Observation Impact and Information Retention in the Lower Troposphere of the GMAO GEOS Data Assimilation System Yanqiu Zhu, Ricardo Todling, and Nathan Arnold Global Modeling and Assimilation Office, NASA Goddard Space Flight Center

5 Corresponding author: Yanqiu Zhu, Yanqiu.Zhu@nasa.gov

ABSTRACT: In this study, we have assessed the effectiveness of the use of existing observing 6 systems in the lower troposphere in the GEOS hybrid-4DEnVar data assimilation system through 7 a set of observing system experiments. The results show that microwave radiances have a large 8 impact in the Southern Hemisphere and Tropical ocean, but the large influence is mostly observed 9 above 925 hPa and dissipates relatively quickly with longer forecast lead times. Conventional data 10 information holds better in the forecast ranging from the surface to 100 hPa, depending on the field 11 evaluated, in the Northern Hemisphere and lowest model levels in the Tropics. Infrared radiances 12 collectively have much less impact in the lower troposphere. Removing surface observations has 13 small but persistent impact on specific humidity in the upper atmosphere, but small or negligible 14 impact on planetary boundary layer (PBL) height and temperature. The model responses to the 15 incremental analysis update (IAU) forcing are also analyzed. In the IAU assimilation window, the 16 physics responds strongly to the IAU forcing in the lower troposphere, and the changes of physics 17 tendency in the lower troposphere and hydrodynamics tendency in the mid- and upper troposphere 18 are viewed as beneficial to the reduction of state error covariance. In the subsequent forecast, 19 the model tendencies continue to deviate further from the original free forecast with forecast lead 20 times around 300-400 hPa, but physics tendency has showed signs of returning to its original free 21 forecast mechanisms at 1-day forecast in the lower troposphere. 22

23 1. Introduction

The planetary boundary layer (PBL) is an important interface between the Earth's surface and 24 the atmosphere, core to the understanding of flux balances across the Earth system components. 25 Its importance is well-established for its applications in weather, climate, and air dispersion, and 26 as such the PBL has been listed as an 'Incubation'-class targeted observable in the 2018 NASEM 27 Earth Science Decadal Survey (National Academies of Sciences and Medicine 2018). Due to the 28 high degree of spatial and temporal heterogeneity of the near surface processes, including diurnal 29 variations and complex interactions between the land/ocean surface and atmosphere, the PBL has 30 been challenging to accurately simulate and observe. 31

Given the capability of advanced data assimilation systems combining model physics with data 32 from multiple observing systems coherently to provide optimal initial conditions for models, an 33 increasingly large number of observations have been assimilated in the Goddard Earth Observing 34 System (GEOS) global hybrid 4D Ensemble-Variational (4DEnVar) data assimilation system at the 35 Global Modeling and Assimilation Office (GMAO). The GEOS data assimilation system is aimed 36 to constrain the PBL atmospheric thermodynamic structure and to reduce the uncertainties of land 37 surface model and PBL parameterization schemes, but in this study we will focus on the lower 38 troposphere for simplicity and set the stage for follow-on PBL work. While each individual available 39 observing system offers unique advantages in measuring the earth, however, there is no perfect 40 observing system for the lower troposphere. Conventional data such as radiosonde data provide 41 reliable temperature, specific humidity and wind profiles, but they are mainly concentrated over land 42 and lack adequate temporal resolution to capture diurnal variations. Global Navigation Satellite 43 System (GNSS) radio occultation (RO) data has high-vertical but coarse along-ray resolution. 44 Furthermore, they are currently not used or assigned very large observation errors in the low 45 troposphere, where super-refraction is common and biases are large. Satellite radiance data have 46 good global coverage, but introduce other challenges. Microwave observations can penetrate 47 through clouds but with broad weighting function and coarse resolution; hyperspectral infrared 48 observations offer high spectral resolution but are unable to provide information beneath clouds. 49 The various limitations in the existing observations, or in our ability to use them, have made it 50 essential to use these observations coherently in the GEOS global data assimilation system. So far, 51

3

no known study has been performed to comprehensively assess the impact of the various observing
 systems on the analysis and forecasts of the lower troposphere.

Several approaches can be used to assess observation impact in data assimilation systems, such 54 as forecast-based sensitivity observation impact (FSOI, Langland and Baker (2004), Gelaro et al. 55 (2010)) and observation-based observation-minus-forecast residuals (Todling (2013). Another 56 commonly used way of studying the impact of different observations in data assimilation systems 57 is to employ the approach of observing system experiments (OSEs). Many previous OSE studies 58 have focused on free atmosphere above the PBL, including the stratosphere. For example, Kelly 59 and Thépaut (2007) and Lord et al. (2016). Recently, Duncan et al. (2021) investigated the impact 60 of microwave sounders on the analysis and model forecast in the ECMWF system; Lawrence et al. 61 (2019) investigated the impact of observations in the polar regions. The present study investigates 62 the impact of observations in the low troposphere using the GEOS atmospheric data assimilation 63 system (ADAS). The goal is to try to identify specific weaknesses of data usages associated with 64 analyzing and predicting thermodynamic structure of the lower troposphere. Additionally, results 65 and discussion are presented to illustrate the model responses to analysis increments. It is well 66 known that rapidly changing physical, rather than hydrodynamical, processes are hard to constrain 67 with data assimilation; basically the model physics tends to forget rather quickly changes induced 68 by the assimilation of observations and falls back into its own mechanisms. The responses of 69 model physics and hydrodynamics tendencies are worth closer examination. 70

This article is organized as the following: section 2 gives an overview of the GEOS global hybrid–4DEnVar data assimilation system; a brief summary of the observations used in GEOS ADAS is given in section 3 by looking at a summary of its FSOI tool. Data denial experiments results are presented in section 4, model responses to analysis increments and evolutions are discussed in section 5, and conclusions are provided in section 6.

76 2. Brief overview of the GEOS hybrid–4DEnVar ADAS

The GEOS atmospheric data assimilation system is a hybrid–4DEnVar system that produces estimates of global atmospheric states by analyzing observations within a 6-hour time window. The deterministic hybrid–4DEnVar uses the Gridpoint Statistical Interpolation (GSI) of Kleist et al. (2009) with the preconditioning strategy of El Akkraoui et al. (2013). Its cost function can be 81 written as

$$J(\delta \mathbf{x}_{k}, \mathbf{a}) = \frac{1}{2} \beta_{c} \delta \mathbf{x}_{c}^{T} \mathbf{B}_{c}^{-1} \delta \mathbf{x}_{c} + \frac{1}{2} \beta_{e} \delta \mathbf{a}^{T} \mathbf{L}^{-1} \delta \mathbf{a}$$

+
$$\sum_{k=1}^{k=K} (\mathbf{H}_{k} \delta \mathbf{x}_{k} - \mathbf{d}_{k})^{T} \mathbf{R}^{-1} (\mathbf{H}_{k} \delta \mathbf{x}_{k} - \mathbf{d}_{k})$$

+
$$J_{d}, \qquad (1)$$

where $\delta \mathbf{x}$ is the total analysis increment; **d** is the observation-minus-background departure vec-82 tor at time t_k ; **H** is the Jacobian of the nonlinear observation operator; **a** is the extension to the 83 control vector account for the ensemble contribution; \mathbf{B}_c and \mathbf{R} are the prescribed climatological 84 background and observation error covariances; L is a localization matrix; β_c and β_e represent 85 weights given to the climatological and ensemble background terms. The last term, J_d , represents 86 additional constraints, for example, a dry mass conservation term (see Takacs et al. 2016). Mini-87 mization of the cost function leads to a four dimensional increment, which is given as the sum of 88 the contribution from the climatological term $\delta \mathbf{x}_c$ and a term composed of linear combination of 89 ensemble perturbations $\delta \mathbf{x}^m$ and optimal coefficients \mathbf{a}^m , that is, 90

$$\delta \mathbf{x}_k = \delta \mathbf{x}_c + \sum_{m=1}^M \mathbf{a}^m \bullet \delta \mathbf{x}_k^m.$$
⁽²⁾

Here the symbol • stands for the Hadamard-Schur (element-wise) product of two vectors, and the 91 ensemble of forecast perturbations $\delta \mathbf{x}_k^m$ are derived from running the ensemble square-root filter 92 (EnSRF) of Whitaker et al. (2008). In the current GEOS ADAS, the coefficients β_c and β_e change 93 with the vertical analysis levels, equally weighting the two terms up to about 5 hPa, and smoothly 94 transitioning to a purely climatological error term above that (see Todling and El Akkraoui 2018). 95 The assimilation of observations in GEOS ADAS is performed through a 4D incremental analysis 96 update (IAU). Instead of using the 4D incremental solution provided by the minimization of (1) 97 to correct model initial conditions and subsequent model states at given frequency (hourly), the 98 incremental solutions are used to form tendency terms that are applied at each model time step 99 during a so-called corrector interval that lines up with the 6-hour assimilation window. In addition, 100 the present formulation of IAU is a revision of the Bloom et al. (1996) version, following Takacs 101 et al. (2018), that guarantees IAU stability by modulating the tendencies with a digital filter. 102

Background fields for the next assimilation cycle are generated by a so-called predictor step that integrates the GEOS atmospheric model for an extra 6–hour period past the IAU corrector with the analysis tendency terms set to zero.

The GEOS Atmospheric General Circulation Model (AGCM) relies on a non-hydrostatic version 106 of the cubed-sphere finite volume hydrodynamics (see Putman and Lin 2007). Its current physical 107 processes include the short- and long-wave components of the Rapid Radiative Transfer Model for 108 GCMs (RRTMG; Clough et al. 2005; Iacono et al. 2008); the deep convection parameterization 109 of Freitas et al. (2018); a catchment land-surface model consistent with the level-4 GMAO SMAP 110 products (Reichle et al. 2018); and gravity wave drag follows McFarlane (1987) and Garcia and 111 Boville (1994). The single-moment cloud physics are based on Bacmeister et al. (2006). Of greatest 112 relevance to the present work are the parameterizations of the boundary layer. More specifically, 113 these consist of a non-local K-profile scheme driven by surface and cloud-top buoyancy fluxes 114 (Lock et al. 2000), and a local scheme for stable conditions based on the Richardson number (Louis 115 and Geleyn 1982). The Lock scheme releases parcels upward from the surface and downward 116 from stratocumulus cloud top to determine the depth of an analytic profile of diffusivity. Above 117 the well-mixed layer defined by the Lock surface-driven diffusivity, shallow cumulus convection is 118 represented by the Park and Bretherton (2009) buoyancy-sorting mass flux scheme. 119

A diagnostic component of GEOS that is of relevance to the motivational part of the present work 120 is its forecast-based sensitivity to observation impact (FSOI) tool. The GEOS FSOI implements 121 a combination of the approaches of Langland and Baker (2004) and Trémolet (2007) that allows 122 assessing the contribution of individual observations to reducing errors in 24-hour forecasts. For 123 that, it employs a linearized moist global energy norm that serves to transform the impact of 124 different quantities into units of energy (J/kg) (e.g., Errico et al. 2004). Use of a *moist* energy 125 component in the norm requires proper representation of linearized moist processes in the model 126 adjoint needed for the produce and the generation of 24-hour forecast sensitivities. Details of the 127 latest version of such processes is found in Holdaway et al. (2015). 128

The near-real-time GEOS ADAS is a 12.5 km system that relies on a 50 km ensemble. This work employs a lower horizontal resolution version of GEOS, that runs the deterministic cycle at 25 km, and the ensemble cycle at 100 km. GEOS uses 72 vertical levels in all its components. Several factors can alter observation impact results, even the rankings of relative importance of

observations. A few examples of such factors include change in the observing system, changes 133 in the data assimilation algorithm, changes in the model, and changes in the weights given to 134 the observations and background fields; horizontal and vertical resolution might also affect the 135 assimilation of observations. The reduced (yet still reasonably high) horizontal resolution used in 136 this study has been carefully chosen and frequently employed to evaluate the operational GEOS 137 system and system upgrades. The impact of such horizontal resolution has been found to be 138 secondary except for extreme weather conditions, and forecast skills and biases approximate those 139 of the operational system. Even in this somewhat reduced resolution configuration the high 140 computational resources requirements and the slow turnaround of experiments, led to the adoption 141 of a conservative approach to conduct the data denial OSEs of this study. That is, the data denial 142 experiments were set up to use the same ensemble backgrounds generated in the control experiment; 143 this latter assimilates the complete set of observations and is set to exercise the entire machinery 144 of the hybrid data assimilation system. The approach of using a given set of ensemble members 145 is referred to as ensemble replay mode. A recent study by Duncan et al. (2021) finds that using a 146 given (fixed) ensemble in various OSEs amounts to about 10% of the total change due to changes in 147 the observing systems introduced in the various experiments, but still reliably represent the impact 148 of such changes. 149

3. GEOS observations and FSOI

The version of GEOS ADAS used in this work is an *upgrade* to the then-current operational 151 system when it was used to process the mid-November-December 2019 period covered here. The 152 upgrade involves only changes to the analysis component, and more specifically to the underlying 153 observing system, by adding: all-sky Advanced Microwave Scanning Radiometer 2 (AMSR-154 2), COSMIC-2 Global Positioning System Radio Occultation (GNSSRO), and the full spectral 155 resolution (FSR) version of the Cross-track Infrared Sounder (CrIS) from both Suomi NPP and 156 NOAA-20 (see Todling et al. (2022)). In the average, each 6-hour cycle assimilates roughly 4.5 157 million observations; the experiments here neglect a two-week spin-up in November 2019. 158

As a motivational introduction to the investigation of how the observing system affects the lower troposphere behavior in GEOS, we start by looking at diagnostics produced by exercising two different configurations of FSOI in the control experiment, which uses the complete set of



FIG. 1. Comparison of FSOI for 24-hour forecasts from all 0000 UTC analyses of December 2019 when two projections (LPO) of the norm are used in the calculations, namely, using the standard set of vertical levels, and using only near surface levels (at and below 850 hPa). The panels show: (a) fractional averaged impacts (%) in each case; and (b) the averaged impact differences obtained after subtracting the standard LPO from the near-surface LPO results (J/kg), in descending order. Error bars show 95% confidence in fractions and differences, respectively.

observations as laid out in Table 1. As mentioned in section 2, FSOI relies on a linearized total 162 moist energy norm. The operator, E, corresponding to this norm is enveloped by a so-called 163 (diagonal) local projection operator (LPO) S, as in $S^{T}ES$, containing zeroes and ones along its 164 diagonal and enabling, for example, restricting the norm to particular variables, regions, or levels. 165 The standard LPO configuration of FSOI in GEOS avoids forecast errors within the sponge layer 166 by excluding the top six levels of the model. For the purposes of the present work, an alternative 167 LPO considers only forecast errors from the lower troposphere, which is set as the lowest eleven 168 model levels (roughly at and below 850 hPa). 169

Evaluation of FSOI using the two LPOs described above for 24-hour forecasts for all 0000 UTC analyses in the month of December 2019 appears in Fig. 1. Panel (a) compares fractional FSOI (%) using the standard LPO (blue bars) with results when the near surface LPO (red bars) is used. Satellite winds, radiosonde observations, and MW radiances from Advanced Microwave Sounding Unit-A (AMSU-A) and Advanced Technology Microwave Sounder (ATMS) are among the top contributors in reducing forecast errors in both LPO configurations. Changing from the standard

Name	Removed Observation	DA strategy
XCTL	None	Deterministic hybrid, full ensemble
XNOIR	Infrared radiances	Deterministic hybrid, ensemble-replay
XNOMW	Microwave radiances	Deterministic hybrid, ensemble-replay
XNOSATW	Satellite winds	Deterministic hybrid, ensemble-replay
XNOCONV	Conventional	Deterministic hybrid, ensemble-replay
XNOSURF	Surface	Deterministic hybrid, ensemble-replay

TABLE 1. Control and OSEs Definitions

LPO to a near-surface LPO configuration leads to a slight reduction in the fractional impact of 182 satellite winds, AMSU-A, Infrared Atmospheric Sounding Interferometer (IASI), and CrIS. The 183 fractional contribution from GNSSRO is considerably reduced in comparison to what is seen in 184 the default settings; this is similar to the reduction seen for aircraft observations. In contrast, the 185 fractional impact of radiosondes, ATMS, Global Precipitation Measurement (GPM) microwave 186 imager (GMI), and Advanced Very High Resolution Radiometer (AVHRR) is slightly increased 187 when compared to the default LPO. The most noticeable increase in fractional impact is seen for 188 land surface observations, followed by Advanced Scatterometer (ASCAT), Advanced Microwave 189 Scanning Radiometer 2 (AMSR2), and ships observations. The error bars in panel (a) show 95% 190 confidence levels in the fractional results. With the exception of results for AVHRR and MODIS 191 winds and drifting buoys, which are not statistically significant, all others are within acceptable 192 levels. Corroboration of the statistical significance of the averaged impact difference (J/kg) between 193 the near-surface and the standard LPO configurations is provided in panel (b). Results are shown to 194 be statistically significant for most of the components of the observing system. Since the standard 195 LPO results have larger negative values and the near-surface LPO results have smaller negative 196 values, where negative values indicate positive impacts, all the differences in panel (b) are positive 197 except AVHRR Wind. The near-surface LPO removes forecast sensitivities above 850 hPa, thus 198 FSOI derived at and below 850 hPa are only affected by the sensitivities at and below 850 hPa -199 this reduces quite significantly the magnitudes of FSOI relative to those derived with the standard 200 LPO. 201

Even with a confined near-surface LPO, both AMSU-A and ATMS still show considerable fractional contribution to forecast error reduction. This is even more peculiar since the GEOS ADAS analysis does not assimilate window channels and very low-peaking temperature sounding

channels (1–3 and 15) from AMSU-A, and corresponding channels (1–4 and 16) from ATMS. 205 Closer examination reveals that the impact from these instruments is dominated by their low-to-206 mid-peaking temperature channels, namely channels 5-7 for AMSU-A, and 5-8 for ATMS, when 207 using the standard LPO. The fact that even under a near-surface LPO these instruments contribute 208 substantially to fractional impact is attributed to the broad weighting functions associated with 209 these channels (not shown). The two other MW sensors, namely AMSR2 and GMI assimilated 210 in all-sky conditions, are also seen to contribute substantially to fractional impact with the near-211 surface LPO. The two window channels (23.8 GHz V¹ and 36.5 GHz V) of AMSR2 and GMI show 212 similar impact as seen from the low-to-mid-peaking AMSU-A and ATMS temperature channels. 213 The remaining three GMI channels (166 GHz V, 183.31 \pm 3 GHz V, and 183.31 \pm 7 GHz V) are 214 sensitive to water vapor and snowfall and are seen to have little impact on 850 hPa and below (not 215 shown). 216

Regarding the impacts of hyperspectral infrared radiances, they are affected by the channel 217 selections from each sensor, data usages over different surface types, and quality control procedures. 218 Compared with AIRS radiances, CrIS radiances are used in a much more conservative way in GEOS. 219 CrIS window channels are not used over non-water surface types, and surface-sensitive radiance 220 observations are also excluded if brightness temperature Jacobians with respect to surface skin 221 temperature are larger than 0.2. Therefore, it is understandable that CrIS's fractional impact in the 222 near surface LPO is lower than in the standard LPO. The seasonal effects of the FSOI results shown 223 in this work have not been studied. To the extent that forecast errors vary seasonally there might 224 be some seasonality in the impacts, but experience from looking at operational impacts suggests 225 that such effects are rather secondary. 226

227 4. Data denial OSEs

Motivated by the differences seen in the FSOI results discussed above, Table 1 lists a set of data denial experiments designed to look more closely at the impact of various observing systems with the primary focus of examining the lower troposphere response. The present work focus exclusively on the layer at and below 850 hPa, considered here to be the lower troposphere. We intend to identify the observing systems that have large impacts in the lower troposphere and that are not used effectively or have small impacts. How deep the observation impact penetrates into the lower

¹V stands for vertical polarization.

troposphere and the length that observation impacts last with the forecast lead time are also exam-234 ined. Evaluations are performed against a control (**XCTL**) experiment that uses all observations 235 and exercises the full deterministic and ensemble ADAS machinery. The OSEs listed in Table 1 236 systematically remove key components of the observing system: **XNOIR**, removes all infrared 237 radiance observations; **XNOMW**, removes all MW radiance observations; **XNOSATW**, removes 238 all satellite-derived wind observations; **XNOCONV**, removes all so-called conventional obser-239 vations², and finally, experiment **XNOSURF**, removes all surface observations, and is designed 240 specifically to evaluate the response of model processes to near-surface observations. Actual 241 evaluation of results is done either with respect to the control experiment or with respect to ERA5 242 analyses (Hersbach et al. 2020), as duly indicated. 243

244 a. Impact on specific humidity

According to the PBL Incubation Study Team Report (Teixeira et al. 2021), a key component to 245 improve modeling of PBL thermodynamics processes is the ability to optimally assimilate PBL 246 observations globally. To this extent, we start by examining the analysis of specific humidity in the 247 model lowest levels. The difference of the control (XCTL) analyzed December 2019 mean, specific 248 humidity at 850 hPa with the corresponding ERA5 monthly mean analysis appears in Fig. 2a. It 249 shows that, at the resolution of the experiments here, GEOS ADAS is drier over Tropical oceans 250 than ERA5; wetter over the southern oceans in the latitude band from roughly 40-60°S and over 251 the Northern Hemispheric Pacific and Atlantic storm tracks. Over South America GEOS ADAS 252 seem wetter than ERA5 in the Amazonian rainy season; over the western African GEOS ADAS is 253 drier than ERA5 in the area's dry season. 254

To facilitate comparison, the remaining panels of Fig. 2 show closeness plots of monthly mean analysis to ERA5 for each of the OSEs in Table 1 and the control experiment. That is, these panels show |OSE - ERA5| - |XCTL - ERA5|; hot colors indicate OSE is further away from ERA5 than the control experiment. With that, it is clear that denying microwave radiances (XNOMW; panel b) exacerbates the differences of the control with ERA5, turning the results further drier in the Tropical oceans. Although results in western Africa seem mixed, results in South America seem to move further away from ERA5. Only minor, mixed, changes are seen in the extratropical

²The wording *conventional observations* is somewhat of a misnomer as it stands for radiosondes, pilot bollons, aircraft and a host of truly traditional observations.



FIG. 2. Panel (a): Difference of analyzed December 2019 mean specific humidity (g/kg) analysis, at 850 hPa, and corresponding ERA5 analysis for XCTL experiment. Panels (b)-(f): closeness of given OSE and CTL to ERA5 monthly mean analysis, that is, difference of the absolute difference of given OSE with ERA5 and the absolute difference of control with ERA5: (b) XNOMW, (c) XNOCONV, (d) XNOIR, (e) XNOSATW, and (f) XNOSURF, at 850 hPa. Notice different color scale in panel (a). Locations below the surface are marked as white.

²⁶⁸ oceans. Generally, all other OSEs suffer considerably less from their corresponding observing ²⁶⁹ system denial than when microwave is denied. Some noticeable exceptional differences can be ²⁷⁰ seen in Europe when conventional observations are removed (panel c), and a slight move in the ²⁷¹ opposite direction to that of microwave, in the tropical oceans, when satellite winds are denied ²⁷² (panel e). No clear signals are seen when surface observations are denied (panel f).

Forecast skill scores for the control experiment and all OSEs have also been calculated, and 273 are discussed here when verified against ERA5 analyses. Each panel of Fig. 3 shows globally-274 averaged root mean square error (RMSE) differences from the control with boxes representing 95% 275 confidence interval for the associated RMSE difference, at selected levels. The largest increase 276 in RMSE is due to denying microwave observations (red curves), with results being statistically 277 significant. Loss of skill due to microwave is felt throughout the 5-day forecast at all levels displayed 278 in the figure, though its significance decreases with increased forecast lead time. To a lesser extent 279 than when denying microwave, loss in skill due to denying conventional (blue curves) and IR 280 (green curves) observations is also statistically significant with the effect lasting throughout the 281 5-day forecast. The significance of denying conventional observations becomes more comparable 282 with that of denying microwave observations as we approach the surface. The impact on specific 283 humidity from denying satellite winds (purple curves) and surface (yellow curves) observations is 284 insignificant at 850 hPa. At lowest levels, satellite winds are seen to have small positive impact in 285 the short forecast lead times, but turn slightly negative at longer forecast lead times; the influence 286 of surface observations is small, with neutral to slightly positive impact observed toward the end 287 of the forecast. 288

The regional influence on specific humidity at low levels from the denial experiments of Table 1 299 is shown for the Northern Hemisphere (NHE) and Southern Hemisphere (SHE) in Figs. 4–5. In 300 the Northern Hemisphere, conventional observations are the most influential data type (Fig. 4a) in 301 terms of mean forecast RMSE. Their impact stretches from the surface to 200 hPa throughout the 302 5-day forecasts (Fig. 4b), with the largest impact in the lower to mid- troposphere. At 925 hPa and 303 below, microwave radiances have much smaller impact, and infrared radiances can be negligible. 304 This may be partially because very limited surface-sensitive radiances are assimilated over land. 305 As expected, microwave radiances contribute the most in the Southern Hemisphere, followed by 306 infrared radiances (Fig. 5a), but the large impact observed from 925 hPa to above 800 hPa decreases 307



FIG. 3. Globally–averaged RMSE difference from the control for all 0000 UTC 5-day forecasts for December 2019 of specific humidity at (a) 850, (b) 925 and (c) 1000 hPa, with boxes representing 95% statistical confidence 2019 interval for each of the RMSE difference curves. The RMSE for the control and each OSE is calculated wrt ERA5 2022 analyses. Curves are for control (black), **XNOMW** (red), **XNOIR** (green), **XNOCONV** (blue), **XNOSATW** 2033 (purple), and **XNOSURF** (yellow).



FIG. 4. Panel (a), as in Fig. 3b, but for Northern Hemisphere. Panel (b), globally-averaged specific humidity RMSE difference (g/kg) between **XNOCONV** and **XCTL**, as a function of pressure levels, for the Northern Hemisphere 0000 UTC forecasts of December 2019. Shaded areas highlight results that are statistically significant with 90% confidence. The darker the shading corresponds to larger differences. The solid, dot-dash, and longdash lines correspond to the confidence intervals of 90%, 95%, and 99%.



FIG. 5. As in Fig 4, but for Southern Hemisphere; and for panel (b) comparing XNOMW with XCTL.

with the forecast lead times (Fig. 5b). In the Tropics (figure not shown), while conventional data have the largest impact at 925 hPa and below, microwave radiances dominate at 850 hPa followed by infrared radiances and conventional data, and the effect of microwave radiances is most noticeable between 875 and 700 hPa but much smaller or neutral impact below. Overall, the impact from MW radiances tends to decrease quickly as forecast lead time increases while the impact of denying conventional observations stands well into the 5-day forecast.

314 b. Impact on temperature field

As displayed in Fig. 6a, the impact of microwave radiances on temperature forecasts can be seen more clearly in the Tropics, where its impact is neutral to negative below 925 hPa throughout the 5-day forecast lead times. Their impact below 900 hPa in the Northern and Southern Hemisphere is also negligible in the first day or two of the forecast.

Similarly, Fig. 6b suggests that infrared radiances mostly contribute to temperature forecast error reduction above 925 hPa in the Tropics (and also Southern Hemisphere). Loss of skill in temperature forecast due to denying infrared observations lasts up to about day 4, whereas considerable losses due to removal of microwave observations are felt throughout the 5-day period between 600 and 925 hPa (Fig. 6a).

Like its impact on specific humidity, conventional data dominate the observation impacts on the lower troposphere in the Northern Hemisphere. When they are removed, forecasts degrade for the 5-day forecast period from surface to 100 hPa with the most severe degradation in the lower troposphere. In Tropics, considerable impacts from conventional data are also observed around 900 and 300-550 hPa (figures not shown).

331 c. Impact on wind field

Although wind is not the focus of the PBL Incubation Study Team report (Teixeira et al. 2021), some of the denial experiments of Table 1 show non-negligible consequences to predicting winds in the lower troposphere. Conventional data and microwave radiances are the two most effective observation sources for reducing wind forecast RMSE globally from the surface to 850 hPa. Infrared radiances have little or neutral impact in this layer. The most interesting result is the positive impact from microwave radiances. While some radiances are affected by surface wind



FIG. 6. Panel (a): similar to Fig. 5b, but for temperature (K) in the Tropics; panel (b): similar to panel (a), but comparing experiment **XNOIR** with **XCTL**.



FIG. 7. As in Fig. 5a, but for meridional wind (ms^{-1}) at 850 hPa.

speed, a considerable impact in the lower troposphere may be through background error covariance
and tracer effect when thermodynamic structure is improved by using the microwave radiances.
For example, Fig. 7 illustrates that in the Southern Hemisphere, microwave radiances have the
largest impact in reducing forecast errors at 850 hPa, followed by conventional data.

However, one of the most unexpected results obtained from examining the wind fields is the im-342 provement in forecast scores when satellite winds are removed. This is seen in Fig. 7 (XNOSATW; 343 purple curve), with the improvement being retained and increasing throughout the length of the 344 5-day forecast. Careful examination reveals this to be the case at other levels, as well, especially 345 along the jet-stream level (not show). Another illustration of the undesirable improvement obtained 346 when satellite winds are removed, from the version of GEOS ADAS used in this work is seen when 347 looking at the ratio of observation-minus-background standard deviations between **XNOSATW** 348 and XCTL, for various instruments. Figure 8 displays this ratio in the Southern Hemisphere for 349 (a) ATMS and (b) IASI radiance observations; improvements appear as the solid black curve falls 350 below 100% (grey, vertical curve). A careful evaluation reveals this unexpected result to be a 351

consequence of a bug in the GEOS system with no thinning being applied to GOES-R satellite
 wind observations; results improve dramatically after the bug is fixed with proper thinning being
 applied.

358 d. Impact on PBL height

The height of the PBL is a relevant parameter used in air quality studies and mixing of aerosols in 359 the turbulence layer. Though careful evaluation of the consequences in changes to PBL height and 360 its diurnal cycle are beyond the scope of the present work, it is still worth seeing how the various 361 OSEs here change this quantity. In the GEOS system, the PBL height uses different definitions over 362 land and ocean. Over land, it is based on the bulk Richardson number with a critical value of 0.25, 363 while over ocean it is based on the profile of diffusivity from the turbulence parameterizations, 364 with a threshold of 10% of the maximum diffusivity. Figure 9 shows the diagnosed December 365 2019 averaged PBL height for the control experiment (panel a), and how PBL height differs for 366 a given OSE from the control (remaining panels). Denial of microwave observation (panel b) 367 tends to lower PBL height in the Southern Hemisphere oceans at this time of the year, and slightly 368 increase it in the Tropics and Northern Hemisphere. This is somewhat similar to what happens 369 when infrared observations are denied (panel d) though an increase of PBL height is observed over 370 tropical lands in this case. The effect from denying conventional observations (panel c) is more 371 visible in the Northern Hemisphere and Tropics with the inner portions of North America and Asia 372 showing a decrease in PBL height and the coastal areas showing an increase. The effects from 373 denying satellite winds is just as large as that of denying microwave radiances, especially in certain 374 areas: noticeably off the Pacific coastal areas of North and South America where stratocumulus 375 clouds play a significant role and are considerably affected by the winds in those regions in this 376 case. It should be noted that some of the effects from satellite winds seen here are caused by the 377 improper handling of GOES-R satellite winds in the GEOS system as discussed in Section 4c. 378 Comparatively speaking, the absence of surface observations (panel f) amounts to relatively small 379 changes in PBL height, which is perhaps indicative of how little the present data assimilation uses 380 such observations to constrain this variable. 381



FIG. 8. Observation-minus-background standard deviation ratio of experiment (**XNOSATW**) and control for (a) ATMS and (b) IASI in the Southern Hemisphere, for December 2019. Bottom x-axis show percentage, magenta shade and top x-axis shows observation count, and bars and grey shades represent 95% significance.



FIG. 9. Averaged December 2019 PBL height (m) for the control experiment (panel a) and difference for each OSE: (b) XNOMW, (c) XNOCONV, (d) XNOIR, (e) XNOSATW, and (f) XNOSURF.

³⁸⁴ e. Impact of surface observations

Early forecast models had low vertical resolution and simply had surface heat exchange, momen-385 tum drag and vertical diffusion, with consequent highly dissipative surface layers. Thus, forecasts 386 in these layers were relatively insensitive to changes of fields aloft which would overwhelm the 387 mechanisms for error growth and vice verse. Modern PBL schemes (e.g. Lock et al. 2000) are 388 more sophisticated, incorporating vertically non-local forcing and effects upward from the surface 389 as well as downward from the layer's top. As removing the surface observations in experiment 390 **XNOSURF** introduces changes mainly to the analyses in the lowest levels, it is worth examining 391 how the atmosphere responds to such changes. 392



FIG. 10. As in Fig. 4b, but for comparing XNOSURF with XCTL in the Tropics.

Figure 10 shows specific humidity RMSE difference between **XNOSURF** and **XCTL** in the 393 Tropics for the month of December 2019. It is seen that removing surface observations degrades 394 upper atmosphere forecast skill from about 150 to 350 hPa in the Tropics persistently. Similar 395 degradation is also observed from 100 to 200 hPa in the Northern and Southern Hemisphere up to 396 day 4. Although the degradation magnitude is small, they are statistically significant at confidence 397 value of 90%. The surface observations have mixed impact on the mid- and lower atmosphere. 398 Removing surface observations makes forecast skill worse below 800 hPa but better in the mid-399 atmosphere in the Tropics, and the forecast skills below 900 hPa become better for up to one 400 and a half days in the Northern Hemisphere. Removing surface observations, however, has no 401 statistically significant impact on temperature and wind fields. In this experiment where surface 402 observations are excluded, the results indicate that changes at or near surface do affect mid- and 403 upper- atmosphere in the GEOS system. As more PBL observations will become available in the 404 future, more studies should be performed to investigate how they affect not only the PBL simulation 405 but also the above free atmosphere. 406

5. Model tendency responses to the IAU forcing

In a traditional data assimilation framework, analysis increments are used to intermittently correct 408 the model's initial condition at every cycle. When the increments change the initial state in a way 409 that is not consistent with the model hydrodynamical and physical processes the model tends to 410 reject the observational information. Geostrophic adjustment, happening in time scales of minutes 411 to hours, is one such well-known dynamical process the model goes through to accommodate to 412 undesirable changes in its state induced by the analysis. When components of the initial state prove 413 inconsistent with the physical processes, the model may reject the analysis information and return 414 to its desired state in a single time step. One such example is discussed in Zhu et al. (2016, Fig. 16 415 there), where parts of the cloud analysis increment are simply rejected after the first pass through 416 the physics term in the model integration. In this example, it was found that an inconsistency 417 between the model clouds and the relative humidity analysis partially explained why the model 418 readily ignores the cloud analysis increments. More generally, the way analysis increments are 419 presented to the model, and whether they are dynamically and physically consistent with the model 420 underlying processes determines how the model retains information from the observations. This 421 consistency is well understood when it comes to dynamical balances, such as geostrophic balance, 422 and it has led to careful development of initialization algorithms (e.g., Kleist et al. 2009, and 423 references therein), and it has also led to procedures to develop dynamically consistent background 424 error covariances (see Bannister 2008, and references therein). 425

As mentioned in Section 2, instead of correcting the model through traditional intermittent initial 426 condition updates, the GEOS data assimilation system employs an IAU procedure that presents the 427 analysis corrections as tendency terms that are continuously applied to the model during the 6-hour 428 assimilation window around the analysis time, [-3h, +3h]. Whether in 3D, or its 4D formulation 429 used in the current GEOS hybrid system, a digital filter modulates the analysis tendencies (Takacs 430 et al. 2018) in a way that guarantees a smooth transition from one 6-hour assimilation cycle to the 431 next. After the first pass of the IAU tendency, model hydrodynamics and physics tendencies start 432 to evolve and depart from the original free model forecast path where IAU forcing is not added. 433 In this section, the changes of model tendencies induced by the IAU forcing in the assimilation 434 window and beyond are examined, and hopefully this information will be helpful for a future study 435 on improving observation retention in model forecast. 436

For a simplified and idealized forecast model, as shown in the Appendix, negative value of the 437 cross-covariance between total model tendency and IAU tendency causes smaller increase of model 438 prediction error from time t_{n-1} to t_n during the IAU [-3h, +3h] assimilation window. Such negative 439 cross-covariance values are also observed over large areas in the complex and nonlinear GEOS 440 system (figure not shown). A closer examination of the two cross-covariance terms between model 441 hydrodynamics/physics tendency (i.e., $\left(\frac{\partial x}{\partial t}\right)_d$, $\left(\frac{\partial x}{\partial t}\right)_p$) and IAU tendency $\frac{\delta x}{\tau}$ are conducted using an 442 ensemble forecast with the IAU forcing for temperature state (right columns of Figs 11–12). δx 443 represents the analysis increment, and τ represents the scaling parameter used to convert increments 444 into tendencies. The cross-covariances using the ensemble forecast without the IAU forcing are 445 also calculated (left columns of Figs 11-12) to help illustrate how the model hydrodynamics and 446 physics tendencies have changed in response to the IAU forcing in the assimilation window. It 447 is shown in Fig. 11 that the patterns of $cov\left(\left(\frac{\partial x}{\partial t}\right)_d, \frac{\delta x}{\tau}\right)$, the cross-covariances between model 448 hydrodynamics tendency and IAU tendency, exhibit little change at 1000 and 925 hPa, but become 449 increasingly negative with height at and above 850 hPa due to the use of the IAU forcing. In contrast, 450 $cov\left(\left(\frac{\partial x}{\partial t}\right)_n, \frac{\delta x}{\tau}\right)$, the cross-covariances between model physics tendency and IAU tendency (Fig. 451 12), indicate relatively small changes at higher vertical levels but substantial changes at 1000, 925 452 and 850 hPa. When IAU forcing is off, these levels show no clear pattern with mixed positive and 453 negative values, but cross-covariance values become strongly negative over large areas when IAU 454 forcing is on. These results indicate that physics tendency tends to evolve much more in response 455 to the IAU forcing than hydrodynamics tendency in the lower troposphere, while the change of 456 hydrodynamics tendency dominates in the middle and upper troposphere. While negative cross-457 covariance values are usually viewed as beneficial to reduce the state error covariance in Equation 458 (A4), they suggest that analysis affects hydrodynamics tendencies more in the desired direction 459 at mid-levels of the troposphere than it does at low levels; conversely, the analysis drives physics 460 tendencies more toward desirable values at low levels than at mid levels of the troposphere. 461

Similar patterns are also noticed in the cross-covariance terms between model hydrodynamics/physics tendency and IAU tendency for specific humidity and wind (figures not shown). The only noticeable pattern variation is seen in the cross-covariance between model hydrodynamics tendency and IAU tendency for specific humidity. While it is still becoming more negative at 850



FIG. 11. Cross-covariance ($\times 1.0e^{-10}K^2s^{-2}$) between ensemble model temperature hydrodynamics tendency and ensemble IAU tendency at 1000 (a, f), 925 (b, g), 850 (c, h), 500 (d, i), and 200 (e, j) hPa at 00UTC December 16, 2019 for the ensemble forecasts with (right columns) and without (left columns) the IAU tendency forcing.

hPa when the IAU forcing is turned on, the changes between with and without IAU forcing are
much smaller than those for temperature and there is little difference at 500 and 200 hPa.

The changes of hydrodynamics and physics tendencies in response to the IAU forcing are also reflected in the spatial correlation coefficients of the model tendencies between the ensemble



FIG. 12. The same as Fig. 11 but for cross-covariance between ensemble model temperature physics tendency and ensemble IAU tendency.

forecast with the IAU forcing and the original free ensemble forecast. A higher correlation coefficient indicates a model tendency is more similar to that of the free model forecast. With the use of IAU forcing, the model tendencies deviate from those of the original free forecast, and the departures are expected to increase with forecast hours. The behaviour of the model tendencies and the degree of similarity to the original free forecast are examined at selected model vertical
levels.

The global correlation coefficients for temperature hydrodynamics and physics tendencies are 481 displayed in Fig. 13 during the 27-hour ensemble forecast, which includes a 6-hour IAU assimilation 482 window (i.e., [-3h, +3h] relative to the analysis cycle time) followed by a 21-hour (i.e., [3h, 24h]) free 483 forecast. In the [-3h, +3h] IAU assimilation window, the correlation coefficient of hydrodynamics 484 tendency (left panel of Fig. 13) dipped slightly at about 100, 300, and 850 hPa, but overall it 485 has relatively small vertical variation globally, and experiences more rapid changes in the second 486 half of the assimilation window than the first half of the window (except for 1000 hPa) and the 487 following free forecast lead hours. In the subsequent [3h, 24h] forecast when the IAU forcing 488 is turned off, the correlation decreases with the forecast lead hours and with the height globally, 489 reaching a minimum of about 0.7 at 300 hPa at 24h, then increases to 0.81 at 200 hPa. At and 490 below 850 hPa, the correlation coefficient has the slowest rate of change after the IAU is turned off. 491 On the other hand, the pattern of the physics tendency correlation coefficient (right panel of 497 Fig. 13) is quite different from that of hydrodynamics tendency. Little departure is observed 498 in physics tendency due to the use of IAU forcing at and above 100 hPa. In the [-3h, 3h] IAU 499 assimilation window, the correlation coefficient of physics tendency experiences relatively smaller 500 vertical variation below 100 hPa and above 850 hPa. However, at and below 850 hPa, it decreases 501 rapidly as the physics tendency deviates from the original forecast model, and the model physics 502 evolves much more significantly in the first half of the assimilation window than the second half. 503 After the IAU forcing is off, two minimum correlation coefficient levels are noticed, one is at the 504 lowest model levels 850-925 hPa, the other is located around 300-400 hPa. While the correlation 505 coefficient still roughly decreases with the forecast lead hours in the mid- and upper troposphere, 506 such pattern doesn't exist in the lower troposphere due to the complexity of physical processes, for 507 example, the correlation coefficients at 6h, 9h, and 12h are higher than 3h, the correlation at 24h 508 is higher than some shorter forecast lead times, and all correlation coefficients of different forecast 509 lead hours cluster together at 1000 hPa. 510

⁵¹¹ Comparing the correlation coefficients in the left and right panels of Fig. 13, it is clearly shown ⁵¹² that the lower troposphere physics tendencies diverge more quickly than the hydrodynamics in both



FIG. 13. Globally-averaged correlation coefficients of model temperature hydrodynamics (left) and physics (right) tendencies between the ensemble forecast with IAU forcing and original free ensemble forecast without IAU forcing during a 27-hour ensemble forecast. The light green line is for the correlation coefficient at the beginning of the assimilation window and therefore the coefficient value is 1. The red/black line is for the coefficient at the middle/end of the assimilation window.

the lower and upper troposphere, which is consistent with the idea that the PBL physics responds
 strongly to the IAU.

The global correlation coefficients of hydrodynamics and physics tendencies between the ensemble forecast with IAU forcing and the original free ensemble forecast are also evaluated for specific humidity and wind (figures not shown). Like the temperature hydrodynamics tendency correlation coefficient, the correlation coefficients for specific humidity and wind decrease significantly in the IAU assimilation window, then continue to decrease gradually with forecast lead times with

the smallest change rate at the lower troposphere and reaching the minimum around 150 hPa for 520 specific humidity and 200–500 hPa for wind. As to the physics tendency correlation coefficients, 521 the patterns for temperature and specific humidity are similar. The correlation coefficients for 522 specific humidity increase at 24h and are even comparable or larger than those at 3h in the lower 523 troposphere, while they decrease gradually with forecast lead times in the mid- and upper tropo-524 sphere with a minimum correlation at 50 hPa. The correlation coefficients for wind decrease the 525 most at 400 hPa in the IAU assimilation window, and decrease slightly with forecast lead times at 526 925 hPa but there is no clear pattern at other levels in the subsequent forecast when the IAU forcing 527 is off. 528

529 6. Conclusions

The GEOS data assimilation system has provided the critical capability of combining model physics and a wide range of observations with various data coverage and spatial/temporal resolutions coherently to improve the global thermodynamic structure and numerical forecast. To prepare for future observing systems of the next decade, we have assessed the effectiveness of the use of existing observing systems in the lower troposphere in the GEOS data assimilation system.

The full set of observations assimilated in the global GEOS data assimilation system is first assessed using the FSOI with the forecast error norm integrated from surface to about 850 hPa. Radiosonde data and microwave radiances from AMSU-A and ATMS are among the top contributors to the GEOS system. Both lower peaking temperature sounding channels from AMSU-A and ATMS and window channels from AMSR2 and GMI are found to be effective in reducing model forecast errors.

Given the FSOI results from the control experiment, a set of data denial experiments are con-541 ducted with selected observing systems of interest being removed. The results of the data denial 542 experiments show that, microwave radiances and conventional data are the two most important data 543 types to improving model forecast skills in the lower troposphere, which is in agreement with the 544 FSOI results. Microwave radiances usually have large positive impact in the Southern Hemisphere 545 and Tropics ocean, but most of the large impact is observed above 925 hPa and at early forecast lead 546 times as the impact dissipates with longer lead times. Microwave radiances are also shown to con-547 tribute much more to specific humidity field than temperature field. Infrared radiances collectively 548

30

have much smaller impact in the lower troposphere, and they have difficulty to influence model 549 levels below 925 hPa. In contrary, conventional data have the largest contribution in the Northern 550 Hemisphere on both specific humidity and temperature fields, and their impact ranges from surface 551 to 100 hPa, depending on the field evaluated. Meanwhile, data denial experiment results also 552 reveal that changes at and near the surface by assimilating surface observations can affect not only 553 lower but also mid- and upper troposphere. They have small but persistently positive impact on 554 specific humidity forecast skill in the upper troposphere but mixed impact in the lower and mid 555 troposphere. However, their impacts on temperature and PBL height are small or negligible. 556

One surprising finding of this study is the obvious inconsistent results between the FSOI and the 557 data denial experiment on satellite winds. FSOI results suggest high positive impact of the satellite 558 winds data, but the data denial experiment indicates negative impact of these data in the GEOS 559 system. Close examinations of the OmF of ATMS and IASI agree with the data denial experiment 560 results. This inconsistency may be partially attributable to the choice of forecast aspect in the 561 FSOI, which may lead to incomplete assessment of the observing system (Todling 2013). The 562 negative impact from the satellite winds is most likely due to the missing of the thinning procedure 563 for a subset of satellite winds. Further testing and tuning of the satellite winds in the GEOS system 564 have been underway in a separate effort. 565

The responses of model hydrodynamics and physics tendencies to the IAU tendency forcing are 566 also investigated in this study. In the GEOS data assimilation system, IAU procedure is employed 567 so piecewise analysis increment tendency is introduced into the forecast model during the 6-hour 568 assimilation window. As the model re-adjusts to the IAU forcing, the IAU tendency is found to 569 contribute to the reduction of state error covariance, mostly noticeable through the interaction 570 with model hydrodynamic tendency in the mid- and upper troposphere and the interaction with 571 model physics tendency in the lower troposphere. The correlation coefficients of temperature 572 hydrodynamics and physics tendencies between ensemble forecast with IAU forcing and free 573 ensemble forecast further illustrate the changes of the model tendencies in the assimilation window 574 and reveal their evolution behaviors in the subsequent free forecast. In the IAU assimilation 575 window, physics tendency correlation coefficient exhibits significant and rapid decrease in the lower 576 troposphere as physics tendency re-adjusts quickly there to the IAU forcing, but hydrodynamics 577 tendency correlation coefficient has much less vertical variation. In the following forecast when 578

⁵⁷⁹ IAU forcing is off, both hydrodynamics and physics tendencies see low correlations around 300-400 ⁵⁸⁰ hPa. In the lower troposphere, while the hydrodynamics tendency has the slowest change rate, the ⁵⁸¹ physics continues to diverge, but the correlation coefficient of physics tendency at 24h becomes ⁵⁸² larger, instead of smaller, than shorter forecast lead times in the lower troposphere, which may ⁵⁸³ suggest that this tendency tends to get back to the original free forecast mechanism.

Overall, there are still a lot of room to improve observation usages in the lower troposphere in 584 the GEOS data assimilation system. GMAO plans to significantly increase the vertical resolution 585 of its GEOS model in the near future, making corresponding adjustments to the model physics 586 and data assimilation components. This near-future upgrade will aim, among other things, to 587 maximize the benefits of using various observations in the lower troposphere through improved first 588 guess thermodynamics. As the complexity and short timescale of PBL processes pose additional 589 difficulties in response to the IAU tendency forcing and retention of information content of PBL 590 observations, future research is also much needed to further improve representation of processes 591 by the analysis and model parameterization schemes and parameters. 592

Acknowledgments. We would like to thank Ronald Errico and Daniel Holdaway for their helpful
 discussions. This study is supported by the Global Modeling and Assimilation Office core funding
 from NASA.

⁵⁹⁶ *Data availability statement*. The GEOS model and data assimilation code and supporting software ⁵⁹⁷ are maintained by the GMAO and publicly available through the NASA Open Source Agreement ⁵⁹⁸ (NOSA) on github (https://github.com/GEOS-ESM). The data generated in this study includes ⁵⁹⁹ output from the GEOS model and data assimilation system. All the unprocessed model output ⁶⁰⁰ were automatically archived and can be accessed on the NCCS Dirac Mass Storage System.

601

APPENDIX

602

A brief derivation of state error covariance with IAU forcing

⁶⁰³ A brief back of the envelop, idealized, calculation provides the rationale to justify why it is ⁶⁰⁴ thought that the correlations between the total model tendency and the IAU tendency should be ⁶⁰⁵ negative.

32

In a very simplified context, and under the most straightforward flavor of IAU, a state variable x_n evolves in a single time step, Δt , from time t_{n-1} to t_n following

$$x_n = x_{n-1} + \Delta t \frac{\partial x}{\partial t} + \Delta t \frac{\delta x}{\tau},$$
(A1)

where the differential in the second term in the rhs represents the total model tendency, which includes hydrodynamics and physics tendencies, $\left(\frac{\partial x}{\partial t}\right)_d$ and $\left(\frac{\partial x}{\partial t}\right)_p$. δx represents the analysis increment, and τ represents the scaling parameter used to convert increments into tendencies.i Subtracting the true state from the equation above, multiplying the resulting expression by itself,

taking the expectation of the result, and assuming that x_{n-1} is not correlated with either the total tendency (i.e., linear dynamics) and the IAU term, we get

$$P_{n} = P_{n-1} + (\Delta t)^{2} Q_{x} + (\Delta t)^{2} Q_{i} + (\Delta t)^{2} cov \left(\frac{\partial x}{\partial t}, \frac{\delta x}{\tau}\right)$$
(A2)

In the above, P is the state error covariance, $Q_x = cov\left(\frac{\partial x}{\partial t}\right)$, $Q_i = cov\left(\frac{\delta x}{\tau}\right)$, and the symbol cov()is used to represent either an autocovariance when only a single entry is in its argument, or a cross-covariance when two arguments are present. In the ideal world, $P_n - P_{n-1} > 0$, that is the error in the predicted state grows in time, therefore,

$$cov\left(\frac{\partial x}{\partial t}, \frac{\delta x}{\tau}\right) > -(Q_x + Q_i)$$
 (A3)

meaning the cross-covariance must be larger than a certain negative value. Any value large than a minimum negative value implies a larger error in the prediction, that is, a large value for $P_n - P_{n-1}$. Therefore the smaller the value of the cross-covariance or the smaller the sum of the cross-covariance and Q_i , the smaller the prediction error. If splitting total model tendency into hydrodynamics and physics tendencies, similar to Equation (A2) we also have

$$P_{n} = P_{n-1} + (\Delta t)^{2} Q + (\Delta t)^{2} Q_{i} + (\Delta t)^{2} cov \left(\left(\frac{\partial x}{\partial t} \right)_{d}, \left(\frac{\partial x}{\partial t} \right)_{p} \right)$$
$$+ (\Delta t)^{2} cov \left(\left(\frac{\partial x}{\partial t} \right)_{d}, \frac{\delta x}{\tau} \right) + (\Delta t)^{2} cov \left(\left(\frac{\partial x}{\partial t} \right)_{p}, \frac{\delta x}{\tau} \right)$$
(A4)

where $Q = cov\left(\left(\frac{\partial x}{\partial t}\right)_d\right) + cov\left(\left(\frac{\partial x}{\partial t}\right)_p\right)$. The last three cross-covariances terms in the rhs affect P_n simultaneously in Equation (A4).

626 **References**

Bacmeister, J. T., M. J. Suarez, and F. R. Robertson, 2006: Rain reevaporation, boundary
 layer-convection interactions, and Pacific rainfall patterns in an AGCM. *Journal of Atmo- spheric Science*, **63**, 3383–3403, https://doi.org/10.1175/JAS3791.1, URL https://doi.org/10.
 1175/JAS3791.1.

Bannister, R. N., 2008: A review of forecast error covariance statistics in atmospheric variational
 data assimilation. II: Modelling the forecast error covariance statistics. *Quarterly Journal of the Royal Meteorological Society*, **134** (637), 1971–1996, https://doi.org/10.1002/qj.340, URL
 https://doi.org/10.1002/qj.340.

Bloom, S. C., L. L. Takacs, A. M. da Silva, and D. Ledvina, 1996: Data assimila tion using incremental analysis updates. *Monthly Weather Review*, **124** (6), 1256–1271,
 https://doi.org/10.1175/1520-0493(1996)124<1256:dauiau>2.0.co;2, URL https://doi.org/10.
 1175/1520-0493(1996)124<1256:dauiau>2.0.co;2.

⁶³⁹ Clough, S., M. Shephard, E. Mlawer, J. Delamere, M. Iacono, K. Cady-Pereira, S. Boukabara,
 ⁶⁴⁰ and P. Brown, 2005: Atmospheric radiative transfer modeling: a summary of the AER codes.
 ⁶⁴¹ *Journal of Quantitative Spectroscopy and Radiative Transfer*, **91** (2), 233–244, https://doi.org/
 ⁶⁴² 10.1016/j.jqsrt.2004.05.058, URL https://doi.org/10.1016/j.jqsrt.2004.05.058.

- ⁶⁴³ Duncan, D. I., N. Bormann, and E. V. Hólm, 2021: On the addition of microwave sounders
 ⁶⁴⁴ and numerical weather prediction skill. *Quarterly Journal of the Royal Meteorological Society*,
 ⁶⁴⁵ https://doi.org/10.1002/qj.4149, URL https://doi.org/10.1002/qj.4149.
- El Akkraoui, A., Y. Tremolet, and R. Todling, 2013: Preconditioning of variational data assimila-
- tion and the use of a bi-conjugate gradient method. *Quarterly Journal of the Royal Meteorological*
- *Society*, **139**, 731–741, https://doi.org/10.1002/qj.1997, URL https://doi.org/10.1002/qj.1997.
- Errico, R. M., K. Raeder, and M. Ehrendorfer, 2004: Singular vectors for moisture measuring norms. *Quarterly Journal of the Royal Meteorological Society*, **130** (**598**), 963–987,
 https://doi.org/10.1256/qj.02.227, URL https://doi.org/10.1256/qj.02.227.
- ⁶⁵² Freitas, S. R., G. A. Grell, A. Molod, M. A. Thompson, W. M. Putman, C. M. S. e Silva, and E. P.
- ⁶⁵³ Souza, 2018: Assessing the grell-freitas convection parameterization in the nasa geos modeling
- system. Journal of Advances in Modeling Earth Systems, 10, 1266–1289, https://doi.org/10.
- ⁶⁵⁵ 1029/2017MS001251, URL https://doi.org/10.1029/2017MS001251.
- Garcia, R. R., and B. A. Boville, 1994: Downward control of the mean meridional circulation and
 temperature distribution of the polar winter stratosphere. *J. Atmos. Sci.*, **51**, 2238–2245.
- Gelaro, R., R. H. Langland, S. Pellerin, and R. Todling, 2010: The THORPEX observation impact
 intercomparison experiment. *Monthly Weather Review*, **138** (11), 4009–4025, https://doi.org/
 10.1175/2010mwr3393.1, URL https://doi.org/10.1175/2010mwr3393.1.
- Hersbach, H., and Coauthors, 2020: The ERA5 global reanalysis. *Quarterly Journal of the Royal*
- Meteorological Society, **146** (**730**), 1999–2049, https://doi.org/10.1002/qj.3803, URL https: //doi.org/10.1002/qj.3803.
- Holdaway, D., R. Errico, R. Gelaro, J. G. Kim, and R. Mahajan, 2015: A linearized prognostic
- cloud scheme in NASA's goddard earth observing system data assimilation tools. *Monthly*
- Weather Review, 143 (10), 4198–4219, https://doi.org/10.1175/mwr-d-15-0037.1, URL https:
- ₆₆₇ //doi.org/10.1175/mwr-d-15-0037.1.
- Iacono, M. J., J. S. Delamere, E. J. Mlawer, M. W. Shephard, S. A. Clough, and W. D. Collins,
 2008: Radiative forcing by long-lived greenhouse gases: Calculations with the AER radiative
 transfer models. J. Geophys. Res., 113.

- Kelly, G., and J.-N. Thépaut, 2007: Evaluation of the impact of the space component of the global 671 observing system through observing system experiments. ECMWF Newsletter, 113, 16–28, 672 https://doi.org/10.21957/ct50muxpx4, URL https://www.ecmwf.int/node/10434. 673
- Kleist, D. T., D. F. Parrish, J. C. Derber, R. Treadon, R. M. Errico, and R. Yang, 2009: Improving 674 incremental balance in the GSI 3dvar analysis system. Monthly Weather Review, 137 (3), 1046– 675 1060, https://doi.org/10.1175/2008mwr2623.1, URL https://doi.org/10.1175/2008mwr2623.1.

676

683

- Langland, R. H., and N. Baker, 2004: Estimation of observation impact using the NRL atmospheric 677 variational data assimilation adjoint system. Tellus, 56A, 189–201, https://doi.org/10.3402/ 678 tellusa.v56i3.14413, URL https://doi.org/10.3402/tellusa.v56i3.14413. 679
- Lawrence, H., N. Bormann, I. Sandu, J. Day, J. Farnan, and P. Bauer, 2019: Use and impact of 680 arctic observations in the ECMWF numerical weather prediction system. Quarterly Journal of 681 the Royal Meteorological Society, 145 (725), 3432–3454, https://doi.org/10.1002/qj.3628, URL 682 https://doi.org/10.1002/qj.3628.
- Lock, A. P., A. R. Brown, M. R. Bush, G. M. Martin, , and R. N. B. Smith, 2000: A new 684 boundary layer mixing scheme. part i: Scheme description and single-column model tests. 685 Monthly Weather Review, **128**, 3187–3199, https://doi.org/10.1175/1520-0493(2000)128<3187: 686 ANBLMS>2.0.CO;2, URL https://doi.org/10.1175/1520-0493(2000)128<3187:ANBLMS>2. 687 0.CO:2. 688
- Lord, S., G. Gayno, and F. Yang, 2016: Analysis of an observing system experiment 689 for the joint polar satellite system. Bulletin of the American Meteorological Society, 690 97 (8), 1409–1425, https://doi.org/10.1175/BAMS-D-14-00207.1, URL https://doi.org/10. 691 1175/BAMS-D-14-00207.1. 692
- Louis, J., and J. Geleyn, 1982: A short history of the pbl parameterization at ecmwf. *Proc. ECMWF* 693 Workshop on Planetary Boundary Layer Parameterization, Reading, United Kingdom, ECMWF. 694
- McFarlane, N. A., 1987: The effect of orographically excited gravity wave drag on the general 695 circulation of the lower stratosphere and troposphere. J. Atmos. Sci., 44 (14), 1775–1800. 696
- National Academies of Sciences, E., and Medicine, 2018: Thriving on Our Changing Planet: 697
- A Decadal Strategy for Earth Observation from Space. The National Academies Press, 698

Washington, DC, https://doi.org/10.17226/24938, URL https://www.nap.edu/catalog/24938/ thriving-on-our-changing-planet-a-decadal-strategy-for-earth.

Park, S., and C. S. Bretherton, 2009: The University of Washington shallow convection and moist
 turbulence schemes and their impact on climate simulations with the community atmosphere
 modell. *Journal of Climate*, 22, 3449–3469.

Putman, W. M., and S.-J. Lin, 2007: Finite-volume transport on various cubed-sphere grids.
 Journal of Computational Physics, 227 (1), 55–78, https://doi.org/10.1016/j.jcp.2007.07.022,
 URL https://doi.org/10.1016/j.jcp.2007.07.022.

Reichle, R. H., and Coauthors, 2018: Soil moisture active passive (SMAP) project assessment
 report for version 4 of the l4_sm data product. Nasa tech. memo., vol. 52, NASA, 72 pp pp. URL
 https://gmao.gsfc.nasa.gov/pubs/docs/Reichle1083.pdf.

Takacs, L. L., M. J. Suárez, and R. Todling, 2016: Maintaining atmospheric mass and water balance
 in reanalyses. *Quarterly Journal of the Royal Meteorological Society*, n/a–n/a, https://doi.org/
 10.1002/qj.2786, URL https://doi.org/10.1002/qj.2786.

Takacs, L. L., M. J. Suárez, and R. Todling, 2018: The stability of incremental analysis update.
 Monthly Weather Review, 146 (10), 3259–3275, https://doi.org/10.1175/mwr-d-18-0117.1, URL
 https://doi.org/10.1175/mwr-d-18-0117.1.

Teixeira, J., and Coauthors, 2021: *Toward a Global Planetary Boundary Layer Observing System: The NASA PBL Incubation Study Team Report*. NASA PBL Incubation Study Team, URL
 https://science.nasa.gov/earth-science/decadal-pbl.

Todling, R., and A. El Akkraoui, 2018: The GMAO hybrid ensemble-variational atmospheric data
 assimilation system: Version 2.0. GMAO Office Note, NASA Goddard Space Flight Center,
 Greenbelt, MD, USA. URL https://gmao.gsfc.nasa.gov/pubs/docs/Todling1019.pdf.

Todling, R., 2013: Comparing two approaches for assessing observation impact. *Monthly Weather Review*, 141 (5), 1484–1505, https://doi.org/10.1175/mwr-d-12-00100.1, URL https://doi.org/
 10.1175/mwr-d-12-00100.1.

- Todling, R., and Coauthors, 2022: A brief report on recent upgrades to the atmospheric analysis
 of the GMAO hybrid 4denvar system: GEOS-5.27 and GEOS-5.29. NASA Tech Memo, *in preparation*, NASA Goddard Space Flight Center, Greenbelt, MD, USA.
- Trémolet, Y., 2007: First-order and higher-order approximations of observation impact. *Meteorol- ogische Zeitschrift*, 16, 693–694.
- ⁷³⁰ Whitaker, J. S., T. M. Hamill, X. Wei, Y. Song, and Z. Toth, 2008: Ensemble data assimilation with
- the NCEP global forecast system. *Monthly Weather Review*, **136** (2), 463–482, https://doi.org/
- ⁷³² 10.1175/2007MWR2018.1, URL https://doi.org/10.1175/2007MWR2018.1.
- 733 Zhu, Y., and Coauthors, 2016: All-sky microwave radiance assimilation in NCEP's GSI
- ⁷³⁴ analysis system. *Monthly Weather Review*, **144** (**12**), 4709–4735, https://doi.org/10.1175/
- ⁷³⁵ mwr-d-15-0445.1, URL https://doi.org/10.1175/mwr-d-15-0445.1.