Characterization of Turbulent Latent and Sensible Heat Flux Exchange between the Atmosphere and Ocean in MERRA

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ABSTRACT

Turbulent fluxes of heat and moisture across the atmosphere–ocean interface are fundamental components of the earth’s energy and water balance. Characterizing both the spatiotemporal variability and the fidelity of these exchanges of heat and moisture is critical to understanding the global water and energy cycle variations, quantifying atmosphere–ocean feedbacks, and improving model predictability. This study examines the variability of the recently completed NASA Modern-Era Retrospective Analysis for Research and Applications (MERRA) product in terms of its turbulent surface fluxes. This assessment employs a large dataset of directly measured turbulent fluxes as well as other turbulent surface flux datasets. The spatial and temporal variability of the surface fluxes are examined in terms of their annual-mean climatologies, their seasonal covariability of near-surface bulk parameters, and their representation of extremes. The impact of data assimilation on the near-surface parameters is assessed through evaluation of the incremental analysis update tendencies. It is found that MERRA turbulent surface fluxes are relatively accurate for typical conditions but have systematically weak vertical gradients in moisture and temperature and a weaker covariability between the near-surface gradients and wind speed than found in observations. This results in an underestimate of the surface latent and sensible heat fluxes over the western boundary current and storm-track regions. The assimilation of observations generally acts to bring MERRA closer to observational products by increasing moisture and temperature near the surface and decreasing the near-surface wind speeds.

1. Introduction

The oceans provide a vast repository of both heat and water that are of critical importance to the earth’s hydrologic and energy cycles. Because of their inherent high heat capacity relative to the atmosphere, the global oceans integrate energy exchanges across the atmospheric interface, providing both “memory” of past fluxes and a potential source of predictability for the atmosphere. These exchanges of moisture and heat with the atmosphere vary richly on a wide range of space and time scales in response to both local and nonlocal balances of physical and dynamical processes. Atmospheric and oceanic circulations are tied to the distributions of these exchanges and work in tandem to minimize equator to pole temperature gradients. Modeling all energy fluxes accurately is obviously crucial to the proper simulation of observed atmospheric and oceanic variability.

In this study, we focus on turbulent oceanic fluxes produced by the National Aeronautics and Space...
Administration (NASA) Modern-Era Retrospective Analysis for Research and Applications (MERRA; Rienecker et al. 2011). As with other reanalyses, surface fluxes in MERRA are the result of parameterized physics representing complicated physical processes of molecular and turbulent diffusion, boundary layer structure, and dynamical processes. Forcing these physical processes through the assimilation of observed state variables of moisture, heat, and momentum yields internally consistent estimates of turbulent and radiative fluxes. However, by construction, all models have tunable parameters and physics biases and the observations themselves have significant uncertainties. Thus, understanding and characterizing the behavior of these assimilated products is a key part of validating the overall performance of MERRA and other reanalyses. Here, we use direct in situ buoy and ship observations along with gridded, observationally based datasets to provide an initial characterization of the NASA MERRA product with respect to its accuracy, climatology, and variability.

In a reanalysis effort, comprehensive global models are combined with sophisticated data assimilation techniques to utilize observations in constraining the model state variables (surface pressure, air temperature, water vapor, and wind) while producing regular gridded state and physics fields (even where observations do not exist). Examples of these products include the National Centers for Environmental Prediction (NCEP; Kanamitsu et al. 2002) reanalysis, the Climate Forecast System Reanalysis (CFSR; Saha et al. 2010), the European Centre for Medium-Range Weather Forecasts (ECMWF) Interim Reanalysis (ERAINT; Dee et al. 2011), and MERRA. These products are differentiated by the use of different physical models, the use of different assimilation strategies, and/or the ingestion of different observational streams. Both CFSR and MERRA employ the three-dimensional gridpoint statistical interpolation (GSI; Kleist et al. 2009) analysis, whereas four-dimensional variational assimilation is used in ERAINT. The end result is a time-varying best-guess state of the atmosphere given the underlying model assumptions and quality of assimilated observations. State variables such as temperature, moisture, and wind speed (WSPD at the lowest model level) are applied to a surface layer parameterization for the production of surface fluxes. A detailed description of surface layer parameterizations, such as Monin–Obukhov similarity theory, can be found in standard texts (Stull 1988; Kraus and Businger 1994). Models vary in the application of surface parameterizations through the choice of several parameters such as roughness lengths, inclusion of ocean-wave effects, and the use of stability functions. Improvements in modeled fluxes can be made through improved estimation of the near-surface variables and/or the improved parameterization of these parameters that effectively control the transfer rates of momentum, heat, and moisture. Sampling problems can also arise in reanalyses because of the incomplete and time-varying nature of the observational system. Changes in the availability and accuracy of observations can lead to time-dependent bias errors (Robertson et al. 2011). Although model reanalyses are constrained to satisfy both model physics and observations, some errors remain. The errors arise from both deficiencies in the surface layer variables (Wang and McPhaden 2001; Cronin et al. 2006; Sun et al. 2003) and turbulent flux parameterizations (Josey 2001; Renfrew et al. 2002). The primary driver of errors in the fluxes may vary regionally and seasonally.

Time-varying, gridded estimates of the turbulent heat fluxes can also be produced through the use of satellite-based observations, in situ observations, and/or combinations of these measurements. Satellite-based products are based heavily on passive or active microwave measurements to derive bulk variables needed to compute the surface fluxes from parameterizations such as the Coupled Ocean–Atmosphere Response Experiment (COARE; Fairall et al. 2003) algorithm. The key variables to be measured are sea surface temperature (SST), near-surface wind speed, specific humidity, and air temperature. A recent review of the abilities to retrieve these quantities is summarized in Bourassa et al. (2010). Products based on in situ observations such as those of the National Oceanography Centre, Southampton (NOC; Berry and Kent 2009) utilize observations of bulk (or mean) variables from dedicated buoys, research vessels, and voluntary observing ships to produce space- and time-averaged fields of turbulent surface fluxes. Gaps in data are often filled through the use of sophisticated optimal interpolation algorithms. Pseudo-observational surface flux products that blend reanalysis, satellite, and in situ data such as objectively analyzed air–sea fluxes (OAFlux) for the global oceans product (Yu and Weller 2007) seek to combine these data sources through objective analysis and use of the observational datasets to determine the optimal combination of products.

Turbulent heat flux estimates based on satellite, in situ, and pseudo-observational methodologies are brought to bear in this analysis of the MERRA ocean turbulent fluxes. The paper is organized as follows: Section 2 details the various datasets used in this analysis and describes in some detail the relevant physical parameterizations in MERRA. Section 3 addresses comparisons of local matchups of in situ data and MERRA through examinations of both the fluxes and near-surface bulk variables. The spatial and temporal characteristics of the MERRA turbulent flux climatology are detailed in section 4, with
an emphasis on both means and extremes of the distribution. Section 5 assesses the impact of the MERRA data assimilation system on near-surface variables that impact the turbulent heat fluxes. The effects of spurious changes arising from observing system inhomogeneities are briefly noted. Discussion and conclusions are presented in section 6.

2. Products and data

Understanding the characteristics and behavior of estimated surface fluxes depends crucially on understanding the methodology of how the fluxes are calculated. There are several key choices to be made regarding the parameterization of the latent heat flux (LHF) and sensible heat flux (SHF). These include both the choice of a bulk flux formula and how to estimate the necessary near-surface variables. A detailed comparison of bulk parameterizations can be found in Brunke et al. (2003). Detailed intercomparisons of both fluxes and near-surface variables between observations and multiple reanalysis- and satellite-based products can be found in C. A. Clayson et al. (2011, unpublished manuscript) and Brunke et al. (2011). In the following, we briefly summarize the key assumptions and choices used in products referenced throughout the remainder of this study.

a. MERRA

The NASA Goddard Earth Observing System version 5 (GEOS-5) atmospheric model (Rienecker et al. 2008) is routinely used to analyze NASA Earth Observing System (EOS) satellite data as well as conventional observations and operational satellite data in support of NASA science and field missions. The MERRA analysis, covering 1979 through the present, is produced over the period of observations where satellite observations are most reliable (Rienecker et al. 2011 provides an overview of MERRA) with an objective to improve upon the representation of the global water cycle in a reanalysis. Several previous reanalyses have shown significant deficiencies in their representation of critical components of the hydrologic cycle such as precipitation, ocean surface evaporation, and water balance closure (i.e., precipitation minus evaporation) (for a recent review, see Trenberth et al. 2011). Preliminary estimates reported by Bosilovich (2008) and a more recent evaluation with MERRA itself (Bosilovich et al. 2011) indicate that MERRA does demonstrate improved skill of spatial distribution of precipitation, especially related to the tropical oceanic regions. Like other reanalysis efforts, MERRA ingests much of the conventional and satellite observational data stream and performs a series of extensive quality checks and bias corrections. An extensive review of these data streams and operational procedures can be found in Rienecker et al. (2008). The MERRA incremental analysis update (IAU) methodology (Bloom et al. 1996; Rienecker et al. 2011) adds forcing terms in the heat, moisture, and momentum equations that smoothly drive the assimilated state variables close to the analyzed values, minimizing spin up–spin down in precipitation, and radiative and turbulent flux quantities. The forcing increments due to the assimilation from the IAU are archived for analysis and are utilized later in this investigation. The GEOS-5 atmospheric model is executed at $1/3^\circ$ latitude by $2/3^\circ$ longitude resolution with a total of 72 vertical levels from the surface to 0.01 hPa.

Sea surface temperature and sea ice are prescribed from the Reynolds dataset (Reynolds et al. 2002). Surface winds are assimilated over the ocean using data from Special Sensor Microwave Imager (SSM/I) and scatterometer retrievals. Atmospheric temperature and moisture at the lowest model level are prognostic variables used for computing the vertical gradients in moisture and temperature needed for calculation of the latent and sensible heat fluxes. These lowest model level variables are affected in part by the planetary boundary layer (PBL) scheme. The PBL parameterization relies on the Lock et al. (2000) scheme during unstable conditions but uses components of the Louis et al. (1982) scheme under stable regimes. Neutral transfer coefficients are computed based on standard similarity relationships using a momentum roughness length based on Charnock (1955), a roughness length for heat based on Beljaars (1995), and a roughness length for moisture that is a factor of 1.5 larger than the roughness length for heat. These transfer coefficients are adjusted for stability in both stable and unstable cases based on the stability functions of Louis (1979). Estimates of surface humidity and temperature at a standard measurement height (10 m) are output as diagnostics based on the computed fluxes and transfer coefficients, being related to the surface lowest-model-level gradient through similarity. The surface layer parameterization as implemented in MERRA does not take into account more recent advances (Fairall et al. 1996, 2003; Zeng et al. 1998; Oost et al. 2002), although an improved surface layer scheme is currently under development (A. Molod 2011 personal communication) for the next revision of the GEOS atmospheric model.

b. NOC 2.0

The production of in situ–based flux products generally makes use of voluntary observing ships (VOS) and moored or floating buoy data. An early example is that of Bunker (1976), who used coarsely gridded VOS data on monthly time scales to estimate the near-surface parameters needed for flux calculation. As more data has
become available, these atlases have steadily improved in both resolution and quality. Still, VOS data varies in quality and often adjustments for bias are needed to take into account variability induced by changes in the observing methodology. NOC developed an in situ observation–based flux dataset in the 1990s at 1° by 1° spatial and monthly temporal resolution (now referred to as NOC1.1; Josey et al. 1999). A new version of this dataset has recently been produced using a different interpolation method and covering a longer period, 1970–2009 (Berry and Kent 2009), which is called NOC2 here. The NOC2 product uses only VOS observations and provides improved uncertainty estimates of the surface heat fluxes. This atlas contains near-surface air temperatures, sea surface temperatures, air specific humidities, wind speeds, sensible heat fluxes, and latent heat fluxes, among others. VOS observations of near-surface variables are used in conjunction with bias adjustments and estimates of error characteristics to optimally interpolate daily average fields. The fields are then used with the bulk flux parameterization of Smith (1980, 1988) to calculate daily averaged estimates of the latent and sensible heat fluxes. These estimates and their uncertainties (with error correlations taken into account) are averaged to a monthly resolution. The improved uncertainty estimates can be used in an inverse analysis procedure to constrain the global net heat flux; however, the current NOC2 remains unconstrained. As reported in Berry and Kent (2011), the NOC2 dataset has a global imbalance of 22 W m\(^{-2}\) over the period 1984–2004.

c. **OAFlux 3.0**

In an effort to capitalize on the benefits of both model and satellite-based methodologies, an optimal estimate of the latent and sensible heat fluxes is employed in the recently developed OAFlux version 3.0 product (Yu et al. 2008). OAFlux is produced at a daily and 1° by 1° temporal and spatial resolution, respectively, over the period of 1985 through the present. In OAFlux, the three reanalyses NCEP1 (Kalnay et al. 1996), NCEP2 (Kanamitsu et al. 2002), and the 40-yr ECMWF Re-Analysis (ERA-40; Uppala et al. 2005) are blended with satellite-retrieved estimates of near-surface variables to determine a best-guess estimate using objective analysis. These surface variables are then used with the COARE 3.0 bulk flux algorithm for the calculation of surface latent and sensible heat flux. Optimally combining the input products requires knowledge of the error covariances of the input data. These are assessed through the use of both VOS-based climatologies (for spatial structure information) and direct comparisons to (primarily) moored buoy data. A comprehensive review of the methodology can be found in Yu et al. (2008). As in NOC2, global net heat flux imbalances also exist in the OAFlux product. Berry and Kent (2011) note an approximately 30 W m\(^{-2}\) imbalance over the 1984–2004 period.

d. **GSSTF2b**

The Goddard Satellite-based Surface Turbulent Flux (GSSTF2b; Shie et al. 2009) product is also used in this study. The GSSTF2b product is a follow-on product to the original GSSTF2 product that was developed originally to cover the period 1987–2000 (Chou et al. 2003). The GSSTF2 product makes use primarily of SSM/I-determined near-surface variables. The bulk flux algorithm used in both GSSTF2 and GSSTF2b follows very closely to that of COARE 2.5 (Fairall et al. 1996), with the GSSTF2b flux algorithm adjusted to include improvements under high wind speed conditions. A review of the bulk flux model and determination of the near-surface variables can be found in Chou et al. (2003). Updates to the GSSTF2 for the GSSTF2b product can be found in Shie et al. (2009). The SSM/I version 4 wind speeds of Wentz (1997) were used in GSSTF2; GSSTF2b uses version 6 SSM/I wind speeds, and brightness temperatures are used in conjunction with estimates of specific humidity following Chou et al. (1995). In GSSTF2b, the sea surface temperatures are based on an updated version of the optimally interpolated SST product (Reynolds et al. 2002). The NCEP2 reanalysis supplies estimates of the near-surface air temperature. The product remains at 1° spatial and daily averaged temporal resolution and is currently produced through a simple binning and averaging approach. The accuracies of the GSSTF2b near-surface variable retrievals are affected by the inherent limitations of satellite retrieval algorithms. In particular, very cloudy or rainy conditions make accurate retrievals of the near-surface wind speed more difficult using SSM/I-based observations (Roberts et al. 2010). As noted in Shie et al. (2009), the GSSTF2 product has regional biases, but it is consistent with patterns of atmospheric seasonal variability and provides a realistic representation of the surface heat fluxes.

e. **Observations**

High-quality in situ measurements of the turbulent heat fluxes remain the ultimate standard in terms of validation purposes. The most accurate methodologies for sampling turbulent fluxes require expensive fast-response equipment capable of directly resolving the turbulent eddy perturbations. Examples of these approaches are the eddy-covariance (EC) and inertial-dissipation (ID) methods (Sjöblom and Smedman 2004). Because of their costly nature, these observations are usually made through dedicated field campaigns. A large set of direct, research-quality field observations...
has been obtained and organized through the auspices of the SEAFLUX program. Flux measurements in the compiled dataset generally originate from research cruises, whereas observations of near-surface variables come from both research cruises and research-quality moored buoys. The surface flux measurements are direct measurements of the turbulent fluxes made using either the EC or the ID methods. These data are quality controlled and adjusted to a standard measurement height of 10 m. The observational data have been collected over the period from 1988 through 2007 and there are approximately 450,000 raw observations, though only about 20,000 observations are direct surface flux measurements. A thorough description of SEAFLUX, available datasets, and sampling methodologies can be found in Curry et al. (2004). The SEAFLUX observational archive is available online (http://seaflux.gfdi.fsu.edu/). A notable drawback of the current observational data is a lack of sampling diversity. Figure 1 depicts the spatial and temporal distribution of observation in the SEAFLUX dataset. The majority of field campaigns have been performed over the tropical Pacific and Atlantic basins. Far fewer have been conducted in high-latitude, high wind conditions. Therefore, the results of the validation section should not be interpreted as representative in all environments, particularly in the subpolar ocean basins. Over the 1988–2007 period, the number of observations in any particular year has varied based on the number of research field campaigns held. A local spike occurs in the early 1990s associated with the Tropical Ocean Global Atmospheric (TOGA) COARE (Weller and Anderson 1996). A secondary uptick in observations occurred in the early 2000s associated with field experiments such as the Eastern Pacific Investigation of Climate Processes (EPIC; Cronin et al. 2002).

3. In situ comparisons

In this section we provide a general overview of results from direct comparisons of matched data with MERRA. The variables to be discussed here are the LHF, SHF, SST, wind speed ($U_{10}$), and near-surface vertical gradients of moisture (Qsqa) and temperature (Tsta) between the surface and measurement height of 10 m. These comparisons represent the most direct evaluation possible and facilitate an understanding of likely bias and random error at high temporal resolution. A detailed discussion of in situ data characteristics and all variables and products used in SEAFLUX can be found in the intercomparison results of C. A. Clayson et al. (2011, unpublished manuscript).

a. Matchup procedure

Comparison to in situ measurements requires the creation of a matchup database (MDB) between observations and the nearest, in space and time, product grid point. The MDB is constructed from all available in situ observations (see above) covering the period 1988 through 2007. The MERRA data is available at hourly temporal resolution. Observations from research cruises and buoys are often sampled at a higher temporal rate. It
is expected that point measurements from these observations will inherently sample increased variability with respect to a smoother, gridded analysis product representative of a larger area. To create one-to-one matches, all in situ observations are placed into their nearest space–time box of the MERRA product and averaged. This procedure is consistent with the representation of the MERRA values that are themselves often an average over some temporal period such as for the surface fluxes. The MERRA surface fluxes will differ from the direct measurements of the observations due both to algorithm and bulk variable errors. It is outside the scope of this investigation to attribute errors to both causes; such a decomposition has been examined in Brunke et al. (2011).

b. Results

Using the MDB, two-dimensional joint density estimates (JDE) are found for both the latent and sensible heat fluxes and bulk parameters used in common parameterizations. These estimates are used instead of traditional scatterplots as they also provide information on the distribution of the total number of observations. Figure 2 displays these plots (normalized to unity) for each of the variables along with a “perfect fit” line. Each value represents the total number of matches that fall within small bins around the axis values. Root-mean-square error (RMSE) and mean bias errors are also given based on all matched observations. Binned scatterplots are provided to show how the bias varies as a function of the observed values. Vertical bars on the binned scatterplot provide an estimate of the variability (standard deviation) of MERRA in each interval. Figure 2 shows that the LHF has a small positive bias of approximately 2 W m\(^{-2}\) based on all observations. The bias of MERRA varies as a function of the strength of the LHF, however, as shown by the binned scatterplot (50 W m\(^{-2}\) intervals). For observed values below 50 W m\(^{-2}\), MERRA overestimates the fluxes by roughly 25 W m\(^{-2}\), but MERRA progressively underestimates the latent heat flux for stronger fluxes with biases as large as 200 W m\(^{-2}\) for observed values greater than 250 W m\(^{-2}\). This results in a cancellation of biases giving the appearance of a small overall bias. Over the most densely observed regions (50–100 W m\(^{-2}\)), the MERRA LHF estimates have small biases of about 10 W m\(^{-2}\). The random error (RMSE) is over 50 W m\(^{-2}\) for all observations but is generally less than 40 W m\(^{-2}\) for observed LHF less than 150 W m\(^{-2}\) and increases to greater than 75 W m\(^{-2}\) for observations greater than 250 W m\(^{-2}\). Shown in Fig. 2, the SHF exhibits a strongly varying bias as a function of the observed SHF strength similar to the latent
heat flux. Binned into intervals of 20 W m\(^{-2}\), MERRA overestimates the sensible heat flux for observed SHF less than \(-15\) W m\(^{-2}\) by 10 W m\(^{-2}\) (i.e., roughly 50\%–75\%), has a small near-zero bias between \(-10\) and 10 W m\(^{-2}\), and progressively underestimates the SHF for values greater than 10 W m\(^{-2}\). MERRA underestimates the observed SHF by about 20 W m\(^{-2}\) for values greater than 40 W m\(^{-2}\) and up to 50 W m\(^{-2}\) for observed magnitudes greater than 100 W m\(^{-2}\). Using all observation, the SHF is biased low by about 4 W m\(^{-2}\) and has an RMSE of about 25 W m\(^{-2}\).

Corresponding joint density estimates are shown for QSQA, TSTA, and WSPD in Fig. 2. All three variables show a positive overall bias based on all available observations. As with the turbulent fluxes, however, the biases of the bulk variables vary as functions of the observed distributions. The bulk variables have relatively small, consistent scatter with RMSE of only 1.1 g kg\(^{-1}\), 1.7 m s\(^{-1}\), and 0.88°C for QSQA, WSPD, and TSTA, respectively. The MERRA wind speed estimates appear to be biased in the most consistent manner. MERRA overestimates wind speeds by about 0.6 m s\(^{-1}\) over the region 3–15 m s\(^{-1}\) though it is biased high by nearly 1.3 m s\(^{-1}\) for observed wind speeds less than 3 m s\(^{-1}\) and about 1 m s\(^{-1}\) for wind speeds greater than 15 m s\(^{-1}\). Conversely, the near-surface moisture temperature and gradients appear to show positive biases for low to mid-range values but are underestimated in the regime of higher values. As with the turbulent fluxes, the magnitudes of the biases scale with the magnitude of the observations. MERRA overestimates QSQA by about 1 g kg\(^{-1}\) for observed values less than 3 g kg\(^{-1}\) and by 0.4 g kg\(^{-1}\) in the region 3–7 g kg\(^{-1}\). MERRA underestimates QSQA by 0.5 g kg\(^{-1}\) between 7 and 9 g kg\(^{-1}\) and by nearly 1.5 g kg\(^{-1}\) at values greater than 9 g kg\(^{-1}\). The near-surface vertical temperature gradient is biased high in MERRA by about 0.75°C for observed negative gradients (air temperature warmer than surface) and has near-zero bias for the most dense portion of the observed TSTA distribution between 1°C and 3°C. MERRA underestimates the TSTA gradient by roughly 1.3°C for observed values greater than 3°C. Given the consistency of the positive wind speed bias, these results suggest that changing systematic biases (in sign) of LHF and SHF originate because of errors in the near-surface vertical gradients. In summary, evidence presented in Fig. 2 suggests that the overall low biases in the latent and sensible heat flux arise from the compensation of biases. MERRA estimates fluxes reasonably well over the most densely observed portion of the observed turbulent flux distributions (i.e., 50–100 W m\(^{-2}\) for LHF and \(-10\) to 10 W m\(^{-2}\) for SHF) but systematically underestimates the amplitude of the fluxes during departures from these typical conditions.

4. Flux distribution

The preceding analysis has provided error characteristics of MERRA as compared to research-quality in situ observations. The use of in situ observations, however, is unable to provide a complete description of the large-scale mean and variability of the turbulent fluxes because of their inherent sampling limitations. To provide a complementary assessment of the large-scale spatial and temporal patterns of variability of MERRA, this section utilizes a suite of observationally based gridded turbulent flux estimates to provide context. Though no perfect calibration target exists at these scales, several reference products using in situ observations, satellite observations, and modeling results are available for intercomparison. Here, we use the NOC2 VOS-based product, the GSSTF2b satellite-based reconstruction, and the pseudo-observational OAFlux product to characterize the salient aspects of the surface flux distribution in MERRA. To avoid contamination of the analysis by ice-covered regions, the following results will neglect regions poleward of 60°N–S latitude.

a. Annual climatology

The products used in this study each covers slightly different time periods. To homogenize the comparisons between one another, the daily resolved climatology is created through averaging over the common period 1987–2007. Any noise in the estimate is reduced using a simple 30-day centered running mean filter. All annual and seasonal mean statistics are based on the smoothed climatological estimates. The surface heat fluxes are most readily related to the near-surface meteorological fields through the bulk aerodynamics formulas

\[
LHF = \rho C_e L_v (Q_s - Q_a)(U_{10}) \quad \text{and} \quad (1)
\]

\[
SHF = \rho C_h C_p (T_s - T_a)(U_{10}) \quad \text{.} \quad (2)
\]

where \(\rho\) is the air density; \(C_e\) and \(C_h\) are the non-dimensional exchange coefficients of moisture and heat, respectively; \(L_v\) is the latent heat of vaporization; \(C_p\) is the specific heat capacity of water; \(Q_s\) is surface specific humidity; \(Q_a\) is air specific humidity; \(T_s\) is sea surface temperature; \(T_a\) is air temperature; and \(U_{10}\) is the 10-m wind speed. To provide additional information on the surface heat flux comparisons, the near-surface gradients of moisture and temperature as well as wind speed are also evaluated. The three observationally based
climatological estimates are averaged together to create a mean observational estimate to which MERRA is compared. There is a range of the observational components and all values of MERRA outside the range of any of the observational estimates are denoted appropriately.

Figure 3 depicts differences between MERRA and the observational estimate of the annual-mean latent heat flux, sensible heat flux, moisture gradient, temperature gradient, and near-surface wind speed. Hatched regions are those where MERRA is higher than the highest or lower than the lowest of the observational products included in this study. Examination of climatologies constructed over the period common to all three products (1987–2007) reveals nearly identical patterns (not shown) between MERRA and the observations. The products capture similar patterns such as higher latent heat release over the western boundary currents, increased fluxes in the trade wind regions, and local minima over the tropical Pacific and Atlantic cold tongues. The primary differences...
are in magnitude. Latent heat fluxes over the Kuroshio and Gulf Stream are about 40 W m\(^{-2}\) lower annually than the observationally based products, whereas sensible heat fluxes are about 15 W m\(^{-2}\) lower. The LHF and SHF from MERRA are within 10 W m\(^{-2}\) of the observational estimate equatorward of 25° latitude. In the extratropics, the latent heat flux is about 10–20 W m\(^{-2}\) lower than the observation estimate but the sensible heat flux is about 5–10 W m\(^{-2}\) larger. The MERRA near-surface moisture gradient is generally larger than the observational products in the tropical and extratropical basins. The MERRA surface specific humidity is controlled by the observationally prescribed sea surface temperature dataset. The higher vertical moisture gradient in comparison to the observational estimates therefore is primarily related to a drier (i.e., less moist) surface layer than the observational products. The MERRA QSOA field varies from about a 0.5 g kg\(^{-1}\) higher value in the middle latitudes to values greater than 1 g kg\(^{-1}\) in the deep tropics. The annual-mean wind speed from MERRA is higher (and outside the range) than the observational products nearly everywhere globally. The MERRA wind speeds are stronger than the observational product by about 1 m s\(^{-1}\) over the lower latitudes but have peak values 3 m s\(^{-1}\) higher in the storm-track regions, particularly over the Kuroshio. During the winter season these difference patterns occur. The covariance of wind and specific heat capacity, the total latent and sensible heat flux is determined from contributions related to the products of annual-mean and anomalous wind speed and vertical gradients. Figures 4 and 5 provide climatological estimates of these terms in the winter [December–January (DJF)] months for the latent and sensible heat fluxes, respectively. The right panels of Figs. 4 and 5 provide the observational estimate, whereas the left panels provide the difference between MERRA and the observational products. From Fig. 4, the largest component of the annual-mean flux with magnitudes generally greater than 100 W m\(^{-2}\) is from the product of the annual-mean components. Many of the long-term mean patterns such as strong western boundary currents, trade wind maxima, and weak cold tongue are carried by this component. Variability associated with the anomalous moisture gradient (\(U\Delta q\)) and wind speed (\(u'\Delta Q\)) is driven by the seasonal evolution of these fields. This is easily seen from the strong hemispheric gradient in these fields during the winter months (Fig. 4) and their seasonal reversal in summer (not shown). Typical amplitudes associated with these seasonally evolving components are 30 W m\(^{-2}\). The bottom panel of Fig. 4 shows the covariance of the anomalous moisture gradient with the anomalous wind speed. Note the maximal values during the winter season are peaked around 20 W m\(^{-2}\) over the western boundary currents, particularly over the Kuroshio. During the winter months, the increase in wind speeds and vertical moisture gradients are associated with midlatitude synoptic systems that advect cold, dry continental air over the warmer ocean waters.

Shown in Fig. 4, the annual-mean component (\(U\Delta Q\)) of MERRA is much higher than the corresponding contribution in the observational products. This might be expected from the discussion of higher QSOA and WSPD values shown in Fig. 3. The contribution from the wintertime moisture anomaly component (\(U\Delta q\)) is about 15–20 W m\(^{-2}\) lower than the observational estimates over the Northern Hemisphere and is about 15 W m\(^{-2}\) larger over the Southern Hemisphere. In both hemispheres, this pattern acts to decrease the amplitude of the seasonal variability related to the near-surface moisture in MERRA with respect to the observational products. Conversely, the anomalous wind speed component (\(u'\Delta Q\)) pattern act to amplify the seasonal variability of MERRA compared to observations. This includes an increase in the wind speed–driven latent heat flux component of 15 W m\(^{-2}\) over the Northern Hemisphere. During the summer months (not shown), a reversal of these difference patterns occurs. The covariance of wind

\[
\text{LHF} = \rho C_v L_a (\bar{\Delta Q} + \Delta q')(\bar{U} + u') \quad \text{and} \quad (3)
\]

\[
\text{SHF} = \rho C_h C_p (\bar{\Delta T} + \Delta T')(\bar{U} + u'), \quad (4)
\]

where overbars represent the annual-mean component and the primes denote anomalies from the mean.
speed and humidity gradient anomalies ($u'q'$) is weaker than in the observational products almost everywhere globally. The largest differences occur over the middle latitudes with MERRA values lower than observations by nearly 25 W m$^{-2}$. The covariability in the summer months (not shown) is also weaker in MERRA than observations.

The corresponding analysis of contributions to the sensible heat flux is provided in Fig. 5. The annual-mean contribution ($U\Delta T$), as for the latent heat flux, carries the largest fraction of the total sensible heat flux with values over the western boundary currents exceeding 150 W m$^{-2}$. The seasonally varying temperature gradient
component \( (U \Delta t') \) provides a significant contribution over the Southern Ocean with decreases in the SHF of nearly 30 W m\(^{-2}\) during the winter season. As with the latent heat flux, the anomalous wind speed and vertical temperature gradient driven contributions \( (u' \Delta T) \) and \( (U \Delta t') \) are characterized by a reversal in sign between summer and winter seasons (not shown). The winter hemisphere is characterized by anomalously high (with respect to annual mean) wind speed and higher temperature gradients, whereas the summer hemisphere is characterized by decreased wind speeds and decreased near-surface temperature gradients. These relationships result in a positive covariance between the anomalous components as seen in the bottom panel of Fig. 5. The
analogous MERRA contributions are very similar in pattern to the observed products but differ in magnitude. The annual component of MERRA is about 30 W m\(^{-2}\) higher than the observational products everywhere outside the tropics. MERRA has a weaker contribution by about 10 W m\(^{-2}\) over the eastern equatorial Pacific. This region corresponds to an area (see Fig. 3) of weaker vertical temperature gradients (i.e., surface air temperature is closer to the sea surface temperature). The wintertime contribution from the anomalous vertical temperature gradient (\(U\Delta T\)) in MERRA is higher over the western boundary currents by approximately 15 W m\(^{-2}\). This component would tend to amplify the seasonal variability in these regions as compared to the observations. The same conclusions can be drawn for the anomalous wind speed forcing (\(u'\Delta T\)), which has a slightly higher (\(-10\) W m\(^{-2}\)) contribution in the winter hemisphere and smaller (10 W m\(^{-2}\)) contribution in the summer hemisphere. As with the latent heat flux, MERRA has weaker covariability between the anomalous wind speeds and anomalous vertical temperature gradients during both the winter and summer months. The reversal of the seasonal components results in a near cancellation of differences such that the seasonally invariant weaker covariances (\(u'\Delta q', u'\Delta T'\)) act to offset the annual-mean biases shown in Fig. 3.

c. Extremes

Climatological-mean values of different datasets provide important information; however, different datasets with very different distributions can still retain similar mean characteristics. The surface heat flux distribution can broadly be described as being composed of at least two very general types of events or situations: fair weather, which is the more frequent case, and stormy weather, which is less frequent. Means of the distribution mix both types of events together. The importance of infrequent (i.e., episodic), high-magnitude events to the turbulent heat fluxes and oceanic processes has been noted as related to midlatitude storms (Moore and Renfrew 2002), cold-air outbreaks over western boundary currents (Garnier et al. 2000), and hurricanes (Shay et al. 2000), among others. At the low extremes, typically driven by calm surface winds, high-amplitude diurnal warming events of the ocean surface temperature can be generated (Clayson and Weitlich 2007), which may play role in coupled air–sea interaction (Qin and Kawamura 2002). Thus, it is important to understand not only the mean but the representation of extremes of the surface heat fluxes. To investigate the extent to which the spread of the turbulent fluxes differ between the datasets, each grid point is evaluated separately. The histogram at each grid point over the entire time series is constructed, and the 5th and 95th percentile values are calculated. Zonal averages of 5th and 95th percentile values and zonal means are shown in Fig. 6. Similar calculations have been performed for SHF, QSQA, WSPD, and TSTA; these results are also shown in Fig. 6. The observational estimate is shown via thin lines and includes an estimate of the range (minimum of products to maximum of products) using thin black lines. The estimates from MERRA are shown using thick lines.

The range of observational estimates (width of horizontal lines) and hence most uncertainty is largest for the 95th percentile values of all parameters. The latent heat flux estimate from MERRA is within the observational range at all latitudes except between 25\(^\circ\) and 35\(^\circ\) of each hemisphere. There, the 95th percentile values from MERRA are nearly 20 W m\(^{-2}\) lower than the observation estimates. This area is also associated with 5 W m\(^{-2}\) lower zonal-mean estimates. Recalling from Fig. 3, this latitude belt encompasses the much weaker (with respect to observations) latent heat flux over the western boundary currents. The values of LHF at the 5th percentile level for MERRA are similar across all latitudes and within the observational range. Only in the tropical regions from roughly 10\(^\circ\)S to 10\(^\circ\)N are there differences in the range of 5 W m\(^{-2}\). In these latitudes, the near-surface vertical moisture gradient from MERRA is nearly 1 g kg\(^{-1}\) higher than the observational products. That is, MERRA is unable to replicate very weakly stratified surface layer moisture gradients in this region as compared to the observational products. A similar problem is seen in the zonal-mean QSQA from MERRA. Elsewhere, the vertical moisture gradient estimates from MERRA appear to be within the observational estimates for the extremes and zonal mean. The amplitudes of sensible heat flux in MERRA appear to be well resolved in the zonal-mean sense for both average and extreme conditions. Figure 3 shows there were several regional biases for the sensible heat flux. The existence of near-zero differences between MERRA and the observation therefore implies a compensation of differences in the zonal-mean calculations. The near-surface temperature gradient closely follows the observational estimates. The largest differences occur in the Southern Hemisphere between 2\(^\circ\) and 40\(^\circ\)S, where MERRA is higher than the observational estimates by about 0.5\(^\circ\)C for both average and extreme conditions. Wind speeds in MERRA show some of the largest deviations from the observational products. For strong, rare events (95th percentile), MERRA wind speeds are higher than and outside the range of observations at all latitudes. The strength of this difference increases with latitude having only 0.5 m s\(^{-1}\) differences in the tropics to 3–5 m s\(^{-1}\) over the middle to high latitudes. A similar pattern is seen
FIG. 6. Zonal-mean average (black), zonal-mean 95th percentile (red), and zonal-mean 5th percentile (blue) values are shown for the LHF, SHF, QSQA, TSTA, and WSPD. Thin and thick solid lines depict the observational and MERRA estimates, respectively. The thin black line superimposed on the observational estimate gives the range (minimum to maximum) of the observational products.
in the zonal mean though differences are somewhat smaller (only a 2–3 m s\(^{-1}\) over the middle latitudes). It is interesting to note MERRA latent heat fluxes are generally smaller than the observational estimate over the 25°–35° band where extreme wind speeds are too large and moisture gradients are similar to observations. This implies that the extremes are uncorrelated in space and/or time, a point emphasized by the weaker covariability of the anomalous components discussed above.

5. Analysis increments

A novel aspect of the MERRA analysis product is the archival of the IAU forcing tendencies. These analysis increments provide the additional tendencies that smoothly nudge the model integration toward the analyzed state over an assimilation window. They provide a measure of the impact of the assimilation of observations on the model reanalysis. Studies such as Robertson et al. (2011) have examined the long-term behavior of these increments and the role of the changing observing system with respect to how the increments affect the global water and energy cycles. The assimilation procedure affects the near-surface moisture, temperature, and momentum fields and hence can impact the turbulent fluxes.

We have evaluated the analysis increments of the two lowest model levels at 1000 and 975 hPa to examine their climatological behavior with respect to the near-surface meteorological variables. The long-term mean increments are given in units of the forcing tendency of each variable (e.g., g kg\(^{-1}\) day\(^{-1}\) for specific humidity). To examine the impact of changes in the observing system, particularly the impact of the Advanced Microwave Sounding Unit (AMSU-A), we have examined the climatological difference of increments before and after 1998, the year AMSU-A was introduced. Figure 7 depicts the annual-mean (left panels) analysis increments for humidity, air temperature, and wind speeds over both the Southern Ocean and Northern Hemisphere. Numerous linear features associated with prominent shipping routes are also seen to be affecting the reanalysis. The analysis increment is on average pumping additional moisture into the analysis at the rate of 0.5–1 g kg\(^{-1}\) day\(^{-1}\) over large stretches of the northern Pacific, northern and tropical Atlantic, and tropical Indian Ocean basins. These values are roughly 5%–10% of the annual-mean surface moisture content. Given annual surface moisture gradients in the range of 4–7 g kg\(^{-1}\), the surface moisture increments are helping maintain roughly 15%–25% of the near-surface moisture gradient per day. Recalling the higher near-surface vertical gradient compared to the observational products (Fig. 3) that implied too dry of a near-surface layer in an annual-mean sense, the analysis increment is generally acting to bring MERRA closer to the observational estimates through moistening. The near-surface air temperature adjustments from the assimilation are strongly correlated with the moisture adjustments. That is, the assimilation is tending to both moisten and warm the near-surface layers. The most notable departure from this general trend is the region stretching from the coast of Peru to the central equatorial Pacific. This is a region associated with a strong transition zone in cloudiness from stratus to stratocumulus to fair-weather cumulus. Along the Peruvian coast, QSQA is smaller (Fig. 3) than the observational estimates, indicating (for similar sea surface temperatures) excessive surface moisture in MERRA. Also, TSTA is larger than the observational estimates indicating that the surface air temperature is cooler in MERRA. Along this coastal region, the analysis acts to cool and moisten the near-surface layers, acting to drive the reanalysis further from the observational products. As one progresses toward the central Pacific, the analysis acts to warm and dry the central equatorial region, also acting to amplify the differences between MERRA and the observational estimates. The analysis increment for wind speeds acts to decrease wind speeds over the Southern Ocean, the central to western equatorial Pacific, and the northern Pacific. There are a few areas where the assimilation of observation generally acts to increase the near-surface wind speeds. This includes a stretch along the tropical Atlantic and northeastern tropical Pacific as well as over the Gulf Stream. The weakening of the near-surface winds generally acts to bring the reanalysis closer to the observational estimates (Fig. 3).

The changes in the observing system associated with the introduction of AMSU-A has been shown to impact several hydrological quantities in reanalyses (Robertson et al. 2011; Wang et al. 2010). The impact of this change, shown in Fig. 7, is felt near the surface as well and therefore will also affect the turbulent heat fluxes. Additional moisture is added to the near-surface layers over much of the Southern Ocean in the post-1998 era. It is perhaps expected that additional satellite measurements may have their largest impacts over data-sparse regions such as the Southern Ocean. Note that much of the traditionally well-sampled North Pacific and North Atlantic show relatively little change before and after 1998 in terms of the moisture increment. Conversely, there is a significant impact on the analysis increments for temperature over both the Southern Ocean and
traditionally well-sampled regions. The post-1998 analysis increment generally reduces warming in the near-surface layers. Compared to the pre-1998 error, wind speed reduction via the increments also decreases in amplitude, especially over much of the North Pacific intertropical convergence zone. However, over the eastern Pacific cold tongue the increments reinforce wind speed decreases. Note also that the dipole structure in moistening–drying in the southeastern Pacific is forced primarily after 1998. Examining the role of these increments in driving the near-surface meteorology of the reanalysis provides a first step at determining how the assimilation of observations impacts the surface fluxes. A useful approach to further investigate the role of specific observational system impacts to increments would be to examine the observed minus forecast (OMF) and observed minus analysis (OMA) statistics for individual observing systems.

6. Summary

In this paper, we have characterized the reanalysis-based MERRA turbulent heat fluxes and have assessed their accuracy, annual and seasonal variability, representation of extremes, and the impact of the data assimilation. Comparisons to direct observations have revealed

Fig. 7. (left) Annual-mean climatological (1988–2007) estimate of the boundary layer (975- and 1000-hPa values) moisture (Q), temperature (T), and WSPD analysis increment. (right) The change in the mean analysis increment after the inclusion of AMSU data in 1998. The analysis increment is applied at a constant rate over a 6-h assimilation window. Values are provided here as the increment applied over a full daily cycle.
that the mean values of the turbulent fluxes are generally modeled accurately. Over the most densely observed intervals of the latent heat flux (50–100 W m$^{-2}$), biases were less than 10 W m$^{-2}$. Similarly, over the $-10$ to 10 W m$^{-2}$ interval, the most densely observed sensible heat flux interval, biases were near zero. The mean accuracy over these regions contrasts with errors at the extremes of the distribution, however.

The latent heat flux is overestimated by MERRA by 25 W m$^{-2}$ for observed values less than 50 W m$^{-2}$ but is progressively underestimated by MERRA by nearly 40–75 W m$^{-2}$ over the range of observed values from greater than 150 W m$^{-2}$ to greater than 250 W m$^{-2}$. Likewise, the sensible heat flux is overestimated by MERRA by nearly 50% for values less than $-10$ W m$^{-2}$ and progressively underestimates the sensible heat flux by 20–50 W m$^{-2}$ for observed magnitudes greater than 40 and 100 W m$^{-2}$, respectively. Examining the near-surface bulk variables used in flux parameterization reveals that this progressive bias (overestimation to underestimation) is controlled by biases in the near-surface vertical gradients of moisture and temperature. Near-surface wind speeds are also biased in MERRA; however, they are consistently high, lacking a similar positive to negative change in bias. It must be emphasized that a majority of these direct observations are from the tropical regions. More comparisons in the extratropics and subpolar basins need to be performed to examine the consistency of these biases in those regions.

The annual-mean climatology of turbulent fluxes in MERRA has also been reviewed. It has been compared to an observational estimate constructed from three observationally derived gridded flux products. These included the VOS-based NOC2, the satellite-based GSSTF2b, and the model- and satellite-based OAFlux. The dominant spatial patterns of latent and sensible heat fluxes are found to correspond quite well with the observational estimates, and the sensible heat fluxes are within the observational range. Analysis of the bulk variables reveals stronger surface wind speeds in MERRA (at the 95th percentile) drive latent heat fluxes of similar amplitude to observational estimates over most latitude with the exception being in the 25°–35°N–S latitude belts consistent with areas frequented by strong synoptic weather systems. In these regions, MERRA tends to underestimate the 95th percentile latent heat fluxes by 20 W m$^{-2}$. The total sensible heat fluxes are within the observational range over all latitudes in the zonal-mean sense, although this is likely the result of compensating regional differences. An analysis of the bulk variables revealed stronger surface wind speeds in MERRA (at the 95th percentile and zonal mean) at nearly all latitudes. Because the near-surface vertical moisture and temperature gradients are within the observational range, this hints again at a different structure to the covariability of the bulk parameters than the observational products.

MERRA is unique in that the analysis increments are also available for study so that the role of analysis corrections compared to physical processes can be analyzed. It is found that the increments tend to moisten the near-surface layers by adding roughly 5%–10% of the total near-surface moisture per day to many regions. The mean temperature and moisture analysis increments are strongest over the well-sampled Northern Hemisphere regions. The surface layer temperature increments strongly
covary with the moisture increments over most of the world oceans in that they tend to warm and moisten or cool and dry. Regional departures from this pattern occur in areas of persistent cloud-topped boundary layers; increments there tend to either warm and dry or cool and moisten. The assimilation of observations usually tends to decrease the surface wind speeds. These corrections, when referenced to the annual-mean climatologies, mostly act to bring MERRA into closer agreement with the observationally based products. Evaluation of changes in the increment before and after 1998 indicated that the inclusion of new satellite sensors, such as AMSU-A, increased the near-surface moisture increment in the Southern Ocean and tended to reduce the required surface air temperature warming and wind speed reduction.

Based on the comparisons presented in this study, it appears that MERRA produces estimates of the turbulent fluxes that agree very well in terms of major patterns with other observationally based estimates. However, MERRA is distinct in terms of amplitude with particularly weak latent and sensible heat fluxes of the western boundary currents. MERRA also has slightly weaker seasonal variability of the latent heat fluxes and may underrepresent the amplitude of extreme events. Several results imply a weaker relationship between the near-surface vertical gradient of moisture and temperature with the near-surface wind speeds than found in observationally based products. Detailed process studies will be helpful in diagnosing what dynamical or physical processes may lead to these particular biases. The availability of the analysis increments of moisture, temperature, and wind is at present unique to MERRA and should assist in gauging uncertainty in the potentially wide variety of applications of MERRA ocean fluxes. Together, these results suggest that MERRA is likely to be a key resource for a number of research applications, though, as with all turbulent flux estimates, the systematic issues are taken into account.

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