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14. ABSTRACT
Sea surface temperature (SST) varies on a range of temporal scales according to variations in insolation, advection, and mixing. A prominent diurnal signal can frequently be identified in the SST of midlatitude to tropical regions, particularly under conditions of high insolation and low wind speed. Case studies in the Gulf of Mexico and Mediterranean Sea are used to examine the impact of such variations on assimilative SST analyses and forecasts. The scenarios provide infrared observations from polar-orbiting or geostationary satellites to an assimilative ocean model using a 24-hour update cycle. SST innovations are determined relative to the prior 24-hour SST forecast or using a first guess at the appropriate time (FGAT) approach which matches each observation to its corresponding time-varying forecast. It was anticipated that the FGAT would have its largest impact in the Gulf of Mexico summer, when the occurrence of the relatively large diurnal cycle maximum is nearly in phase with the nowcast. In contrast, FGAT was anticipated to have relatively little impact in the Mediterranean summer, where the diurnal maximum and nowcast are 90° out of phase. The impact of FGAT in the fall-spring seasons would be more affected by the skill in forecasts of the non-diurnal trend, as the diurnal signal is smaller in these seasons. FGAT is found to have its largest benefit in reduction in the mean error of the SST forecasts; its impact on standard deviation is mixed. It is also found to have larger impact in the cases assimilating observations from geostationary satellites, which give a broad sample of SST over all times of the day. Observations from the polar orbiter come at a sun-synchronous 10:00 AM or PM, sampling near the midpoints of the diurnal variation. The effectiveness of FGAT is dependent on model forecast skill and effective only if the model is able to adequately predict diurnal or other dominant variations between analysis times.

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IMPACT OF DIURNAL WARMING ON ASSIMILATION OF SATELLITE OBSERVATIONS OF SEA SURFACE TEMPERATURE

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ABSTRACT

Sea surface temperature (SST) varies on a range of temporal scales according to variations in insolation, advection, and mixing. A prominent diurnal signal can frequently be identified in the SST of midlatitude to tropical regions, particularly under conditions of high insolation and low wind speed. Case studies in the Gulf of Mexico and Mediterranean Sea are used to examine the impact of such variations on assimilative SST analyses and forecasts. The scenarios provide infrared observations from polar-orbiting or geostationary satellites to an assimilative ocean model using a 24-hour update cycle. SST innovations are determined relative to the prior 24-hour SST forecast or using a first guess at the appropriate time (FGAT) approach which matches each observation to its corresponding time-varying forecast. It was anticipated that the FGAT would have its largest impact in the Gulf of Mexico summer, when the occurrence of the relatively large diurnal cycle maximum is nearly in phase with the nowcast. In contrast, FGAT was anticipated to have relatively little impact in the Mediterranean summer, where the diurnal maximum and nowcast are 90° out of phase. The impact of FGAT in the fall-spring seasons would be more affected by the skill in forecasts of the non-diurnal trend, as the diurnal signal is smaller in these seasons. FGAT is found to have its largest benefit in reduction in the mean error of the SST forecasts; its impact on standard deviation is mixed. It is also found to have larger impact in the cases assimilating observations from geostationary satellites, which give a broad sample of SST over all times of the day. Observations from the polar orbiter come at a sun-synchronous 10:00 AM or PM, sampling near the midpoints of the diurnal variation. The effectiveness of FGAT is dependent on model forecast skill and effective only if the model is able to adequately predict diurnal or other dominant variations between analysis times.

1. Introduction

The Mediterranean Sea and the Gulf of Mexico are similarly-sized semi-enclosed sea basins in the midlatitudes of the northern hemisphere, with the central latitude of the Mediterranean falling near 30°N, close to the northernmost latitude in the Gulf of Mexico. Both encompass a range of sub-regional SST climates. The Gulf is dynamically divided into eastern and western regions, with the east dominated by the warm Loop Current and the west more strongly influenced by weather systems moving eastward off the coast and westward-propagating Loop Current eddies. The Gulf of Campeche to the west is somewhat sheltered from all but the southernmost eddy paths and dynamically distinct from the wind-driven circulation on broad shelf to the north. The northern boundary has strong freshwater inflow concentrated in centrally-located Atchafalaya and Mississippi River plumes. The Gulf domain in this study also extends into the northwestern Caribbean and Atlantic waters north of Cuba and east of Florida, adding to the diversity obscured within a single number measuring Gulf-wide performance.

The Mediterranean includes greater distinctions among an even wider range of subregions. The western Mediterranean includes regions west of Corsica and Sardinia. At the extreme southwest, the Alboran Sea is dominated by the Alboran gyres and exchange with the North

Atlantic through the Strait of Gibraltar. It is connected by the westward flowing Algerian Current to the Algerian Basin, which produces prominent regions of cool upwelling when it is pushed offshore. To the north, the Balearic Sea, Gulf of Lion, and Ligurian Sea also show episodic upwelling, most strongly evident when strong Mistral winds blow from the northwest across the Gulf of Lion. The central Mediterranean from Sardinia east to Greece includes Tyrrhenian, Adriatic, and Ionian Sea subdivisions with their own local characteristics. The eastern region tends to have the warmest Mediterranean SSTs. These occur under conditions of high insolation in the southeast, and conditions can be significantly cooler to the north in the Aegean Sea, a region exposed to cold continental wind outbreaks and inflow of cool, fresh Black sea water through the Turkish Straits. The diversity of conditions in the Mediterranean leads a larger range of SST variability with potentially higher uncertainty for SST predictions and verification.

Diurnal warming adds an additional complication to accurately analyzing and forecasting SST. Performance of daily SST predictions is assessed relative to independent *in situ* SST measurements matched to model fields interpolated to be valid at each observation time and location. If the SST field remains fairly constant between daily analyses, then observations at any time of the day are equally useful as measures of model-ocean difference, valid to estimate system performance to calculate model-ocean mismatches to be minimized through variational data assimilation. If diurnal variations are present, then the range of temperature over the course of the day often exceeds the difference from one daily analysis time to the next. Such diurnal and other sub-daily excursions increase the impact of non-uniform temporal sampling in the observations and representativeness errors associated with the analysis and performance increments.

2. Experiments

Experiments in the two domains from December 2009 to December 2011 are configured to evaluate satellite data streams and data assimilation approaches. In particular, three sets of source SST observations are defined in each domain: polar orbiting observations, geostationary observations, and combined satellite observations. The NOAA AVHRR sensors provide the polar satellite observations, while the NOAA Geostationary Operational Environmental Satellite (GOES-East) and the European Meteosat Second Generation (MSG) provide the geostationary observations for the Gulf of Mexico and Mediterranean, respectively. The AVHRR and GOES SST estimates are produced by the U.S. Naval Oceanographic Office, while the MSG SST estimates are produced by IFREMER/METEO-France.

These satellite data are assimilated into cycling NCOM/NCODA (Barron et al 2010) forecast models on a 3-km grid forced with COAMPS atmospheric fields. The models are run with the First Guess at Appropriate Time (FGAT; Massart et al., 2010) option on or off. With FGAT off, the assimilation interpolates the satellite observations to the analysis time and calculates an innovation based on the difference between the interpolated observed and model nowcast SSTs. With FGAT on, model-observation differences are calculated at the time and location of each observation and the differences are interpolated to estimate a nowcast innovation.

Model analyses and forecasts are output at three-hour frequency with forecasts to 72 hours after the 0:00 UTC analysis/nowcast time. To assess performance, model SST is interpolated in space and time to match corresponding independent SST observations from drifting buoys. While all *in situ* surface-only observations are withheld from the assimilative model forecasts and thereby offer independent estimates of the ocean state, only the surface drifters are used in the performance metrics reported in this article. Other, similarly withheld surface *in situ* observations such as those from fixed buoy locations or shipboard observations might be used, but the drifting buoys are selected as having the best

combination of broadly distributed geographic coverage, reducing geographic sampling bias, sampling bias, and accurate measurements at a fairly uniform near-surface depth. Results are compiled by local time of day and combined seasonally, annually, and multi-annually.

3. Results

Bias and standard deviation of the errors are evaluated for all cases, where standard deviation is the square root of the mean squared error after the mean differences are removed. In the Gulf of Mexico (Table 1), standard deviations of the analysis errors are near 0.50°C for all satellite and FGAT combinations, with standard deviation of the forecast errors increasing to about 0.55°C . FGAT tends to produce slightly larger deviations, near 0.57°C , again similar among all satellite alternatives. Bias in the Gulf of Mexico differs significantly among the satellite options. With FGAT on (best case), AVHRR-based analyses show 0.03°C bias (warm) while GOES-E gives -0.17°C bias (cold) and -0.11°C bias for the combined case. FGAT makes a significant impact, as the FGAT-off biases in these cases are about 0.10°C cooler. Forecast adds an additional cold bias, near 0.23°C cooling after 72 hours. In the Mediterranean (Table 2), the nowcast with FGAT bias is 0.03°C cold for AVHRR-only and 0.15°C warm for MSG, with a combined result near 0.04°C . FGAT adds a warm bias near 0.05°C , about half of the Gulf of Mexico impact. Model forecast has a cold bias of about half of the Gulf of Mexico case, near 0.10°C cold after 72 hours. The FGAT forecast appears best in the MSG case, but this is misleading as the warm MSG bias counteracts the cold forecast bias.

Breaking the results down seasonally (Table 3), the impact of FGAT is unambiguously positive in summer but slightly negative in winter. This result reflects seasonal changes between the dominant processes causing temperature variations between successive analyses. If the model has no skill in representing variations on scales shorter than a day, our assimilation approach should ignore these sub-daily variations and treat the temporal mean of the observations as an estimate of the ocean state at the nowcast time, using the difference between the observation mean and the nowcast SST as the basis for calculating assimilation increments. On the other hand, when the model does have some skill in predicting sub-daily variations, then we can benefit from FGAT, calculating the observation-model differences at the time of the observations and averaging these differences to estimate the true model-observation increment at the analysis time. FGAT shows its most positive impact during the northern hemisphere spring and summer. These are times of maximum solar heating and corresponding diurnal warming. Thus, the model has skill in representing the diurnal variations and providing a sound basis for an FGAT approach. In the fall and winter, insolation and diurnal warming are smaller, allowing other contributors to sub-daily SST variations to increase in relative importance. The cold forecast bias, stronger in the Gulf of Mexico but also evident in the Mediterranean, reduces the fidelity of short-term SST forecasts. The effect of this bias and inadequate representation of the cumulative effects of short-time scale processes other than diurnal warming provide an insufficient basis for effective FGAT assimilation during the fall and winter.

	Gulf of Mexico 196,740 obs	Bias °C (model-ob)		Standard Deviation °C	
		FGAT on	FGAT off	FGAT on	FGAT off
Nowcast analysis - observation	Both Polar and Geostationary	-0.11	-0.21	0.54	0.5
	Polar only	0.03	-0.07	0.54	0.51
	Geostationary only	-0.17	-0.26	0.54	0.52
51-72 hr forecast - observation	Both Polar and Geostationary	-0.34	-0.41	0.57	0.55
	Polar only	-0.25	-0.30	0.57	0.55
	Geostationary only	-0.39	-0.46	0.57	0.57

Table 1: SST matchups between cycled NCODA analyses, NCOM forecasts, and independent drifting buoy observations in the Gulf of Mexico over years 2010-2011. NCODA analyses are daily at 0:00 UTC while forecasts are interpolated to the observation time from 3-hourly NCOM output spanning 51-72 hours after each nowcast.

	Mediterranean 95,179 obs	Bias °C (model-ob)		Standard Deviation °C	
		FGAT on	FGAT off	FGAT on	FGAT off
Nowcast analysis - observation	Both Polar and Geostationary	0.04	0.10	0.70	0.70
	Polar only	-0.03	0.03	0.71	0.71
	Geostationary only	0.15	0.18	0.72	0.72
51-72 hr forecast - observation	Both Polar and Geostationary	-0.06	-0.01	0.82	0.82
	Polar only	-0.12	-0.07	0.82	0.84
	Geostationary only	0.04	0.06	0.82	0.83

Table 2: SST matchups as in Table 1 but for Mediterranean Sea.

A significant cold bias reduces the skill of the forecast over the 51-72 hour range in the Gulf of Mexico, with bias in the best seasonal cases from -0.05 to -0.52°C. The cold bias is less evident in the Mediterranean over most seasons, with 51-72 hour forecast bias in the best cases generally ranging from -0.05 to 0.03°C. The best cases as determined over the 51-72 hour forecast range in the Mediterranean obscure the cold forecast bias by emphasizing runs relying on the geostationary MSG observations, observations that lead to a warm bias at the analysis time. Nevertheless, most seasons are found to have only a small forecast bias. However, comparisons with observations during Autumn 2013 indicate a Mediterranean 3-day forecast bias near to -0.3°C, much colder than other months. This result appears to be a consequence of sampling bias. The surface drifters providing the matchups in this season (Fig. 1) are clustered in the southern parts of the western Mediterranean with a disproportionate presence in the cool upwelling north of Algeria. This sampling bias is identified as the likely cause of the apparent cold bias during the Autumn of 2011; prior seasons showed broader coverage across the sea and few observations immediately north of the Algerian coast.

	Season and years	Min Analysis Bias (model-ob)			Min 51-72 hr. Fcst Bias (mod-ob)			Number of obs
		Satellites	FGAT	°C bias	Satellites	FGAT	°C bias	
Gulf of Mexico	Winter 2010	AVHRR	same	±0.03	AVHRR+GOES	off	-0.12	4148
	Spring 2010	AVHRR	off	-0.01	AVHRR	on	-0.17	17764
	Summer 2010	AVHRR	on	0.07	AVHRR	on	-0.21	76562
	Autumn 2010	AVHRR	same	-0.03	AVHRR	off	-0.25	45052
	Winter 2011	GOES	off	-0.07	AVHRR+GOES	off	-0.25	23725
	Spring 2011	GOES	off	0.00	AVHRR	on	-0.05	16461
	Summer 2011	AVHRR	on	-0.15	AVHRR	on	-0.52	8796
	Autumn 2011	AVHRR+GOES	on	-0.16	AVHRR+GOES	on	-0.38	4956
	2010	AVHRR	same	±0.06	AVHRR	on	-0.24	146699
	2011	AVHRR	on	-0.04	AVHRR	on	-0.28	50041
	2010-2011	AVHRR	on	0.03	AVHRR	on	-0.25	196740
Mediterranean Sea	Winter 2010	AVHRR+MSG	off	-0.02	MSG	off	-0.01	5174
	Spring 2010	MSG	off	0	MSG	off	0.03	3113
	Summer 2010	AVHRR+MSG	on	0.03	MSG	off	-0.01	7653
	Autumn 2010	AVHRR	on	0.03	AVHRR+MSG	on	-0.01	28960
	Winter 2011	AVHRR	on	-0.01	AVHRR	same	±0.01	19100
	Spring 2011	AVHRR	on	-0.02	AVHRR+MSG	off	-0.05	11340
	Summer 2011	AVHRR+MSG	on	0.03	MSG	same	±0.02	11490
	Autumn 2011	MSG	off	-0.09	MSG	off	-0.29	8561
	2010	AVHRR	on	-0.01	AVHRR+MSG	on	-0.03	46714
	2011	AVHRR+MSG	on	0	MSG	off	-0.01	48465
	2010-2011	AVHRR	on	-0.03	AVHRR+MSG	off	-0.01	95179

Table 3: Seasonal SST matchups between cycled NCODA analyses, NCOM forecasts, and independent drifting buoy observations in the Gulf of Mexico over years 2009-2011. NCODA analyses are daily at 0:00 UTC while forecasts are interpolated to the observation time from 3-hourly NCOM output spanning 51-72 hours after each nowcast.

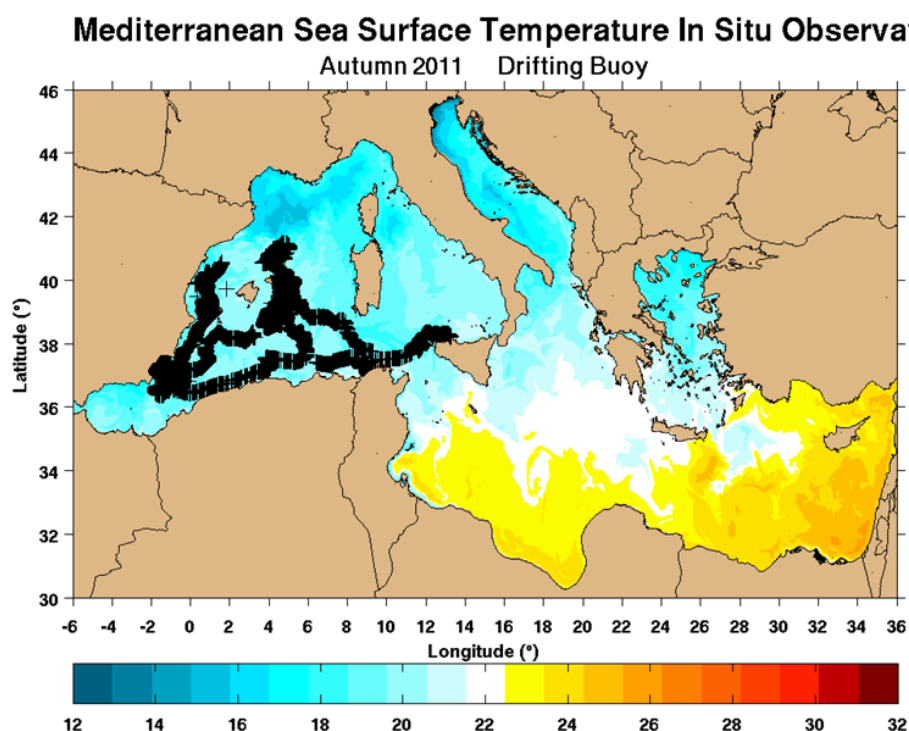


Figure 1: Locations of drifting buoy matchup observations superimposed on mean model sea surface temperature during Autumn 2011 in the Mediterranean Sea. The concentration of the observations in the western Mediterranean and in particular the cool upwelling along the coast of Algeria introduces as sampling bias relative to the true errors averaged over the entire Mediterranean domain.

4. Conclusion

Evaluations of regional NCOM forecasts using 3DVAR NCODA assimilation in the Gulf of Mexico and Mediterranean demonstrate the impact of diurnal variations on analyses and forecasts of sea surface temperatures. The FGAT approach mitigates the errors introduced by sub-daily variations if the model is able to skillfully forecast evolution over these time scales. It is shown that the models do have skill to sufficiently simulate the mean diurnal signals which are most important in the spring and summer seasons of maximum insolation. Differences between assimilation of observations from geostationary and polar-orbiting platforms are reduced by FGAT but problems associated with intra-sensor bias persist. Sampling bias introduces additional complexities to interpreting the statistics associated with matchups between model analyses and forecasts and independent SST measurements from surface drifters. An overall cold forecast bias is a persistent source of error that will be addressed in future research efforts.

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