q_k^{-1} (x_{(k+1)} - M_k x_k)$$  \hspace{1cm} (1.10)

where $M_k$ is a known model linear operator, and $Q_k$ is the model error covariance matrix. The model error is assumed to be uncorrelated in time, and uncorrelated with the observations and background errors (Talagrand, 2014). This adds further complexity to the 4D-Var process whereby the model error covariance matrix just like $B$ and $R$ needs to be represented in an
efficient and simplified manner.

To improve the efficiency of implementation rather than searching for the minimum of $J[x]$ the cost function directly, it is better to instead search for the gradient of $J[x]$ that is equal to zero i.e. $\frac{\partial J(x)}{\partial x} = 0$ (Lorenc, 2014). Figure 1.1 visually demonstrates how this gradient can be used to find the minimum of the cost function.

![Figure 1.1: Cost function $J[x]$ against $x$ demonstrating how successive estimates of $\frac{\partial J(x_n)}{\partial x_n}$ can be used to determine the minimum $J[x]$. Adapted from the lecture notes of Lawless (2014).](image)

The most common way to perform such a procedure is an iterative gradient method which requires the explicit determination of the local gradient $\frac{\partial^2 J(x_n)}{\partial x_n^2}$ at each iteration (Talagrand, 2014). The quasi-Newton formulation of this approach is demonstrated below (Lorenc, 2014); however, one is not restricted to this method as a conjugate gradient can also be used (Lawless, 2014). The quasi-Newton method is a conventional mathematical technique used to find successively better approximations to roots of functions and can be formulated for 4D-Var as;

$$x_{(n+1)} = x_n - \left[ \frac{\partial^2 J(x_n)}{\partial x_n^2} \right]^{-1} \frac{\partial J(x_n)}{\partial x_n}$$

(1.11)

where $x_n$ is the nth iteration of a best estimate and $x_{(n+1)}$ is the improved estimate.

The term $\left[ \frac{\partial^2 J(x_n)}{\partial x_n^2} \right]^{-1}$, the true Hessian, is evidently impossible to calculate but can be ap-
proximated effectively using a descent algorithm with further iterations (Lorenc, 2014). For conjugate gradient methods, this Hessian approximation is typically used in preconditioning to accelerate the convergence of the solution rather than in minimization process itself (Tshimanga et al., 2008). To determine the local gradient $\frac{\partial J(x_n)}{\partial x_n}$ at every iteration a powerful mathematical technique can be utilised known as the adjoint method. It allows the computation of the gradient of a function at a cost much less than the direct calculation of the function (Talagrand, 2010).

Thus the process for determining the gradient $\frac{\partial J(x_0)}{\partial x_0}$ is summarized in Talagrand (2010) as follows;

1. Starting from $x_o$ integrate the basic equation and store $x_k$;

2. Starting from the final condition $x_k$ at time $k$, integrate the adjoint equations backward in time until the required gradient is found.

According to this method, it is required that the model is run forwards and backwards at every iteration (the inner loops), meaning the adjoint method can be computationally expensive. An approximation to a whole DA system is applied in an incremental approach (Talagrand, 2014), to make the adjoint more efficient. Here the non-linear problem is replaced by a sequence of approximately linear least-squares problems (Lahoz and Schneider, 2014); thus the minimisation can be performed using the tangent linear model at lower computational cost. This is known as Incremental 4D-Var, the variant that is utilised for this thesis.

1.3 The Angola Basin

The eastern equatorial Atlantic Ocean is a complex region highlighted by its system of ocean currents (Figure 1.1). The major oceanographic features are well-known within the area, following extensive observational studies by Eisma and van Bennekom (1978); Van Bennekom and Berger (1984); Jansen et al. (1984); Signorini et al. (1999); Stramma and Schott (1999).
1.3. The Angola Basin

These oceanic features include the Equatorial Under Current (EUC), Gabon-Congo Undercurrent (GCUC), South Equatorial Under Current (SEUC), South Equatorial Current (SEC), the South Equatorial Counter Current (SECC) which branches to become the Angola Current (AC) moving south along the coast, the Benguela Current (BC) and its coastal branch the Benguela Coastal Current (BCC) moving north along the coast, the Angola dome (AD), the Angola-Benguela front (ABF) and the Congo River (Stramma and Schott, 1999).

The equatorial SEC and easterly boundary BC broadly form part of the northern and eastern sections of the Southern Atlantic subtropical gyre (Peterson and Stramma, 1991). They are driven by the prevailing trade winds (Pitcher et al., 2010) and primarily fed by the Agulhas Current and the South Atlantic Current (Bachêlery et al., 2016).

Counter currents (a current that opposes the prevailing wind direction) such as the SECC is formed from the pressure gradient force (PGF) acting towards the east. This PGF develops as the water 'piles up' from the westward currents (SEC) and is blocked by the landmasses along the western boundaries (Brown et al., 2001a). The counter currents driven by this eastward PGF can overcome the prevailing wind direction in equatorial areas of light winds known as the Doldrums. Furthermore, convergence around 4°N creates a slope in the sea-surface which drives a geostrophic current towards the east (such as for the North Equatorial Countercurrent). Another way for a counter current to overcome the prevailing wind is at depth via the sloping thermocline (a transition layer between the mixed layer at the surface and the deep water layer) that also induces an eastward PGF. Beneath the influence from the prevailing wind this PGF at depth can create very strong currents known as undercurrents (Brown et al., 2001a). The EUC for example, is the fastest of the equatorial currents at 1.5 m/s (Brown et al., 2001a). The south easterly winds driving the BC (coloured arrows in Figure 1.2) also force coastal upwelling and Ekman offshore transport creating a highly productive oceanic ecosystem known as the Benguela Upwelling System (BUS) (Bachêlery et al., 2016). With Ekman transport 90° to the left of any longshore equatorial winds (southern hemisphere), net offshore divergence of the Ekman layer flow results in the upwelling of cold nutrient rich waters to replace the diverging flow (Brown et al., 2001b). The AC is a southward flowing current (mean flow of 58 cm/s) fed by the equatorial EUC, SECC and GCUC (Kopte et al., 2017). Ostrowski et al. (2009) suggests
The variability in strength is associated with coastally trapped waves that propagate poleward and interact with the AC. The sharp boundary then separating the warm saline AC from a cold up-welling system of the BC is known as the Angola-Benguela front (ABF), situated 15-17°S off the coast of Africa. The front exhibits an annual cycle of position and intensity where it is southernmost (north-most) and strongest (weakest) in austral summer (winter). Colberg and Reason (2006) directly studied the ABF front and investigated the sensitivity of its location and position. Colberg and Reason (2006) argued that the location is determined by the opposing coastal currents, the Angola Current (AC) and Benguela Coastal Current (BCC) which are subsequently driven by local wind stresses. In particular the AC is driven by the negative wind stress curl north of the ABF which has a significant effect on the strength of the AC, and hence the location of the ABF (Xu et al., 2013). The AD is a thermal upwelling dome that was first identified by Mazeika (1967) associated with cyclonic flow inducing upwelling. Recently, Doi et al. (2007) used a high resolution ocean model (10 km) to study the seasonality of the AD, where they found the dome developed from May to September owing to the divergence of heat transport associated with upwelling. The complicated interplay of these currents makes accurate simulations of the regional circulation a challenging prospect (Denamiel et al., 2013).

Some more challenging features to simulate realistically are the Congo River plume and the sea surface temperature south-east of the Angola Basin. The Congo River plume can reach as far as 800 km from the source (Hopkins et al., 2013a), influencing a substantial section of the basin. Previous studies have analysed the Congo River plume and notable features. Yankovsky and Chapman (1997) noted that the plume could be classified as surface-advected; with identifiable near- and far-field regions. Variations in the near-field have been identified with the speed of outflow, the orientation of the estuary mouth and local coastal currents (Eisma and van Bennekom, 1978; Denamiel et al., 2013). For the far-field, a more complex situation arises through the interaction between the wind stress, ocean circulation patterns, tidal currents and river discharge variations that contribute to different scenarios of the Congo River plume dispersion (Signorini et al., 1999). Denamiel et al. (2013) performed the first numerical simulation of the Congo River plume where they found the plume had a northward extension for the majority of the year except during February-March where the plume had a
1.3. The Angola Basin

Figure 1.2: Schematic of all the major oceanographic features of the Angola Basin. Warm surface currents (solid lines with black arrowheads) are the South Equatorial Current (SEC), South Equatorial Counter Current (SECC), Angola Current (AC). Warm undercurrents (dashed lines with black arrowheads) are the Equatorial Undercurrent (EUC) and Gabon-Congo Undercurrent (GCUC). Cold surface currents (solid lines with white arrowhead) are; the Benguela Oceanic Current (BOC) and Benguela Coastal Current (BCC). Also shown, The Angola Dome (AD), the Angola-Benguela Front (ABF) and the Congo River (solid white line in land). Overlaid as vector velocities (m/s) are the ERA-I (JFM) averaged winds averaged over January-March 2013. Adapted from Pérez et al. (2001)

A sizeable westward expansion (800 km). Subsequent model studies have focused on the plume’s buoyancy-driven dynamics (Vic et al., 2014; Palma and Matano, 2017), the effect of the Congo on ocean temperatures (White and Toumi, 2014), and a complete simulation of the Congo river-to-sea continuum with a multi-scale unstructured mesh model (Bars et al., 2016). A significant warm SST bias has been identified in various model studies of this region (White and Toumi, 2014), yet its origin is not well understood and remains highly debated (Xu et al., 2013). Previous studies (reviewed in Xu et al. (2013)) have suggested this bias stems from systematic errors in atmospheric models in reproducing the correct surface heat flux and coastal winds. Xu et al. (2013) suggested systemic errors in ocean models also make a notable contribution, proposing two oceanic mechanisms. The first is related to an overshooting of the Angola Current
(AC in Figure 1.2) which subsequently shifts the position of the Angola-Benguela Front (ABF in Figure 1.2) forming an SST bias. The second is related to difficulties in simulating the sharp thermocline along the Angola coast. Here, a substantial subsurface warm bias subducts underneath the Benguela Coastal Current (BCC in Figure 1.2) upon the collision of the AC and BCC. This subducted warm bias is then brought to the surface by the Benguela up-welling system forming a coastal SST bias.
Chapter 2

Models and Data

2.1 Regional Ocean Modelling System (ROMS)

2.1.1 Equations of Motion

ROMS is a hydrostatic, primitive equation, Boussinesq ocean general circulation model where the Reynolds-averaged Navier-Stokes (RANS) equations under the hydrostatic and Boussinesq assumption are the fundamental equations of motion. The momentum balance in the x- and y-directions in Cartesian coordinates are as follows;

\[
\frac{\partial u}{\partial t} + \vec{v} \cdot \nabla u - f v = -\frac{\partial \phi}{\partial x} - \frac{\partial}{\partial z} \left( w'w' - \nu \frac{\partial u}{\partial z} \right) + F_u + D_u \tag{2.1}
\]

\[
\frac{\partial v}{\partial t} + \vec{v} \cdot \nabla v - f u = -\frac{\partial \phi}{\partial y} - \frac{\partial}{\partial z} \left( v'v' - \nu \frac{\partial v}{\partial z} \right) + F_v + D_v \tag{2.2}
\]

where \( u, v, w \) are the \( x,y \) (horizontal coordinates) and \( z \) (vertical coordinate) components of the vector velocity \( \vec{v} \), \( t \) is the time, \( f(x,y) \) is the Coriolis parameter, \( \phi(x,y,z,t) \) is the dynamic pressure which is equal to \( P \) the total pressure divided by \( \rho_0 \) the characteristic density, \( \nu \) is
the molecular viscosity, $F_{u,v}$ are the forcing/source terms and $D_{u,v}$ are the optional horizontal diffusive terms. Note also the overbar represents a time average and a prime represents a fluctuation about the mean.

Here, a Reynolds decomposition (decomposing the turbulent flow into average and fluctuating components (Reynolds, 1895)) has been applied to the full Navier-Stokes (NS) equations averaged over time, simplifying the problem into solving the RANS Equations 2.1 and 2.2. This simplification is crucial for the practical solution of the NS equations to which a full 3D solution remains the subject of on-going research in mathematics (Xu et al., 2017). During this simplification a new set of terms of the form $\overline{uv'w'}$ arise from decomposing the non-linear terms in the original NS equations. These terms are known as Reynolds stresses representing the vertical flux of streamwise momentum ($\overline{uv'w'}$ and $\overline{uw'w'}$) or mass ($\overline{Cv'w'}$).

With the addition of these Reynolds stresses, the RANS equations are not a closed set of equations. Therefore this 'closure problem' is addressed by parametrising the Reynolds stresses as follows;

$$
\overline{uv'w'} = -K_M \frac{\partial u}{\partial z}; \quad \overline{vw'w'} = -K_M \frac{\partial v}{\partial z} \tag{2.3}
$$

where $K_M$ is the vertical eddy viscosity. ROMS contains several options for this coefficient ranging from choosing fixed values to the K-profile Parametrization (KPP) (Large et al. [1994]), generic length scale (GLS) and Mellor-Yamada turbulence closure schemes.

Density variations are excluded in the momentum equations following the Boussinesq approximation. However, they still contribute to the buoyancy force in the vertical momentum equation. The vertical pressure gradient then balances the buoyancy force following the hydrostatic approximation as follows;

$$
\frac{\partial \phi}{\partial z} = -\frac{\rho g}{\rho_o} \tag{2.4}
$$
where $\rho_o + \rho(x, y, z, t)$ is the total in-situ density and $g$ is the acceleration of gravity.

Furthermore, the continuity equation for an incompressible fluid is as follows;

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

(2.5)

where the vertical velocity $w$ is computed diagnostically from continuity rather than prognostically.

Additionally, the advective-diffusive equation governs the change in the scalar concentration fields, i.e. temperature and salinity, over time;

$$\frac{\partial C}{\partial t} + \vec{v} \cdot \nabla C = -\frac{\partial}{\partial z} \left( C' w' - \nu_{\theta} \frac{\partial C}{\partial z} \right) + F_C + D_C$$

(2.6)

where $C(x, y, z, t)$ is a scalar quantity, $\nu_{\theta}$ is the molecular diffusivity, $F_C$ a forcing/source term and $D_C$ is an the optional horizontal diffusive term.

This equation is then also closed by parametrising the Reynolds stress;

$$C' w' = -K_C \frac{\partial C}{\partial z}$$

(2.7)

where $K_C$ is the vertical eddy diffusivity.

Finally, an equation of state completes the governing equations as;

$$\phi = \phi(T, S, P)$$

(2.8)

where $T(x, y, z, t)$ is the potential temperature and $S(x, y, z, t)$ is the salinity.
2.1.2 IS4D-Var Module

4D-Var in ROMS

Throughout this thesis ROMS version 3.7 revision 737 was utilised. The capability and extensiveness for a data assimilation system within ROMS have grown substantially over the last decade, moving towards 4D-Var. To date, ROMS can employ a primal formulation of incremental, strong 4D-Var (IS4D-Var), a dual formulation through physical-space statistical analysis (4D-PSAS) and dual formulation method of representers (R4D-Var). These act to find the optimal value and combination of three primary control variables; the initial conditions, surface forcing and boundary conditions that best estimate the analysis circulation (Moore et al., 2011b).

The terminology 'primal' and 'dual' refer to the space in which the search for the minimisation of the cost function is performed. The primal space is spanned by the full model control vector while the dual space is spanned by the observations (Moore et al., 2011b).

ROMS can be constructed into several different models, all of which are required for the 4D-Var algorithms. The main non-linear model, NLROMS is the starting point to which all successive model versions of ROMS can be derived from and can be stated as follows;

\[ x(t_i) = M(t_i, t_{i-1})x(t_{i-1})f(t_i)b(t_i) \]  

(2.9)

where \( M \) is nonlinear ROMS acting on the initial conditions, \( x \) subject to forcing, \( f \) and boundary conditions, \( b \). The whole equation is known as the NLROMS. For the case of weak constraint, an additional vector of control variables is introduced \( \eta(t_i) \) representing sources of errors and uncertainty associated with the model dynamics as well as unresolved scales (Moore et al., 2011b).

The other ROMS models are known as follows; TLROMS which represents the perturbation tangent linear of the above equation, ADROMS which represents the matrix transpose of TL-
ROMS and finally RPROMS that relates to the finite-amplitude linearization of ROMS (only utilized in the method of representers).

For IS4D-Var, successive iterations of TLROMS and ADROMS (known as the inner loops) are solved using a preconditioned Lanczos formulation of the conjugate gradient method (Moore et al., 2011b). The larger the number of loops, the more likely the convergence of the cost function and the closer to the most likely analysis $x_a$. An outer loop can be added so that the non-linear model solution can be redefined to account for non-linearities, thus with a new initial condition the inner loops are rerun. This approach is only implemented for strong constraint due to the potentially impractically large dimension of the increment, whereby weak constraint adds an extra dimension, at every model time step (Moore et al., 2011b).

**IS4D-Var**

For this thesis, IS4D-Var adjusting the initial conditions, surface forcing and boundary conditions was utilised within ROMS. Moore et al. (2011b) describes a comprehensive outline of the numerical algorithms of ROMS IS4D-Var. The cost function is based on Courtier et al. (1994) described in Moore et al. (2011b) as;

$$J(\delta z) = \frac{1}{2} \delta z^T D^{-1} \delta z + \frac{1}{2} (G \delta z - d)^T R^{-1} (G \delta z - d)$$

(2.10)

where $\delta z$ represents the incremental control vector comprised of the initial condition increment $\delta x(t_0)$, the surface forcing increment $\delta f(t)$ and open boundary condition increment $\delta b(t)$; $D$ is the block diagonal background error covariance matrix consisting of the initial condition $B_x$, surface forcing $B_f$, and open boundary $B_b$ background error covariance matrices; $R$ is the block diagonal observation error covariance matrix; $G$ is the operator that maps the tangent linear model solution at the observations points; $d = (y - H(x^b(t)))$ is the innovation vector where $y$ is a vector of the observations; $H(x^b(t))$ is the background state vectors at the observation points; and $H$ is the observation operator that maps the model state vector at observational
points in time via the model integration and space via interpolation (Courtier et al., 1994). The minimization of Equation 2.10 gives the analysis increment $\delta z^a$, to which the optimal circulation estimate $\hat{z}$, can be obtained by $\hat{z} = z^b + \delta z^a$, where $z^b$ is a vector of background control variables.

**Background Error Covariance Matrix**

The background error covariance matrices, $B_x$, $B_f$ and $B_b$ are modeled in ROMS following Weaver and Courtier (2001).

$$B = K_b \Sigma C \Sigma^T K_b^T$$  \hspace{1cm} (2.11)

where $K_b$, is a lower block triangular matrix describing the balanced components of the background errors. Balance in data assimilation assumes that state variables in a balanced circulation are mutually correlated, while the unbalanced residual is expected to be uncorrected (Moore et al., 2011b). $\Sigma$ is a diagonal matrix of standard derivations, and $C$ is the correlation matrix.

Following Weaver et al. (2006), balance relationships are based on $\delta T$, the temperature increment. Therefore, the linear balance equations are as follows;

$$\delta T^k = \delta T^k$$
$$\delta S^k = K_s^k \delta T^k + \delta S_U$$
$$\delta \zeta^k = K_{\zeta T} \delta T^k + K_{\zeta S} \delta S^k + \delta \zeta_U$$  \hspace{1cm} (2.12)
$$\delta u^k = K_{uT} \delta T^k + K_{uS} \delta S^k + K_{u\zeta} \delta \zeta^k + \delta u_U$$
$$\delta v^k = K_{vT} \delta T^k + K_{vS} \delta S^k + K_{v\zeta} \delta \zeta^k + \delta v_U$$

where $\delta T, \delta S, \delta \zeta, \delta u$ and $\delta u$ are the increments of temperature, salinity, the surface elevation,
and horizontal velocity components respectively. \( k \) is the number of outer-loops and \( K_{xy} \) is the linear balance relationship between variable \( x \) and \( y \). The subscript \( U \) refers to the unbalanced component. These linear balance relationships are based on the hydrostatic balance, geostrophic balance and T-S relationships.

There are numerous approaches for modelling error covariance matrices and for ROMS, \( C \) is modelled using the diffusion operator approach as described by Weaver and Courtier (2001) such that \( C = C_v C_h \), the vertical and horizontal correlation matrices with;

\[
\begin{align*}
C_h &= \Lambda_h L_h^{(\frac{1}{2})} W_h^{-1} (L_h^{(\frac{1}{2})})^T \Lambda_h \\
C_v &= \Lambda_v L_v^{(\frac{1}{2})} W_v^{-1} (L_v^{(\frac{1}{2})})^T \Lambda_v 
\end{align*}
\]  

(2.13)

where \( W \) is a diagonal matrix representing grid box areas for \( W_h \) and level thickness for \( W_v \); \( L \) represents the action of the matrix obtained by the solution of the 1D (v) or 2D (h) diffusion equation with assigned decorrelation length scales and \( \Lambda \) is a diagonal matrix of normalization coefficient to ensure that \( C_v \) and \( C_h \) remain in the range of \( \pm 1 \).

This highlights a crucial part of the ROMS 4D-Var formulations, whereby \( B \) is often highlighted as a significant contributor to the success of the assimilation process (Bannister, 2008a). Note that \( B \) modelled here is static in time and homogeneous in space, and thus has limited flow dependence (Moore et al., 2011b).

**Multivariate Characteristics**

Besides the balance implemented within ROMS 4D-Var \( B \) covariance via \( K_b \), the tangent linear (TL) and adjoint (AD) models achieve multivariate characteristics as discussed by Carrier et al. (2016) for the Navy Coastal Ocean Model 4D-Var system (NCOM-4DVAR). They show that the assimilation of velocities can impact the model sea surface height without the need for a balance operator \( K_b \) via two mechanisms.

Firstly, a forcing of velocity in the adjoint model will propagate to force the adjoint of the
surface elevation via the geostrophic balance relationship. This is the same mechanism as in the ROMS 4D-Var system. Following Carrier et al. (2016), the horizontal pressure gradient terms in Reynolds-averaged Navier-Stokes momentum equations are isolated (first and fourth terms in Equations 2.1 & 2.2) and the first-order derivative is taken:

\[
\frac{\partial \delta u}{\partial t} = \ldots - \frac{1}{\rho_o} \frac{\partial \delta P}{\partial x} + \ldots
\]

(2.14)

\[
\frac{\partial \delta v}{\partial t} = \ldots - \frac{1}{\rho_o} \frac{\partial \delta P}{\partial y} + \ldots
\]

with all components previously defined. Note the switch from dynamic pressure \( \phi \) to \( P \), total pressure for clarity.

The adjoint is then:

\[
- \frac{\partial \lambda_P}{\partial t} = \frac{1}{\rho_o} \left( \frac{\partial \lambda_u}{\partial x} + \frac{\partial \lambda_v}{\partial y} \right)
\]

(2.15)

where \( \lambda_P \) is the adjoint pressure, and \( \lambda_{u,v} \) are the adjoint velocities.

Furthermore, taking only the components of differences in the surface elevation \( \zeta \) from the equation of the horizontal pressure gradient field (derived from the vertical pressure gradient, Equation 2.4) and similarly taking the first-order derivative gives:

\[
\frac{1}{\rho_o} \frac{\partial \delta P}{\partial x} = \ldots + g \frac{\partial \delta \zeta}{\partial x} + \ldots
\]

(2.16)

\[
\frac{1}{\rho_o} \frac{\partial \delta P}{\partial y} = \ldots + g \frac{\partial \delta \zeta}{\partial y} + \ldots
\]

where \( \zeta \) is the surface elevation.
The adjoint is then:

\[
-\frac{\partial \lambda_\zeta}{\partial x} = -\rho_o g \frac{\partial \lambda_P}{\partial x}
\]

\[
-\frac{\partial \lambda_\zeta}{\partial y} = -\rho_o g \frac{\partial \lambda_P}{\partial y}
\]  

(2.17)

where \(\lambda_\zeta\) is the adjoint surface elevation.

Thus a forcing in the adjoint velocity will generate a forcing on the adjoint of the pressure field (Equation 2.15) and subsequently the adjoint surface elevation (Equations 2.17). The tangent linear model (initialized by the adjoint model) then propagates this information forward in time.

Additionally, the tangent linear model provides another forcing mechanism via the depth-integrated continuity equation given by integrating Equation 2.5 between the sea floor and the free surface \(\zeta\):

\[
\frac{\partial \zeta}{\partial t} = -\frac{\partial D \tilde{u}}{\partial x} - \frac{\partial D \tilde{v}}{\partial y}
\]

(2.18)

where \(D\) is the total depth and \((\tilde{u})\) and \((\tilde{v})\) are the depth integrated baroclinic velocities. This suggests a flow into or out of a volume of water must have an associated change in water depth. Therefore, a perturbation in the tangent linear velocity will also induce a perturbation on the tangent linear surface elevation.

### 2.1.3 Lagrangian Module

The ROMS online particle trajectory module was used to simulate drifter trajectories during the model forecast. This module uses a fourth-order Milne predictor and fourth-order Hamming corrector scheme to time-step the float trajectory (Lapidus and Seinfeld, 1971). Random walk (simulates sub-grid scale vertical diffusion) is also available in the ROMS float module but was not activated here for similar comparisons with other studies that only use advection (i.e.
the forcing of the ocean currents alone). Clusters of floats can be defined by the user with customizable distributions. To partially account for model error, a small localised cluster of 21 particles centred on the exact location of the observed drifters of 4km width was utilised. The advantage of using the ROMS online module over the numerous offline options available (Thyng and Hetland, 2014) is that the time-stepping of the numerical particle scheme is of the same order as that of the model integration.

### 2.1.4 Angola Basin Domain

Previous studies have utilised various versions of this ROMS model of the Angola Basin in understanding the Congo River plume dynamics (Denamiel et al., 2013) and effects on ocean temperature (White and Toumi, 2014). The model domain extends between $1^\circ S - 21^\circ S$ and $3.7^\circ E - 13.8^\circ E$ with a 10km resolution and 40 terrain-following vertical levels. To determine the degree of vertical stretching, ROMS employs a generalised topography-following coordinate system with user-defined $\sigma$ parameters. ROMS $\sigma$ parameters were as follows: $h_c = 200m$ is the critical depth applied to both the surface and bottom boundary layer where there is an enhanced resolution, and $\sigma_s = 10$ and $\sigma_b = 2$ control the degree of enhanced resolution at the surface and bottom boundary layer respectively. Thus, the vertical levels were compressed at the surface to increase the vertical resolution of the surface currents (Figure 2.1). Realistic bathymetry was obtained from the Global Topography data set (Smith and Sandwell, 1997) with a minimum depth set to 5m (Figure 2.2).

Sub-grid mixing was prescribed using the generic length-scale (GLS) scheme of Warner et al. (2005). The Multidimensional Positive Definite Advection Transport Algorithm (MPDATA) (Smolarkiewicz, 1984) scheme is employed for the advection of tracers. The horizontal advection of momentum is determined using a third-order upwind scheme, with the Smagorinsky-like viscosity, while vertical momentum advection is determined through the fourth-order centred scheme.

Lateral boundary and initial conditions for temperature, salinity, ocean current velocities and sea surface height were obtained from the HYCOM reanalysis (Chassignet et al., 2007).
Regional Ocean Modelling System (ROMS)

Figure 2.1: The vertical levels of ROMS Angola Basin for a cross-section at around 11° with ROMS σ parameters highlighted below.

Atmospheric forcing at the surface for downward radiative surface fluxes, sea level pressure, 2m specific humidity, 2m air temperature, 10m winds, and total precipitation were obtained from European Centre for Medium-Range Weather Forecasts (ECMWF) reanalysis ERA-Interim re-analysis data (ERA-I) at approximately 80 km resolution (Dee et al., 2011). A sponge area is also defined in such a way that the horizontal viscosity is larger at the boundary than seven grid points away from it by four times. This ‘sponge’ will then damp out any spurious interactions with the boundary of the domain. Note there is no tidal forcing to simplify the assimilation of sea surface height.

River Inputs

Seven rivers (Nyanga, Kouilou, Kwanza (Cuanza), Kuene, and the Congo) are incorporated into ROMS as boundary conditions. For each river channel, several source points are assigned a unique outflow rate with a constant temperature (15 degrees) and near-zero salinity (0.1
PSU). Following White and Toumi (2014), river flow rates were obtained from various sources, including the RivDIS v1.1 database (Vorosmarty et al., 1998), the Global Environmental Monitoring System/Global River Inputs (GEMS/GLORI) database (Meybeck and Ragu, 2012), the EIB ERE and the University of Brazzaville available at (http://hmf.enseeiht.fr/travaux/CD0809/bei/beiere/groupe5/node/53). The Congo represents the largest of the rivers in the model domain with a channel of 20km (width) x 60km (length) (2 x 6 grid points) containing 8 source points. Figure 2.3 shows the average annual cycle of the Congo River discharge computed from the observed monthly mean discharge between 1902 and 2005 provided by the BEI ERE (http://hmf.enseeiht.fr/travaux/CD0809/bei/beiere/groupe5/node/53) in collaboration with the University of Brazzaville. These two peaks have been previously attributed to the seasonal migration of the Intertropical Convergence Zone (ITCZ) enhancing local convection (Alsdorf et al., 2016). However, more recently, Jackson et al. (2009) found that the
seasonal migration of the Northern and Southern Africa Easterly Jets bounding mesoscale convec-
tive systems (MCSs) that are in turn enhanced by the local orography could contribute to the seasonal rainfall patterns across central Africa.

![Figure 2.3: The average annual cycle of the Congo River discharge with standard deviation error bars computed from the observed monthly mean discharge between 1902 and 2005 provided by the BEI ERE in collaboration with the University of Brazzaville. Red error bars highlight the specific months analysed in Chapter 5 regarding the Congo River plume modelling.](image)

Figure 2.3: The average annual cycle of the Congo River discharge with standard deviation error bars computed from the observed monthly mean discharge between 1902 and 2005 provided by the BEI ERE in collaboration with the University of Brazzaville. Red error bars highlight the specific months analysed in Chapter 5 regarding the Congo River plume modelling.

![Figure 2.4: The yearly average Congo River discharge computed from the observed monthly mean discharge between 1902 and 2005 provided by the BEI ERE in collaboration with the University of Brazzaville.](image)

Figure 2.4: The yearly average Congo River discharge computed from the observed monthly mean discharge between 1902 and 2005 provided by the BEI ERE in collaboration with the University of Brazzaville.
Despite the significant amount of data (more than 100 years), the measurements stop at 2005. Therefore, the average discharge (Figure 2.3) is employed for the Congo River within the simulations presented here (study periods are 2013-onwards). There is significant variation from year to year (Figure 2.4). The inter-quartile range of monthly discharge over the entire 100 years is 4377 m³/s (10% the value of the mean). Although this constraint (data gap of from 2005 onwards) is not ideal and could be a significant source of error, this dataset represents the only reliable source of the Congo River discharge.

### 2.2 Data for Assimilation

For ROMS version 3.7, \( R \) contains a singular assigned observational error for each observation assumed to be homogeneous, and spatially and temporally uncorrelated. This singular observational error is made up of the instrument error \( E \), the representative error \( F \) (modelled representation of an observation) (Janjić et al., 2017), and some subjective adjustment to firstly, obtain the appropriate relative weightings between \( R \) and \( B \) and secondly, to inflate the impact of a limited number of observations (Broquet et al., 2009; da Rocha Fragoso et al., 2016). Following (Broquet et al., 2009; Moore et al., 2011a), all observations within each 10km grid cell of ROMS Angola Basin and 6 hours temporally were combined to form 'super observations'. The standard deviation of the observations that contribute to each cell is then used as proxy for the representative error. The single observation error \( R \) is then assigned as whichever error, \( E \) or \( F \) is largest (Broquet et al., 2009; Moore et al., 2011a). Note for many of the observations discussed below \( F = 0 \) as the observations themselves are both temporally and spatially coarse. It should also be noted that the creation of super observations does not eliminate representative error (van Leeuwen, 2015). Instead it provides a framework to reduce data redundancy (when too many observations are providing the same information) and in some cases an estimate of representative error.
2.2.1 Currents

Satellite Sea Surface Currents

Ocean Surface Current Analysis Real-time (OSCAR) is a surface current analysis product. The analysis combines geostrophic, Ekman and Stommel shear dynamics along with a term from the surface buoyancy gradient (Bonjean and Lagerloef, 2002). These terms were estimated from satellites observing sea surface height anomalies from AVISO (Archiving, Validation and Interpretation of Satellite Oceanographic Data), surface vector winds from the Special Sensor Microwave Imager (SSM/I) (Atlas et al., 1996) and QScat (Pegion et al., 2000), and SST from the Reynolds Smith O.I.v2. (Reynolds et al., 2002).

Bonjean and Lagerloef (2002) provides an in-depth formulation of the model used to construct the analysis, some of the core equations are expanded here. They start with a quasi-linear and steady flow in a surface layer where the velocity $\mathbf{U} \equiv (u, v)$ can vary with depth, $z$. Vertical turbulent mixing is then characterised by an eddy viscosity $A$ uniform in depth. The vertical shear $\mathbf{U}' \equiv \mathbf{U}_z$, is set to reach zero at a constant scaling depth, $z = -H$ (selected as 70 km). A simplified buoyancy force, $\theta$ is formulated as solely a function of sea surface temperature (SST) and is retained in the vertical hydrostatic balance. The equations for such a model (in complex notation with $\mathbf{U}(x, y, z, t) \equiv u + iv$ and $\nabla \equiv \partial/\partial x + i\partial/\partial y$) are;

$$if\mathbf{U} = -\frac{1}{\rho_m} \nabla p + A\mathbf{U}_z \quad (2.19)$$

$$\frac{1}{\rho_m} p_z = -g + \theta \quad (2.20)$$

$$\nabla \theta = g\chi_T \nabla SST \quad (2.21)$$
with $-H \leq z \leq 0$, and boundary conditions;

$$
\mathbf{U}'(z = 0) = \frac{\tau}{A}
$$

(2.22)

$$
\mathbf{U}'(z = -H) = 0
$$

where $\rho_m = 1025 \text{ kg m}^{-3}$ represents the characteristic density constant, $g = 9.8 \text{ ms}^{-2}$ the gravity acceleration, $\chi_T \approx 3 \times 10^{-4} \text{ K}^{-1}$ the coefficient of thermal expansion, $f$ the Coriolis parameter ($2\Omega \sin \varphi$) and $\tau = \tau^x + i\tau^y$ a complex vector of the surface wind stress divided by $\rho_m$.

$A$, the eddy viscosity is proportional to the square of the wind speed at the surface and is formulated empirically following (Santiago-Mandujano and Firing, 1990);

$$
A = \alpha |W|^{b} \quad |W| \geq 1 \text{ ms}^{-1}
$$

$$
A = \alpha \quad |W| < 1 \text{ ms}^{-1}
$$

(2.23)

where $W_1 = 1 \text{ ms}^{-1}$, $\alpha = 8 \times 10$ and $b = 2.2$.

From Equations 2.19, 2.20 and 2.21 and setting $|\theta/g| \ll 1$ the velocity averaged between the interface and depth, $h = 30m$ can be derived as;

$$
if \mathcal{U} \equiv \frac{if}{h} \int_{-h}^{0} \mathbf{U}(z) \, dz
$$

$$
= -g \nabla \zeta + \frac{h}{2} \nabla \theta + \tau - \frac{A \mathbf{U}'(-h)}{h}
$$

(2.24)

where $\mathcal{U}$ represents the average velocity over $h$ and $\zeta$ the displacement of the ocean-atmosphere interface (known from $dh + \text{de-meaned SSH}$).

The first term on the RHS of Equation 2.24 mainly represents the pressure gradient force with an additional contribution from the second term via the buoyancy gradient. The final term relates to the net drag force from vertical diffusion applied to the layer of thickness $h$. Each
2.2. Data for Assimilation

The term can be calculated from remote sensing satellites via altimetry (SSH), radiometry (SST) and scatterometry (Wind Stress). Since \( f = 0 \) at the equator, a singularity is evident in Equation 2.24. Therefore, this solution is not applied within 5° of the equator. Instead, velocities within this latitude band are obtained via a weak formulation of the momentum equations using a linear combination of orthogonal polynomials.

The resulting gridded analysis represents the mean velocity of the upper 30 m ocean and has a resolution of 1/3° spatially and 5-day average temporally. This coarse spatial resolution of 1/3° is much larger than the model resolution of 10km and therefore ROMS Angola Basin should be able to capture the scales of OSCAR currents with a negligible representative error, \( F = 0 \).

No errors were provided as part of the OSCAR dataset. However, Johnson et al. (2007) compared the OSCAR currents to in-situ data (surface drifters, moored current meters and acoustic Doppler current profilers) and showed within the tropics typical errors of 0.12 m/s. In the absence of any error analysis this validation could represent an approximation of the OSCAR errors for \( E \). This ‘instrument’ error \( E \) can then be assumed to be a combination of the spatial mapping/averaging technique, the simplifications in the derived model and the actual instrument errors from the three input observations. A simplified diagnostic model of the surface circulation, as used in the formulation of OSCAR currents, is clearly an unusual choice to assimilate into ROMS (a full physics ocean model). For example, the assimilation could conceivably cause a discrepancy with the OSCAR model lacking some intricacies (local acceleration and non-linearities) that ROMS can represent. Nevertheless with an appropriate assigned error structure for both the observations \( R \) and the model \( B \), the OSCAR assimilation could still have a positive impact on the forecast correcting some of the large scale circulation problems within ROMS while having relatively little impact on the smaller scales absent from OSCAR.

Two of the observational data sets used in the formulation of OSCAR (AVISO gridded SSH and daily SST) are also assimilated separately from OSCAR in this thesis (Section 2.2.3 and 2.2.4). Therefore, to ascertain the extent of any multivariate corrected errors (\( corr(R) \)), the OSCAR model as described in Equation 2.24 is reproduced in Matlab (Matlab, 2015) for a random white noise (uncorrelated in space and time) SSH and SST error field.
Figure 2.5a and 2.5b shows a typical white noise error field and distribution for an SSH instrument error of 0.04 m. From Equation 2.24, Figure 2.5c and 2.5d then represents the resulting OSCAR error field and distribution. Note the equation only holds for up to 5° from the equator. As expected areas of large SSH gradient have the largest impact on the OSCAR errors which gradually increases towards the equator as high as 1.5 m/s.

Figure 2.5: White noise error for SSH (a and b) and the associated OSCAR errors (c and d).

While Figure 2.5 demonstrates a typical white noise error field for SSH, more samples can be repeatedly generated and the correlation between the resulting OSCAR current error field can
be investigated. For example, with 10,000 different SSH error fields the correlation between the SSH errors and the OSCAR errors is extremely weak (Figure 2.6).

![Figure 2.6: Domain wide correlation between 10,000 samples of the white noise error for SSH (m) and resulting OSCAR error (m/s)](image)

This weak correlation can be explained by a simplified example of two points in the SSH error field at two different times. At $t_1$, the difference between two sample points of the SSH error field, say 0.04 m and -0.02 m will produce the same gradient as say 0 m and -0.06 m at $t_2$. So while the errors in SSH have substantially changed, the gradient has remained the same, with the subsequent errors in OSCAR (determined by the gradient of SSH) also remaining the same. Therefore, under the assumption that the underlying SSH errors are uncorrelated in time and space i.e. a white noise process, SSH errors will be uncorrelated with OSCAR errors. This assumption breaks down if the SSH errors have a consistent bias that would likely propagate into the OSCAR errors via a constant error in the SSH gradient. Term 2 in the RHS of Equation 2.24 represents the contribution to the surface currents from buoyancy via SST. Using the same methodology as above the resulting currents are much weaker and the correlation (now between the SST errors and OSCAR errors) remains near zero.
Surface Drifters

Surface current in-situ velocity observations were obtained from Surface Velocity Program (SVP) drifters maintained by the Global Drifter Program’s (GDP) Drifter Data Assembly Centre (Lumpkin and Pazos, 2007). Figure 2.7 shows the drifter trajectories and spatial coverage over the study period (January - March 2013). Note the drifters are roughly evenly distributed throughout the domain although the majority remain away from the coast. Positions and velocities for all drifters were smoothed using a 24 hour 6th order low-pass Butterworth filter to eliminate tidal currents (Roberts and Roberts, 1978). These velocities have been derived from 6 hourly interpolated drifter positions and centred finite differences representing the currents at 15 m at the drogue depth. This 6-hourly temporal resolution restricts the formation of super observations and therefore cannot provide an approximation of the representative error $F$.

Janjić et al. (2017) briefly explored the representative error in surface drifters and showed how local wind-forced inertial oscillations could account for velocity errors of as much as 0.1 m/s. For all experiments presented in this thesis the wind forcing is provided by ERA-I at approximately 80 km resolution. It is therefore very likely that local inertial oscillations would be absent from the resulting simulations. In their study on Lagrangian predictability and ocean DA, Muscarella et al. (2015) assimilated a different drifter data set (Grand Lagrangian Deployment Drifters). Here they assigned a representative error of 0.03 m/s diagnosed by comparing their 6km ocean model with a higher resolution 3km ocean reanalysis. For the Angola Basin ROMS at 10km resolution this representative error of the surface velocities is likely to be even higher. Furthermore through an error analysis of the GLAD drifter positions they concluded a maximum instrument error of 0.02 m/s.

Here for the SVP drifter velocities, exact contributions to $E$ and $F$ are challenging to diagnose, especially so in a region without any reference values (da Rocha Fragoso et al., 2016). Therefore the SVP drifter velocities was assigned an overall observation error $R$ of either 0.04 or 0.08 m/s. At this lower limit of 0.04 m/s, clearly the instrument and representative error is much larger however some subjective adjustment is performed to artificially inflate the impact of the assimilation of sparse data (Broquet et al., 2009), especially against superior the coverage of
satellite data. With such subjectivity the sensitivity of this assigned error is later explored through the two choices of observation errors (0.04 and 0.08 m/s).

Furthermore correlated errors ($\text{corr}(\mathbf{R})$) spatially and temporally are present due to the auto-correlations in Lagrangian data (Janjić et al., 2017). However, as previously mentioned ROMS IS4D-Var only supports a $\mathbf{R}$ covariance matrix that is spatially and temporally uncorrelated.

![Figure 2.7: Location of all the drifters from January to March 2013.](image)

### 2.2.2 Salinity

**Satellite Sea Surface Salinity**

The Soil Moisture and Ocean Salinity (SMOS) mission is a satellite launched in November 2009 to measure sea surface salinity (SSS) remotely. The level 3 (L3) product consisting of a regularly
gridded processed SSS map was utilised. Very recently (as of May 2017), the Barcelona Expert Centre (BEC) released an updated version of SMOS (available at http://bec.icm.csic.es) with the aim to correct two known issues in previous versions of the dataset. Firstly, the systematic biases created by land masses (land contamination) and radio interference (RF), and secondly, significant data gaps due to the non-convergence of the retrieval algorithm. This new filtering strategy is based on the quality of the individual brightness temperature signals each processed separately; rather than a global threshold used to filter data based on a Chi-square test criteria (Olmedo et al., 2017). The resulting gridded product has a spatial resolution of 0.25° and time averaging window of 9 days, outputted daily. For the tropics, the validation with in-situ data (Argo floats) provided by BEC shows that between 2011-2016 the RMSE is 0.24 PSU (SMOS-BEC Team, 2017). Previous versions of SMOS error statistics has been studied by (Vinogradova et al., 2014), who notably gave an estimate of errors at the coastal regions (1-2 PSU). More recently Hoareau et al. (2018) performed an error characterization of different sea surface salinity products including SMOS. Hoareau et al. (2018) then concluded SMOS had an average error of around 0.2 PSU (open ocean) with a representative error contributing approximately 15 to 50 %. With a relatively course resolution (0.25°) as in OSCAR (0.3°) the representative error in assimilating SMOS into the ROMS Angola Basin (10km) would be negligible, $F = 0$. An instrument error $E$ was assigned as 1.2 PSU, much larger than some previously noted errors (Lu et al., 2016; SMOS-BEC Team, 2017; Hoareau et al., 2018) but similar to (Vinogradova et al., 2014) for along the coasts (1-2 PSU). The variability of the Congo River plume requires a larger assigned error and is discussed in more detail in Section 5.2.1. The observational error $R$ was therefore assigned as 1.2 PSU. Correlated errors, $(corr(R))$ are challenging to diagnose and could be present for SMOS both spatially and temporally. For example, the plume region of SMOS which has different characteristics to the open ocean, is likely to have temporal errors associated with the shifting of the plume from one regime to another i.e. westward to north-westward orientated.
2.2. Data for Assimilation

2.2.1 In Situ Salinity

In situ salinity profile observations (sampling a depth of up to 2000 m) were obtained from the EN4 dataset provided by the Met Office Hadley Centre (Good et al., 2013). This dataset collates all types of ocean profiling instruments such as expendable bathythermographs (XBT), Argo floats, and Conductivity Temperature Depth (CTD) profiles from several data compilation sources including World Ocean Data (WOD09) and the Argo global data assembly centres (GDACs). Upon compilation, the data set is then subject to several quality control procedures. As typical for in-situ observations the spatial and temporal coverage is variable, however the temporal resolution is artificially prescribed within the assimilation via the creation of the super observations to every 6 hours. An instrument error $E$ of 0.01 PSU was assigned following (Broquet et al., 2009; Moore et al., 2011a; da Rocha Fragoso et al., 2016). This rather low error was assigned to inflate the sparse in-situ data relative to satellite data such as SMOS (Broquet et al., 2009). The analysis of the super observations standard deviation reveals an average proxy representative error $F$ of 0.01 PSU. Therefore $R$ was assigned as 0.01 PSU. Correlated errors ($corr(R)$) are likely reduced when designing super observations (binned into 6 hourly data instead of extremely frequent) however the transport of salinity is a slow process, with the Congo River plume sometimes shifting several 100s of km over a period of around 10 days (Hopkins et al., 2013b). Nevertheless, the direct impact of these correlated errors ($corr(R)$) in ROMS IS4D-Var is still unknown.

2.2.3 Temperature

2.2.3.1 Satellite Sea Surface Temperature

Sea surface temperature (SST) observations were obtained from a blended analysis product, the NOAA Optimum Interpolation SST (daily OISST). The resolution is 0.25° spatially and daily temporally. This analysis combines observations from satellites such as the Advanced Very High-Resolution Radiometer (AVHRR), ships and buoys (Reynolds et al., 2007). As with previously mentioned satellite products the representative error in assimilating the coarse STT
product into the ROMS Angola Basin (10km) would be negligible, $F = 0$. An instrument error $E$ of 1°C was assigned. This is larger than what is typically used in the literature (0.4°C) (Broquet et al., 2009; Moore et al., 2011a; da Rocha Fragoso et al., 2016), but was applied to relax the contribution of SST for better convergence in $J$. Ultimately, $R$ determines the contribution of the observations to $J$ in relation to the model background $B$ (Broquet et al., 2009). Therefore if the SST $R$ is reduced, the cost function is required to fit the evolution of the observations more closely and the convergence will be negatively effected. Together with the in situ data (Section 2.2.2 and 2.2.3), SST is assimilated as a typical observations and is not subject to same scrutiny as the assimilation of either the OSCAR or drifter currents, and sea surface height observations. Furthermore, the model at 10 km is able to capture smaller scale structures than the observations, perhaps requiring an inflated error to provide less weight to the assimilation as compared to the model. Correlated errors ($corr(R)$) are likely present from the use of in situ temperature data (buoys) (Section 2.2.3) to construct the blended analysis. Note this data set is used in the construction of OSCAR currents (via the buoyancy gradient) to which the correlated errors are discussed in Section 2.2.1.

**In Situ Temperature**

In situ temperature profile observations were obtained from the EN4 dataset provided by the Met Office Hadley Centre (Good et al., 2013) as described in Section 2.2.2 for in situ salinity. The spatial resolution is variable and temporally at 6 hours (via super observation binning) as for in situ salinity. A similarly low instrument error $E$ was assigned as 0.1°C to inflate the sparse in-situ data relative to the high spatial coverage of the satellite data (Broquet et al., 2009). The analysis of the super observations standard deviation reveals an average proxy representative error $F$ of 0.09°C. Therefore $R$ was assigned as 0.1°C. Janjić et al. (2017) provides an alternative insight of in situ temperature representative errors with tropical moored arrays. They analysis two time series at 40m and 100m depth and note quasi-daily fluctuations of the order 0.25°C and 0.5°C respectability. This suggests the proxy representative error of $F = 0.09°C$ is too optimistic. However, increasing $F$ and therefore increasing $R$, would relax the contribution over SST in $J$, with the in situ temperature then providing little impact in the assimilation.
Again as for in situ salinity correlated errors ($corr(R)$) were likely reduced when designing super observations (binned into 6 hourly data instead of extremely frequent).

### 2.2.4 Sea Level

**Satellite Sea Surface Height**

Gridded sea surface height (SSH) observations consisted of a merged Ssalto/Duacs data-set (TOPEX/Poseidon, Jason-1&2, Envisat, ERS-1&2, and GFO measurements) distributed by Aviso with support from the Centre National dEtudes Spatiales (CNES). ROMS does not resolve the global steric signal. This signal was removed from SSH using a database provided by Willis (2004). Furthermore, SSH was calibrated to ensure ROMS and AVISO dynamic topography were spatially and temporally equal over a long-term average. The resolution is 0.25° spatially and daily temporally. This gridded product is an interpolation of the along-track counterpart over 10 days. The along-track data has a 4km resolution with an orbital period of around 10 days. While some accuracy is lost in this interpolation, the assimilation of a smooth field rather than a sparse, localised impulse avoids the generation of surface gravity waves (Ngodock et al., 2016). Furthermore, at a resolution of approximately 25 km, ROMS Angola Basin (at 10 km resolution) should be able to capture the eddies with a negligible representative error, $F = 0$. Oke and Sakov (2008) presented a comprehensive global estimate of the representative error $F$ of along track sea level anomaly for a 100 km model grid. By visual inspection for their analysis the Angola Basin has a representative error $F$ of up to 0.03 m. The instrument error $E$ was assigned as 0.04 m slightly higher than commonly used in literature, typically 0.02 m (Broquet et al., 2009; Moore et al., 2011a; da Rocha Fragoso et al., 2016). An additional 0.02 m of uncertainty was added since the model resolves more smaller scale structures at than captured by the observations. Restricting the instrument error to 0.02 m could have a negative impact on smaller scales features within the model (Kerry et al., 2016). Therefore the observation error $R$ of 0.04 m was assigned. Correlated errors ($corr(R)$) are likely present in the SSH observations. Areas that are under sampled by the satellite would likely contain larger errors that would have some time dependency until a new orbit passes. Note
this data set is also used in the construction of the OSCAR currents (via the pressure gradient force) to which the correlated errors are discussed in Section 2.2.1.
Chapter 3

Satellite Current Assimilation

3.1 Introduction

The remote sensing of ocean currents from satellites such as Topex/Poseidon and ERS-1/2 in the early 1990s was considered a breakthrough for ocean modelling, especially for ocean DA (Isern-Fontanet et al., 2017). To date, there have been numerous studies on the assimilation of altimetry, shown to improve model circulation (via geostrophy) in various parts of the ocean (Fukumori et al., 1999; Dorofeev and Korotaev, 2004; Dombrowsky et al., 2009; Moore et al., 2011a; da Rocha Fragoso et al., 2016).

More recently, Bonjean and Lagerloef (2002) developed an operational synthesis product of ocean currents denoted the Observing Surface Current Analysis Real-Time (OSCAR). This satellite-derived surface current analysis product (Johnson et al., 2007) combines the computed geostrophic component explicitly from satellite altimetry with a wind-induced Ekman surface current component derived from satellite scatterometer wind and an additional contribution from the buoyancy term via satellite sea surface temperature.

OSCAR has been previously assimilated using a nudging technique for the Indian Ocean by Santoki et al. (2013), where surface current improvements were demonstrated. However, no further studies of the impact of OSCAR assimilation had since been reviewed, with some
critical questions left unanswered;

1. What is the impact of OSCAR assimilation via an advanced data assimilation technique such as 4D-Var?

2. How would the assimilation of OSCAR compare to the assimilation of traditional observation streams such as the closely related satellite altimetry?

With the latter providing the most intriguing proposition of whether a DA system could generate a geostrophic current comparable to the direct assimilation via the OSCAR velocities.

The chapter is organised as follows: first, the methodology of assimilating OSCAR and altimetry via the ROMS 4D-Var set up and experiment procedures are introduced. The results follow firstly presenting the validation of the DA system in general, the forecast skill and the Lagrangian predictability of the currents. The discussion is then presented before finally a conclusion of the chapter.

### 3.2 Method

#### 3.2.1 ROMS 4D-Var Parameters

Table 3.1 summarises important parameters in the 4D-Var system for the experiments outlined in Section 3.2.2. The horizontal decorrelation length scale for the background error covariance (100 km) was chosen as the approximate average of the Rossby radius of deformation for the region, as suggested by Broquet et al. (2009). The Rossby radius of deformation ranges from approximately 60 km at 21° S to 230 km at 1° S (Chelton et al., 1998).

A model climatology run with no assimilation from 2004-2008 was used to estimate standard deviations for the initial conditions for each month (Figure 3.1) and surface forcing background error covariances. HYCOM boundary conditions were used to calculate standard deviations for open boundary background error covariance. This monthly separation of B allows some
Table 3.1: A summary of important parameters required by the IS4D-Var ROMS module. The decorrelation length scales (horizontal and vertical) are outlined in (a), the method for estimating the background error standard deviation (initial conditions, surface forcing and open boundary) in (b) and the observational information (error and frequency) in (c).

(a) Decorrelation Length Scales

<table>
<thead>
<tr>
<th>B</th>
<th>Horizontal</th>
<th>Vertical</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Condition</td>
<td>100 km</td>
<td>30 km</td>
</tr>
<tr>
<td>Surface Forcing</td>
<td>100 km</td>
<td>30 km</td>
</tr>
<tr>
<td>Open Boundary</td>
<td>100 km</td>
<td>30 km</td>
</tr>
</tbody>
</table>

(b) Background Error Standard Deviations

<table>
<thead>
<tr>
<th>B</th>
<th>Method for estimation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Condition</td>
<td>Model climatology run (2004-2008)</td>
</tr>
<tr>
<td>Surface Forcing</td>
<td>Model climatology run (2004-2008)</td>
</tr>
<tr>
<td>Open Boundary</td>
<td>HYCOM boundary conditions</td>
</tr>
</tbody>
</table>

(c) Observational Information

<table>
<thead>
<tr>
<th>Data</th>
<th>Error</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>In-situ Temperature</td>
<td>0.1 °C</td>
<td>6-hourly</td>
</tr>
<tr>
<td>In-situ Salinity</td>
<td>0.01 PSU</td>
<td>6-hourly</td>
</tr>
<tr>
<td>Sea Surface Temperature (SST)</td>
<td>1 °C</td>
<td>Daily</td>
</tr>
<tr>
<td>Gridded Sea Surface Height (SSHG)</td>
<td>0.04 m</td>
<td>Daily</td>
</tr>
<tr>
<td>OSCAR velocities</td>
<td>0.12 ms$^{-1}$</td>
<td>5-daily</td>
</tr>
</tbody>
</table>

sense of seasonality into the background forecast. However, this $B$ is considered static with some rudimentary flow dependency via the propagation of $B$ by the forecast model over the assimilation window (Bannister, 2008a,b). Note this propagated $B$ reverts back to a static matrix at the start of every assimilation cycle. Therefore there may be a discrepancy in the statistics of the variance over a long time window of 4 years as compared when cycling 4D-Var assimilation with a short window length (4-7 days). The use of ensembles clearly has an advantage when computing $B$, where covariance statistics of the differences between each ensemble member and the mean are used to form a flow-dependent $B$ (Bannister, 2008a). Nevertheless, the use of a static $B$ within 4D-Var by approximating the diagonal elements of matrix $\Sigma$ with a long climatology run is a standard approach to ocean DA (Moore et al., 2011a).

Multivariate balance options for momentum (geostrophic balance) were not enforced. For the stability of ROMS domains boarding the equator, the equatorial adjustment of the geostrophic balance within $B$ is required. However, this has yet to be implemented into the ROMS 4D-Var balance. Instead, the tangent linear and adjoint models achieve multivariate characteristics as described by Carrier et al. (2016) and Section 2.1.2.
Chapter 3. Satellite Current Assimilation

Figure 3.1: The daily standard deviation of the model a) SSH, b) surface U velocity and c) surface V velocity for January computed from a climatology run (2004-2008).

OSCAR was assimilated at a depth of 15 m and every five days as per the temporal resolution. After a series of sensitivity experiments, it was found that assimilating at the same frequency as this 5-day output provided the best convergence of $J$. An interpolated daily output was considered and subsequently trialled, but the solution of the DA was not converging in this case. It was likely that daily adjustments of the entire velocity field were too extreme, causing convergence problems. An error of 0.12 m/s was assigned for OSCAR following a validation of OSCAR provided by Johnson et al. (2007).

The number of inner and outer loops control the convergence of the cost function, $J[x]$. After a series of sensitivity experiments for the inner loops (not shown), it was determined 25 inner loops was sufficient for the convergence of the cost function (reduced by a factor of 80-90%). A constant outer loop of one was chosen. While previous studies have shown that multiple outer loops can have a beneficial effect on the assimilation of ocean currents (Sperrevik et al., 2015), the computational cost of an extra outer loop is significant. A single outer loop was, therefore, a computational compromise. A 4-day assimilation window length was chosen for this study, slightly shorter than Moore et al. (2011a). This was chosen as long enough to allow the multivariate characteristics of the model to evolve (Section 2.1.2) and short enough to keep computational costs low.
3.2.2 Satellite Current Assimilation Experiments

Assimilation was performed sequentially using Angola Basin ROMS (Section 2.1.4) with IS4D-Var (Section 2.1.2) beginning on 1st Jan 2013 (initialised from a one year model spin up without assimilation) using four-day assimilation windows ending on 10th March (17 cycles) adjusting the initial conditions, surface forcing and boundaries conditions. Prior initial conditions for each cycle were taken from the final posterior analysis from the previous cycle, except for the first DA cycle in which all experiments were initialised from HYCOM data. The prior boundary conditions and surface forcing were from HYCOM and ERA-I. Alongside the assimilation cycles, a series of four-day forecast cycles were run starting from the end of every DA cycle to assess the short-term forecast skill of the model.

The first experiment was the assimilation of the baseline observations, SST and T&S profiles, often assimilated in operational centres. This observational dataset is expected to have only a marginal impact on the upper ocean current circulation. The subsequent two experiments were the addition of either satellite altimetry or OSCAR velocities (Table 3.2).

To assess the performance of the assimilation system, a normalised error metric was used (Carrier et al., 2014; da Rocha Fragoso et al., 2016), described here as:

\[ J_{fit} = \frac{1}{N} \sum_{n=1}^{N} \frac{|y_n - H_n X_a|}{\sigma_n} \]  

(3.1)

where \( y_n \) is the \( n \)th observation; \( X_a \) is the model analysis mapped to the observations location by \( H_n \), the observation operator; and \( \sigma_n \) is the error standard deviation of the \( n \)th observation. \( J_{fit} \) represents a unit-less measure of the fit of the observations to the model information within one standard deviation of the observation error. If \( J_{fit} \) is less than 1, then the analysis residual is, on average, within observation error bounds.

To assess the performance of the forecast, standard error metrics are used including the time average root mean squared error (RMSE) and the correlation coefficient (R). Here, assimilated observations are also used during the forecast cycle to understand how well the adjustments
made to the initial conditions by the assimilation system are maintained. Independent ocean current observations are also utilised in the form of 4-16 Lagrangian drifters with velocities and positions every 6 hours (Section 2.2.1, Figure 2.7).

Table 3.2: Summary of the DA experiments. X indicates the experiment was assimilating the corresponding observational data set. SSHG is the gridded altimetry product, OSCAR is the analysis surface currents, SST is satellite sea surface temperature, and TS are profile measurements of temperature and salinity. B refers to the baseline observational dataset to which additional observations are added.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>OSCAR</th>
<th>SSHG</th>
<th>SST</th>
<th>TS</th>
</tr>
</thead>
<tbody>
<tr>
<td>TS-SST (B)</td>
<td></td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>B-SSHG</td>
<td>X</td>
<td></td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>B-OSCAR</td>
<td></td>
<td>X</td>
<td></td>
<td>X</td>
</tr>
</tbody>
</table>

Table 3.3: Summary of Lagrangian metrics used within the study. \( x_{\text{obs}}(t) \) represents the longitudinal and \( y_{\text{obs}}(t) \) the latitudinal position at time \( t \) (hours) for the observed drifter and \( x_{\text{ROMS}}(t)/y_{\text{ROMS}}(t) \) for the ROMS simulated floats. \( \text{ang}_{\text{obs}}(t) \) represents the angle between the starting position and position at time, \( t \) for the observations and \( \text{ang}_{\text{ROMS}}(t) \) for ROMS simulated floats. \( n \) represents the threshold for skill score \( S \).

<table>
<thead>
<tr>
<th>Metric</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Separation Distance</td>
<td>( D(t) = \sqrt{(x_{\text{obs}}(t) - x_{\text{ROMS}}(t))^2 + (y_{\text{obs}}(t) - y_{\text{ROMS}}(t))^2} )</td>
</tr>
<tr>
<td>Growth Rate of Separation Distance</td>
<td>( D[0 : t]/[0 : t] )</td>
</tr>
<tr>
<td>Angular Difference</td>
<td>( \text{ang}<em>{\text{obs}}(t) - \text{ang}</em>{\text{ROMS}}(t) )</td>
</tr>
<tr>
<td>Cumulative Distance Difference Skill Score</td>
<td>( S(t) = \begin{cases} 1 - c, &amp; (c &lt; 1) \ 0, &amp; (c &gt; 1) \end{cases} ) ( c(t) = \sum D[0 : t]/n \sum D_0[0 : t] ) ( D_0(t) = \sqrt{(x_{\text{obs}}(t) - x_{\text{obs}}(t-1))^2 + (y_{\text{obs}}(t) - y_{\text{obs}}(t-1))^2} )</td>
</tr>
</tbody>
</table>

Assessing the Lagrangian predictability of the ocean currents via the observed drifters then provides a convincing test of the ocean circulation of ROMS. Therefore, simulated floats were released into the ROMS at the start of every new forecast cycle using the ROMS Lagrangian
Module described in Section 2.1.3. With these simulated float trajectories, four skill metrics were used to assess the Lagrangian flow (Table 3.3): average separation distance after 24 hours between the drifters and ROMS simulated floats; the average growth rate of separation distances (linear fit applied to the average separation distances over the entire 4 day forecast); an average angular difference after 24 hours (Muscarella et al., 2015), and a normalized 3 day cumulative distance difference skill score i.e. the ratio of the cumulative separation between drifters and simulated floats and cumulative distance travelled by the observed drifter after 3 days (Liu and Weisberg, 2011). The latter can be modified via a threshold number $n$ dictating the weight of the denominator in the ratio. For example, a threshold number of $n = 2$ inflates the cumulative distance travelled by the observed drifter by two, allowing for a less stringent skill score.

3.3 Results

3.3.1 Validation of the Assimilation System

The asymptote of the cost function was reached before the 25 iterations of the inner loops and one outer loop for all experiments. Over the entire study period, the cost function decreased on average by approximately 93% indicating the data assimilation system has converged to a solution that has optimised the difference between the observation and model information. The non-linear cost function decreased on average by 80%, suggesting the tangent linear assumption held well over the four-day assimilation windows.

Table 3.4: The average $J_{fit}$ of each analysis cycle (17) over the four days. Significant improvements over TS-SST (B) are shown in bold.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>OSCAR-U</th>
<th>V</th>
<th>DRIFT-U</th>
<th>V</th>
<th>SSH</th>
<th>SST</th>
<th>In-Situ T</th>
<th>In-Situ S</th>
</tr>
</thead>
<tbody>
<tr>
<td>CONTROL</td>
<td>0.95</td>
<td>0.92</td>
<td>3.12</td>
<td>2.59</td>
<td>0.71</td>
<td>1.23</td>
<td>7.43</td>
<td>14.89</td>
</tr>
<tr>
<td>TS-SST (B)</td>
<td>0.99</td>
<td>1.01</td>
<td>3.23</td>
<td>3.01</td>
<td>0.98</td>
<td>0.23</td>
<td>2.25</td>
<td>4.73</td>
</tr>
<tr>
<td>B-SSHG</td>
<td>0.78</td>
<td>0.80</td>
<td>2.65</td>
<td>2.44</td>
<td>0.27</td>
<td>0.24</td>
<td>2.32</td>
<td>5.17</td>
</tr>
<tr>
<td>B-OSCAR</td>
<td>0.56</td>
<td>0.52</td>
<td>2.57</td>
<td>2.42</td>
<td>0.76</td>
<td>0.22</td>
<td>2.22</td>
<td>5.22</td>
</tr>
</tbody>
</table>
In all three observational data sets that were assimilated in the baseline experiment (TS-SST), the fit improved over the control as expected (Table 3.4).

Note the relatively high values of $J_{fit}$ for in-situ T and S, shows the model is struggling to fit the observations within the error bounds. This results suggests the representative error is likely much larger than estimated in Section 2.2.2 and 2.2.3. Here, the model cannot effectively fit the observations since, at 10km it is missing the physical processes at finer scales. However, these small errors were chosen to inflate the impact of sparse observations, a technique that is widely used for in-situ measurements (Broquet et al., 2009). The difficulty in fitting such observations has been recognised in previous studies (da Rocha Fragoso et al., 2016).

$J_{fit}$ reduced either below or close to 1 in B-SSHG and B-OSCAR for each observation that was assimilated (black bold in Table 3.4). The assimilation system was therefore on average, fitting each observation within the observational error bounds. $J_{fit}$ also improved for the drifter velocities (observations not assimilated) in both, B-SSHG and B-OSCAR on average, with a reduction over the baseline of approximately 15%.

Furthermore, in B-SSHG, the OSCAR velocities $J_{fit}$ reduced on average, although only half as much reduction as in B-OSCAR. Furthermore, in B-OSCAR the SSH $J_{fit}$ also reduced on average, similarly half as much as in B-SSHG. The time-series of the SSH $J_{fit}$ for B-OSCAR (Figure 3.2) reveals this reduction was not consistent for all cycles. During the first four cycles, the assimilation of the OSCAR velocities was unable to reduce the fit to SSH as compared to the control, even degrading the fit during cycle three. However, this subsequently improves as time progresses. Since the assimilation of OSCAR velocities covers the whole domain, this dramatic shift in a large-scale velocity field may require more time to adjust before the assimilation becomes more efficient after several cycles. These reductions for non-assimilated observations highlight the capability of multivariate characteristics within the model.
Figure 3.2: The SSH $J_{fit}$ time series for two experiments, B-SSHG, B-OSCAR in dashed black lines. The bold black line in each figure represents the $J_{fit}$ for experiment TS-SST the baseline, B for comparison. The vertical dashed lines in light grey indicate the start of a new assimilation cycle.

### 3.3.2 Forecast Skill

Similar to the $J_{fit}$ statistics, the average forecast RMSE over each 4-day forecast reduced in each experiment for each observation that was assimilated (black bold in Table 3.5). For non-assimilated observations the RMSE was also reduced, the drifter velocities RMSE for example reduced by approximately 17-20%. The average R is similar to the RMSE and $J_{fit}$ statistics (Table 3.6). Therefore, the forecasts on average managed to retain some of the skill generated by the initial adjustments from the assimilation over the four days.

Interestingly, the average RMSE for the OSCAR velocities in the B-OSCAR forecasts were larger than that in the B-SSHG forecasts, by approximately 0.8 cm/s. The time-series of OSCAR velocities RMSE (Figure 3.3) reveals that a more substantial increase in error from the start of the forecast cycle (up to 40%) occurs during the forecast cycles 7, 8, 10 and 15. Therefore, despite an initially smaller OSCAR velocities RMSE in B-OSCAR than B-SSHG, this improvement is rapidly lost, becoming on average a slightly worse forecast.
Table 3.5: The average RMSE ($\text{cms}^{-1}$ for OSCAR and drifter velocities, $\text{cm}$ for SSH, $\text{°C}$ for SST and in-situ T, and PSU for in-situ S) of each forecast cycle (17) over the four days. Significant improvements over TS-SST (B) are shown in bold.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>OSCAR-U</th>
<th>V</th>
<th>DRIFT-U</th>
<th>V</th>
<th>SSH</th>
<th>SST</th>
<th>In-Situ T</th>
<th>In-Situ S</th>
</tr>
</thead>
<tbody>
<tr>
<td>CONTROL</td>
<td>15.3</td>
<td>14.4</td>
<td>15.5</td>
<td>13.2</td>
<td>3.5</td>
<td>1.36</td>
<td>1.08</td>
<td>0.23</td>
</tr>
<tr>
<td>TS-SST (B)</td>
<td>15.8</td>
<td>15.9</td>
<td>16.2</td>
<td>15.0</td>
<td>4.5</td>
<td>0.63</td>
<td>0.87</td>
<td>0.19</td>
</tr>
<tr>
<td>B-SSHG</td>
<td>14.1</td>
<td>13.2</td>
<td>13.4</td>
<td>12.5</td>
<td>2.3</td>
<td>0.62</td>
<td>0.89</td>
<td>0.20</td>
</tr>
<tr>
<td>B-OSCAR</td>
<td>14.7</td>
<td>14.0</td>
<td>13.6</td>
<td>13.0</td>
<td>3.5</td>
<td>0.62</td>
<td>0.82</td>
<td>0.20</td>
</tr>
</tbody>
</table>

Table 3.6: The average R of each forecast cycle (17) over the four days. Significant improvements over TS-SST (B) are shown in bold.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>OSCAR-U</th>
<th>V</th>
<th>DRIFT-U</th>
<th>V</th>
<th>SSH</th>
<th>SST</th>
<th>In-Situ T</th>
<th>In-Situ S</th>
</tr>
</thead>
<tbody>
<tr>
<td>CONTROL</td>
<td>0.14</td>
<td>0.09</td>
<td>0.10</td>
<td>0.29</td>
<td>0.83</td>
<td>0.95</td>
<td>0.99</td>
<td>0.91</td>
</tr>
<tr>
<td>TS-SST (B)</td>
<td>0.19</td>
<td>0.10</td>
<td>0.11</td>
<td>0.27</td>
<td>0.85</td>
<td>0.98</td>
<td>0.99</td>
<td>0.94</td>
</tr>
<tr>
<td>B-SSHG</td>
<td>0.31</td>
<td>0.28</td>
<td>0.40</td>
<td>0.41</td>
<td>0.96</td>
<td>0.98</td>
<td>0.99</td>
<td>0.92</td>
</tr>
<tr>
<td>B-OSCAR</td>
<td>0.24</td>
<td>0.22</td>
<td>0.29</td>
<td>0.32</td>
<td>0.88</td>
<td>0.98</td>
<td>0.99</td>
<td>0.93</td>
</tr>
</tbody>
</table>

Over the entire study period, the OSCAR currents show three distinct dynamical features (Figure 3.4a). A strong coastal current forming part of the Gabon-Congo Undercurrent (GCUC) which feeds the Angola Current (AC). A distinctive semi-persistent anti-cyclonic eddy at 11°S 8°E spanning approximately 200 km and three strong zonal currents flowing east to west making up part of the SEC from 13°S to 21°S. Absent from the OSCAR analysis currents is the South Equatorial current and Angola Dome (Figure 1.2).

Table 3.7 summaries how well each experiment captures these distinctive flow features and reproduce the approximate flow (Figures 3.4b, 3.4c and 3.4d). For the GCUC all experiments except in B-OSCAR experience a weaker coastal jet. It is reasonable to assume boundary conditions from HYCOM could affect the magnitude of this jet as the outflow/inflow will likely differ to that of OSCAR. The dominant eddy is best reproduced in location for B-SSHG and shape in for B experiments. B-SSHG had an eddy more elliptical and a weakened southern edge. Finally, the set of zonal currents are best differentiated in B-SSHG.
3.3. Results

Figure 3.3: The OSCAR velocities (U & V) RMSE time series (cm/s) for two experiments, B-SSHG, B-OSCAR in dashed black lines. The bold black line in each figure represents the OSCAR velocities RMSE for the baseline experiment TS-SST for comparison. The vertical dashed lines in light grey indicate the start of a new assimilation cycle.

Table 3.7: Summary of the OSCAR circulation forecast features captured by each experiment.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>Location</th>
<th>Strength</th>
<th>GCUC / AC</th>
<th>Dominant Eddy (9°E,12°S)</th>
<th>Zonal Currents (&lt;13°S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Control</td>
<td>Y</td>
<td>N - Weaker</td>
<td>Y</td>
<td>N - Incomplete</td>
<td>Y - N - Broader and less defined</td>
</tr>
<tr>
<td>TS-SST (B)</td>
<td>Y</td>
<td>N - Weaker</td>
<td>Y</td>
<td>Y</td>
<td>Y - N - Broader and less defined</td>
</tr>
<tr>
<td>B-SSHG</td>
<td>Y</td>
<td>N - Weaker</td>
<td>Y</td>
<td>Y</td>
<td>Y - N - Broader and less defined</td>
</tr>
<tr>
<td>B-OSCAR</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y - N - Broader and less defined</td>
</tr>
</tbody>
</table>

3.3.3 Lagrangian Predictability of the Ocean Currents

For all simulated ROMS trajectories over each 4-day forecast, the Lagrangian predictability of the ocean currents was evaluated quantitatively using the four skill metrics (Table 3.3). Table 3.8 summarises the average values of each metric in all the experiments. Two-sample Kolmogorov-Smirnov tests were performed in all experiments to test the significance of distributions. $p < 0.05$ indicates that the null hypothesis (the two samples come from the same distribution) is rejected. The KS test is a non-parametric test which is necessary for skewed data samples (Massey, 1951). The spatial distributions of all Lagrangian metrics were independent of location (not shown).
Figure 3.4: Ocean current speeds (m/s) and velocity vectors averaged over all forecast cycles (5th January-13th March) and the top 30 meters depth for OSCAR analysis, TS-SST (B), B-SSHG and B-OSCAR
3.3. Results

Table 3.8: Summary of Lagrangian metric statistics. For $\hat{D}(24)$ and $D_{Linear}(96)$ mean values are displayed with the interquartile range in brackets. For $AD(24)$ the mean value is displayed with the standard deviation. For both $S(72)$ $n = 1$ and $n = 2$ the mean values are displayed with the percentage of positive value skill scores in square brackets.

<table>
<thead>
<tr>
<th>Metric</th>
<th>CONTROL</th>
<th>TS-SST (B)</th>
<th>B-SSHG</th>
<th>B-OSCAR</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\hat{D}(24)$ (km)</td>
<td>15.3 (11.1)</td>
<td>16.3 (12.4)</td>
<td>13.4 (10.2)</td>
<td>13.5 (9.4)</td>
</tr>
<tr>
<td>$D_{Linear}(96)$ (km/day)</td>
<td>13.5 (11.4)</td>
<td>14.1 (10.6)</td>
<td>10.9 (8.6)</td>
<td>10.7 (7.1)</td>
</tr>
<tr>
<td>$AD(24)$ (degrees)</td>
<td>5 ± 92</td>
<td>−5 ± 94</td>
<td>12 ± 83</td>
<td>10 ± 84</td>
</tr>
<tr>
<td>$S(72)$ $n = 1$</td>
<td>0.16 [45%]</td>
<td>0.13 [44%]</td>
<td>0.24 [58%]</td>
<td>0.22 [60%]</td>
</tr>
<tr>
<td>$S(72)$ $n = 2$</td>
<td>0.42 [79%]</td>
<td>0.41 [81%]</td>
<td>0.51 [87%]</td>
<td>0.51 [90%]</td>
</tr>
</tbody>
</table>

Averaged over the entire study period, the experiments with the smallest average separation distance between the simulated trajectories and the observed drifter trajectories after 24 hours $\hat{D}(24)$ was equally B-SSHG (13.4 km) and B-OSCAR (13.5 km). As suggested by their close mean values the difference between these distributions of separation distance was not significant ($p = 0.6$). This is a significant improvement of 17% over the baseline experiment TS-SST with an average separation distance of 16.3 km.

The experiment with the smallest average separation growth rate $D_{Linear}(96)$ was equally B-OSCAR (10.7 km/day) and B-SSHG (10.9 km/day), an average improvement of 3.2 and 3.4 km/day (23%) over the baseline experiment TS-SST. Again these distributions are not significantly different. Nevertheless, it can be recognised that the inter-quartile range differs by as much as 1.5 km/day (smaller for B-OSCAR). This difference can be seen graphically by a more compact group of grey lines representing the average $D_{Linear}(96)$ for each cycle (Figure 3.5).

The angular differences between each observed 24-hour drifter angle (the angle between the starting position and position after 24 hours) and 24-hour simulated trajectory angle within each forecast are shown in Figure 3.6. Since the spread was more significant for $AD(24)$ than previous metrics, it was useful to note improvements regarding the reduction of the standard deviation in $AD(24)$.

The experiment with the smallest standard deviation of the angular difference $AD(24)$ was
Figure 3.5: The average and spread of the growth rate in separation per day (km/day) for TS-SST (B), B-SSHG, and B-OSCAR. Each grey line represents the average separation over the entire domain (drifter averaged) within one forecast cycle. The black line represents the average over all drifters and forecasts. The dashed line shows the CONTROL (free run without assimilation) averaged over all drifters and forecasts for comparison.

equally B-SSHG (83°) and B-OSCAR (84°), an average improvement of 11° and 10° (12%) over the baseline experiment TS-SST. Despite the similarity in the average statistics, the wind rose (Figure 3.6) can provide visually additional useful information. For example, for B-SSHG the −20° to 20° sector contains 12% of the drifter forecasts as compared to only 5 % for B-OSCAR.

For the normalised three-day cumulative distance difference skill score $S'(72)$, B-OSCAR had the largest skill score (0.22) on average closely followed by B-SSHG (0.24). Again, the differences between these distributions are not significant. It was expected that a forecast evaluation would likely yield lower skill scores (Liu and Weisberg, 2011) than for an analysis evaluation such as
3.3. Results

Figure 3.6: Wind roses of the spread of angular differences between each observed 24-hour drifter angle (the angle between the starting position and position at 24 hours) and 24-hour simulated trajectory angle for TS-SST (B), B-SSHG and B-OSCAR.

used by Berta et al. (2015a) and Liu et al. (2014a). The threshold number, \( n \) (see Table 2) can thus be increased to compensate for increased forecast error. The increased threshold \( (n = 2) \) average cumulative skill score for B-SSHG and B-OSCAR was 0.51, an average improvement of 0.1 (25%).

Unique to \( S(72) \), the percentage of positive value skill scores can be evaluated. This positive value percentage \( (n = 1) \) increases the most in B-OSCAR by 16% and B-SSHG by 14%. This indicates that previously simulated drifters with ‘no skill’ \( (S(72) = 0) \) can now be assigned skill with the assimilation of altimetry or OSCAR.
3.4 Discussion

Here OSCAR was assimilated for the first time in an advanced data assimilation system (4D-Var). The assimilation of OSCAR currents and subsequent forecast validation against the OSCAR currents surprisingly performed worse than the B-SSHG forecast on average. Here, the SSH assimilation is notably efficient at capturing the geostrophic currents through the multivariate characteristics of these models, while the forecast for the OSCAR assimilation had some deficiencies. From the analysis validation (via $J_{fit}$), the OSCAR forecast was initially closer to OSCAR observations than B-SSHG as expected. However, ROMS is unable to maintain these substantial domain-wide velocity adjustments from the OSCAR assimilation as the forecast progresses. It is plausible that this was due to the frequency of the OSCAR observations, which were assimilated only every five days while SSHG was assimilated daily. This discrepancy in frequency could then have a potentially significant impact on the retention of skill.

Another potential influencer is the difference in parameters of the background error covariance matrix between the velocity and sea level variables, notably the standard deviation. For both U & V velocities, the standard deviation is higher than 0.12 m/s approximately north of 9° (Figure 3.1). Therefore, with an assigned OSCAR error of 0.12 m/s, the observations have a stronger weighting in the north of the domain than the south. This is reflected in the comparison of the model fields (Table 3.7 and Figure 3.4) which shows the B-OSCAR assimilation best captured the northern GCUC/AC. On the other hand, the sea level standard deviation is higher than 0.04 m (the assigned observation error for SSH) in the south (Figure 3.1). This larger weighting for SSH is then, in turn, converted into a stronger velocity adjustment, reflected in the B-SSHG forecasts best representing the zonal currents in the south (Table 3.7 and Figure 3.4). If the assigned observation error was decreased in the U & V velocities in order to inflate the influence of OSCAR, this perhaps could influence this results.

The addition of assimilating OSCAR velocities or satellite altimetry (to in-situ temperature and salinity profiles, and satellite sea surface temperature) significantly improves the Lagrangian predictability of the ocean currents on average. This represents the first time OSCAR assim-
imulation has shown improvements in Lagrangian flow. Still, these improvements (for OSCAR velocities and satellite altimetry) are roughly equivalent and statistically not different. The extra independent information in OSCAR such as the Ekman and Stommel shear dynamics (Bonjean and Lagerloef, 2002) is not enough to provide improvements over just the sea surface height information which was also assimilated four times more often than OSCAR. Aside from the reduced frequency of assimilation, it is also possible that without the multivariate balance of momentum, significant domain-wide adjustments of velocities are too extreme for ROMS to balance via the tangent linear and adjoint. This is indicated from the forecast of SSH where the error is approximately 50% larger for B-OSCAR than B-SSHG. The B-SSHG forecast of OSCAR velocities was similar to that of B-OSCAR. An alternative hypothesis is the impact of the assimilation on different oceanic modes. While the B-SSHG assimilation experiment will excite geostrophic modes (via the multivariate characteristics within 4D-Var), B-OSCAR will update on the full current field which contains both geostrophic and ageostrophic modes. The ageostrophic modes have a shorter memory and thus the impact of the B-OSCAR assimilation may be shorter. Furthermore, the wind surface forcing (ERA-I) is the same in the forecast for both B-OSCAR and B-SSHG. Therefore, any benefits from Ekman component in OSCAR could be quickly reversed as the forecast currents adjust. Despite these abundant limitations (lack of frequency, momentum balance for the equator, short-time scale modes and imposed surface forcing), credit should be given to the OSCAR assimilation forecast for Lagrangian predictability of the ocean currents on a par with altimetry assimilation forecast.

Previous studies of broad velocity field assimilation such as from HR radar can be compared with these results. Sperrevik et al. (2015) assimilated HR radar observations into a ROMS model of the Northern Norway coastline also using IS4D-VAR. They also perform the same skill score metric utilised here for seven drifters and show a skill score improvement of 0.12 over a control run, 50% larger than that for OSCAR (0.06) in this study. Hoteit et al. (2009) assimilated HR radar into a high-resolution MITgcm model of the San Diego Bay. They show the forecast exceeds persistence for up to 20 hours. It is hard to compare these results as they perform the assimilation in challenging area of highly ageostrophic conditions. In the only previous study of OSCAR assimilation, Santoki et al. (2013) assimilated OSCAR via a nudging
scheme into a model of the Indian Ocean. Unconventionally, they compared and computed errors statistics of their forecast runs to the OSCAR assimilated analysis. A standard approach would be to compare against a control run. Nevertheless, they found the RMSE of surface currents for 1-day and 5-day forecasts to be around 17 cm/s and 19 cm/s respectively thus, in four days the RMSE increases by 12%. With no control run, a relative improvement cannot be easily compared. Here, the average RMSE of drifter velocities over the entire four-day forecast is around 13 cm/s with an average RMSE increase of around 13% in four days.

3.5 Conclusion

The comparison of assimilating OSCAR velocities and satellite altimetry was studied for the first time. This was achieved by directly comparing the addition of either satellite altimetry and OSCAR velocities to a set of baseline observations assimilated into the ROMS 4D-Var system of the Angola Basin.

The assimilation system was first verified through cost function analysis and the $J_{fit}$ metric. The cost function reached the asymptote by 25 iterations, decreasing by 93% on average. For the experiment assimilating altimetry, the model sea surface height $J_{fit}$ reduced below one improving against the baseline assimilation by approximately 70% on average. Similarity for the experiment assimilating the OSCAR velocities, the OSCAR velocities $J_{fit}$ reduced below 1. The assimilation system was therefore concluded to be correctly fitting all observations within observational error bounds.

The forecast skill was also evaluated. The forecasts maintained perturbations from the assimilation system and exhibited an increased forecast skill from the assimilation system over four days. Interestingly, the domain-wide OSCAR velocities were best reproduced in the forecast by altimetry assimilation and not by the OSCAR assimilation itself. It is likely that the frequency of the OSCAR assimilation (every five days), the absence of the momentum balance in the background error covariance matrix and the imposed surface forcing has a detrimental impact on the performance as compared to the daily assimilated altimetry.
Trajectory forecasts were computed for independent drifters for every forecast cycle, and four different Lagrangian predictability metrics were used for robustness. Despite the aforementioned limitations OSCAR assimilation improves the Lagrangian predictability of the ocean currents in the forecast on par with altimetry.
Chapter 4

Drifters for Assimilation and Persistence Forecasts

4.1 Introduction

Lagrangian trajectory forecasts offer a stringent test for an ocean model’s circulation. While the Eulerian based framework focuses on a specific location with fluid parcels moving past with time, the Lagrangian framework focuses on following a fluid parcel over time and space (Batchelor, 2000). Therefore in a Lagrangian framework, at some time $T + x$, the associated forecast error has been influenced by the previous error at time $T$. Such errors include those associated with the wind forcing, initial and boundary conditions, as well as approximations in model physics and sub-grid scale parameterisations (Griffa et al., 2004a).

Lagrangian trajectory forecasts can also serve as a proxy for tracking surface based ‘floats’ such as ocean debris, in search and rescue missions, and marine pollution. Perhaps following the Deepwater Horizon incident, interest in predicting Lagrangian trajectories has expanded, especially with a focus on the utilisation of surface-drifting floats for improving forecasts (Poje et al., 2014). Surface drifters sample numerous scales of the ocean circulation (Lumpkin et al., 2017) and their assimilation has also been shown to improve model circulation and predictability (Molcard et al., 2003; Özgökmen, 2003; Fan et al., 2004; Molcard et al., 2005; Nodet, 2006;
4.1. Introduction

Salman et al., 2006; Nilsson et al., 2012; Carrier et al., 2014).

More recently, research on the assimilation of drifter velocities has concentrated on the Gulf of Mexico (GOM) due to a large quantity of available drifter data. Muscarella et al. (2015) and Carrier et al. (2016) utilised the Grand Lagrangian Deployment (GLAD) data set (300 drifters released in a short period in a localised region in the GOM) and have shown that assimilating drifter inferred velocities improves both the Lagrangian predictability of the ocean currents and sea level forecast in a 4D-Var system.

Here, this study sought to quantify the relative importance of assimilating limited drifter data separately and combined with common observation streams such as altimetry and more uniquely OSCAR velocities within the Angola Basin. The Angola Basin has limited drifter coverage. While the GOM and GLAD drifter data remains valuable for the community, this isolated abundance of observations is not typical. Typically for other regions, the drifter coverage would be considerably less, and in a catastrophic event of marine pollution, would require some form of targeted deployment (Sharma et al., 2010). Therefore this study focused on the impact of local changes near the drifters and not how information spreads to unobserved regions, with no data denial experiments performed. In a more realistic drifter limited region, the impact of assimilating the drifters together with other observations was not apparent.

Assimilating combinations of ocean current information such as drifters and altimetry has been previously shown to improve forecast predictability (Fan et al., 2004; Carrier et al., 2016). However, it has yet to be established in an advanced DA system if such combinations would improve upon the substantial benefits from assimilating drifters alone (Muscarella et al., 2015). It was expected a combination should produce an improved result since combining extra information should complement each other. Despite concluding in Chapter 3 that the assimilation of OSCAR velocities exhibits Lagrangian skill on par with the assimilation of SSH, both are included in combination with drifters for a more comprehensive view.

A simple scenario is conceptualised to highlight the importance of studying these interactions for an example of marine pollution.
1. An oil rig off the coast of Angola suffers an oil well blow-out and a catastrophic marine pollution event occurs.

2. The government acts quickly to forecast the marine pollution trajectory, deploying drifters in the vicinity of the event (Sharma et al., 2010). Once in place, Lagrangian predictions of the oil spill can now be informed with the most up-to-date current fields.

3. An advanced assimilation system would form the basis of the most sophisticated forecast possible that can utilise this data. However, is not yet known whether the assimilation of additional information such as altimetry or OSCAR in combination with the drifters will benefit the forecast.

This reiterates the potential importance of a comprehensive quantification of the impact of assimilating available observations on ocean current forecasting, specifically the Lagrangian flow. To define these impacts, many metrics can be employed. For example, in Chapter 3, the observed drifter paths were compared with simulated trajectories from the model in various ways, providing a stringent test due to the accumulation of errors and the chaotic nature of Lagrangian flow (Özgökmen et al., 2000). However, these drifter paths could be utilised in the formulation of a new, more novel assessment of ocean current forecasting via persistence forecasts.

Persistence has been widely adopted in meteorology as a performance benchmark (Van den Dool, 2007) but less in oceanography (Oey et al., 2005; Shriver et al., 2007; Vandenbulcke et al., 2009; Farrara et al., 2013; Rowe et al., 2016; Solabarrietaa et al., 2016). For quantifying improvements in the Lagrangian flow of the ocean, persistence has been typically taken as either a constant last known position (Ullman et al., 2006; Barron et al., 2007; Kuang et al., 2012; Schmidt and Gangopadhyay, 2013) or constant last known velocity (Paldor et al., 2004; Rixen and Ferreira-Coelho, 2007) of an observed drifter. So far the evaluation of such persistence has been given as an error or skill score for different times which lacks a clear physical interpretation. Therefore, a new diagnostic in quantifying improvements in ocean modelling, denoted as the crossover time is proposed. This represents the timescale at which the model equals the performance of persistence for any chosen metric.
The chapter is organised as follows: first, the methodology of assimilating the drifter observations via the ROMS 4D-Var set up, experiment procedures and the formulation of the crossover time are introduced. The results follow firstly presenting the validation of the DA system in general, the forecast skill, the Lagrangian predictability of the currents, sensitivity to different parameters and finally a global and regional demonstration of the crossover time metric. The discussion is then presented before finally a conclusion of the chapter.

### 4.2 Method

#### 4.2.1 ROMS 4D-Var Parameters

Following Chapter 3, many of the same 4D-Var parameters in the background error and observational error covariance matrices are also utilised for this study (repeated for clarity in Table 4.1). Similarly, 25 inner loops were chosen for the cost function convergence as well as an assimilation window length of 4 days. Multivariate balance options for momentum (geostrophic balance) were also not enforced. Notable differences include the addition of drifter velocities with an assigned observation error of 0.04 or 0.08 m/s, and multiple choices of the horizontal decorrelation length scale of 50, 100 or 150 km. These multiple choices represent the sensitivity experiments performed to understand the relative impact on the results of changes in these parameters. The bold values (0.04 m/s and 100 km) denotes the initial choice which all results in Chapter 4 are based upon; Section 4.3.4 describes the sensitivity experiments.

#### 4.2.2 Drifter Assimilation Experiments

To compare with Chapter 3, where altimetry and OSCAR was assimilated, the same experimental procedure was undertaken. Assimilation was therefore similarly performed sequentially using Angola Basin ROMS (Section 2.1.4) with IS4D-Var (Section 2.1.2) over the same 17 cycles (1st Jan 2013 - 10th March). The first experiment is identical from Chapter 3, the assimilation
Table 4.1: A summary of important parameters required by the IS4D-Var ROMS module. The decorrelation length scales (horizontal and vertical) are outlined in (a), the method for estimating the background error standard deviation (initial conditions, surface forcing and open boundary) in (b) and the observational information (error and frequency) in (c). The bold values denote the initial choice over a selection that is later explored.

<table>
<thead>
<tr>
<th>(a) Decorrelation Length Scales</th>
<th>(b) Background Error Standard Deviations</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>B</strong></td>
<td><strong>Method for estimation</strong></td>
</tr>
<tr>
<td>Horizontal</td>
<td>Vertical</td>
</tr>
<tr>
<td>Initial Condition</td>
<td>50/100/150 km</td>
</tr>
<tr>
<td>Surface Forcing</td>
<td>100 km</td>
</tr>
<tr>
<td>Open Boundary</td>
<td>100 km</td>
</tr>
<tr>
<td>Initial Condition</td>
<td>Model climatology run (2004-2008)</td>
</tr>
<tr>
<td>Surface Forcing</td>
<td>Model climatology run (2004-2008)</td>
</tr>
<tr>
<td>Open Boundary</td>
<td>HYCOM boundary conditions</td>
</tr>
</tbody>
</table>

(c) Observational Information

<table>
<thead>
<tr>
<th>Data</th>
<th>Error</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>In-situ Temperature</td>
<td>0.1 °C</td>
<td>6-hourly</td>
</tr>
<tr>
<td>In-situ Salinity</td>
<td>0.01 PSU</td>
<td>6-hourly</td>
</tr>
<tr>
<td>Sea Surface Temperature (SST)</td>
<td>1 °C</td>
<td>Daily</td>
</tr>
<tr>
<td>Gridded Sea Surface Height (SSHG)</td>
<td>0.04 m</td>
<td>Daily</td>
</tr>
<tr>
<td>OSCAR velocities</td>
<td>0.12 ms⁻¹</td>
<td>5-daily</td>
</tr>
<tr>
<td>Drifter velocities</td>
<td>0.04/0.08 ms⁻¹</td>
<td>6-hourly</td>
</tr>
</tbody>
</table>

of the baseline observations, SST and temperature and salinity profiles (TS). In three experiments the additional assimilation of observed surface drifters (Section 2.2.1) and combined with either altimetry (Section 2.2.4) or OSCAR velocities (Section 2.2.1) were performed (Table 4.2). The same control simulation (no assimilation) was also compared throughout.

A series of four-day forecast cycles were also run starting from the end of every DA cycle to assess the short-term forecast skill of the model. Simulated floats were also released into the ROMS at the start of each new forecast cycle using the ROMS Lagrangian Module described in Section 2.1.3. Here, the same observed drifters assimilated within the assimilation cycles are used in evaluating the subsequent forecast cycles. Outside assimilation cycles, these drifter observations become approximately independent (Carrier et al., 2014). As outlined earlier this study focuses on local changes close to the drifters and therefore this only approximate independence was not considered a problem.

To assess the performance of the assimilation system, the forecast and the Lagrangian predictability of the ocean currents; the same metrics as described in Chapter 3 were also employed.
Table 4.2: Summary of the DA experiments. $X$ indicates the experiment was assimilating the corresponding observational data set. DRIFT is the drifter inferred velocities, SSHG is altimetry, OSCAR is the analysis surface currents, SST is satellite sea surface temperature, and TS are profile measurements of temperature and salinity. B refers to the baseline observational dataset to which additional observations are added.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>OSCAR</th>
<th>DRIFT</th>
<th>SSHG</th>
<th>SST</th>
<th>TS</th>
</tr>
</thead>
<tbody>
<tr>
<td>TS-SST (B)</td>
<td></td>
<td>X</td>
<td></td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>B-DRIFT</td>
<td></td>
<td>X</td>
<td></td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>B-SSHG-DRIFT</td>
<td>X</td>
<td>X</td>
<td></td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>B-OSCAR-DRIFT</td>
<td>X</td>
<td>X</td>
<td></td>
<td>X</td>
<td>X</td>
</tr>
</tbody>
</table>

This included $J_{fit}$, RMSE, $R$, $D(24)$, $D_{Linear}(96)$, $AD(24)$ and $S$.

### 4.2.3 Drifter Persistence in A New Evaluation Metric: The Crossover Time

In addition to the Lagrangian skill metrics already introduced in Chapter 3, an alternative metric is proposed to assess ocean model skill with respect to the benchmark forecast of persistence, denoted the crossover time (Phillipson and Toumi, 2018). Persistence is formulated as keeping the last known velocity of the drifter, $V_0$. This constant velocity is then persisted throughout the prediction, representing a simplistic forecast for a numerical model to outperform. The crossover time is then defined as the time, $T_c$, at which the model is just about to outperform persistence, i.e. when the model and persistence performance are equal:

$$T_c \mid M(T_c)_p - M(T_c)_m = 0$$  \hspace{1cm} (4.1)$$

where $M$ is a measure of goodness as a function of time, which can be flexibly defined and based on any chosen error or skill metric. The subscripts $p$ and $m$ denote that $M$ has been estimated using the persistence and model results respectively, and $T_c$ is the crossover time.
given the persistence ($M_p$) and model ($M_m$) performance are now equal, i.e. the moment the model is about to ‘crossover’, becoming the best predictor.

The better the model performs, the shorter time it takes to outperform persistence (shorter $T_c$). Conversely, the better persistence performs (linked to the memory of the local circulation), the more challenging it is for the model (longer $T_c$). An example of a reasonable choice of $M$ is the commonly used Lagrangian separation distance, $D$ (Castellari et al., 2001; Barron et al., 2007; Rixen and Ferreira-Coelho, 2007; Liu et al., 2014b; Berta et al., 2015b; Muscarella et al., 2015; Phillipson and Toumi, 2017). For illustration, Figure 4.1 is a schematic of the crossover time calculated using the separation distance $T_c(D)$, between a model, persistence and drifter trajectory. Here, $T_c(D)$ occurs where the separation distance for the model is equal to the separation distance for persistence. $T_c(D)$ is about three days here. For a perfect model, the drifter would represent the exact path and therefore always outperform persistence with $T_c(D)$ equal to zero.

Figure 4.1: A schematic of the crossover time $T_c$ framework in terms of the Lagrangian separation distance (d). The drifter is in light red with time markers in days, the model in blue and persistence in black. The black cross denotes the approximate location of $T_c$ for this example.

Diverging from the Angola Basin, the concept of the $T_c$ is first demonstrated on a global-scale, providing a more thorough quantification and test of $T_c$. This is achieved by assessing the
4.3. Results

4.3.1 Validation of the Assimilation System

Comparable to the experiments in Chapter 3, the asymptote of the cost function was also reached for all drifter experiments before the 25 iterations of the inner loops and one outer loop.

Table 4.3: The average $J_{fit}$ of each analysis cycle (17) over the four days. Significant improvements over TS-SST (B) are shown in bold.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>OSCAR-U V</th>
<th>DRIFT-U V</th>
<th>SSH</th>
<th>SST</th>
<th>In-Situ T</th>
<th>In-Situ S</th>
</tr>
</thead>
<tbody>
<tr>
<td>CONTROL</td>
<td>0.95</td>
<td>0.92</td>
<td>3.12</td>
<td>2.59</td>
<td>0.71</td>
<td>1.23</td>
</tr>
<tr>
<td>TS-SST (B)</td>
<td>0.99</td>
<td>1.01</td>
<td>3.23</td>
<td>3.01</td>
<td>0.98</td>
<td>0.23</td>
</tr>
<tr>
<td>B-DRIFT</td>
<td>0.98</td>
<td>1.00</td>
<td>1.08</td>
<td>0.98</td>
<td>0.96</td>
<td>0.24</td>
</tr>
<tr>
<td>B-SSHG-DRIFT</td>
<td>0.83</td>
<td>0.81</td>
<td>1.04</td>
<td>0.96</td>
<td>0.29</td>
<td>0.25</td>
</tr>
<tr>
<td>B-OSCAR-DRIFT</td>
<td>0.58</td>
<td>0.53</td>
<td>1.24</td>
<td>1.20</td>
<td>0.76</td>
<td>0.22</td>
</tr>
</tbody>
</table>

$J_{fit}$ also reduced either below or close to 1 in B-DRIFT, B-DRIFT-OSCAR and B-DRIFT-SSHG for each observation that was assimilated (black bold in Table 4.3). Additional ob-
servations add extra strain to the convergence algorithm (more observations to fit), however this result reveals adding additional observation streams did not hinder the assimilation system for any individual observation. The drifters in this study were too sparse to impact the non-assimilated SSHG observations for the domain average statistics of SSH $J_{fit}$ (Table 4.3). However, their assimilation locally improved the fit (within 1° of the assimilated drifters) decreasing the SSH $J_{fit}$ by approximately 11%.

![Figure 4.2](image.png)

Figure 4.2: Column left to right: Prior (background forecast), posterior (updated forecast from the assimilation system) and increments (posterior minus prior) of model SSH (m) averaged over the first assimilation cycle, 1st to 5th January. Overlaid are the model velocity vectors. Top to bottom: The B-SSGH experiment (as discussed in Chapter 3) and B-DRIFT experiment. Highlighted in the B-DRIFT field in magenta are the drifters available for assimilation in the first cycle.

In addition to $J_{fit}$, a more visual approach highlighting the direct impact of the assimilation in ROMS is the increment fields describing the posterior circulation minus the prior circulation
During the 1st assimilation cycle (1st to 5th January 2013) the prior circulation captured the coastal current (GUCU), however, over-estimated the size and strength of an anticyclonic eddy. From AVISO observations of SSH (not shown), this large eddy slowly evolved east to west over the span of a few months and thus has considerable influence on the surrounding circulation. The assimilation of SSH (those individual assimilation experiments are detailed in Chapter 3) corrected this deficiency in the prior by weakening a strong anti-cyclonic eddy at around 10°S, 11°E while strengthening another further south, shifting the positions as well as the size. The B-DRIFT assimilation similarly achieved these two critical adjustments with only four drifters, illustrating how the assimilation of few drifter velocities can have a relatively significant spatial influence. Note this spatial influence is naturally highly dependent on the assigned decorrelation length (the sensitivity of results of this length scale is explored in Section 4.3.4). Nevertheless, the drifters within this cycle were still too few to constrain the entire domain and even generating spurious changes. As the coverage of drifters increased with time (4 to 16), the SSH $J_{fit}$ for B-DRIFT improved (Figure 4.3). However, beyond cycle 9, $J_{fit}$ rapidly degraded. This deterioration is likely due to the emergence of an isolated drifter, north of 5°S. This drifter is in a critical area where the GUCU is active (Figure 1.1) and cannot adequately constrain the feature alone.

4.3.2 Forecast Skill

The average forecast RMSE reduced in B-DRIFT, B-DRIFT-OSCAR and B-DRIFT-SSHG for each observation that was assimilated (black bold in Table 4.4), similar to the experiments in Chapter 3. As in the $J_{fit}$ statistics, the B-DRIFT forecasts also only exhibit RMSE improvements locally to the SSHG (5%) and OSCAR (6%) observations. The average R is similar to the RMSE and $J_{fit}$ statistics (Table 4.6), except that the B-DRIFT forecast unveiled a domain-wide improvement in the R of OSCAR velocities (not assimilated in B-DRIFT) and not merely locally. This improvement indicates that the drifters are more able to correct eddy and ocean current locations and directions rather than the absolute magnitudes. For example, while the main OSCAR current features are present in the TS-SST forecasts (Figure 4.4), the eddy lo-
Figure 4.3: The SSH $J_{fit}$ time series for three experiments, B-DRIFT, B-SSHG-DRIFT and B-OSCAR-DRIFT in dashed black lines. The bold black line in each figure represents the $J_{fit}$ for experiment TS-SST the baseline for comparison. The vertical lines indicate new DA cycles.

cation remains erroneously shifted by 3°N. The subsequent addition of the drifters (B-DRIFT) then improved the predicted location of this dominant eddy, correctly displacing the position southwards, although the size is erroneously decreased.

### 4.3.3 Lagrangian Predictability

A visual example of the TS-SST (B), B-SSHG, B-OSCAR, B-DRIFT, B-SSHG, B-OSCAR-DRIFT trajectory forecasts from the 22nd to 26th February 2013 (forecast cycle 13) is presented
4.3 Results

Table 4.4: The average RMSE (cm$^{-1}$ for OSCAR and drifter velocities, cm for SSH, °C for SST and in-situ T, and PSU for in-situ S) of each forecast cycle (17) over the four days. Significant improvements over TS-SST (B) are shown in bold.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>OSCAR-U</th>
<th>V</th>
<th>DRIFT-U</th>
<th>V</th>
<th>SSH</th>
<th>SST</th>
<th>In-Situ T</th>
<th>In-Situ S</th>
</tr>
</thead>
<tbody>
<tr>
<td>CONTROL</td>
<td>15.3</td>
<td>14.4</td>
<td>15.5</td>
<td>13.2</td>
<td>3.5</td>
<td>1.36</td>
<td>1.08</td>
<td>0.23</td>
</tr>
<tr>
<td>TS-SST (B)</td>
<td>15.8</td>
<td>15.9</td>
<td>16.2</td>
<td>15.0</td>
<td>4.5</td>
<td>0.63</td>
<td>0.87</td>
<td>0.19</td>
</tr>
<tr>
<td>B-DRIFT</td>
<td>15.8</td>
<td>16.2</td>
<td><strong>12.4</strong></td>
<td><strong>12.0</strong></td>
<td>4.4</td>
<td>0.63</td>
<td>0.91</td>
<td>0.20</td>
</tr>
<tr>
<td>B-SSHG-DRIFT</td>
<td><strong>14.6</strong></td>
<td><strong>13.6</strong></td>
<td>11.1</td>
<td><strong>10.7</strong></td>
<td>2.4</td>
<td>0.63</td>
<td>0.91</td>
<td>0.21</td>
</tr>
<tr>
<td>B-OSCAR-DRIFT</td>
<td><strong>14.5</strong></td>
<td><strong>14.0</strong></td>
<td>11.7</td>
<td><strong>11.6</strong></td>
<td><strong>3.5</strong></td>
<td>0.61</td>
<td>0.82</td>
<td>0.20</td>
</tr>
</tbody>
</table>

Table 4.5: The average RMSE (%) increase of each forecast cycle (17) after 4 days with respect to the initial forecast RMSE.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>OSCAR-U</th>
<th>V</th>
<th>DRIFT-U</th>
<th>V</th>
<th>SSH</th>
</tr>
</thead>
<tbody>
<tr>
<td>B-DRIFT</td>
<td>1%</td>
<td>1%</td>
<td>113%</td>
<td>109%</td>
<td>−1%</td>
</tr>
<tr>
<td>B-SSHG-DRIFT</td>
<td>8%</td>
<td>10%</td>
<td>139%</td>
<td>111%</td>
<td>100%</td>
</tr>
<tr>
<td>B-OSCAR-DRIFT</td>
<td>10%</td>
<td>13%</td>
<td>76%</td>
<td>100%</td>
<td>10%</td>
</tr>
</tbody>
</table>

in Figure 4.5. Note that B-SSHG and B-OSCAR (as discussed in Chapter 3) are also included in this example for additional context. Black lines represent the observed trajectory, and red lines represent the simulated float. A smaller section of the domain highlights five drifters, and their difference from the simulated ROMS floats.

The B-SSHG-DRIFT forecast best-represented Drifters 1 and 2. For Drifter 1, the B-SSHG forecast predicted the position of the eddy too far west. For the B-DRIFT forecast, a substantial broad current (generated from the assimilation of Drifter 2) was erroneously influencing the local region of Drifter 1. However, when combined in B-SSHG-DRIFT, the eddy was more pronounced, with Drifter 1 correctly positioned on the northern side of the eddy (in anticyclonic flow). For Drifter 2 both the B-OSCAR-DRIFT and B-DRIFT forecasts were able to capture the correct direction of the influencing current, but only the combination of SSHG and DRIFT accurately replicated the along track speed. Drifters 3 and 4 show that this interaction was not always advantageous with a degradation of the forecast as compared to B-DRIFT. For Drifter 3, the B-SSHG-DRIFT forecast had spurious southward flow while for
Table 4.6: The average R of each forecast cycle (17) over the four days. Significant improvements over TS-SST (B) are shown in bold.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>OSCAR-U</th>
<th>DRIFT-U</th>
<th>SSH</th>
<th>SST</th>
<th>In-Situ T</th>
<th>In-Situ S</th>
</tr>
</thead>
<tbody>
<tr>
<td>CONTROL</td>
<td>0.14</td>
<td>0.10</td>
<td>0.83</td>
<td>0.95</td>
<td>0.99</td>
<td>0.91</td>
</tr>
<tr>
<td>TS-SST (B)</td>
<td>0.19</td>
<td>0.11</td>
<td>0.85</td>
<td>0.98</td>
<td>0.99</td>
<td>0.94</td>
</tr>
<tr>
<td>B-DRIFT</td>
<td>0.25</td>
<td>0.48</td>
<td>0.52</td>
<td>0.84</td>
<td>0.98</td>
<td>0.92</td>
</tr>
<tr>
<td>B-SSHG-DRIFT</td>
<td>0.30</td>
<td>0.56</td>
<td>0.52</td>
<td>0.96</td>
<td>0.98</td>
<td>0.92</td>
</tr>
<tr>
<td>B-OSCAR-DRIFT</td>
<td>0.28</td>
<td>0.46</td>
<td>0.47</td>
<td>0.88</td>
<td>0.98</td>
<td>0.93</td>
</tr>
</tbody>
</table>

Drifter 4, the position of the eddy was predicted too far north. Both these drifters resided in weaker currents where the assimilation tends to alter the boundaries of the sharper currents in proximity. This alludes perhaps to a forecast preference for the combination with altimetry (B-SSHG-DRIFT) or singular assimilation of drifter observations (B-DRIFT). Finally, Drifter 5 was best represented by the B-OSCAR-DRIFT forecast. Here, the B-OSCAR forecast showed some skill for Drifter 5 and in combining with the drifters further improved the skill by correctly shifting the boundaries of local currents.

This specific example has demonstrated how B-DRIFT, B-SSHG-DRIFT and B-OSCAR-DRIFT can each provide unique local improvements producing the best trajectory forecast for a particular drifter. For a more encompassing outlook Table 4.7 summarises the average values (all drifters for each cycle) of each Lagrangian metric (as used in Chapter 3) for each drifter experiment. Two-sample Kolmogorov-Smirnov (K-S) tests were similarly performed in all experiments to test the significance of distributions with \( p < 0.05 \) indicating that the null hypothesis is rejected.

Both the B-DRIFT and B-SSHG-DRIFT forecast had the smallest average separation distance after 24 hours \( \hat{D}(24) \) equally at 9.5 km. In comparison to the baseline forecast TS-SST (B), this was an average improvement of 6.8 km (42%) in predictability after 24 hours. B-OSCAR-DRIFT closely followed this with an improvement of 6.4 km (40%). The differences between B-DRIFT, B-SSHG-DRIFT and B-OSCAR-DRIFT \( \hat{D}(24) \) distributions were not significant \( (p = 0.4) \).
4.3. Results

Figure 4.4: Ocean current speeds (m/s) and velocity vectors averaged over all forecast cycles (5th January-13th March) and the top 30 meters depth for OSCAR analysis, TS-SST (B), and B-DRIFT. The GUCU is highlighted in the OSCAR analysis.

The B-OSCAR-DRIFT forecast had the smallest average separation growth rate $D_{\text{Linear}}(96)$ with a rate of 8.2 km/day, an average improvement of 5.9 km/day (42%) over the baseline (Figure 4.6). B-SSHG-DRIFT and B-DRIFT closely followed this with an improvement of 5.8 km/day (41%) and 5.4 km/day (38%). Similar to $\bar{D}(24)$, the differences between these $D_{\text{Linear}}(96)$ distributions were not significant ($p = 0.35$).

The B-DRIFT forecast had the smallest standard deviation of the angular difference after 24 hours $AD(24)$ at 54°, an average improvement of 40° (43%) over the baseline (Figure 4.7). This improvement was approximately four times larger than for B-SSHG and B-OSCAR (12%, Chapter 3), the largest difference between B-SSHG/B-OSCAR and B-DRIFT among all Lagrangian metrics. The assimilation of drifters is valuable for correcting the angle of the local currents. B-SSHG-DRIFT and B-OSCAR-DRIFT followed this with a mean improvement of 32° and 33° (34%). Despite a 10% difference the differences between these $AD(24)$ distributions were still not significant ($p = 0.26$).

The B-OSCAR-DRIFT forecast had the largest normalised three-day cumulative distance dif-
Figure 4.5: Ocean current speeds (m/s) and velocity vectors for a sub-section of the Angola Basin domain averaged over the four-day forecast from 22nd to 26th February 2013 for TS-SST (B), B-SSHG, B-OSCAR, B-DRIFT, B-SSHG-DRIFT and B-OSCAR-DRIFT. Simulated float forecasts for each experiment within the sub-domain are shown as red lines. Real observations of the drifters are shown as black lines. The labels 1-5 for each drifter are displayed in TS-SST (B).

Difference skill score $S(72)$ on average at 0.36, an average improvement of 0.23 (176%) over TS-SST (B). B-DRIFT and B-SSHG-DRIFT very closely followed this with an average improvement of 0.22 (169%). For increased threshold ($n = 2$) average cumulative skill score for B-OSCAR-DRIFT, B-SSHG-DRIFT and B-DRIFT were 0.62 and 0.61, an average improvement of 0.21 and 0.20 (50%) over TS-SST (B). Again, the differences between these $S(72)$ distributions were not significant ($p = 0.93$). The positive value percentage ($n = 1$) increases the most in B-OSCAR-DRIFT by 38%, followed by B-DRIFT by 32%, B-SSHG-DRIFT by 31%.

Similar to the Chapter 3 experiments (B-SSHG and B-OSCAR) the spatial distributions of the aforementioned Lagrangian metrics were approximately independent of location. For example, when focusing on the differences between B-SSHG-DRIFT and B-DRIFT for the skill
4.3. Results

Table 4.7: Summary of Lagrangian metric statistics. For $\hat{D}(24)$ and $D_{\text{Linear}}(96)$ mean values are displayed with the interquartile range in brackets. For $AD(24)$ the mean value is displayed with standard deviation. For both $S(72)$, $n = 1$ and $n = 2$ the mean values are displayed with percentage of positive value skill scores in square brackets.

<table>
<thead>
<tr>
<th>Metric</th>
<th>CONTROL</th>
<th>TS-SST (B)</th>
<th>B-DRIFT</th>
<th>B-SSHG-DRIFT</th>
<th>B-OSCAR-DRIFT</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\hat{D}(24)$ (km)</td>
<td>15.3 (11.1)</td>
<td>13.5 (9.4)</td>
<td>9.5 (8.2)</td>
<td>9.5 (7.0)</td>
<td>9.9 (8.6)</td>
</tr>
<tr>
<td>$D_{\text{Linear}}(96)$ (km/day)</td>
<td>13.5 (11.4)</td>
<td>14.1 (10.6)</td>
<td>8.7 (6.8)</td>
<td>8.3 (5.1)</td>
<td>8.2 (5.8)</td>
</tr>
<tr>
<td>$AD(24)$ (degrees)</td>
<td>5 ± 92</td>
<td>−5 ± 94</td>
<td>7 ± 54</td>
<td>15 ± 62</td>
<td>7 ± 63</td>
</tr>
<tr>
<td>$S(72)$ $n = 1$</td>
<td>0.16 [45%]</td>
<td>0.13 [44%]</td>
<td>0.35 [77%]</td>
<td>0.35 [75%]</td>
<td>0.36 [82%]</td>
</tr>
<tr>
<td>$S(72)$ $n = 2$</td>
<td>0.42 [79%]</td>
<td>0.41 [81%]</td>
<td>0.61 [93%]</td>
<td>0.62 [93%]</td>
<td>0.62 [94%]</td>
</tr>
</tbody>
</table>

score statistics, improvement (B-SSHG-DRIFT outperforms B-DRIFT) and degradation was spatially variable (Figure 4.8). Nevertheless, a small consistent cluster of degradation is present just south of the dominant eddy around 12°S 9°E. This consistency perhaps suggests the position, shape and strength of this eddy (that has been shown to be constrained by the assimilation of only drifters in Figure 4.4) could be critical in determining the skill improvements for the local region. However, with such few data points, specific conclusions cannot be adequately verified. Instead, the variability throughout the domain is noted.

**Dependency on Current Speed**

Due to the lack of data, identifying robust differences between B-SSHG-DRIFT and B-DRIFT or B-OSCAR-DRIFT and B-DRIFT is challenging. Furthermore, this makes forming dynamical hypothesis rooted in robust statistical relationships just as challenging. Therefore, to further investigate forecast skill differences, a probabilistic perspective is adopted. Here, improvements (B-SSHG-DRIFT outperforms B-DRIFT) or degradation (B-DRIFT outperforms B-SSHG-DRIFT) were categorised as the percentage of positive and negative values of the difference of $D(t)$ between B-SSHG-DRIFT and B-DRIFT (Figure 4.9). This percentage distribution is additionally divided into two categorises; faster and weaker currents based on the median of the observed drifter speed distribution (upper and lower 50%). This separation follows from the example outlined earlier (Figure 4.5), hinting at the possibility of a dependence on the current speed.
Figure 4.6: The average and spread of the growth rate in separation per day (km/day) for TS-SST (B), B-DRIFT, B-SSHG-DRIFT and B-OSCAR-DRIFT. Each grey line represents the average separation over the entire domain (drifter averaged) within one forecast cycle. The black line represents the average over all drifters and forecasts. The dashed line shows the CONTROL (free run without assimilation) averaged over all drifters and forecasts for comparison.

The difference between weaker and stronger current distributions becomes significant (K-S test) beyond 30 hours. At this time in the forecast, the weaker currents distribution (blue line) peaks at almost 15% more B-DRIFT forecast improvements over B-SSHG-DRIFT (negative values). This later decreases to 5%, where it remains constant. This degradation (B-DRIFT outperforms B-SSHG-DRIFT) is in contrast to the stronger currents distribution (red dashed line) which steadily remains around 10% more B-SSHG-DRIFT forecast improvements over B-DRIFT (positive values) peaking later in the forecast at 88 hours at around 12%. Therefore, after 30 hours for weaker currents, it is more likely (5% to 15%) that the B-DRIFT forecast
4.3. Results

Figure 4.7: Wind roses of the spread of angular differences between each observed 24-hour drifter angle (the angle between the starting position and position at 24 hours) and 24-hour simulated trajectory angle for TS-SST (B), B-DRIFT, B-SSHG-DRIFT and B-OSCAR-DRIFT.

will outperform B-SSHG-DRIFT. While for stronger currents it is more likely (10%) that the B-SSHG-DRIFT forecast will outperform the B-DRIFT forecast. The B-OSCAR-DRIFT and B-DRIFT forecast skill differences were similarly investigated (not shown) and interestingly the $D(t)$ percentage difference revealed no dependence on the current speed. The same analysis was performed for metrics $AD(t)$ and $S(t)$ (not shown). The $AD(t)$ percentage difference revealed no dependence on the current speed, favouring the B-DRIFT forecast for both stronger and weaker distributions. The $S(t)$ percentage difference revealed the same dependence on the current speed as for $D(t)$. Further to the mean current, a dependence on the velocity variance (a measure of turbulence) and latitude (less than and greater than $-10^\circ$) was also considered, both of which showed no significance between distributions.
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Figure 4.8: The spatial distribution of the cumulative skill score metric, $S$ differences between B-SSHG-DRIFT and B-DRIFT. Overlaid in light grey is the OSCAR current streamlines averaged over the entire study period. Positive values are circles and negative values are triangles.

4.3.4 Sensitivity to Assimilation Parameters

This section describes the sensitivity of the results to two critical parameters of the data assimilation system. Note only B-SSHG-DRIFT and B-DRIFT are subject to this sensitivity. While expanding to the whole set of experiments, i.e. additionally for TS-SST (B) and B-OSCAR-DRIFT would be preferable, a computational compromise was made with regards to the large cost of running cycling 4D-Var for three months.

Decorrelation Length Scale Sensitivity

The choice of the decorrelation length scale in the initial condition background error covariance matrix $B^{-}x$ determines the extent of influence for the assimilated data. Initially, the length scale
4.3. Results

Figure 4.9: The positive to negative percentage difference of $D(t)$ between B-SSHG-DRIFT and B-DRIFT as a function of time. Positive values denote that the B-SSHG-DRIFT has a larger proportion of improved trajectory forecast than B-DRIFT. Conversely, a negative value denotes that B-DRIFT has a greater proportion of improved trajectory forecast than B-SSHG-DRIFT. The distributions of $D(t)$ are split into three categories; total, weaker and stronger currents based on the median of the observed drifter speed distribution (upper and lower 50%).

was chosen as 100km, the average Rossby Radius. Four additional experiments were performed to investigate whether the results were sensitive to changes in this length scale. The first two represented the experiments B-DRIFT and B-SSHG-DRIFT with a change in the decorrelation length scale to 50 km (decreasing by half the original length scale) and the second two changing the scale to 150 km (increasing by half the original length scale).

Decreasing the decorrelation length scale by 50 km increased the Lagrangian predictability of the ocean currents for both B-SSHG-DRIFT and B-DRIFT experiments (Table 4.8). The statistical significance of this increase varied between the two experiments and different metrics (Bold in Table 4.8). Conversely, increasing the decorrelation length scale by 50 km slightly decreased the Lagrangian predictability of the ocean currents for both B-SSHG-DRIFT and B-DRIFT experiments in almost every Lagrangian metric. However, this slight decrease in
Table 4.8: Summary of Lagrangian metric statistics for different decorrelation length scale. Bold values denote that the difference between the original 100km experiments and the changed decorrelation length experiments are significant \((p < 0.05)\). \((*)\) denotes significance at \(p < 0.1\).

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(D(24)) (km)</td>
<td>8.4 (6.6)</td>
<td>8.3 (6.5)</td>
<td>10.2 (9.0)</td>
<td>9.5 (7.3)</td>
</tr>
<tr>
<td>(D_{Linear}(96)) (km/day)</td>
<td>7.3 (5.3) *</td>
<td><strong>7.0 (6.1)</strong></td>
<td>8.9 (6.6)</td>
<td>8.1 (6.1)</td>
</tr>
<tr>
<td>(AD(24)) (Degrees)</td>
<td>7 ± 52</td>
<td>10 ± 52</td>
<td>7 ± 59</td>
<td>11 ± 60</td>
</tr>
<tr>
<td>(S(72)) (n = 1)</td>
<td>0.4 [82%]</td>
<td><strong>0.43 [85%]</strong></td>
<td>0.32 [77%]</td>
<td>0.36 [77%]</td>
</tr>
<tr>
<td>(S(72)) (n = 2)</td>
<td>0.66 [94%]</td>
<td><strong>0.67 [95%]</strong></td>
<td>0.60 [92%]</td>
<td>0.62 [94%]</td>
</tr>
</tbody>
</table>

The increased error did not significantly change the Lagrangian predictability of the ocean currents for both B-SSHG-DRIFT and B-DRIFT, and the difference between B-DRIFT and B-SSHG-DRIFT remained insignificant. Therefore, the results presented here were robust to doubling the drifter velocities error.

**Drifter Velocity Observation Error Sensitivity**

Another critical component of the data assimilation system is the choice the assigned observational error \(R\) determining the weight given to the observations as compared to the background in the assimilation. Two additional experiments were performed to investigate the sensitivity of the drifter velocities error. Here, the drifter velocities errors in B-DRIFT and B-SSHG-DRIFT were doubled to 0.08 m/s.
4.3.5 Demonstrating the Crossover Time

Analysis of the Global MERCATOR Model

The crossover time was earlier introduced as a new metric defined as the time it takes for a numerical model to equal the performance of persistence. The analysis of the global MERCATOR model is first presented.

Figure 4.10: Global median separation distance (km) between observed and modelled drifter positions, comparing the simulated trajectories of the MERCATOR forecast (blue dashed) and analysis (blue solid) model, and persistence (black solid) as a function of forecast time (days). The average observed drifter displacement (km) is overlain in light red. The stem (vertical lines from 0) is the difference between the MERCATOR model forecast and persistence (crosses) and MERCATOR analysis and persistence (circles). The dashed lines in light grey mark the \( T_c(\hat{D}) \) and the corresponding drifter displacement (km) for the MERCATOR analysis.

The persistent trajectories outperformed both the MERCATOR analysis and forecast trajectories, for the majority of the prediction regarding the average separation distance \( \hat{D} \) (Figure 4.10). This \( T_c(\hat{D}) \), of 6 days, represents the limits of persistence as a useful predictor compared to the average MERCATOR analysis. The average MERCATOR forecast fails to ever reach a crossover time for the entire span of the available prediction. During the study period, the average decorrelation times of the drifter velocities were found to be 1.2 days (not shown) in approximate agreement with Poulain et al. (1996); LaCasce (2008); Döös et al. (2013); Lump-
kin and Johnson (2013). This timescale is very similar to the e-folding timescale of persistence (Black line in Figure 4.10).

Computing $T_c$ in terms of the average separation distance $\bar{D}$ is useful to represent an average global crossover visually (dashed lines in Figure 4.10). However, an alternative perhaps more appealing approach would be to compute the $T_c(D)$ of all individual trajectories regarding each separation distance $D$ and subsequently form an average $T_c(D)$. This usefully allows for a distribution of crossover times (Figure 4.11) with further insights such as the percentage of forecasts that are assigned the maximum time, i.e. the percentage that have failed to crossover and outperform persistence for the entire prediction. Here, the median $T_c(D)$ for the MERCATOR analysis reduces to 4 days with a percentage of successful crossover at approximately 62-64%. This decrease is similarly observed for the MERCATOR forecast with a median $T_c(D)$ of 4.5 days and 57-60%. Although this result differs from the interpretation of $T_c(\bar{D})$, the persistent trajectories still outperformed both the MERCATOR analysis and forecast trajectories on average over more of the trajectory prediction (62-70%).

The spatial variability of crossover times is next explored (Figure 4.12). On day three the MERCATOR analysis trajectories (Figure 4.12a) generally have more skill in the open ocean and less skill in the more active regions such as the boundary currents. Similarly, the persistence trajectories (Figure 4.12c) also have higher relative separation distances in active regions. However, in a direct comparison (comparing Figure 4.12a and 4.12c), persistence shows more skill over the MERCATOR analysis independent of location to first order.

On day six the MERCATOR analysis trajectories (Figure 4.12b) perform significantly better in comparison to the persistence trajectories (Figure 4.12d) than at day 3 with now a similar proportion of lower separation distance regions. At this later stage in the prediction, the inhomogeneity of the differences becomes more noticeable. Regions of higher kinetic energy (Ishikawa et al., 1997) were better captured by the MERCATOR analysis especially the energetic region of Atlantic Circumpolar Current (ACC). However, it should be noted that even at this later prediction time some regions are still strongly favoured by persistence such as the Peru Basin, South Equatorial current, the subpolar North Pacific and central sub-tropical
4.3. Results

Figure 4.11: Total crossover time (days) distribution for both the MERCATOR analysis (a,b) and forecast (c,d) model (January and July) over each forecast cycle. The median is denoted by the black vertical line in each. A box-and-whisker diagram is displayed above each histogram, denoting the mean (red cross), the median (red line), the 25th and 75th percentiles (ends of the box), 9th and 91st percentile (whiskers) and outliers beyond (dots).

North Atlantic.

Figure 4.12e shows the spatial distribution of $T_c(D)$. The majority of the MERCATOR analysis has a $T_c(D)$ of greater than three days. However, large local variability is evident; such is the case for the Pacific Ocean for example. Qualitatively some regions can be highlighted where the $T_c(D)$ is consistently large or small. The Peru Basin, for instance, has the most uniform cluster of larger $T_c(D)$. Conversely, groups of shorter $T_c(D)$ were located in parts of the ACC between South America and Africa.
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Figure 4.12: The separation distance (km) for the model analysis trajectories (a,b) and persistence trajectories (c,d), after 3 days (a,c) and 6 days (b,d) and the associated crossover time, $T_c(D)$ (e). The data is averaged into 20 degree bins over January and July.

Analysis of Angola Basin ROMS

The results of the crossover time are next explored for the experiments outlined in Table 4.2 using Angola Basin ROMS (Section 2.1.4) with IS4D-Var (Section 2.1.2), summarised in Table 4.9. Figure 4.13 depicts the distribution of crossover time for each experiment and every observed drifter. The B-OSCAR-DRIFT has the shortest median crossover time of 44 hours with 75% of the Lagrangian forecasts achieving a crossover. B-DRIFT follows with a crossover of 49 hours with 71% and B-SSHG-DRIFT of 56 hours with 70%. Although this represents a more considerable difference between the three experiments than previous metrics (especially B-SSHG-DRIFT and B-OSCAR-DRIFT at 12 hours), the difference between the distributions
Table 4.9: Summary of $T_c(D)$ median values with the percentage of forecasts achieving a crossover within the entire four-day prediction in square brackets.

<table>
<thead>
<tr>
<th>Metric</th>
<th>CONTROL</th>
<th>TS-SST (B)</th>
<th>B-DRIFT</th>
<th>B-SSHG-DRIFT</th>
<th>B-OSCAR-DRIFT</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_c(D)$ (hours)</td>
<td>96 [54%]</td>
<td>96 [56%]</td>
<td>49 [71%]</td>
<td>56 [70%]</td>
<td>44 [75%]</td>
</tr>
</tbody>
</table>

of crossover times remains not significant. Nevertheless, the improvement over the baseline is significant, with TS-SST (B) forecast exhibiting a median crossover time of 96 hours with just 56% achieving a crossover.

It is telling to note that despite the assimilation and subsequent forecast of the drifters that still up to 25-30% of the forecasts are outperformed (in terms of Lagrangian skill) by a simple persistence forecast for the entire four-day prediction. This compares to 44% for the baseline experiment. Furthermore, crossover times of less than one day only occur for 21% of B-OSCAR-DRIFT forecast, and 22% for B-DRIFT and B-OSCAR-DRIFT; however, this is significantly larger than the baseline forecast with just 9%.

4.4 Discussion

The assimilation of drifter velocities locally improves the forecast skill of sea surface height (within 1 degree of the drifters) on average. The positive impact of assimilating drifter inferred velocities with a 4D-Var assimilation system on model SSH has been previously studied by Carrier et al. (2016). They describe two mechanisms in support of the multivariate properties of the adjoint and linear tangent model within the Navy Coastal Ocean Model 4D-Var system, that can be similarly applied to ROMS. The mathematical details of these mechanisms are outlined in Chapter 2.1.2 describing the IS4D-Var module within ROMS.

This effect of velocity assimilation on SSH is highlighted by the similar increments (posterior minus prior) produced for the drifter and altimetry assimilation (Figure 4.2). Here the drifter coverage is too sparse to improve the SSH domain-wide but can still influence large areas of the circulation such as shifting and forming eddies (Figure 4.4).
Furthermore, the addition of assimilating drifter velocities (either to in-situ temperature and salinity profiles and satellite sea surface temperature, or additionally with satellite altimetry) improves the Lagrangian predictability of the ocean currents in the Angola Basin significantly on average. To allow for robust conclusions a variety of skill metrics were used (Table 4.7). This improvement is in agreement with previous work in the Gulf of Mexico (Fan et al., 2004; Muscarella et al., 2015; Carrier et al., 2016) and Mediterranean (Nilsson et al., 2012). Comparing with the results from the individual addition of satellite altimetry or OSCAR velocities from Chapter 3 reveals the addition of the drifter velocities provides almost double the benefit locally. Superior improvements for drifters is unsurprising as the drifter trajectories are
discussion simulated in the vicinity of the assimilation.

The combination of satellite altimetry or OSCAR velocities with drifter velocities does not on average significantly improve the Lagrangian predictability of ocean currents than using the drifter velocities alone. This result is somewhat unexpected as the combination of these observations has been previously shown to complement each other (Fan et al., 2004; Carrier et al., 2016). However, Carrier et al. (2016) never present the essential baseline of assimilating the drifters individually. Although Fan et al. (2004) does present this comparison, their conclusions (that the combined assimilation of SSH, SST and drifter data improves the analysis over the assimilation of drifter alone) is only valid for the analysis and not for any subsequent forecasts which they did not perform. Additionally, the DA scheme adopted by Fan et al. (2004) is less sophisticated (optimal interpolation for SSH and nudging for drifters).

For drifters in stronger currents, the combined altimetry and drifter assimilation is more likely to improve Lagrangian predictably by as much as 12% in the forecast as compared to assimilating just the drifters alone. Conversely, for the drifters in weaker currents, this combination is more likely to degrade the Lagrangian predictability of the ocean currents by as much as 15%. No such significant probabilities were found for the combined OSCAR and drifter assimilation. A hypothesis for this absence is the lack of frequency of the OSCAR assimilation (5-daily) as compared to the drifters (6 hourly). Therefore, the observational data-set assimilated is dominated by the more frequent drifters, and thus only a subtle difference between B-DRIFT and B-OSCAR-DRIFT is apparent. Conversely, the daily assimilated altimetry provides a more frequent adjustment in the observational data-set for better or worse.

A few possible hypotheses can be put forth to explain this dependence on current speed and overall skill variability. Concerning the sampling of the satellite observing system; stronger currents with increased kinetic energy usually act on larger scales, which are better sampled by the satellite-inferred geostrophic currents. Weaker currents on the other hand usually act on smaller scales better sampled by the drifters. Therefore, the assimilation of drifter could produce a better forecast in weaker currents.

Besides the sampling accuracy, the variable coverage (spatially and temporally) of a satellite
observing system (alongtrack orbital repeat period is approximately 10 days) could also reduce skill in the combination. Berta et al. (2015a) used this to explain the variance in skill scores when using geostrophic velocity estimates in the Gulf of Mexico, suggesting that periods of low satellite altimetry coverage could correspond to lower skill scores. Therefore, in areas of low coverage, the drifter velocities are combined with a geostrophic current derived from satellite altimetry that is less accurate, diminishing the performance of trajectory forecast skill. This issue is directly related to the utilisation of the gridded satellite altimetry as compared to the use of the along-track altimetry (where low coverage areas would apply no assimilation at all, a different and challenging issue in its own right). Gridded satellite altimetry maps are an interpolated product and thus contain some estimate of the error covariance used to spread the information (Ngodock et al., 2016). There are no prior criteria for the choice of altimetry product and the impact between gridded and along track assimilation of altimetry has not been directly quantified.

Furthermore, the assumptions that relate to the 4D-Var system are uncertain. For example, the construction of the background $B$ and observational error $R$ covariance matrices (determining the relative weighting of background and observational information) is subject to much ambiguity. Information on the background and observational error statistics, and the scales of influence are both uncertain, yet are required in this construction. da Rocha Fragoso et al. (2016) highlighted the different approaches to determining the decorrelation length scale within $B$ such as; semivariogram analysis, the length scales of the main dynamic features, and consideration of the model resolution and subjective adjustment to optimise the performance of 4D-Var. Additionally, the simplification of physics in the tangent linear and adjoint models could restrict the propagation of non-linear ageostrophic modes. However, Sperrevik et al. (2015) have previously shown that even in the presence of non-linear ageostrophic forcing ROMS 4D-Var can perform well.

Some of the results have been shown to be sensitive to the decorrelation length scale within $B$. For B-DRIFT and B-SSHG-DRIFT, Lagrangian predictability of the ocean currents significantly improves when reducing the length-scale by 50km. The smaller decorrelation length scale reduces the filtering effect on the smaller scales captured by the drifter (Liu et al., 2014a),
and thus local velocities (where the subsequent forecast of the observed drifters reside) are likely to improve. Nevertheless, the difference between B-DRIFT and B-SSHG-DRIFT remain insignificant.

The sensitivity of only the drifters observation error $R$ values were explored. Clearly, an exploration of all observation errors would be more beneficial, however computational resources were restricted by the substantial cost of running 3 months of 4D-Var simulations. Nevertheless the sensitivity of the results to $R$ in the drifters provided some insights where none of the results was sensitive to doubling of the drifter velocity observation error. Ultimately, the correct specification of $R$ could improve the forecasts. For example, an ideal $R$ for SSH would give less weight to areas under-sampled by the along-track interpolation. This $R$ however would then require some spatial dependence that currently not implemented within ROMS IS4D-Var. Currently, the development of $R$ in complexity is lagging behind $B$ (Waller et al., 2016) and is often assumed uncorrected in time and space for ease of implementation. The limitation of this assumption has been shown previously shown (Stewart et al., 2013) and more complicated iterations of $R$ could certainly improve the results.

The results of the crossover time for the global ocean model are discussed next. Persistence uses the observations directly with no interpolation. Thus, persistence can initially capture scales of motion not represented by the MERCATOR model horizontal grid-scale resolution of about 8 km. Many studies (Griffa et al., 2004b; Huntley et al., 2011; Putman and He, 2013) have noted the effect of the horizontal grid resolution in ocean models on Lagrangian flow highlighting the importance of unresolved sub-grid-scale processes on the Lagrangian predictability of ocean currents.

Despite the resolved initial conditions, a significant limitation of persistence is the linear nature of the prediction with no dynamical circulation and thus wholly depends on retaining the memory of the local ocean velocity. Thus, persistence typically has very high skill at the start of the forecast, $t_0$ which naturally degrades as the correlation between $t_0$ and $t_{0+i}$ reduces. The extent of this correlation can be quantified via the decorrelation time of the drifter velocities (1.2 days on average). Therefore, the advantage of the resolved initial condition for first 1.2
days is accumulated, translating to a more extended improvement in the Lagrangian framework where the average crossover time is approximately 4-6 days. An alternative interpretation is that $T_c(D)$ depicts the scale at which the observed drifters are no longer following a straight line. The influence of larger scale circulation patterns is then much more important which can be captured by a dynamical numerical model. This decorrelation time also corresponds closely to the secondary maxima exhibited in the distribution of crossover times (Figure 4.11).

A large $T_c(D)$ can be due to the actual local motion (high persistence) and/or model error. Therefore, the MERCATOR analysis trajectory error may produce variability in $T_c(D)$ that cannot be explained regarding local dynamical features. However, some dynamical features can be broadly recognised. Gille and Kelly (1996) concluded that local instability mechanisms determine the ACC scales with a short spatial decorrelation scales of about 85 km and longer time-scales of 34 days. Shorter $T_c(D)$ present in many parts of the ACC could be linked to these shorter spatial scales. Lumpkin and Johnson (2013) have identified regions of ‘eddy deserts’ with significantly low time-mean eddy speeds. Here, these regions, i.e. the Peru Basin, South Equatorial current, the subpolar North Pacific and Central sub-tropical North Atlantic typically have larger $T_c(D)$. The local circulation memory is likely maintained for longer in slowly evolving dynamics, improving the performance of persistence trajectories.

Using the crossover time to compare the drifter assimilation experiments as presented in this Chapter, revealed some insights into the impacts of drifter assimilation. Here, percentages of successful crossovers can be usefully interpreted as the probability of a successful prediction for ROMS as compared to the simplest possible forecast, persistence. From this perspective, the addition of drifters in the IS4D-Var assimilation system (by perhaps a targeted deployment system) is approximately 14-19% more likely to additionally improve the trajectory prediction upon persistence over a 4-day prediction and 12-13% for a 1-day prediction as compared to a control forecast. This result was consistent with the other Lagrangian metrics employed in this Chapter. Similarly, the combination of satellite altimetry or OSCAR velocities with drifter velocities did not significantly change the distribution of crossover time as compared to the assimilation of drifters alone.
4.5 Conclusion

The relative importance of assimilating combinations of altimetry, OSCAR and drifter observations for ocean current forecasts were quantified for the first time. This was achieved by directly comparing the addition of drifter inferred velocities and combinations with either satellite altimetry or OSCAR velocities to a set of baseline observations assimilated into the ROMS IS4D-Var system of the Angola Basin.

In first analysing the assimilation system (ROMS IS4D-Var) via the cost function and the $J_{fit}$ metric, ROMS IS4D-Var was concluded to be correctly fitting all observations within observational error bounds. The Lagrangian predictability of the ocean currents was analysed via trajectory forecasts (computed for every forecast cycle for each observed drifter) and five different Lagrangian predictability metrics. Drifter velocity assimilation is shown on average to significantly improve the Lagrangian predictability of the ocean currents within the Angola Basin in agreement with previous studies (Nilsson et al., 2012; Muscarella et al., 2015; Carrier et al., 2016).

A surprising finding is that when assimilating the combination of either altimetry or OSCAR and drifter velocities, the Lagrangian predictability of the ocean currents may degrade just as equally as improve compared to the assimilation of drifter velocities alone, and on average these combinations do not significantly improve the predictability. For the assimilation of altimetry combined with drifters, it is found in stronger currents the combination is more likely to increase (15%) the probability of improvement in the trajectory forecast. Conversely, for weak currents, a combination is more likely to decrease the probability of improvement. This distinction is thought to be attributed to the drifter observations ability to sample the smaller scales more effectively, which are associated with weaker currents as compared to the variable sampling and coverage of the satellite altimetry. This study adds further support for the role of drifter data in an assimilation system. However, caution should be exercised when combining this information with other data streams.

Independent to these results, one of the metrics adopted in the study; the crossover time was
newly introduced to examine the performance of the ROMS IS4D-Var forecast against a simple benchmark, persistence (last known velocity of the drifter persisted). To adequately demonstrate the concept, the crossover time was also estimated for a high-resolution global ocean model forecast and analysis, where the average crossover time for the model analysis was found to be approximately four to six days. The crossover time can be used to evaluate different ocean models (MERCATOR and ROMS) while providing a simple, intuitive and physical insight. Here, persistence is an excellent short-term predictor of Lagrangian trajectories but as numerical models improve (increased resolution, improved model physics, etc.) the crossover time is excepted to shorten.
Chapter 5

Satellite Salinity Assimilation for River Plume Modelling

5.1 Introduction

The ten largest rivers transport a combined 40% of the freshwater and particulate material into the oceans (Dagg et al., 2004; Chen et al., 2008; Kang et al., 2013; Hopkins et al., 2013a). Some larger rivers can generate offshore plumes of significant distance (Braga et al., 2004; Hopkins et al., 2013a) with high levels of biological productivity, due to the vast amount of supplied nutrients (Higgins et al., 2006; Kouame et al., 2009). Therefore, the accuracy of modelling these river plumes is especially crucial for fishing communities. Furthermore, terrestrial material, both suspended and dissolved are transported via river plumes, affecting sediment and pollutant distributions and the biogeochemistry of carbon (Kang et al., 2013). The second largest river (regarding the annual mean daily discharge) is the Congo in West Africa, outputting approximately 40,000 m$^3$/s of fresh water per month into the Angola Basin. Such extensive outflow produces a plume as large as 800 km from the river mouth (Braga et al., 2004; Hopkins et al., 2013a).

Data assimilation (DA) is a powerful tool that, until recently, could not easily be utilised in the context of river plume modelling. While the more traditional Argo floats provide relatively
accurate in-situ salinity profiles, their lack of spatial coverage is a significant limitation. In 2009 the European Space Agency (ESA) launched the first satellite to monitor surface sea salinity under the Soil-Moisture-Ocean Salinity (SMOS) mission (Lu et al., 2016) providing global coverage of surface salinity.

SMOS has been utilised for data assimilation by two previous studies; in a pilot attempt Köhl et al. (2014) assimilated SMOS but found no benefits to the model salinity. Conversely, Lu et al. (2016) found that SMOS data plays a complementary role in model salinity simulations with an Ensemble Optimal Interpolation DA scheme (EnOI). Note Lu et al. (2016) used a version of the Barcelona Expert Centre (BEC) SMOS data (Font et al., 2013) which suffered from radio frequency interference (RFI) and land contamination, significantly reducing data near the coast. In May 2017, BEC released a new version of SMOS that dramatically improves this land/sea interference (Olmedo et al., 2017). Here, large plumes can be fully analysed on a 9-daily scale instead of monthly, which expands the scope of the data for use in coastal assimilation, particularly for large river plumes such as the Congo River plume.

In this chapter, this recent SMOS data is assimilated to study the impact on the Congo River plume. This will be the first time this particular data set has been used in the context of DA and the first time the Congo River plume forecast has been a focus of improvement in forecasting via DA. Furthermore, satellite altimetry measuring sea surface height (SSH) is also assimilated individually and in combination with SMOS, to explore whether these two data streams could compliment each other. The ocean circulation (shown in Chapter 3 to improve with the assimilation of SSH) may be important for the plume dynamics in the far-field (up to 800 km from the coast).

This chapter is set up as follows: first, the methodology of assimilating SMOS via the ROMS 4D-Var set up and the river plume detection model based on Hopkins et al. (2013a) is introduced. The results follow, firstly presenting the validation of the DA system regionally, and then focusing on the plume specifically. The discussion is then presented before finally a conclusion of the chapter.
5.2 Method

5.2.1 ROMS IS4D-Var Parameters

Following Chapters 3 and 4, despite a shift in focus on river plume modelling, many of the same 4D-Var parameters were employed in this study (repeated for clarity in Table 5.1). Notable similarities include the choice of inner loops for the convergence of the cost function (kept at 25), multivariate balance options for momentum remaining absent, and the observation error for satellite altimetry measuring sea surface height, maintained as 0.04 m.

Table 5.1: A summary of important parameters required by the IS4D-Var ROMS module. The decorrelation length scales (horizontal and vertical) are outlined in (a), the method for estimating the background error standard deviation (initial conditions, surface forcing and open boundary) in (b) and the observational information (error and frequency) in (c).

<table>
<thead>
<tr>
<th>(a) Decorrelation Length Scales</th>
<th>(b) Background Error Standard Deviations</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>B</strong></td>
<td><strong>Method for estimation</strong></td>
</tr>
<tr>
<td>Horizontal</td>
<td>Vertical</td>
</tr>
<tr>
<td>Initial Condition</td>
<td>100 km</td>
</tr>
<tr>
<td>Surface Forcing</td>
<td>100 km</td>
</tr>
<tr>
<td>Open Boundary</td>
<td>100 km</td>
</tr>
<tr>
<td><strong>(c) Observational Information</strong></td>
<td></td>
</tr>
<tr>
<td>Data</td>
<td>Error</td>
</tr>
<tr>
<td>Sea Surface Temperature (SST)</td>
<td>1 °C</td>
</tr>
<tr>
<td>Gridded Sea Surface Height (SSH)</td>
<td>0.04 m</td>
</tr>
<tr>
<td>Sea Surface Salinity (SSS)</td>
<td>1.2 PSU</td>
</tr>
</tbody>
</table>

During the testing phase of the data, i.e. proof of concept assimilation tests and optimisation, it became apparent that the standard deviation used in the background error covariance for the initial condition of salinity required specific tuning.

To re-iterate, the background error covariance matrix for the initial condition is formulated following (Weaver et al., 2006) via a combination of multivariate balance relationships, the standard deviations of the of model via a long climatology run, and a diffusion operator (Equation 2.11). Here the standard deviation field represents a spatially varying parameter controlling
Chapter 5. Satellite Salinity Assimilation for River Plume Modelling

the relative weighting of the model in the data assimilation system, whereas the relative weight-
ing of the observations is controlled via a single assigned observational error. Both are kept
constant throughout the DA procedure.

Therefore the significant difference in the estimated standard deviation in salinity for the open
ocean (0.2-0.5 PSU) compared to that of the area surrounding the Congo plume (of up to 10
PSU) caused issues.

Previous studies assimilating SMOS (Lu et al., 2016) have used an observation error of 0.1
PSU. However, this study is confined to the open ocean. In fact, no studies of data assimilation
for such extensive river plumes exist, and so this challenge is unique to modelling the Congo
River (as also likely for Amazon River). The initial tests of the assimilation of SMOS using a
‘typical’ error of 0.1 PSU and the original estimated standard deviation from the climatology
run drastically over-fit the observations near the river plume (0.1 PSU ≪ 10 PSU). Moore
et al. (2013) noted a similar issue in developing an operational ROMS 4D-Var analysis system
for the California current. Moore et al. (2013) suggested that the salinity standard deviation
could be capped at a certain level to account for this. Therefore following (Moore et al., 2013)
the salinity standard deviation within B was capped at 0.6 PSU. This cap was chosen in order
isolate the area of the plume, i.e. most of north of 12 degrees longitude (Figure 5.1). After
further testing, an observational error of 1.2 PSU for the SMOS observations were assigned
(double that of the applied salinity cap). Lower errors (< 1.2 PSU) resulted in over-fitting
SMOS, especially near the river plume mouth. Therefore, an error of 1.2 PSU enabled the
SMOS observations to have the most substantial impact near the plume without over-fitting
the observations.

This highlights the problems of using the (Weaver et al., 2006) formulation of the background
error covariance. Typically error covariance modelling is challenging and limited alternatives
have been implemented in 4D-Var for ocean models.

Although this error is much larger than the typical error of SMOS in the open ocean (a quality
report from BEC noted an error of 0.24 PSU in the tropics SMOS-BEC Team (2017)), this was
adopted as a pilot approach for the assimilation of SMOS in river plume modelling. Note the
standard deviations for the initial condition and surface forcing of all other variables except salinity $< 0.6$ PSU were similarly estimated using a model climatology run (as previously described in Chapter 3).

Figure 5.1: The daily standard deviation of the model salinity (PSU) for January computed from a climatology run (2004-2008) with a cap of 0.6 PSU

5.2.2 Satellite Salinity Assimilation Experiments

Assimilation was performed sequentially (four-day assimilation window) using Angola Basin ROMS (2.1.4) with IS4D-Var (2.2.2) for four experiments during January, April, July and August 2013. During each month, four cycles of DA were performed (16 days) with the initial conditions for each new cycle obtained from the final posterior analysis from the previous cycle, a similar procedure as in Chapters 3 and 4. The first cycle was initialised with a minimum one-year spin-up of the model without assimilation. Although simulating the whole year would be preferable to capture the whole season of the Congo River plume, four months was a compromise of computational resources to examine the impact of assimilating SMOS. These four months cover a range of different discharges (Figure 2.1). January represents a month of peak discharge, April represents the transition into the secondary peak and July and August represent low discharge months.

Four experiments were undertaken (Table 5.2); firstly a control run (CNTRL) without any
Table 5.2: Summary of the DA experiments. $X$ indicates the experiment was assimilating the corresponding observational data set. SSH is the gridded sea surface height dataset from AVISO satellite altimetry (previously used in Chapters 3 and 4) and SMOS is the sea surface salinity dataset from SMOS.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>SSH</th>
<th>SMOS</th>
</tr>
</thead>
<tbody>
<tr>
<td>SSH</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>SMOS</td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>SMOS-SSH</td>
<td>X</td>
<td>X</td>
</tr>
</tbody>
</table>

assimilation was simulated throughout each month studied. The subsequent three experiments were; the assimilation of either satellite altimetry (SSH); satellite sea surface salinity (SMOS) or the combination of both (SMOS-SSH). Here; the focus is on the analysis (i.e. the direct outcome of the assimilation) and not a subsequent forecast as produced in previous Chapters. Although expanding this Chapter to include the forecasts would be ideal, time restrictions limited the study to the analysis. Nevertheless, this study provides a pilot attempt at assimilating the recent SMOS data with applications to modelling a river plume.

To validate the assimilation system familiar metrics (as used throughout Chapters 3 and 4) were also utilised, i.e. the $J_{fit}$, RMSE and R. Note, because of a lack of independent data, a domain-wide regional validation of the experiments were performed with the same observations as assimilated. Therefore, the results of the RMSE and R error metrics can only compliment $J_{fit}$ in further confirming that the assimilation system is successfully fitting the observations and does not provide additional information about the improvements of the salinity field and plume. However, a few select Argo floats are present in Angola Basin near the plume. The RMSE and R were computed for these vital few that represent the only independent data in this study.

5.2.3 Validating the Congo River Plume: Gaussian Mixture Model

Two broad methodologies exist to define a river plume. Firstly, a simple pre-defined choice of isohaline (a line of the same salinity), for example, Jiang and Xia (2016) used the 27 PSU
isohaline as the definition. A more complex methodology is to use a Gaussian mixture model (GMM) (McLachlan and Peel, 2000). Gaussian mixture models are composed of an assigned amount of multivariate normal density components, with each component containing a mean, covariance matrix, and a mixing proportion determining the proportion of each component. Hopkins et al. (2013a) used GMM fitting to deduce an optimal isohaline automatically for the Congo River plume from an older generation of SMOS observations. Here the GMM was fit to monthly salinity fields from $2^\circ - 10^\circ$S from SMOS. The resulting GMM then consisted of two normal density components with the first representing the open ocean and the second component representing the open ocean. Following Hopkins and Polton (2012), a GMM is also applied to define the Congo River plume for this study (Figure 5.2). To expand upon the reasoning behind this choice; firstly, the use of a GMM will enable an absolute maximum extent of the plume. Secondly, since Hopkins et al. (2013a) applied the use of a GMM also for the Congo River, this provides a useful reference for comparison. Finally, the GMM fitting is moderately simple to implement and fast to execute.

The Matlab Statistics and Machine Learning Toolbox\textsuperscript{TM} function fitgmdist (Matlab, 2015) is used to fit the SMOS data for $k = 2$, where $k$ represents the number of multivariate normal density components i.e the open ocean and the plume salinities. The resulting fitted PDF $f(x)$ can be described as in (Hopkins et al., 2013a) as follows;

$$f_n(x) = \sum_{k=1}^{K} a_k \theta(x|\mu_k, \sigma_k)$$

(5.1)

where $\mu_k$ and $\sigma_k$ are vectors of the mean and standard deviation of $K = 2$ normal distributions, $\theta(x|\mu_k, \sigma_k)$ and $a_k$ are the weights applied to each function.

This function (fitgmdist) fits GMMs to data using an iterative expectation-maximisation (EM) algorithm (Prescher, 2004); obtaining the maximum likelihood of parameters in statistical models. Initial values for component means, covariance matrices, and mixing proportions are estimated by partitioning $n$ observations into $k$ clusters via k-means clustering (Kanungo et al., 2002) with a randomized seeding technique via a k-means ++ algorithm (Arthur and Vassil-
vitskii, 2007).

To validate $fitgmdist$, the same SMOS data used by Hopkins et al. (2013a) (an older version processed the by Centre Aval de Traitement des Donnes SMOS) was utilised. Through a qualitative analysis for December 2010 the optimal isohaline, separating the open ocean and the river plume was identified as the same with the Matlab function $fitgmdist$ as in Hopkins et al. (2013a) (not shown). Therefore, $fitgmdist$ was deemed sufficient for use in this study.

GMMs were fit to the recent SMOS (Chapter 2.2.2) for January, April, July and August 2013 (Figure 5.2). There are distinct differences in the plume isohaline deduced by Hopkins et al. (2013a) during 2010 as compared to this study (2013), specifically, April (Figure 5.2c) with a notably low plume isohaline $< 33$ PSU. During April 2013 the plume was significantly more widespread in SMOS which possibly caused $fitgmdist$ to assign April with a smaller isohaline more related to the near-field (deep blue salinity in Figure 5.2b $< 33$ PSU) than the maximum extent of the plume. Note the recent SMOS data (Chapter 2.2.2) has an increased abundance of data near the coast and therefore, a higher proportion of deeper near-field saline waters will be present in the distribution. Nevertheless, since the isohaline is compared to the model simulation, a maximum value is not necessarily essential, and despite this limitation, $fitgmdist$ is still a useful and consistent approach.

With this calculated plume isohaline, the area bounded by the isohaline and the model domain, i.e. the approximate area of the plume can be estimated. The average salinity inside and outside the plume can also be determined. It is worth noting that these metrics are not independent of the computed isohaline. For example, a drastic difference in the calculated isohaline will then have a substantial impact on the area and salinity of the estimated plume.

Furthermore, a novel approach to validating the model results with SMOS was recognised, unique for river plume modelling. The standard procedure perhaps is to apply the same isohaline as computed for the observed SMOS data as for the model results. However, the SMOS data cannot capture the near-field salinity which would typically have lower salinities simulated in the model results. This limitation creates an inconsistency in comparing the SMOS and ROMS simulated salinity fields where the two distributions display different characteristics.
5.2. Method

(a) January
(b) April
(c) July
(d) August

Figure 5.2: A demonstration of computing the optimal plume isohaline between the Congo River plume and the open ocean for a) January, b) April, c) July and d) August computed using the Matlab Statistics and Machine Learning Toolbox™ function fitgmdist (Matlab, 2015) with SMOS. For each month, the top left represents the resulting optimal isohaline (black line) overlaid with the SMOS salinity field (PSU). The top right represents a stem histogram of the SMOS data with a red line denoting the optimal isohaline. The bottom left depicts the GMM model fit to the SMOS data. The bottom right represents the GMM model split into the two components (plume and open ocean).
For the SMOS observations, the distribution cuts off at 30 PSU, while the modelled salinity within ROMS has a more extended tail towards 0 PSU. An alternative methodology is then to account for the absence of low salinities in the observations by comparing the quantiles of the observed and simulated salinity distributions. As an example, for January the SMOS plume isohaline of 34.14 PSU (calculated from fitgmdist) corresponds to a quantile of 0.32. Therefore, for a ROMS simulated salinity field, the quantile of 0.32 would correspond to a different plume isohaline consistent with the model simulation with lower salinity. Each experiment (CNTRL, SSH, SMOS and SMOS-SSH) would, therefore, have a unique isohaline to which the area and average salinity inside and outside the plume can be computed. Again, it is worth emphasising that while these metrics specifically target the validation of the plume, they use the SMOS data that is also being assimilated for several experiments. Therefore, they can also only compliment $J_{fit}$, RMSE and $R$ in further confirming that the assimilation system is successfully fitting these observations and replicating the specific features.

5.3 Results

5.3.1 Validation of the Assimilation System

The cost function reduced by 60-80% for all experiments reaching an asymptote after 25 iterations. The SMOS $J_{fit}$ reduced to well below one as compared to the control for all experiments assimilating SMOS over each month analysed (Table 5.3). Similarly, the SSH $J_{fit}$ reduced for all experiments assimilating SSH (not shown). This reduction indicates the observations were being successfully fit well within the assigned error bound by the 4D-Var system.

The SMOS RMSE reduced for each experiment assimilating SMOS as expected (Table 5.3). Interestingly, the combined assimilation SMOS-SSH experiment had the smallest SMOS RMSE for three of the four months analysed, at 12-22% less than the SMOS experiment. This result was mirrored in the correlation coefficient (R); although, the difference between the experiments was much smaller at around 3% improvement in R for SMOS-SSH as compared to SMOS.
Table 5.3: The average SMOS $J_{fit}$, root mean squared error (RMSE) and correlation coefficient (R) of each analysis cycle (4) over the four days, for each month analysed.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>$J_{fit}$</th>
<th>RMSE (PSU)</th>
<th>R</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNTRL</td>
<td>1.13</td>
<td>2.76</td>
<td>0.54</td>
</tr>
<tr>
<td>SSH</td>
<td>1.18</td>
<td>2.61</td>
<td>0.71</td>
</tr>
<tr>
<td>SMOS</td>
<td>0.19</td>
<td>0.61</td>
<td>0.92</td>
</tr>
<tr>
<td>SMOS-SSH</td>
<td>0.19</td>
<td>0.48</td>
<td>0.95</td>
</tr>
<tr>
<td>CNTRL</td>
<td>1.35</td>
<td>2.33</td>
<td>0.76</td>
</tr>
<tr>
<td>SSH</td>
<td>1.44</td>
<td>2.35</td>
<td>0.79</td>
</tr>
<tr>
<td>SMOS</td>
<td>0.18</td>
<td>0.38</td>
<td>0.94</td>
</tr>
<tr>
<td>SMOS-SSH</td>
<td>0.19</td>
<td>0.43</td>
<td>0.93</td>
</tr>
<tr>
<td>CNTRL</td>
<td>0.48</td>
<td>0.88</td>
<td>0.70</td>
</tr>
<tr>
<td>SSH</td>
<td>0.48</td>
<td>0.84</td>
<td>0.71</td>
</tr>
<tr>
<td>SMOS</td>
<td>0.12</td>
<td>0.25</td>
<td>0.95</td>
</tr>
<tr>
<td>SMOS-SSH</td>
<td>0.12</td>
<td>0.22</td>
<td>0.96</td>
</tr>
<tr>
<td>CNTRL</td>
<td>0.56</td>
<td>1.4</td>
<td>0.51</td>
</tr>
<tr>
<td>SSH</td>
<td>0.49</td>
<td>1.0</td>
<td>0.61</td>
</tr>
<tr>
<td>SMOS</td>
<td>0.13</td>
<td>0.31</td>
<td>0.94</td>
</tr>
<tr>
<td>SMOS-SSH</td>
<td>0.13</td>
<td>0.28</td>
<td>0.95</td>
</tr>
</tbody>
</table>

experiment. Similarly, the SMOS RMSE and R also reduced and increased respectively, for the SSH experiment as compared to the control for the majority of the study period. This supports the benefits of altimetry assimilation in modelling the regional salinity field.

Quantile comparisons of the observation and model distributions (Figure 5.3) indicate that the control experiment struggled to represent the lower tail of the distribution with excessive low extreme salinities, i.e. the lowest 5% of the distribution is fresher. Furthermore, while the assimilation of satellite altimetry (SSH) helps to correct the majority of the distribution, it fails to adjust these lower tail extremes. Only with the assimilation of SMOS is this lowest 5% adequately replicated, although some fresh bias remains.

Finally the increment (posterior minus the prior) of the SMOS assimilation experiment during the first assimilation cycle in January (Figure 5.4) reveals that assimilation produced the most significant impact near the river mouth, increasing the salinity by greater than 6 PSU. Further afield the salinity increment is smaller but still as much as 3 PSU. A dipole feature of negative and positive salinity increment changes close to the river mouth also suggests a shift of the salinity plume south-westerly. Through assessing the $J_{fit}$, RMSE, and R statistics,
Figure 5.3: Quantile-Quantile plots of the observed and modelled (CNTRL, SSH, SMOS, SMOS-SSH) salinity distributions snapshots of a) January 8th 2013, b) April 8th 2013, c) July 8th 2013 and d) August 8th 2013.
quantile-quantile comparisons and the assimilation increments, it can be concluded that the
data assimilation is successfully fitting the observations within the region.

Figure 5.4: Prior (background forecast), posterior (updated forecast from the assimilation
system) and increments (posterior minus prior) of model salinity (PSU) averaged over the first
assimilation cycle, 1st to 5th January 2013 for the SMOS assimilation experiment.

5.3.2 Evaluating the Congo River Plume

While the previous section focused on the regional domain-wide metrics ($J_{fit}$, RMSE, and R),
this section utilises the three previously described plume evaluation metrics. These comprise of
the plume isohaline (via fitting the GMMs and quantile comparisons) and the associated mean
salinity and area of the plume (bounded by the model domain).

Plume Isohaline

In comparing the mean plume isohaline between experiments (Table 5.4), it is clear that the
assimilation of SMOS, whether assimilated alone or in combination with SSH, produces an
analysis of the plume isohaline most consistent with observations. This is in agreement with the
quantile-quantile comparisons (Figure 5.3) whereby the quantiles of the observations most agree
with the quantiles of the SMOS-SSH assimilation experiment. Unlike the regional statistics of
the SMOS RMSE and R, the difference between the plume isohaline of the SMOS and SMOS-
SSH experiments were insignificant ($< 1\%$ difference). The SMOS and SMOS-SSH experiments
also exhibited limited variation of the plume isohaline between cycles (blue and orange lines
in Figure 5.5) for all months analysed, staying close to the observations (Black line in Figure
5.5). Instead, significant variations from cycle to cycle are only present for the CNTRL and SSH experiments. For example, in January, the plume isohaline of the CNTRL experiment steadily shifts towards the observations over time and conversely, for July, shifts away from the observations.

Table 5.4: The mean plume isohaline of the plume extent (bounded between the model domain) computed via the quantile comparison during the assimilation cycles for each month analysed for each experiments as compared to the observations (PSU). The closest plume isohaline to the observations between experiments are shown in bold for every month.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>Plume isohaline (PSU)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Jan</td>
</tr>
<tr>
<td>OBS</td>
<td>34.14</td>
</tr>
<tr>
<td>CNTRL</td>
<td>33.80</td>
</tr>
<tr>
<td>SSH</td>
<td>33.31</td>
</tr>
<tr>
<td>SMOS</td>
<td><strong>34.04</strong></td>
</tr>
<tr>
<td>SMOS-SSH</td>
<td>34.01</td>
</tr>
</tbody>
</table>

**Plume Salinity**

Similar to the mean plume isohaline, the mean salinity inside the plume is closer to the observations with the assimilation of SMOS, reducing the bias consistently for all months analysed (Table 5.5) as compared to the control. The difference between SMOS and SMOS-SSH remained insignificant. This improvement is largest during April at around 5 PSU (98%), considerably larger than the other analysed months (2 PSU for January, 0.1 PSU for July and 1 PSU for August). The smaller observed plume isohaline in April (Figure 5.2) restricts the average salinity much closer to the river mouth where the fresher water resides. This represents the lower tail of the distribution of salinity where the fresh bias in the CNTRL is most evident (Figure 5.3). Again cycle to cycle variations are only present for experiments not assimilating SMOS (Figure 5.6).
5.3. Results

![Graphs showing salinity (PSU) over time for OBS, CNTRL, SSH, SMOS, and SMOS-SSH experiments during January, April, July, and August.]

Figure 5.5: The average daily plume isohaline as a function of time for OBS, CNTRL, SSH, SMOS, and SMOS-SSH experiments during January, April, July, and August.

**Plume Area**

Finally, for the mean area of the plume, the results were far less consistent, presenting a more ambiguous view (Table 5.6). Here, the experiments assimilating the combined SMOS-SSH produced the closest plume area to the observations for only January and July, improving upon the control by 7139 km² (80%) and 5775 km² (94%) respectively. Within these months, changes in the plume area from cycle to cycle (black line in Figure 5.7) are closely replicated by all experiments, except with a consistent negative bias in the control and a slight consistent bias (negative for January and positive for July) in the SSH experiment. For August, the control has the closest plume area to the observations, with both SMOS experiments exhibiting biases in either the first or second half of the assimilation period. For April, both SMOS-SSH and SMOS experiments have a consistent negative bias, a perhaps misleading result that is next investigated.

Alternatively, the plume salinity and area can be graphically represented and compared to the average plume statistics in Tables 5.4, 5.5 and 5.6, crucially enabling the spatial structures to
Table 5.5: The mean surface salinity within and outside the plume during the assimilation cycles for each month analysed (PSU). The closest surface salinity within and outside the plume to the observations between experiments are shown in bold for every month.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>Inside Plume Salinity (PSU)</th>
<th>Outside Plume Salinity (PSU)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Jan</td>
<td>Apr</td>
</tr>
<tr>
<td>OBS</td>
<td>32.7</td>
<td>31.7</td>
</tr>
<tr>
<td>CNTRL</td>
<td>30.7</td>
<td>26.7</td>
</tr>
<tr>
<td>SSH</td>
<td>30.0</td>
<td>26.7</td>
</tr>
<tr>
<td>SMOS</td>
<td><strong>32.6</strong></td>
<td><strong>31.6</strong></td>
</tr>
<tr>
<td>SMOS-SSH</td>
<td><strong>32.6</strong></td>
<td>31.4</td>
</tr>
</tbody>
</table>

Table 5.6: The mean area of the plume (bounded between the model domain) during the assimilation cycles for each month analysed for each experiments as compared to the observations (km²). The closest plume area to the observations between experiments are shown in bold for every month.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>Plume area extent (km²)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Jan</td>
</tr>
<tr>
<td>OBS</td>
<td>182,385</td>
</tr>
<tr>
<td>CNTRL</td>
<td>173,435</td>
</tr>
<tr>
<td>SSH</td>
<td>178,732</td>
</tr>
<tr>
<td>SMOS</td>
<td>180,855</td>
</tr>
<tr>
<td>SMOS-SSH</td>
<td><strong>180,574</strong></td>
</tr>
</tbody>
</table>

be compared as well as the area (Figure 5.6). As an example, for a snapshot of January 8th, the CNTRL and SSH experiments (second and third columns in Figure 5.8) produce a plume structure that is often too stretched either along the coast (January, July and August) or too dispersive as a whole (April). Notably, the salinity is also fresher than the observations (first column in Figure 5.8). Here, the coastal currents of CNTRL are perhaps unreasonably influential with the mixing of the fresh water too diffuse, allowing the plume to spread significantly along the coast while maintaining a lower salinity. The assimilation of SMOS improves the results, with a structure similar to the observations and a resulting salinity better mixed.

This comparison also highlights a fundamental issue with interpreting the plume area statistics.
Figure 5.6: The average daily plume salinity as a function of time for OBS, CNTRL, SSH, SMOS, and SMOS-SSH experiments during January, April, July and August.

For example, during August, the control has the closest plume area to the observations; however, Figure 5.8c shows the plume structure is inaccurate as compared to the SMOS assimilation. Note also that the R of SMOS observations (a spatial measure) improves as SMOS is assimilated (Table 5.3). Therefore, it is vital to take into account several metrics while also graphically comparing the plume to establish structural differences.

This comprehensive improvement in the majority of the plume assessment metrics for the SMOS assimilation validates the ability of the assimilation system to fit the observations and improve the representation of the plume. This complements the results of the previous section (5.3.1) that highlighted the ability of the assimilation system to fit the observations on a region domain-wide scale.
Argo Floats

A few in-situ Argo salinity profile floats (Chapter 5.3.2) were available for comparison during this study period. These represent valuable independent data not assimilated in the experiments. The RMSE computed for all Argo floats during each month reduced as compared to the CNTRL (15-53%) with the assimilation of SMOS, either together with SSH or individually (Table 5.7). However, due to a shortage of data, only during April was this reduction statistically significant. Additionally, all Argo floats were located in the local vicinity of the plume and not inside. These two difficulties (lack of data and imperfect location) makes validating the plume independently a challenging task. Nevertheless, the spatial extent of this reduction can still be evaluated despite the lack of data (Figure 5.9).

During April, several of the Argo floats were situated south of the defined plume. Note that the plume extent (Bold black line in Figure 5.8), calculated via the fitting of a GMM to SMOS observations (Section 5.2.3), was smaller than expected for April (Figure 5.2b). Furthermore,
5.3. Results

(a) January 8th 2013

(b) April 8th 2013

(c) July 8th 2013

(d) August 8th 2013

Figure 5.8: Snapshots of the SMOS observation fields (OBS) and model fields for each experiment (CNTRL, SSH, SMOS, SMOS-SSH) with the superimposed plume isohaline during January, April, July and August assimilation cycles.

observing Figure 5.8b, the plume extent was evidently much larger than depicted here. Therefore, the assimilation of SMOS has a substantial impact on the error for these more distant floats, reducing the negative biases of up to 2 PSU for the CNTRL, i.e. decreasing the spread of the plume.

During July, one Argo float was situated next to the far tip of the plume, and it follows that a reduction in error for the assimilation of SMOS was evident, although much less than for during April. Several floats further south exhibited a limited change in the error between experiments. Unlike April, the plume during July was much more restrained and oriented north-west, notably away from these floats.

During August, two features can be recognised. Firstly, the assimilation of SMOS reduces a positive bias (enhancing fresher waters) in the north for one Argo float, and secondly enhances negative biases further south in two Argo floats. This is the first time the assimilation of SMOS
Figure 5.9: The bias (PSU) of Argo Salinity floats (surface) analysed for each experiment (CNTRL, SSH, SMOS, SMOS-SSH) during January, April, July and August. Overlain in black is the optimal plume isohaline computed using fitgmdist (Matlab, 2015) with SMOS observations.
Table 5.7: The RMSE of Argo Salinity floats (surface) during each month analysed (PSU). Significant improvements over the CNTRL are shown in bold ($p < 0.05$). (*) denotes significance at $p < 0.1$.

<table>
<thead>
<tr>
<th>Exp. Name</th>
<th>In-situ Argo Salinity RMSE (PSU)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNTRL</td>
<td>0.25 0.80 1.04 0.52</td>
</tr>
<tr>
<td>SSH</td>
<td>0.35 1.28 0.67 0.49</td>
</tr>
<tr>
<td>SMOS</td>
<td>0.05 0.42* 0.55 0.44</td>
</tr>
<tr>
<td>SMOS-SSH</td>
<td>0.02 0.40 0.57 0.45</td>
</tr>
</tbody>
</table>

has been detrimental and is perhaps unsurprising. From previous metrics (R, RMSE, plume isohaline, and associated area and salinity value) it has been established that the assimilation is successfully fitting the SMOS observations. However, the observations themselves are subject to limitations. Here, the independent data suggests that the SMOS observations imply a plume with too strong an influence in the south.

Despite this degradation, the error reduction across all months (Table 5.7) is encouraging and shows that the assimilation of SMOS can improve the state of the salinity field (especially for April) in the vicinity of the plume as compared to the control without assimilation. The difference between the individual assimilation of SMOS and then combined with SSH was minimal.

## 5.4 Discussion

The assimilation system successfully fits the SMOS observations, reducing the regional SMOS $J_{fit}$, RMSE and R metrics during the four analysed months. Furthermore, the improvement in the majority of the plume specific metrics (plume isohaline and associated area and mean salinity), demonstrates that the assimilation of SMOS improves the representation of the Congo River plume structure and salinity magnitude. Finally, independent data via the in-situ Argo
Chapter 5. Satellite Salinity Assimilation for River Plume Modelling

float salinity profiles affirms that the assimilation of SMOS is beneficial for the model salinity near the plume as compared to a control (model run without assimilation) and sole assimilation of satellite altimetry.

The control and SSH assimilation experiments inadequately reproduced observations of the Congo River plume (via SMOS and Argo float comparisons). Notably, a significant bias in the plume salinity was exhibited throughout all months, especially so during April (Figure 5.8b). A few hypotheses can be put forth to explain this discrepancy. Firstly, the discharge of the plume is incorrect. The river input (as described in Chapter 2.1.4) is based on 103 years of data which ends in 2005. This provides only an approximation of the average of the annual Congo discharge where the standard deviation ranges from 10-15% of the mean value (red error bars in Figure 2.1).

However, an average variation of 13% (as during April) is still unlikely to account for the extreme differences between the observations and the control (Figure 5.8). Therefore, perhaps deficiencies in the mixing schemes could hinder the plume especially at the sub-grid scale near the river mouth. The Angola Basin ROMS has a resolution of 10 km with two grid points representing the opening of the Congo River channel. Recently, Bars et al. (2016) employed a multi-scale unstructured mesh model to simulate the Congo river-to-sea continuum, with elements as small as 200 m in the river and estuary and as large 20 km in the deep ocean. They note the river flow is characterised by smaller length scales that require a higher resolution. Therefore, it is clear that the resolution of the Congo within Angola Basin ROMS could be restricting the mixing of fresh water, and thus enabling a very fresh bias to expand into the open ocean where the general ocean circulation could propagate the bias into the basin. Furthermore, extreme gradients in the bathymetry such as those found near the Congo Canyon (originating downstream of the river) are particularly challenging (Bars et al., 2016). However, despite these apparent difficulties, the assimilation of SMOS can successfully constrain the plume and correct any prior bias in the model salinity as seen in the control.

This improvement is in agreement with Lu et al. (2016) who shows that the assimilation of SMOS globally plays a complementary role in model salinity simulations with an Ensemble
Optimal Interpolation DA scheme (EnOI). Specifically, Lu et al. (2016) show that for the assimilation of SMOS the mean RMSE of the modelled sea surface salinity field compared with Argo float salinity data within the tropics (20°S - 20°N) reduced by approximately 30% as compared to a control. This result held only for the open ocean as Lu et al. (2016) used an older version of the BEC data (Font et al., 2013) which suffered from RFI and land contamination issues. Nevertheless, this percentage improvement is similar to the experiments presented in this study with a limited number of available Argo floats (15-53 %). Köhl et al. (2014) also assimilated a different SMOS product (processed by the University of Hamburg) globally but found conflicting results to Lu et al. (2016) and this study (negative to neutral impacts on the salinity field for the open ocean). Lu et al. (2016) noted differences in the observation error covariance, models and data assimilation methods and SMOS datasets as possible reasons for this discrepancy.

Lu et al. (2016) also found assimilating traditional data sets such as satellite altimetry (SSH), sea surface temperature (SST), and subsurface temperature and salinity profiles (T/S) reduced errors as compared to the control (21 %). Furthermore, the combined assimilation of these data sets (SSH, SST & T/S) with SMOS additionally reduced the error as compared to the individual assimilation of SMOS (7% additional improvement). Lu et al. (2016) describe how adjustments in the SST and SSH could alter the salinity field via the correlations in ensembles.

In this study, the SSH assimilation similarly improves the regional domain-wide SMOS RMSE on average for 3 of the four months studied (4-30%), and regional SMOS R for all months (1 -30%). Furthermore, the RMSE and R further reduced and increased for the combined assimilation of SMOS with SSH respectively, as compared to the assimilation of SMOS individually (12-22% for RMSE, 3% for R).

This result suggests; firstly that the combination with satellite altimetry has a positive impact on fitting the observations as compared the sole assimilation of SMOS, and secondly that this combination has more influence on the absolute error of the regional salinity (via the RMSE error metric) rather than the spatial error (via R). However, the plume evaluation metrics revealed minimal differences (< 1%) between the individual assimilation of SMOS and combined
with SSH. If the assimilation of SSH improves the large-scale ocean circulation (Fukumori et al., 1999; Dorofeev and Korotaev, 2004; Dombrowsky et al., 2009; Moore et al., 2011a; da Rocha Fragoso et al., 2016) then it follows that the salinity field further away from the river mouth is more influenced by the SSH assimilation, thus affecting the regional salinity statistics more than the plume metrics. Still, with such a large plume stretching as far as 600 km (Figure 5.2), this is perhaps a surprising result.

Contrary to an Ensemble DA scheme, the ROMS IS4D-Var system could improve the salinity field via a few mechanisms. Firstly, the linear balance relationships within $B$ (Section 2.1.2). Secondly, multivariate characteristics within the adjoint and tangent linear models (as discussed in Section 2.1.2). Finally, the assimilation of SSH would improve the surface circulation that, in turn, could improve the far-field of the river plume.

In the first realistic numerical simulation of the Congo plume Denamiel et al. (2013) studied the effects of the geomorphology, wind and ocean circulation on the plume. They conclude the northward extension can be explained via a buoyancy-driven upstream coastal current linked closely to the Congo River estuary and the combination of ocean currents and wind stress. Furthermore, they also conclude the westward extension of the plume during February-March was due to the ocean circulation via the South Equatorial Counter Current (SECC) and Angola Current (AC). In their observational study, Hopkins et al. (2013a) argued that the march westward plume extent is instead driven by Ekman currents turning more west. They point out that bias in the wind forcing and lack of accurately simulated currents in the Denamiel et al. (2013) study could be influencing the resulting conclusions. However, despite this disagreement, they note that ocean circulation patterns could theoretically enhance the westward flow. Therefore, it is feasible to suggest that with the assimilation of SSH improving the general ocean circulation, a better simulation of the plume follows. More simulations than presented here are required to validate whether SSH combined with SMOS could further improve the representation of the Congo plume than the assimilation of SMOS alone.
5.5 Conclusion

The impact of assimilating satellite salinity with applications to modelling the Congo River plume has been assessed. The latest version of SMOS (May 2017), a satellite salinity product, was processed with an updated technique to reduce errors near the coast. This allows more frequent coastal data, which could be employed in a DA system of the Congo River plume. This assessment was then achieved using the ROMS Angola Basin configuration with IS4D-Var, comparing the assimilation of SMOS with a control run (without DA) during four months. Furthermore, the combination with satellite altimetry measuring sea surface height (SSH) was undertaken to evaluate if any additional benefits would be observed.

The metrics applied to assess the assimilation system’s ability to fit the observations, i.e. SMOS $J_{fit}$, RMSE and R revealed that the SMOS observations were successfully fit to the region during each month. The combined assimilation of SMOS and SSH additionally improved regional domain-wide SMOS RMSE statistics suggesting a complementary role for the assimilation of SSH on a regional scale, particularly on the absolute magnitude of salinity. Specific plume evaluation metrics consisted of the plume isohaline (determined from fitting a Gaussian Multi-Mean Model and quantile comparisons) and the associated mean plume salinity and area (bounded by the model domain). The plume isohaline and mean salinity were closer to the SMOS observations with the assimilation of SMOS where the SMOS structure was well replicated within the model. Contrary to the regional statistics, the combined assimilation of SMOS and SSH exhibited minimal differences as compared to the assimilation of SMOS individually. Note the cyclic nature of this evaluation, i.e. SMOS observations were used for both validation and assimilation, implies the results mentioned above only concludes that the ROMS IS4D-Var system is correctly fitting the observations to sufficiently reproduce the observed plume structure and salinity magnitude, complimenting the regional $J_{fit}$, RMSE and R metrics.

However, some completely independent data (Argo float salinity profiles) was available, although very limited in both quantity and spatial extent. Despite this limitation, the RMSE computed for all Argo floats during each month reduced as compared to the control (15-53%) with the assimilation of SMOS, however, only during April was this reduction statistically sig-
significant. The spatial extent of this reduction was also investigated, and some broad features were noted. This affirms the beneficial role of assimilation SMOS for the model salinity field that is in agreement with previous studies. For the first time, it has been shown that the current generation of satellite salinity observations can be successfully used to constrain a large river plume such as that produced by the Congo River.
Chapter 6

Discussions, Conclusions and Future Work

This thesis contained a comprehensive study of different data assimilation (DA) applications within the Angola Basin using the Regional Ocean Modelling System and 4D-Var DA.

6.1 Satellite Current Assimilation

Firstly, the impact of assimilating a novel observational data set, satellite-derived currents (OSCAR), in an advanced DA system on ocean current forecasts was investigated (Phillipson and Toumi, 2017). This represents an application that could influence operational forecasting during real-time events such as an oil spill. The objective was to compare any impacts of assimilating OSCAR to more traditional observations, namely sea surface height (SSH), which has previously been shown to improve current forecasts. Only one previous study with a simplistic DA scheme (nudging) has assimilated OSCAR. Thus a fundamental question remained as to whether its assimilation in a more advanced DA system such as 4D-Var, could produce a better forecast than assimilating SSH. These two remote observations (OSCAR and SSH) are not entirely independent, as OSCAR uses the same satellite altimetry to derive part of the velocity field.
This objective was then achieved by conducting several experiments comparing 17 simulated and observed drifter floats over January-March 2013. The results revealed that the assimilation of either OSCAR or SSH equally improved the forecast upon a control (forecast without any assimilation), and the assimilation of sea surface temperature (SST) and in situ temperature and salinity profiles (T/S). Therefore, there was no significant benefit between the assimilation of one over the other in the Lagrangian predictability of the ocean currents. Based on insights gained through the course of this research, this behaviour was attributed to a combination of the reduced frequency of the OSCAR velocities as compared to the SSH observations, differences in the background/error covariance matrix parameters and the consistent assigned surface forcing to all experiments.

6.2 Drifters for Assimilation and Persistence Forecasts

Motivated by a recent study by Muscarella et al. (2015) showing that the assimilation of drifter velocities improves the Lagrangian predictability of the ocean currents, the impact of combining the aforementioned remote-sensing observations (OSCAR or SSH) with drifters was investigated. The objective was to assess whether this combination could improve upon assimilating the drifters alone. This was an important question left unanswered by Muscarella et al. (2015) and similar to the OSCAR assimilation experiments, could influence the use of observations during operational forecasting of a major marine event. Here, the impact on the local circulation in the vicinity of the assimilated drifters was investigated and not the impact of independent drifters far away. The assumption is that in a realistic event, targeted deployment of drifters would be favourable (Sharma et al., 2010; Novelli et al., 2017). Thus the forecast would be in the vicinity of the deployed drifters. This assumption is reasonable given the coverage of drifters is typically very poor, especially in the tropics and the Angola Basin.

This objective was then achieved by conducting more experiments comparing 17 simulated and observed drifter floats over January-March 2013. The results revealed that while the drifter assimilation improved upon a control (forecast without any assimilation), the assimilation of
SST and T/S profiles, and the assimilation of either SSH or OSCAR; combinations with any of the aforementioned data sets showed no further significant benefit. It was also found that differences in the current speed either improves (stronger currents) or degrades (weaker currents) the probability of a more beneficial forecast for the combined assimilation of drifters with SSH as compared to the assimilation of drifters alone. This difference, and the skill variability in general, could have been due to the sampling differences between the variable coverage of the remote-sensing satellite and the drifters, and uncertain assumptions that relate to the 4D-Var system.

Besides for assimilation, the drifter velocities were also utilised in the formation of a new evaluation metric denoted the crossover time. The objective was to develop a new metric to examine the performance of an ocean model with respect to persistence. This was then achieved by first demonstrating the crossover time concept in a global ocean model evaluated separately from ROMS. This global model had a crossover time of approximately four to six days, varying spatially. Spatial variations in the crossover time are explained in terms of the model error and some regional dynamical features. Furthermore, the crossover time for the experiments exploring the impact of combining the remote-sensing observations with drifters in the Angola Basin was also compared. With the assimilation of drifters the crossover time shortened and the percentage of failed crossovers, i.e. the percentage of forecasts that did not improve upon persistence for the entire prediction, reduced.

The crossover time joins a community of existing Lagrangian evaluation metrics. In some aspects, the crossover time in terms of the Lagrangian separation distance is similar to the skill score of Liu and Weisberg (2011). For this skill score, the observed drifter distance normalises the cumulative drifter separation distance of the model. Whereas, for the crossover time, the drifter separation distance of the persistence forecast ‘normalises’ the drifter separation distance of the model. However, due to its unique flexibility, it is not limited to the Lagrangian framework. Therefore, the crossover time concept could also be useful to evaluate the forecast performance of any other ocean variables such as sea surface temperature and the mixed layer depth. Furthermore, the allocation of a timescale means the interpretation can provide some dynamical logic, i.e. in relating to the decorrelation time scale of the drifters.
6.3 Satellite Salinity Assimilation

The impact of assimilating satellite salinity on the Congo River plume was also investigated. Recently, an advanced version of a satellite salinity product (SMOS), was made available that contained significantly more observations near the coast. This development improved the frequency of observations for the Congo River plume and therefore the objective was to explore, for the first time, coastal DA applications with SMOS. This objective was achieved by conducting experiments assimilating SMOS and comparing the resulting analysis with different metrics (specifically focusing on validating the Congo River plume) and limited in-situ observations. The results revealed the ability of the assimilation system to fit the SMOS observations successfully. The independent in-situ observations verified that the assimilation of SMOS could improve the modelled regional salinity fields in agreement with previous studies. Furthermore, in combining with SSH, some results indicated a complementary role on a regional scale, although the effect on the plume remains inconclusive.

6.4 Future Work

The assimilation of SSH and the resulting impact on the currents (by multivariate characteristics in the adjoint and tangent linear model) is similar to the direct assimilation via the OSCAR velocities. Therefore, perhaps there is a case for utilising the assimilation of OSCAR in future studies. The assimilation of SSH has had many more years of research as compared to satellite-derived current analysis products (such as OSCAR) that are a relatively recent concept (Isern-Fontanet et al., 2017). Therefore, when considering the numerous limitations of OSCAR (frequency, background error unknowns) as compared to SSH, it was very encouraging to see that the assimilation forecasts performed on par, thus advocating its development in a DA system.

In a significant marine pollution event, drifters could be released in an area where the forecast is of most interest (Sharma et al., 2010; Novelli et al., 2017). This study has then provided some insight into what different observations may need to be assimilated to improve the Lagrangian
predictability of the ocean currents, advocating the use of drifters in an assimilation system. However, caution must be taken when combining such data with satellite remote-sensing, where both improvements and degradation were exhibited.

Drifter positions could be assimilated instead of the drifter inferred velocities. Previous studies on drifter position assimilation have shown to have a positive impact on the resulting circulation (Molcard et al., 2003; Nodet, 2006). One clear advantage would be in bypassing the required approximations in the reconstruction of Eulerian velocity information (Salman et al., 2008). However, no such comparison between the two methodologies (assimilating either drifter positions or the inferred velocities) for the same ocean model has been assessed. It is also unknown whether combining this drifter position assimilation with the assimilation of multiple different observations would yield similar results as presented here. Despite such unknowns, it is simply worth recognising that different methodologies exist that could have been applied to this study.

Recently, the Consortium for Advanced Research on Transport of Hydrocarbon in the Environment (CARTHE) drifter was designed as a low-cost and biodegradable alternative to a standard drifter (Novelli et al., 2017). These unique qualities enabled 1100 units to be deployed during the Lagrangian Submesoscale Experiment (LASER) campaign, January-February 2016 (Novelli et al., 2017). Such large deployments covering much broader areas could be very beneficial for a DA system.

The Surface Water and Ocean Topography (SWOT) mission (launching in 2021) is expected to be able to measure the SSH at a higher resolution of 15-25 km using unique swath altimetry of up to 120 km wide (Durand et al., 2010). This potentially unprecedented improvement could then dramatically improve both the SSH and the subsequent SWOT-derived current analysis. As well as perhaps better complimenting the assimilation of drifter velocities, in moving towards smaller scales. Such current DA systems will likely need to adapt to assimilate this unique data alongside traditional data streams. For example, (Liu et al., 2014a) demonstrated for spatially high-resolution observations combined with sparse data, the multi-scale implementation of the background error covariance matrix $B$ improves upon the standard single-scale approach in a 3D-Var system, reproducing finer velocity structures observed in high-frequency (HF) radar
velocity fields. The dilemma of combining such information for a single-scale $B$ is that the choice of the decorrelation length scale needs to be both small (to reduce filtering effects for the spatially high-resolution observations) and large (to increase the spread the information for the sparse data). In the future, one could then imagine a similar study as undertaken here but instead utilising 1000s of biodegradable drifters (Novelli et al., 2017) and the SWOT-SSH swaths (Durand et al., 2010).

For the SMOS assimilation experiments only the analysis was investigated. Therefore, a logical next step would be to assess the forecast with the potential for substantial improvements. One could also imagine how the assimilation of SMOS could potentially also have an impact on other variables besides salinity via the multivariate characteristics. Recently, Palma and Matano (2017) showed that eddy-to-eddy interaction is an essential mechanism for the spreading of a Near-Equatorial River Plumes (NERP) and the re-stratification of the basin. Therefore, prolonged assimilation of the plume could dramatically influence local eddies and hence the circulation within in the region.

A unique application that could be later considered is in estimating the Congo discharge rate with parameter estimation. Parameter estimation is the process of finding optimal parameter values given a set of measurements and dynamical model with known uncertainty (Evensen, 2009). The assumed Congo discharge rate represents a notable limitation of the study with observed monthly discharges ending at 2005. Variational parameter estimation within ROMS could be theoretically achieved with the use of the adjoint model through state augmentation, a process where parameters are assigned an uncertainty so that they can be examined like dynamic variables (Powell, 2009).

### 6.5 Final Remarks

To conclude, some possible general improvements are highlighted. A more advanced DA system could improve the results of all experiments. Despite, a suitably advanced methodology, the ROMS IS4D-Var system utilised here, has some further recent improvements that could be
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useful. For example, a spatially varying decorrelation length scale would be beneficial in the Angola Basin domain, where the natural length scale varies dramatically by up to 100km (Moore et al., 2013). The addition of an equatorial adjustment for the geostrophic balance within B may also help. However, previous studies (Carrier et al., 2016; Neveu et al., 2016) including as presented in this thesis (Phillipson and Toumi, 2017) suggest that this is not necessarily required to achieve multivariate characteristics within 4D-Var. In the future, advanced hybrid methodologies implemented within ROMS are also likely to improve results, such as combining the current IS4D-Var algorithm with an Ensemble Kalman Filter (EnKF) which updates the background error covariance matrix as the system evolves using an ensemble of non-linear model runs at each assimilation time (Desroziers et al., 2014). Finally, although the results exhibited significance, more data (i.e. more drifter observations) over more seasons (say the entire year) would be ideal. Unfortunately, ROMS IS4D-Var is computationally expensive and has a fundamental limitation to the user’s available computational set-up. Scalable DA is an on-going area of research (D’Amore et al., 2014; Phillipson et al., 2016).

The conclusions presented within this thesis highlight the first insight into data assimilation within the Angola Basin. Multiple observations, both novel and conventional were assimilated with a focus on improving the modelling capabilities of two unique aspects of the Angola Basin; the diverse ocean currents and the Congo River plume. Additionally, a new metric was introduced as an evaluation of ocean models against persistence.
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