Potential sources of a priori ozone profiles for TEMPO

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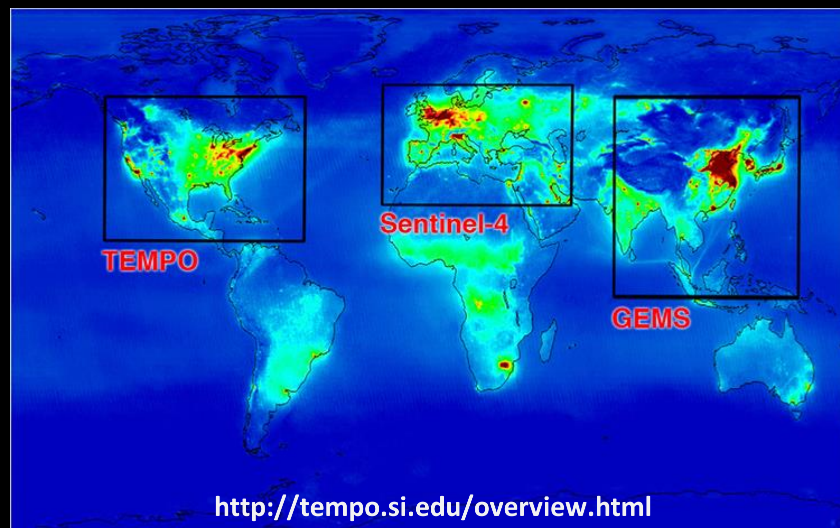
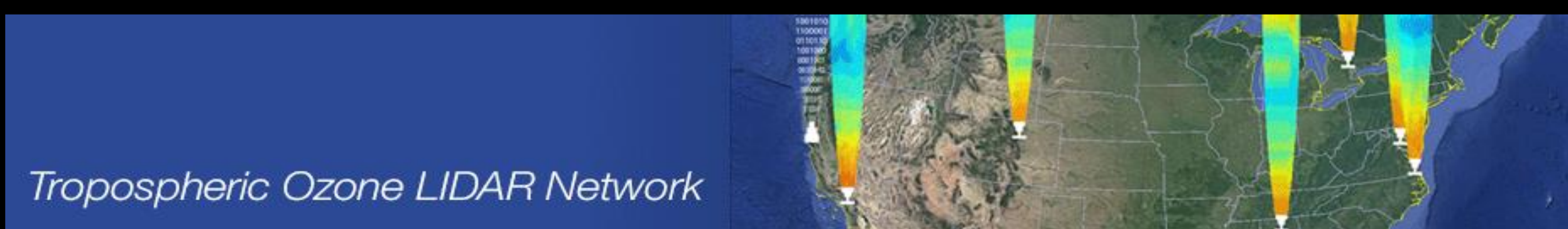


Harvard-Smithsonian Center for Astrophysics
TEMPO Science Team Meeting
May 31 – June 1, 2017



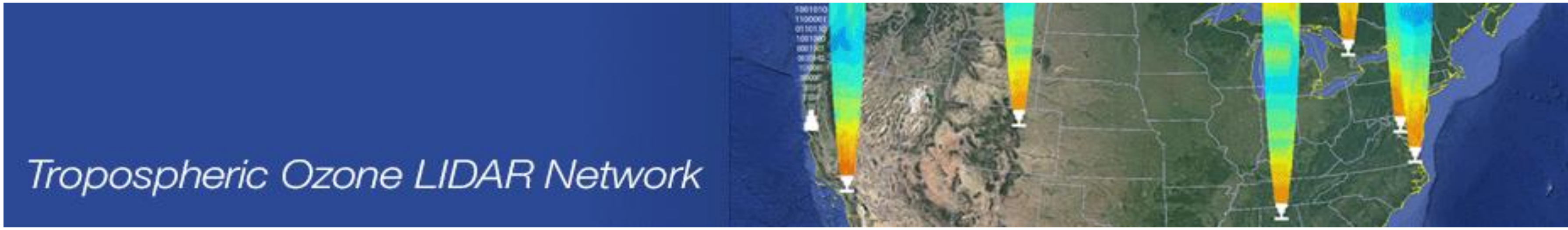
Science Questions and Objectives

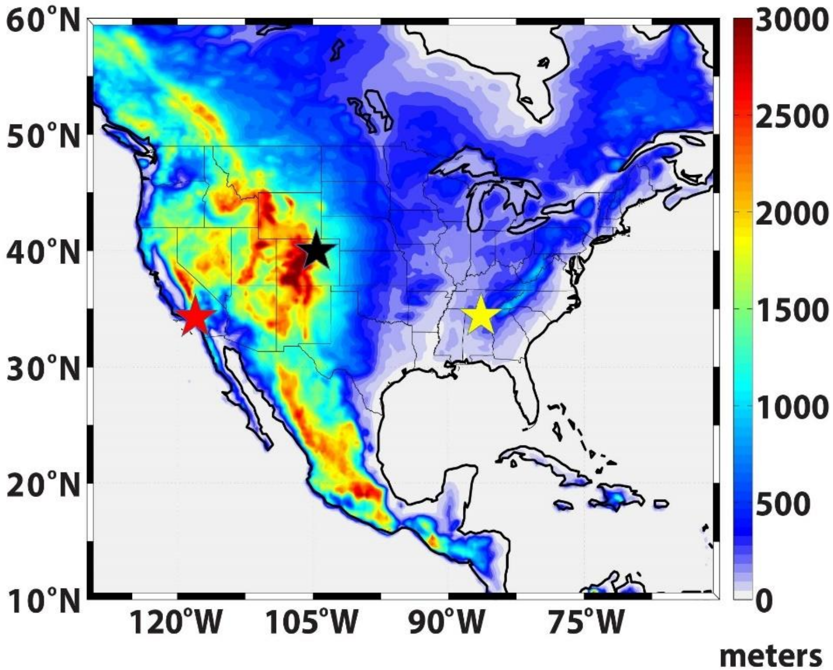
Science/Validation Questions:

1. How well does the suggested a priori ozone (O_3) profile dataset to be used in TEMPO retrievals capture the spatial and temporal variability of tropospheric O_3 in North America?
2. How might different sources of a priori O_3 profiles (e.g., ozonesonde datasets, various models) impact the accuracy of TEMPO retrievals in the troposphere?

Objectives:

1. Demonstrate the utility of TOLNet tropospheric O_3 observations in evaluating/validating TEMPO.
2. Evaluate the accuracy of tropospheric O_3 vertical profiles from the tropopause-based (TB-Clim) and the Labow-Logan-McPeters (LLM) O_3 climatology datasets.
3. Evaluate vertical profile information from two near-real-time (NRT) data assimilation (DAS) models (GEOS-5 FP and MERRA2) and a full chemical transport model (CTM) (GEOS-Chem).
4. Determine the theoretical impact of different a priori profile products on TEMPO O_3 retrievals (Xr) in the troposphere (0-10 km) and at the surface (0-2 km).





Location of the GSFC TROPOZ (black star), JPL TMF (red star), and the UAH RO3QET (yellow star) TOLNet observation sites during the summer of 2014.

TOLNet System	Latitude (°N)	Longitude (°W)	Elevation (m)[a]	# of observations[b]
TROPOZ	40.6	105.1	1569.0	21
JPL TMF	34.4	117.7	2285.0	26
RO3QET	34.7	86.6	206.0	12

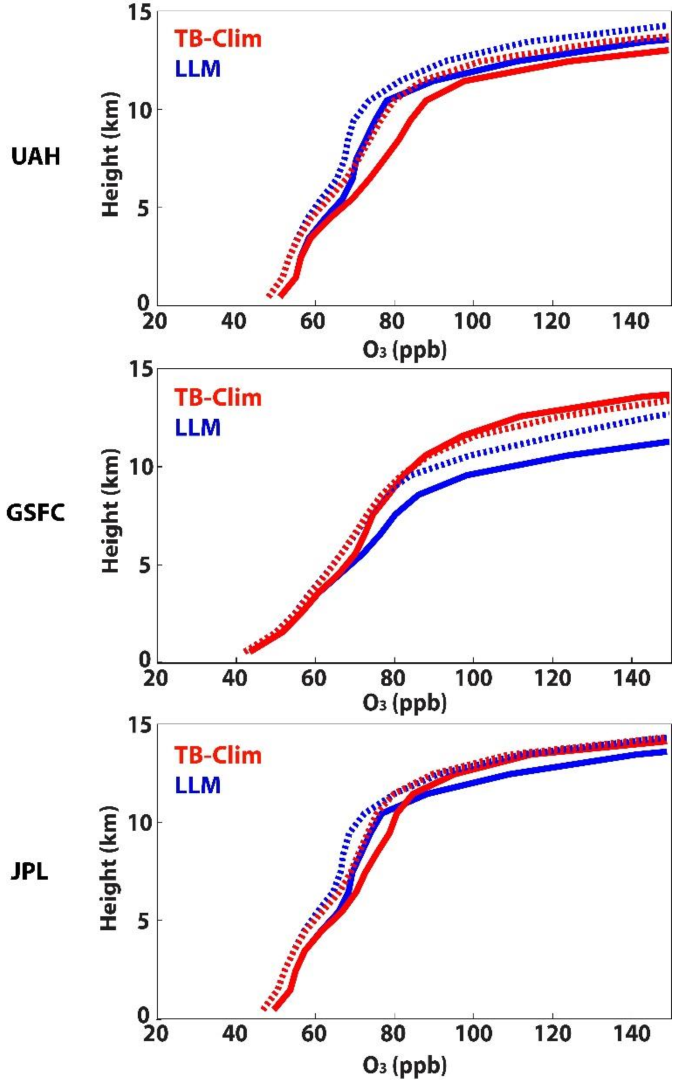
[a] Elevation of the topography above sea level.
[b] Number of days of lidar observations between July – August 2014.

- **TOLNet sites selected due to data availability and to represent regions of North America with differing topography, meteorology, and atmospheric chemistry conditions.**
- **The TROPOZ and JPL TMF lidars provide data from near the surface to ~10 km above ground. The RO3QET lidar system provides O_3 data from 0-5 km during the summer of 2014.**

TOLNet data is applied in this study to:

1) **evaluate a priori O_3 profile datasets to be, or potentially be, used in TEMPO retrievals.**
2) **represent the "true" atmospheric O_3 profile in theoretical TEMPO Xr calculations.**

TB-Clim and LLM O_3 Profiles



Profiles of O_3 (ppb) from TB-Clim and LLM at the location of the UAH RO3QET, GSFC TROPOZ, and JPL TMF TOLNet sites for July (solid lines) and August (dashed lines).

- TB-Clim climatological dataset (currently suggested to be used in TEMPO O_3 profile retrievals)
  - based on 51,736 ozonesondes.
  - monthly-averaged profiles with 1 km vertical resolution in 18 10° latitude bins.
  - TB-Clim profiles were derived applying daily-averaged GEOS-5 FP tropopause heights.
- LLM climatological dataset (used in OMI O_3 profile retrievals)
  - based on 23,400 ozonesondes and satellite data.
  - monthly-averaged profiles with 1 km vertical resolution in 18 10° latitude bins.
- Both a priori datasets have similar shape and magnitudes throughout the troposphere and have identical values in the first 2 km above the surface.

* TB-Clim and LLM profiles are vertically sampled to match the TEMPO averaging kernel and interpolated using a 3rd order polynomial fit.

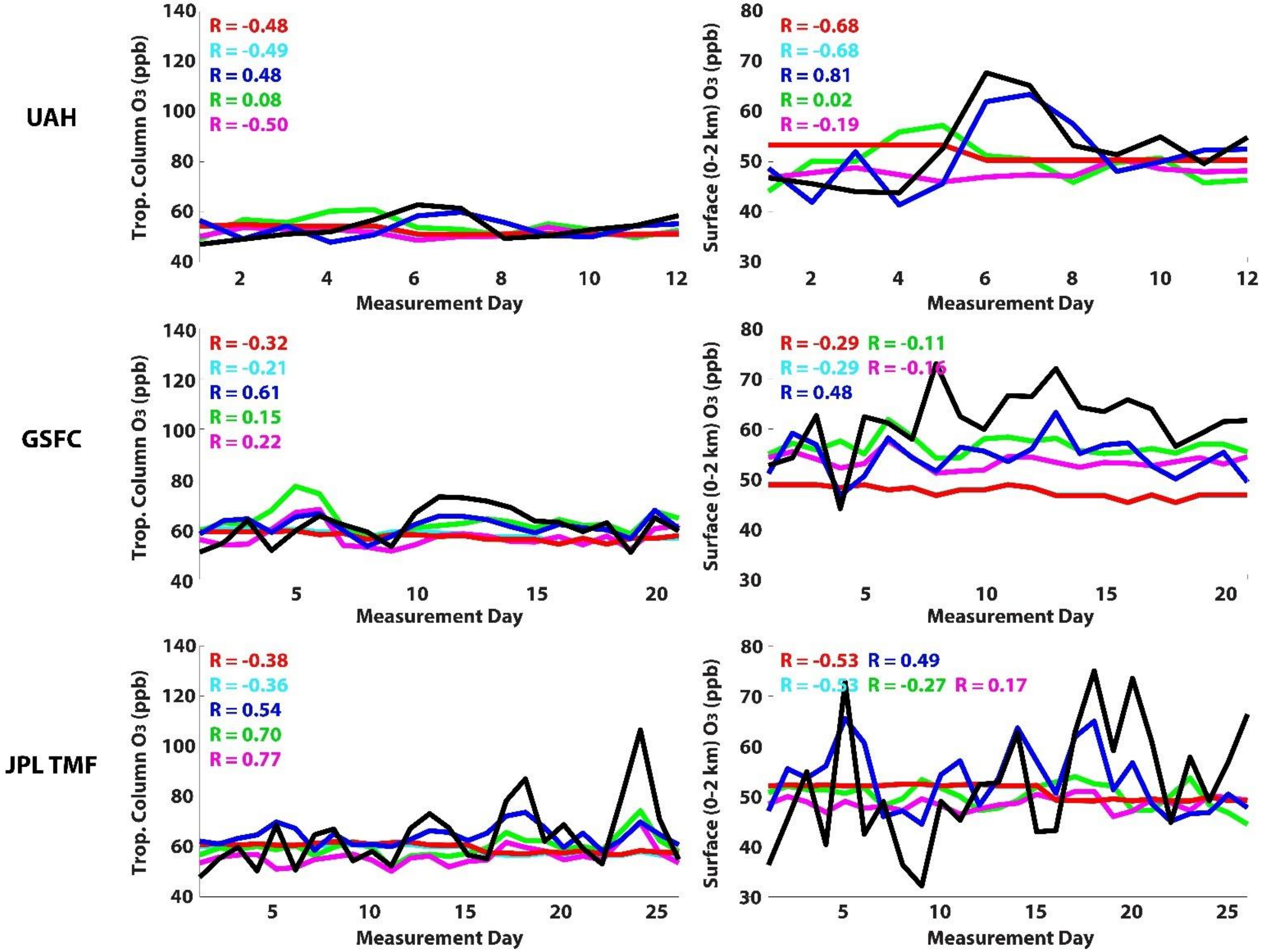
Models Used for O_3 Profile Information

1. GEOS-5 FP (v1.1)
   - operational product from NASA's Global Modeling and Assimilation Office (GMAO) GEOS-5 atmospheric general circulation model (AGCM) and data assimilation system (DAS)
   - 0.25° × 0.3125° spatial resolution and 72 hybrid terrain following vertical levels
   - assimilates roughly 2×10^6 observations for each analysis
   - highly simplified atmospheric chemistry and no surface emissions

2. MERRA version 2 (MERRA2)
   - reanalysis product produced using the NASA GMAO GEOS-5 AGCM
   - 0.50° × 0.667° spatial resolution and 72 hybrid terrain following vertical levels
   - assimilates roughly 2×10^6 observations for each analysis
   - highly simplified atmospheric chemistry and no surface emissions

3. GEOS-Chem (v9-01-03)
   - applied in this work as a proxy for full chemistry CTMs or air quality models
   - purpose of this work is not to evaluate the performance of the GEOS-Chem model, or to suggest GEOS-Chem as the only model with the ability to provide a priori information in TEMPO O_3 retrievals
   - 0.25° × 0.3125° spatial resolution and 47 hybrid terrain following vertical levels
   - state-of-the-art atmospheric chemistry modules and surface emissions data

Daily-averaged Time-series Evaluation



Time-series of daily-averaged tropospheric and surface column O_3 (ppb) from the TB-Clim, LLM, GEOS-5 FP, MERRA2, GEOS-Chem, and TOLNet at the location of UAH RO3QET, GSFC TROPOZ, and JPL TMF.

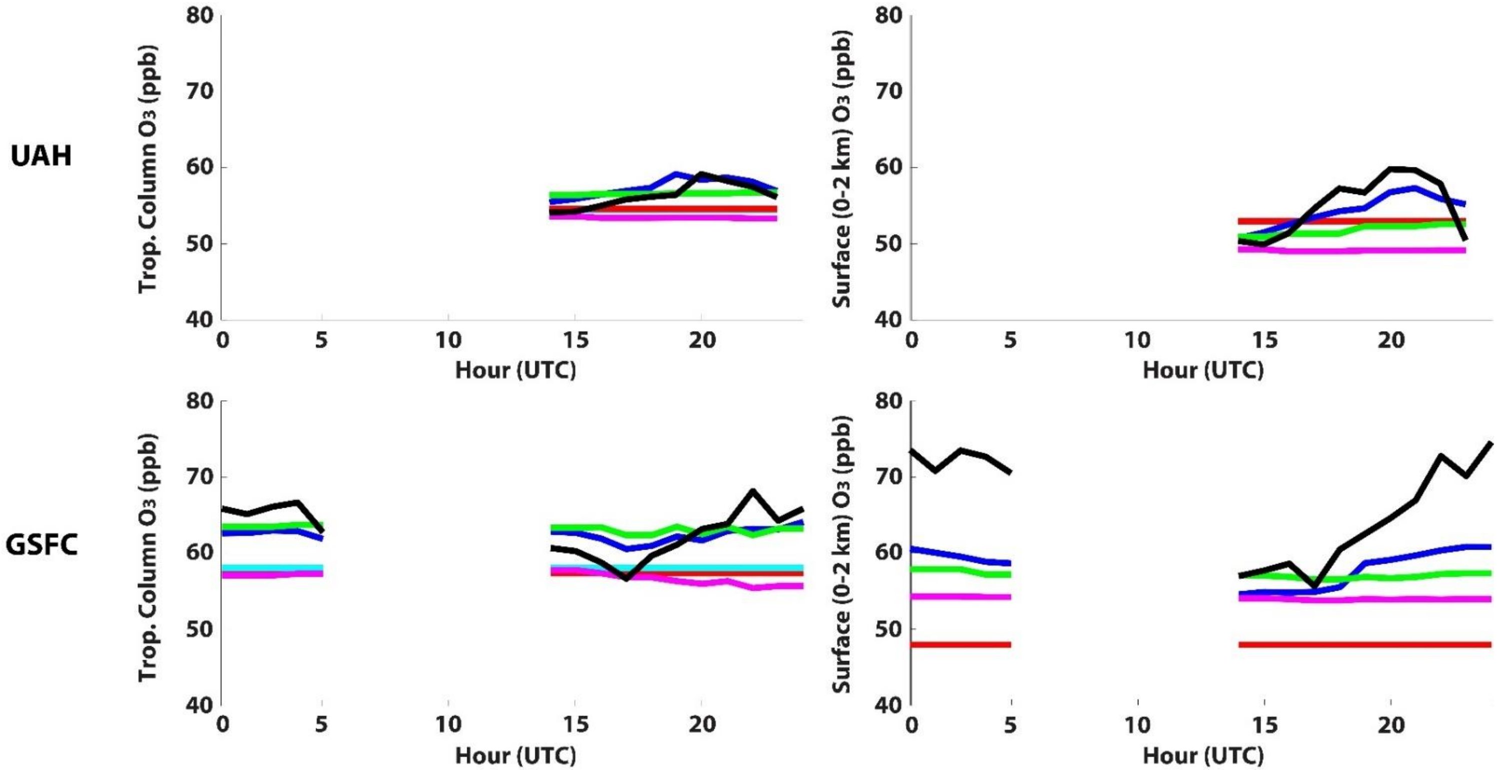
- Large tropospheric/surface O_3 daily variability observed by GSFC and JPL systems.
- Due to climatological datasets (TB-Clim and LLM) having constant monthly O_3 values, they can not replicate the daily variability of observed tropospheric and surface O_3.

Daily-averaged Time-series Evaluation

RO3QET	TB-Clim	LLM	GEOS-5 FP	MERRA2	GEOS-Chem
			Tropospheric Column O_3 (0-5 km)		
Correlation (R)	-0.48	-0.49	0.08	-0.50	0.49
Bias ± 1σ (ppb)	-1.3 ± 6.1	-1.5 ± 6.1	0.4 ± 6.1	-2.3 ± 6.0	1.1 ± 4.6
RMSE (ppb)	5.97	5.97	5.81	6.21	4.57
			Surface-level O_3 (0-2 km)		
Correlation (R)	-0.68	-0.68	0.02	-0.19	0.82
Bias ± 1σ (ppb)	-0.9 ± 8.8	-0.9 ± 8.8	-2.7 ± 8.5	-4.7 ± 7.9	-1.3 ± 4.5
RMSE (ppb)	8.47	8.47	8.58	8.93	4.49
TROPOZ	**TB-Clim**	**LLM**	**GEOS-5 FP**	**MERRA2**	**GEOS-Chem**
			Tropospheric Column O_3 (0-10 km)		
Correlation (R)	-0.32	-0.21	0.15	0.22	0.61
Bias ± 1σ (ppb)	-4.4 ± 7.4	-3.7 ± 7.4	1.6 ± 7.8	-4.7 ± 7.2	-0.2 ± 5.4
RMSE (ppb)	8.50	8.11	7.75	8.49	5.28
			Surface-level O_3 (0-2 km)		
Correlation (R)	-0.29	-0.29	-0.11	-0.16	0.59
Bias ± 1σ (ppb)	-14.0 ± 6.8	-14.0 ± 6.8	-4.9 ± 6.8	-8.0 ± 6.8	-7.5 ± 5.1
RMSE (ppb)	16.05	16.05	8.29	10.35	9.32
JPL TMF	**TB-Clim**	**LLM**	**GEOS-5 FP**	**MERRA2**	**GEOS-Chem**
			Tropospheric Column O_3 (0-10 km)		
Correlation (R)	-0.38	-0.36	0.70	0.77	0.54
Bias ± 1σ (ppb)	-4.6 ± 13.9	-5.3 ± 13.9	-4.2 ± 10.6	-8.1 ± 10.4	0.2 ± 11.4
RMSE (ppb)	14.42-0.53	14.62	11.22	12.97	11.21
			Surface-level O_3 (0-2 km)		
Correlation (R)	-0.53	-0.53	-0.27	0.17	0.49
Bias ± 1σ (ppb)	-1.7 ± 12.7	-1.7 ± 12.7	-2.3 ± 12.7	-3.9 ± 11.7	1.0 ± 10.5
RMSE (ppb)	12.54	12.54	12.67	12.07	10.19

- **All products display low biases at the surface (0-2 km) compared to the GSFC lidar.**
- **CTM predictions generally capture the daily-variability of TOLNet observations most accurately, but not always.**

Hourly-averaged Time-series Evaluation



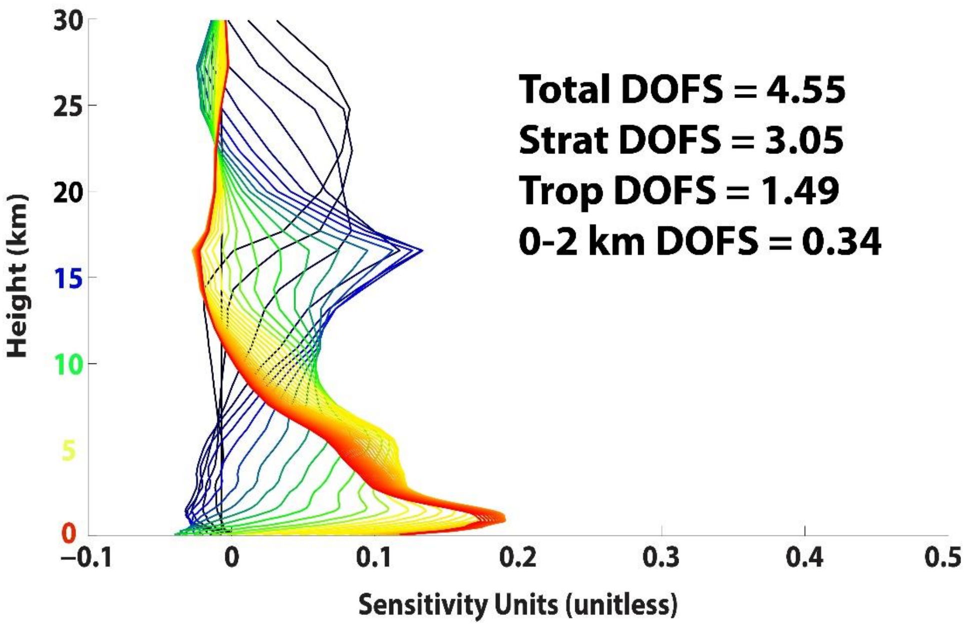
Diurnal time-series of hourly-averaged tropospheric and surface column averaged O_3 from the TB-Clim, LLM, GEOS-5 FP, MERRA2, GEOS-Chem, and TOLNet at the locations of UAH and GSFC sites

- **Climatological datasets (TB-Clim and LLM) currently have constant daily O_3 values, therefore are unable to reproduce observed diurnal variability.**
- **Forward model CTM predictions have highest correlation, lowest mean biases and bias standard deviations, and lowest RMSE values.**
- **Large low mean biases (> 8 ppb) from all products at the surface compared to GSFC TOLNet observations with largest low biases in the afternoon hours (3pm to 8pm MDT).**

TEMPO Tropospheric O_3 Calculations

$$X_r = X_a + A(X_t - X_a) + \varepsilon$$

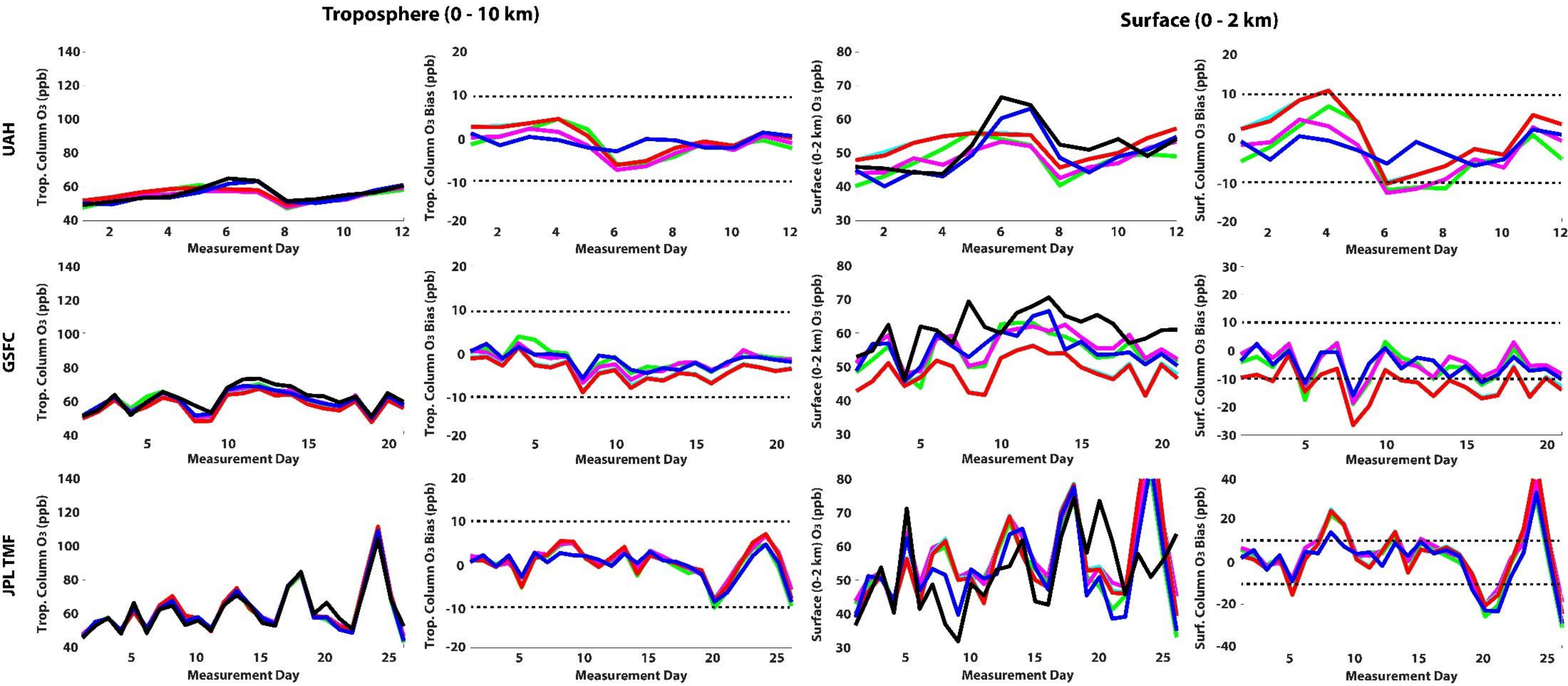
- Optimal estimation is used to calculate theoretical TEMPO profiles (Xr).
- Xa is the a priori profile, A is the averaging kernel, Xt is the true O_3 profile, and ε is the instrument noise.
- ε is neglected during this study



Normalized averaging kernel for UV+VIS wavelengths (290-345 nm, 540-650 nm) from the surface to 30 km at the UAH RO3QET TOLNet site.

- UV+VIS wavelengths to be used in TEMPO O_3 retrievals have enhanced sensitivity in the lower troposphere.
- Degrees of Freedom (DOFS) are a factor of 2 larger near the surface (0–2 km) compared to just UV wavelengths.
- 0–2 km O_3 will be a standard TEMPO product and will provide important information for air quality monitoring.

Daily Tropospheric Column and Surface Xr



Time-series of daily-averaged tropospheric and surface column O_3 Xr values (ppb) when using TB-Clim, LLM, GEOS-5 FP, MERRA2, and GEOS-Chem profiles as a priori information compared to TOLNet at the location of UAH RO3QET, GSFC TROPOZ, and JPL TMF.

- Tropospheric Xr profiles are well constrained using all a priori profile sources.
- Large differences in surface (0-2 km) Xr values are predicted when using different sources of a priori profiles.
- Daily-averaged Xr values at the surface exceed the desired ± 10% threshold.

Daily Tropospheric Column and Surface Xr

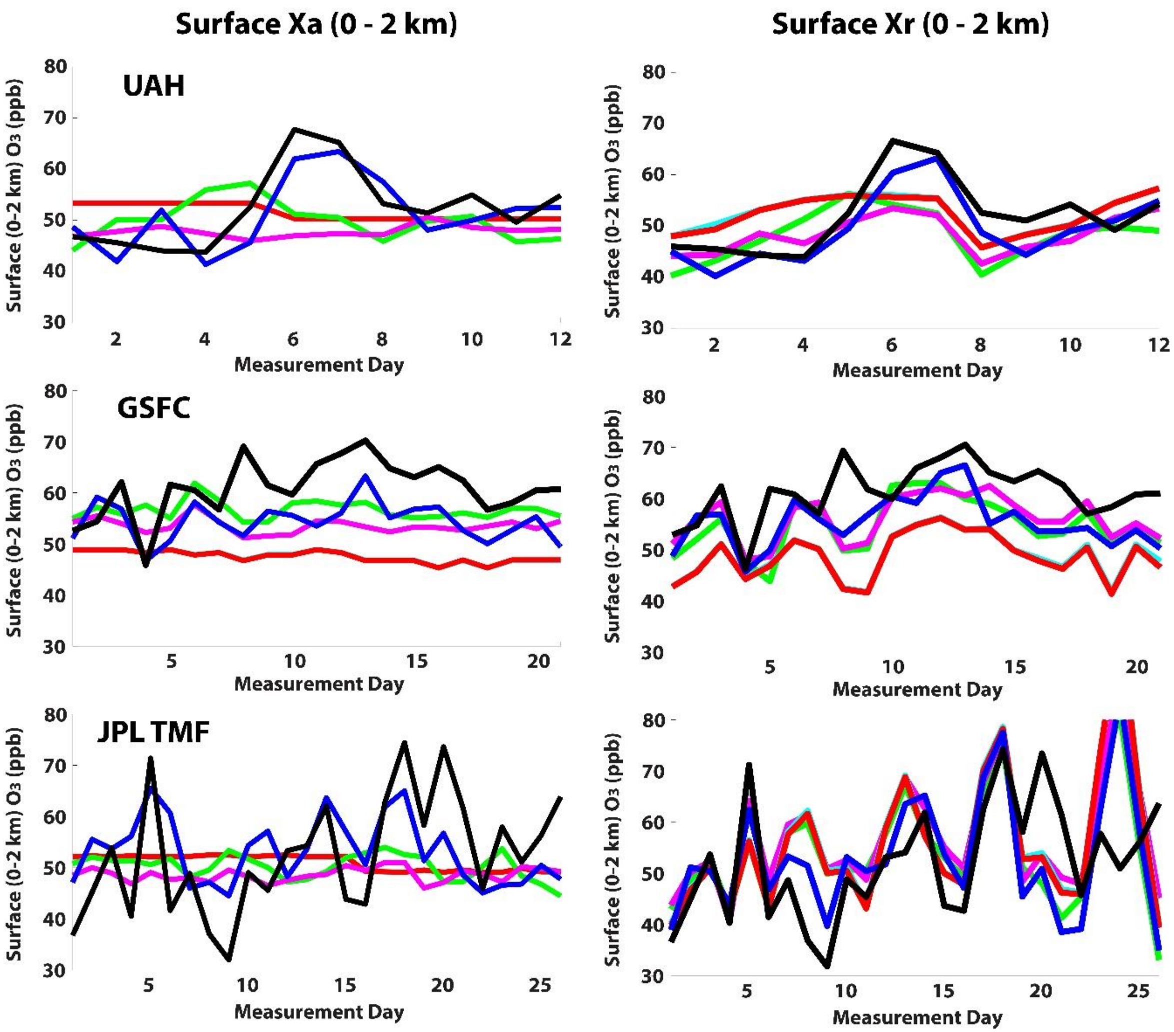
RO3QET	TB-Clim	LLM	GEOS-5 FP	MERRA2	GEOS-Chem
			Tropospheric Column O_3 (0-5 km)		
Bias ± 1σ (ppb)	-0.2 ± 3.4	-0.1 ± 3.4	-1.3 ± 3.3	-1.7 ± 3.0	-0.8 ± 1.5
RMSE (ppb)	3.28	3.28	3.42	3.39	1.66
10 ppb error exceed.	0	0	0	0	0
			Surface-level O_3 (0-2 km)		
Bias ± 1σ (ppb)	0.3 ± 7.0	-0.2 ± 7.0	-3.8 ± 6.5	-3.7 ± 5.8	-2.5 ± 2.9
RMSE (ppb)	6.71	6.71	7.32	6.69	3.75
10 ppb error exceed.	2	2	3	2	0

TROPOZ	TB-Clim	LLM	GEOS-5 FP	MERRA2	GEOS-Chem
			Tropospheric Column O_3 (0-10 km)		
Bias ± 1σ (ppb)	-4.2 ± 2.5	-4.0 ± 2.5	-1.4 ± 2.5	-2.1 ± 2.3	-1.8 ± 2.1
RMSE (ppb)	4.84	4.63	2.86	3.08	2.70
10 ppb error exceed.	0	0	0	0	0
			Surface-level O_3 (0-2 km)		
Bias ± 1σ (ppb)	-12.6 ± 5.5	-12.4 ± 5.5	-6.5 ± 6.0	-5.1 ± 5.5	-5.8 ± 4.7
RMSE (ppb)	13.70	13.46	8.72	7.46	7.42
10 ppb error exceed.	15	14	5	3	5

JPL TMF	TB-Clim	LLM	GEOS-5 FP	MERRA2	GEOS-Chem
			Tropospheric Column O_3 (0-10 km)		
Bias ± 1σ (ppb)	0.5 ± 3.9	0.6 ± 3.9	-0.1 ± 4.0	0.8 ± 3.4	-0.1 ± 3.5
RMSE (ppb)	3.86	3.83	3.97	3.48	3.40
10 ppb error exceed.	0	0	1	0	0
			Surface-level O_3 (0-2 km)		
Bias ± 1σ (ppb)	3.5 ± 14.5	3.9 ± 14.5	1.8 ± 13.6	4.7 ± 12.4	0.9 ± 12.6
RMSE (ppb)	14.70	14.70	13.44	13.06	12.41
10 ppb error exceed.	9	9	9	10	7

- Tropospheric and surface Xr values generally have smaller biases (and bias standard deviations) and RMSE values in comparison to Xa profiles.
- Climatological datasets lead to the most, and CTM predictions lead to the least, occurrences of error exceeding the desired ± 10% threshold.

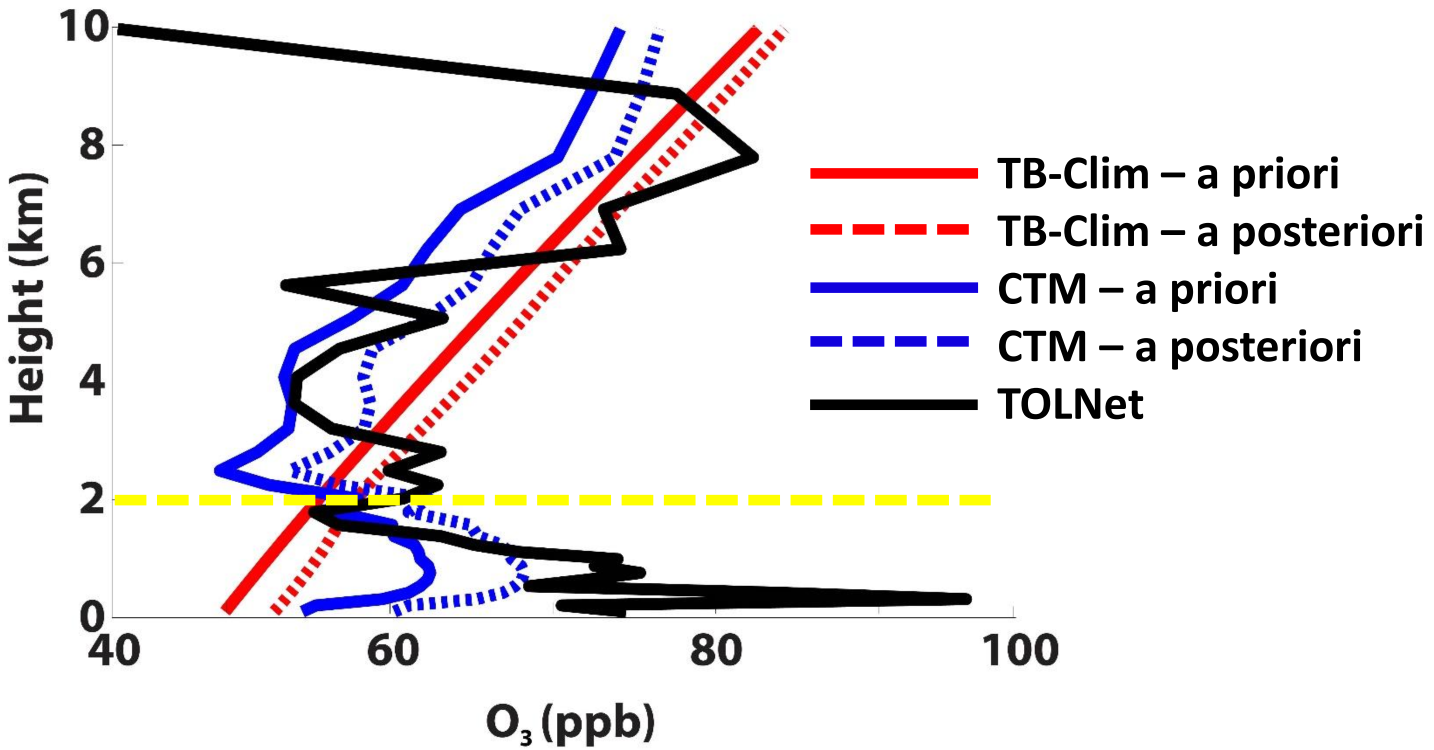
Daily Surface Xa and Xr Time-series



Time-series of daily-averaged surface column Xa and Xr O_3 (ppb) from the TB-Clim, LLM, GEOS-5 FP, MERRA2, GEOS-Chem and TOLNet at the location of UAH RO3QET, GSFC TROPOZ, and JPL TMF.

- **In general, surface Xr values replicate TOLNet observations better in comparison to Xa.**
- **Xr values have much larger daily variability in comparison to Xa values.**
- **When large daily 0-2 km O_3 (>65 ppb) is observed, Xr values using GEOS-Chem a priori profiles have smallest biases 60% of occurrences, followed by MERRA2 (30%) and GEOS-5 FP (10%).**
- ***What is happening when surface Xr values demonstrate large (>20 ppb) errors at the JPL TMF location?***

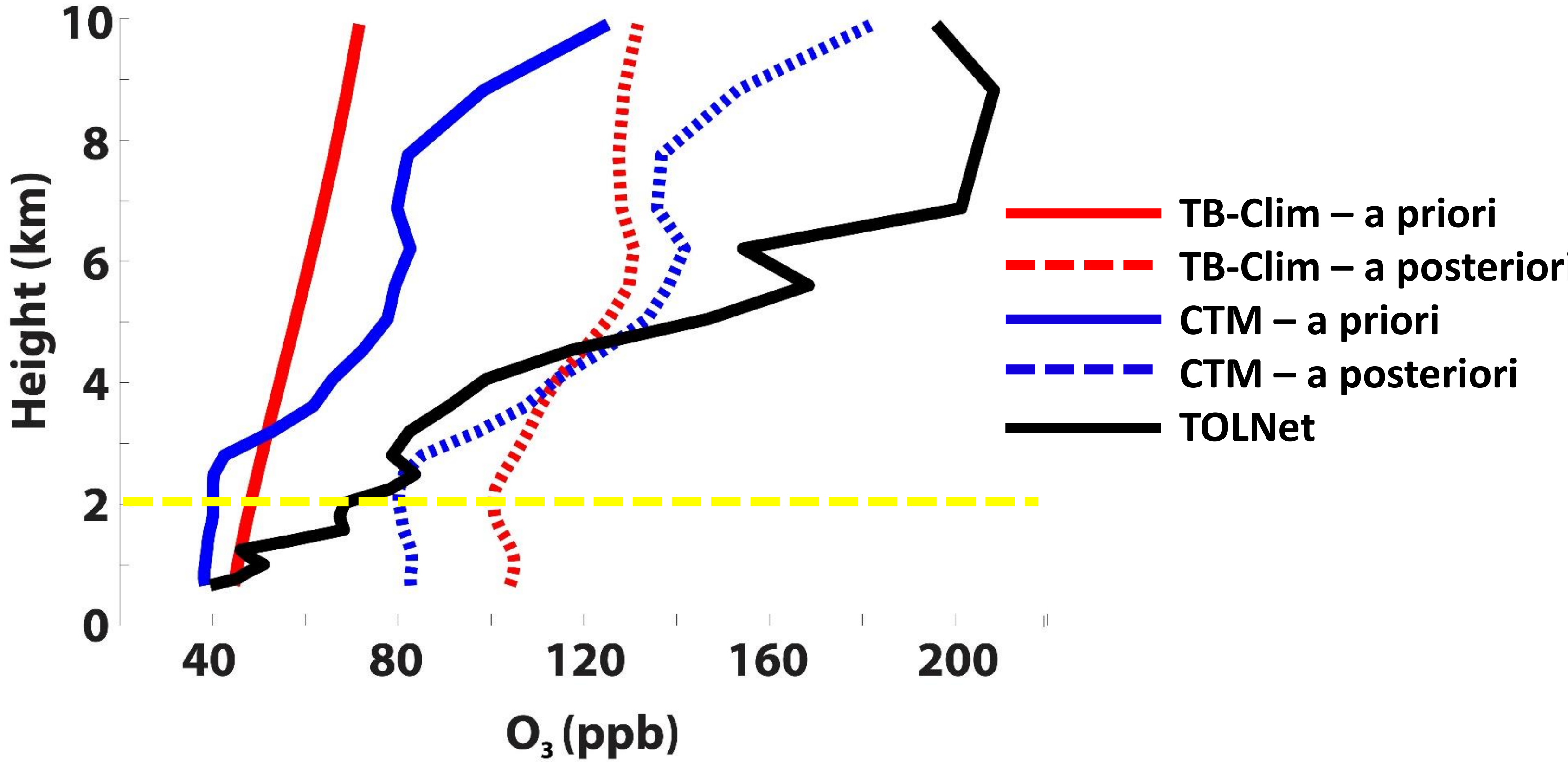
Boundary Layer Enhancement Case



Daily-averaged Xa (solid line) and Xr (dashed lines) O_3 profiles from TB-Clim and GEOS-Chem compared to TOLNet observations at the location of JPL TMF on 20140708.

- Large PBL enhancement (up to ~100 ppb) observed by TOLNet.
- Tropospheric column Xa values from CTM predictions and TB-Clim are both low compared to TOLNet, but CTM a priori profile captures the PBL O_3 enhancement shape.
- TEMPO surface Xr values using the CTM a priori (65.6 ppb) profile compares better to TOLNet at the surface (72.5 ppb) compared to when using the TB-Clim (54.4 ppb) profile.

Stratospheric Intrusion Case



Daily-averaged Xa (solid line) and Xr (dashed lines) O_3 profiles from TB-Clim and GEOS-Chem compared to TOLNet observations at the location of JPL TMF on 20140821.

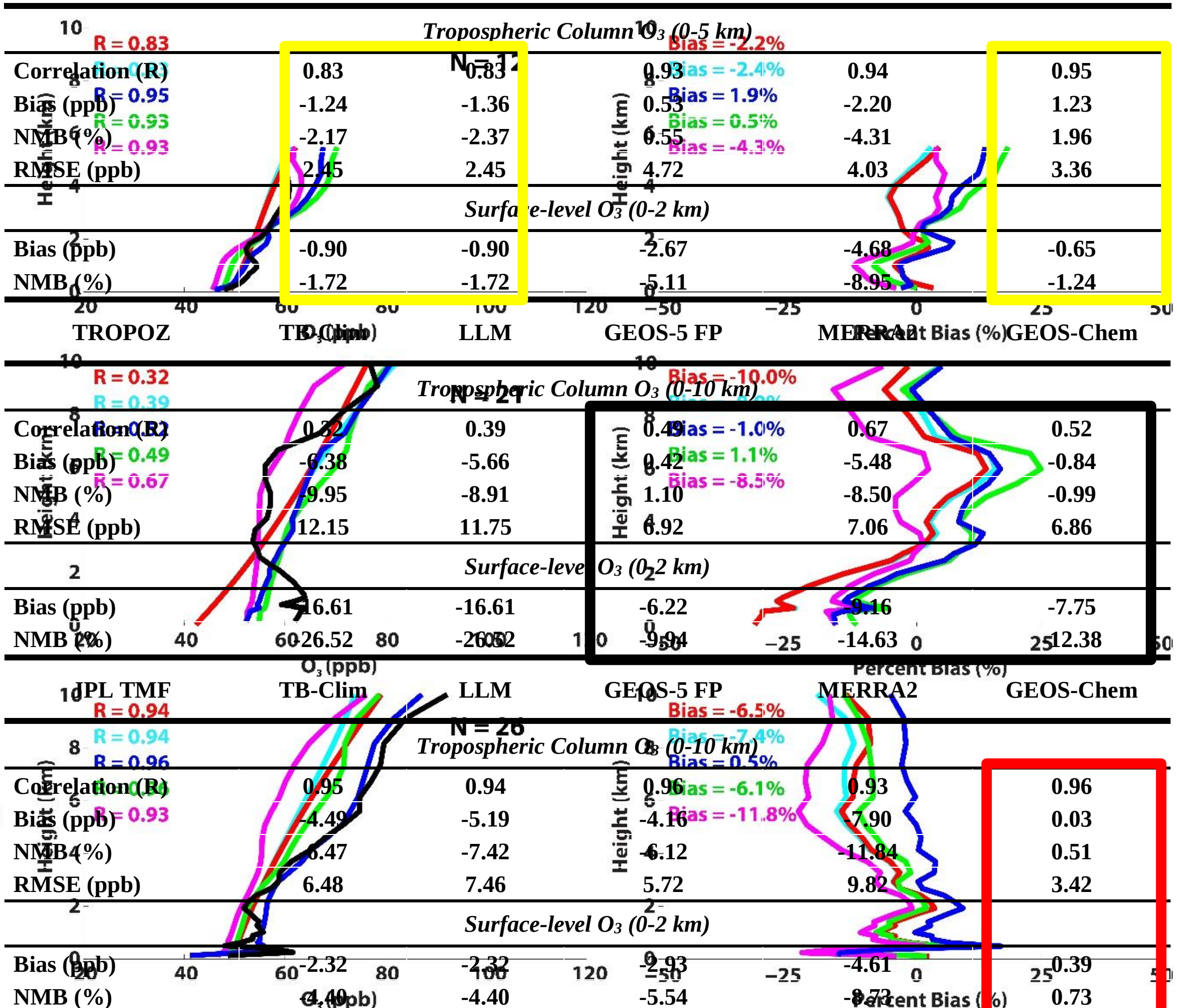
- Large STE event (~200 ppb) observed by TOLNet.
- Tropospheric column Xa values from CTM predictions and TB-Clim are both very low compared to TOLNet, but CTM a priori profile displays some characteristics of the STE.
- TEMPO surface Xr value using CTM a priori (83.2 ppb) and TB-Clim (99.4 ppb) profiles are much higher than TOLNet (48.9 ppb) due to over-correction caused by the large low bias of Xa profiles in the free/upper troposphere.

Conclusions and Next Steps

- TOLNet tropospheric O_3 observations are used to evaluate a priori profiles which could be used in TEMPO retrievals.
- CTM predictions (GEOS-Chem) generally reproduce the spatio-temporal variability of observed O_3 in comparison to DAS models (GEOS-5 FP and MERRA2) and climatological O_3 datasets (TB-Clim and LLM).
- The ability of CTM predictions to better replicate daily and diurnal variability of vertical O_3 profiles results (on average) in more accurate TEMPO retrievals in the troposphere (0-10 km) and the surface (0-2 km).
- A priori profile shape is critical in order to accurately retrieve tropospheric and surface-level O_3.
- Potential next steps:
  1. Determine if forward model data can be trusted in TEMPO retrievals.
  2. Perform inter-model comparison to determine what model, or models, would be most trusted.
  3. Develop an operational DAS CTM to provide a priori data?
  4. Can we produce a "look-up" table of a priori profile shapes/magnitudes to be chosen based on real-time meteorology/chemistry observations?
  5. Explore the many other methods to produce accurate a priori profiles.

EXTRA SLIDES

Summer-time Vertical Profile Evaluation



UAH (N = 12)

	TB-Clim	LLM	GEOS-5 FP	MERRA2	GEOS-Chem
Tropospheric Column O_3 (0-5 km)					
Correlation (R)	0.83	0.83	0.93	0.94	0.95
Bias (ppb)	-1.24	-1.36	0.53	-2.20	1.23
NMB (%)	-2.17	-2.37	0.55	-4.31	1.96
RMSE (ppb)	2.45	2.45	4.72	4.03	3.36
Surface-level O_3 (0-2 km)					
Bias (ppb)	-0.90	-0.90	-2.67	-4.68	-0.65
NMB (%)	-1.72	-1.72	-5.11	-8.95	-1.24

GSFC (N = 21)

TROPOZ	TB-Clim	LLM	GEOS-5 FP	MERRA2	GEOS-Chem
Tropospheric Column O_3 (0-10 km)					
Correlation (R)	0.32	0.39	0.49	0.67	0.52
Bias (ppb)	-6.38	-5.66	0.42	-5.48	-0.84
NMB (%)	-9.95	-8.91	1.10	-8.50	-0.99
RMSE (ppb)	12.15	11.75	6.92	7.06	6.86
Surface-level O_3 (0-2 km)					
Bias (ppb)	-16.61	-16.61	-6.22	-9.16	-7.75
NMB (%)	-26.52	-26.52	-9.94	-14.63	-12.38

JPL TMF (N = 26)

JPL TMF	TB-Clim	LLM	GEOS-5 FP	MERRA2	GEOS-Chem
Tropospheric Column O_3 (0-10 km)					
Correlation (R)	0.95	0.94	0.96	0.93	0.96
Bias (ppb)	-4.49	-5.19	-4.16	-7.90	0.03
NMB (%)	-6.47	-7.42	-6.12	-11.84	0.51
RMSE (ppb)	6.48	7.46	5.72	9.82	3.42
Surface-level O_3 (0-2 km)					
Bias (ppb)	-2.32	-2.32	-2.93	-4.61	0.39
NMB (%)	-4.40	-4.40	-5.54	-8.72	0.73

Summer-time averaged O_3 from TB-Clim, LLM, GEOS-5 FP, MERRA2, GEOS-Chem, and TOLNet at the locations of UAH RO3QET, GSFC TROPOZ, and JPL TMF.

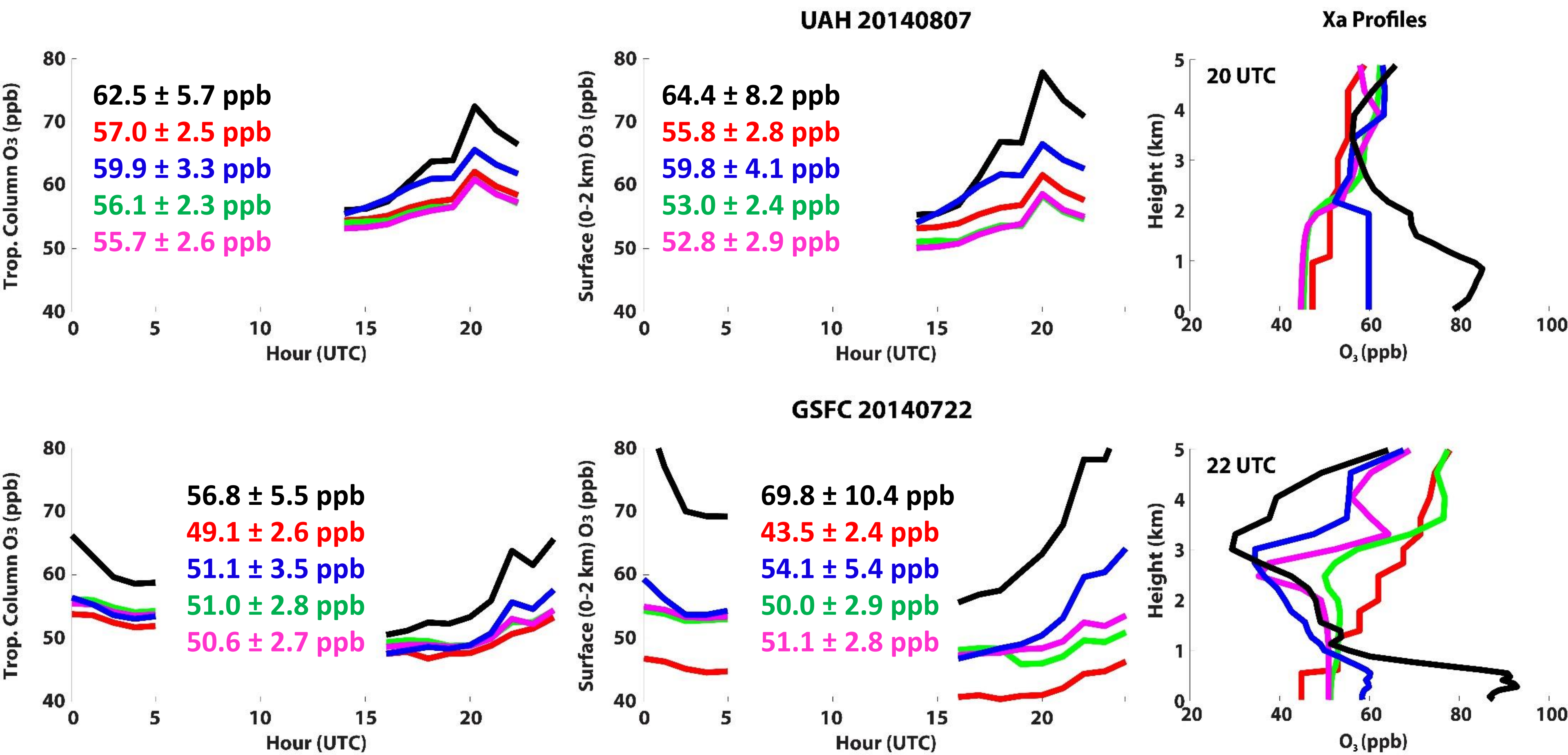
- TB-Clim, LLM, and GEOS-Chem perform best at UAH TOLNet site location.
- All profile sources demonstrate a low bias compared to the GSFC TROPOZ lidar but modeled (GEOS-5 FP and CTM predictions) profiles compare best.
- CTM predictions reproduce TOLNet observations most accurately at JPL TMF.

Hourly-averaged Time-series Evaluation

RO3QET	TB-Clim	LLM	GEOS-5 FP	MERRA2	GEOS-Chem
Tropospheric Column O_3 (0-5 km)					
Correlation (R)	0	0	0.68	-0.57	0.85
Bias ± 1σ (ppb)	-1.7 ± 1.7	-1.9 ± 1.7	0.3 ± 1.6	-2.8 ± 1.7	1.0 ± 0.9
RMSE (ppb)	2.35	2.45	1.52	3.27	1.37
Surface-level O_3 (0-2 km)					
Correlation (R)	0	0	0.57	-0.36	0.82
Bias ± 1σ (ppb)	-1.8 ± 4.0	-1.8 ± 4.0	-3.0 ± 3.6	-5.7 ± 4.0	-0.6 ± 2.5
RMSE (ppb)	4.19	4.19	4.57	6.84	2.44
TROPOZ	**TB-Clim**	**LLM**	**GEOS-5 FP**	**MERRA2**	**GEOS-Chem**
Tropospheric Column O_3 (0-10 km)					
Correlation (R)	0	0.21	0.25	-0.41	0.89
Bias ± 1σ (ppb)	-5.7 ± 3.2	-5.0 ± 3.2	0.1 ± 3.2	-6.3 ± 3.6	-0.6 ± 2.7
RMSE (ppb)	6.51	5.91	3.06	7.22	2.64
Surface-level O_3 (0-2 km)					
Correlation (R)	0	0.26	0.73	0.57	0.74
Bias ± 1σ (ppb)	-18.4 ± 6.8	-18.4 ± 6.8	-9.2 ± 6.5	-12.3 ± 6.7	-8.1 ± 4.7
RMSE (ppb)	19.52	19.52	11.14	13.92	9.31

- **GSFC TOLNet lidar observed large average diurnal variability in surface O_3.**
- **Due to taking into account emissions and atmospheric chemistry, CTM predictions tend to reproduce the diurnal variability of TOLNet observations most accurately.**
- **No a priori O_3 products are able to replicate the large diurnal variability of GSFC lidar O_3 observations near the surface (15-20 ppb).**

Hourly Tropospheric Column and Surface Xr



Case studies of hourly-averaged tropospheric and surface column O_3 Xr values (ppb) when using TB-Clim, LLM, GEOS-5 FP, MERRA2, and GEOS-Chem profiles as a priori information compared to TOLNet at the location of UAH RO3QET and GSFC TROPOZ.

- TOLNet observations display more diurnal variability compared to TEMPO Xr calculations when using all source of a priori profiles.
- Diurnal Xr values compare best to TOLNet when applying CTM predicted a priori profiles.

Suggestions for O_3 Profiles used in TEMPO

1. **Climatologically-averaged ozonesonde profile datasets may not be beneficial for application as a priori information in high spatio-temporal space-based observations of tropospheric O_3.**
2. **CTM (forward model only) predictions on average produce the most accurate TEMPO tropospheric and surface column O_3 retrievals.**
3. **Forward model simulations in CTMs do demonstrate times when they lead to worse TEMPO retrievals in comparison to simple DAS models and climatological datasets.**
   - **Emphasizes the need to use a trusted model.**
   - **Assimilate chemistry observations into CTMs to produce a priori profiles?**
4. **Use real-time remote-sensing and in situ observations of meteorological and chemistry conditions to select a pre-determined a priori profile shape. e.g.:**
   - **Elevated O_3 measurements from surface networks would justify using a profile with a boundary layer enhancement.**
   - **Large UTLS O_3 and low RH from satellites would justify using a profile replicating an STE event.**
5. **Other options?**