Data-Driven Inference and Investigation of Thermosphere Dynamics and Variations

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Major Contributions

- ✓ New methodology for data-driven inference and investigation of thermosphere dynamics and variations.
- ✓ Reduced order modeling and self-consistent calibration using mass and number density observations simultaneously.

Introduction

Modal decomposition or variance reduction methods offer an opportunity for data-driven investigation of thermosphere dynamics and variations and for self-consistent calibration of the thermosphere models. We develop the methodology using the MSIS model and infer oxygen-to-helium transition as a validation by simultaneously assimilating discrete TIMED/GUVI and CHAMP/GRACE observations [1,2,3].

Methodology

We generate hourly model output (snapshots), x_i, for each input sample generated using a latin-hypercube ($F_{10.7} \in [60, 250], A_p \in [0, 50], DOY \in [1, 365]$) to cover the full range of inputs. We use a total of 365 + 8 (corner samples of the latin-hypercube) = 373 samples. A SVD decomposition is performed on the snapshot matrix, $\mathrm{X} = [\mathrm{x}_1, \mathrm{x}_2, \dots, \mathrm{x}_m]$, to derive the optimal set of basis vectors, U ($\mathrm{X} = \mathrm{USV}^T$), for O, O_2, N_2, and He. We do not tune N and H under the assumption that the CHAMP and GRACE observations do not contain any signal about the minor species and that the partial pressure of H is negligible. The spatial basis vectors or modes, U, can then be combined with time-dependent coefficients, c, such that $\mathrm{x}(\mathbf{s}, t) = \sum_{i=1}^{r} c_i(t)\mathrm{U}_i(\mathbf{s})$, where r is the order or rank of truncation. The first ($r = 3$) modes for each species captures more than 98% of the total variance. The coefficients, c, are derived by projecting the data, x, onto the spatial modes, U. We model their daily temporal variations using a sum of three *cosine* terms $c(t) = \sum_{i=1}^{3} a_i \cos(\omega_i t + \zeta_i)$ and fit a, ω, ζ for each mode and species using Gaussian Process Regression for prediction at any new set of inputs.

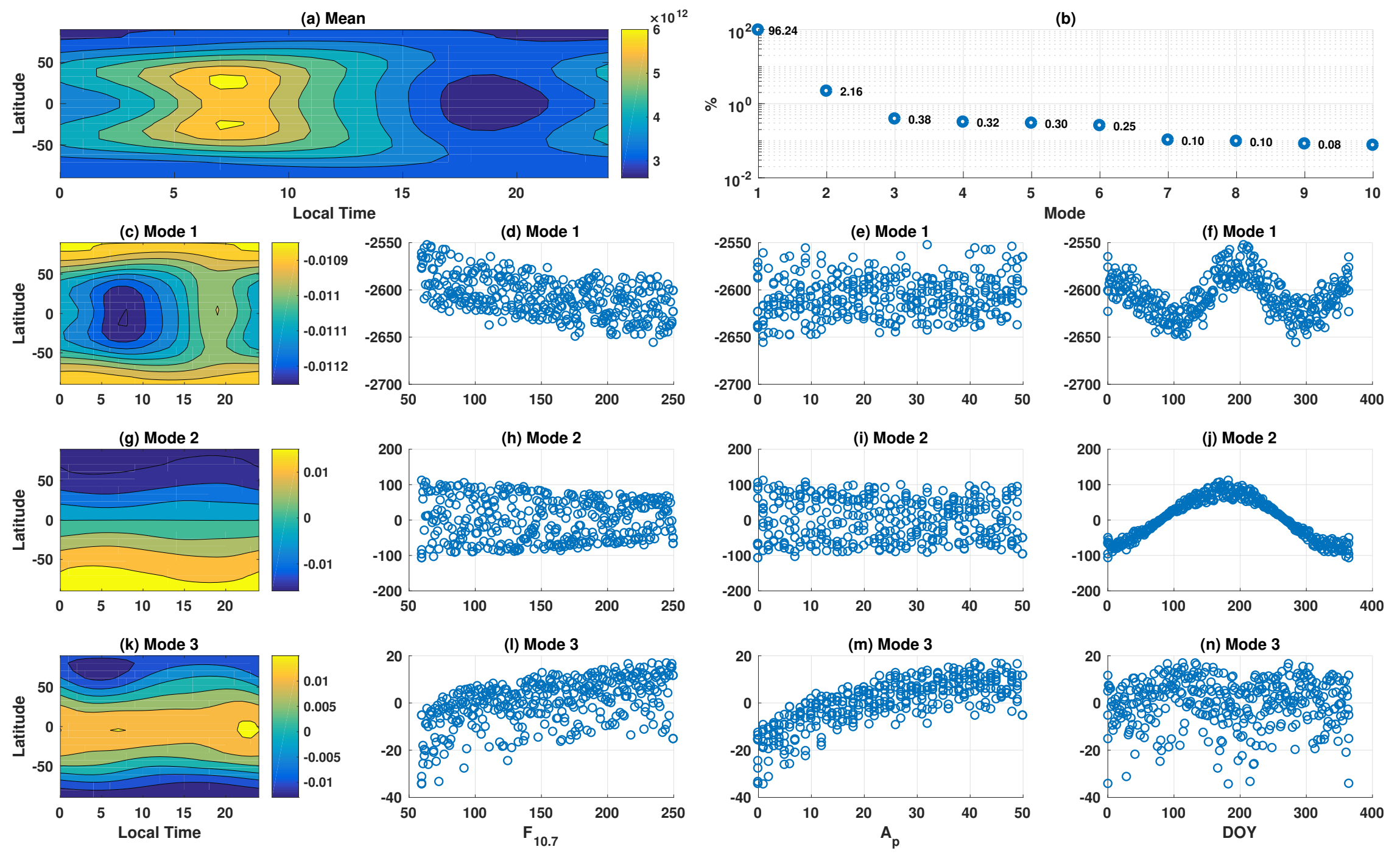

Figure: Mean and first 3 dominant modes for He.

Measurement Intercalibration

Typically, reliable data assimilation requires the observations to be intercalibrated. The CHAMP and GRACE observations are first intercalibrated by multiplying the GRACE densities with a yearly scale factor to match the mean and variance of the observation-to-model ratio.

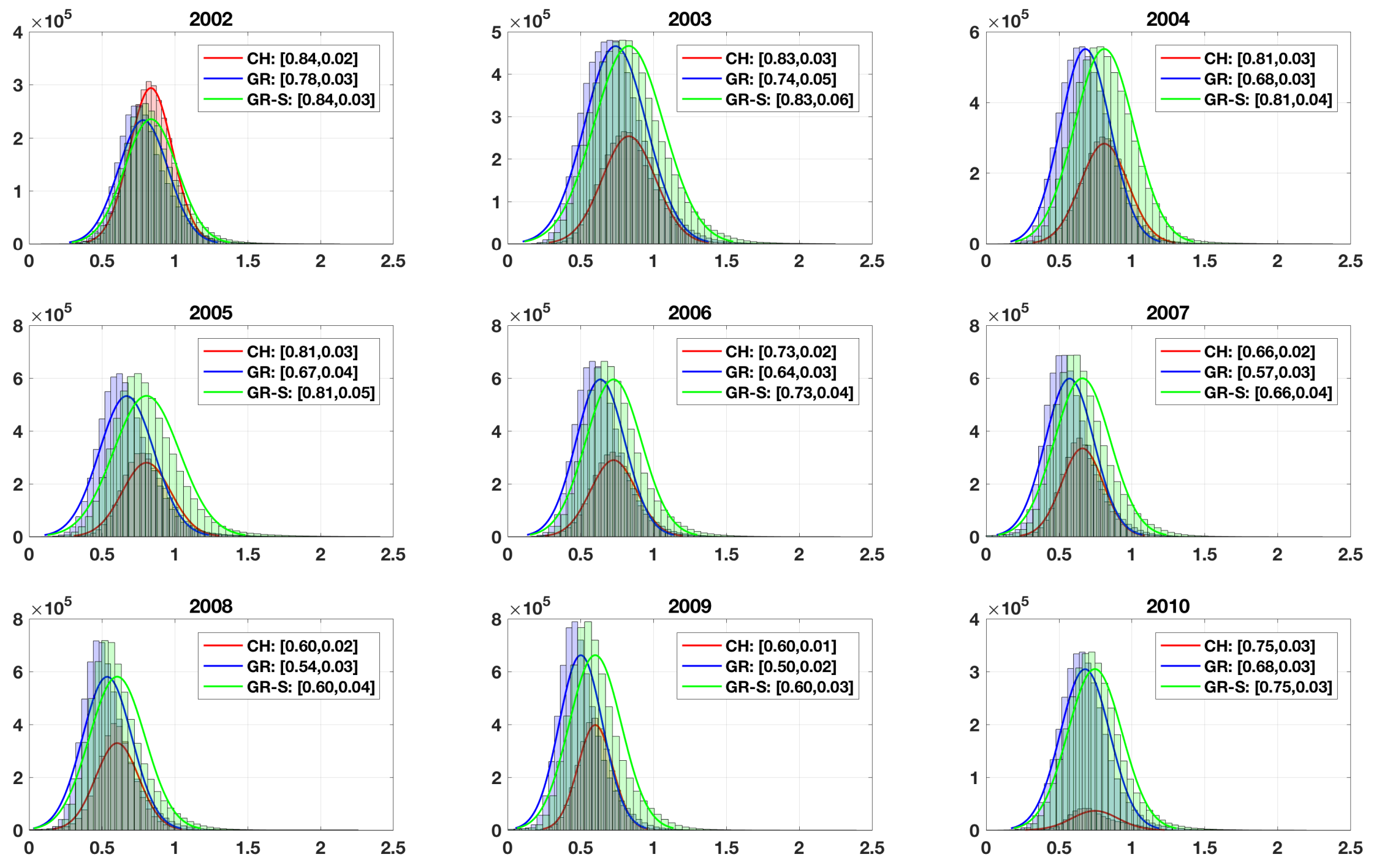

Figure: Observations/MSIS; CH = CHAMP, GR = GRACE, GR-S = GRACE Scaled, [mean,variance].

The GUVI number density and intercalibrated CHAMP/GRACE mass density observations are then calibrated daily to the reference GUVI observation-to-model value (based on mass density computed with O, N_2, and O_2) at ~200 km, where the uncertainties are minimum.

Model or Measurement Calibration?

Intercalibration (IC) of observations accounts for biases with respect to a given model; however, it keeps the calibration from the *true* state by modifying the observations. The real goal is to calibrate the model to the observations, even if it means relaxing certain model assumptions. We first validate the data assimilation process with intercalibrated observations for representative days (2002270 and 2007034 for high and low solar activity, respectively) using 3, 5, and 10 modes. We find that using 5 modes provides optimal results while avoiding overfitting. We then perform assimilation w/o IC of the observations using 5 modes. All results presented are derived using 5 modes.

Table: RMS values. CH: CHAMP, GR: GRACE, GV: GUVI

Assimilate → *Validate* ↓	*CH* (%)	*GR* (%)	*CH+GR* (%)	*GV* (%)	*CH+GV* (%)	*GR+GV* (%)	*CH+GR* +GV (%)
2002270							
CH w/ IC	6.9	10.8	9.7	14.3	8.7	11.7	10.5
GR w/ IC	16.3	10.0	10.1	14.1	15.2	10.8	10.7
CH w/o IC	6.2	12.0	9.1	14.8	9.5	13.5	12.4
GR w/o IC	24.1	9.1	9.3	14.8	17.1	10.5	10.5
2007034							
CH w/ IC	7.5	16.8	10.7	27.6	8.8	16.1	10.7
GR w/ IC	18.1	12.5	13.2	34.5	20.4	12.2	12.5
CH w/o IC	7.0	17.4	9.2	16.8	8.8	15.1	11.3
GR w/o IC	29.1	11.2	11.7	18.4	22.7	11.5	12.1

Oxygen-to-Helium Transition

We use the methodology to infer He dynamics and O-to-He transition. Assimilation shows that the O-to-He transition occurs at significantly lower altitudes, as inferred by Thayer et. al., [4] using CHAMP and GRACE observations.

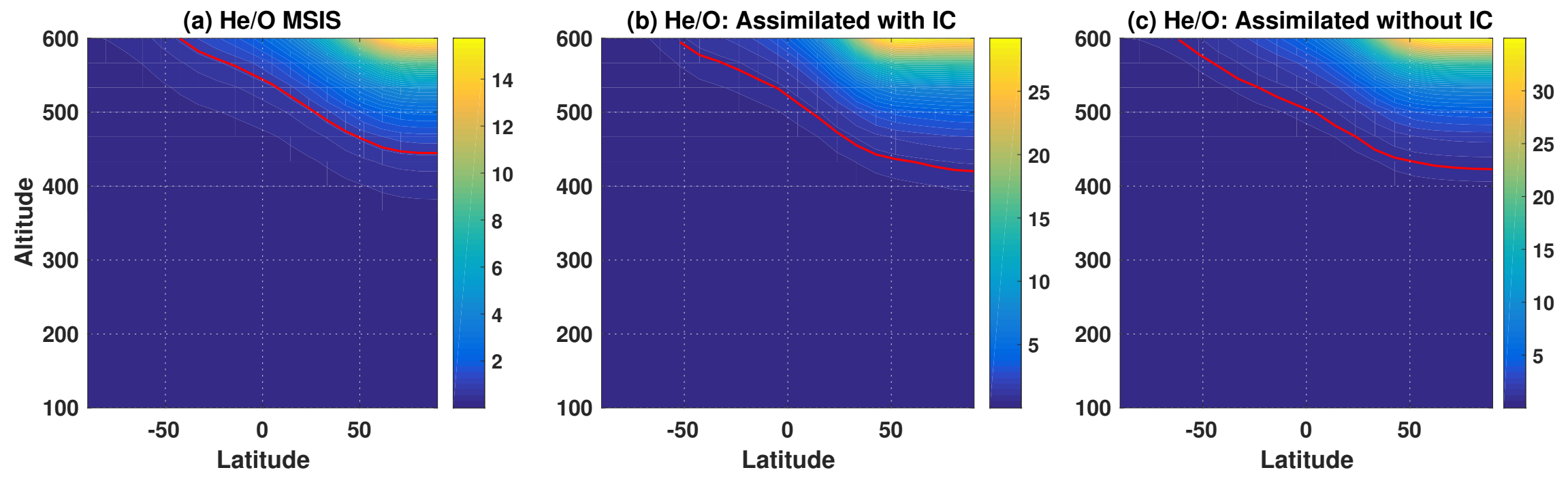

Figure: Helium-to-Oxygen ratio on 2007034.

The amount of O and He at higher altitudes differ significantly between the two different cases (w/ and w/o IC). This difference is caused by the IC of observations with the case w/o IC providing the *true* state of the thermosphere. For both cases, MSIS underpredicts the amount of He at higher altitudes in the winter polar region.

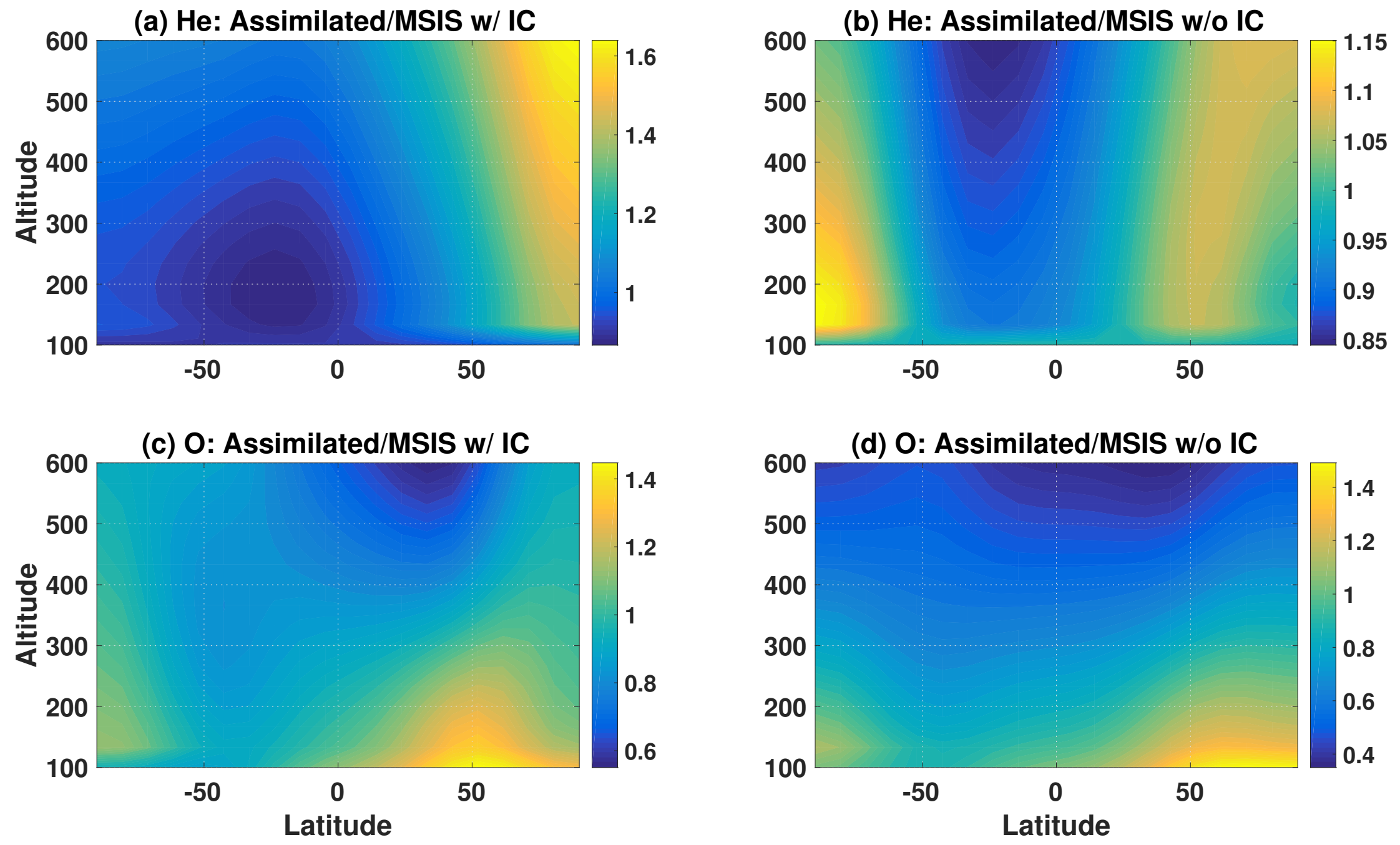

Figure: He and O Assimilated/MSIS ratio on 2007034.

The spatially and temporally averaged daily vertical profiles of He and O are used to estimate the contribution of lower boundary composition and temperature effects under the diffusive equilibrium assumption. Assimilating observations with IC suggests over and underprediction by MSIS close to GRACE altitudes for O and He, respectively. Assimilating without IC suggests that MSIS models He accurately, however, significantly overpredicts O at GRACE altitudes.

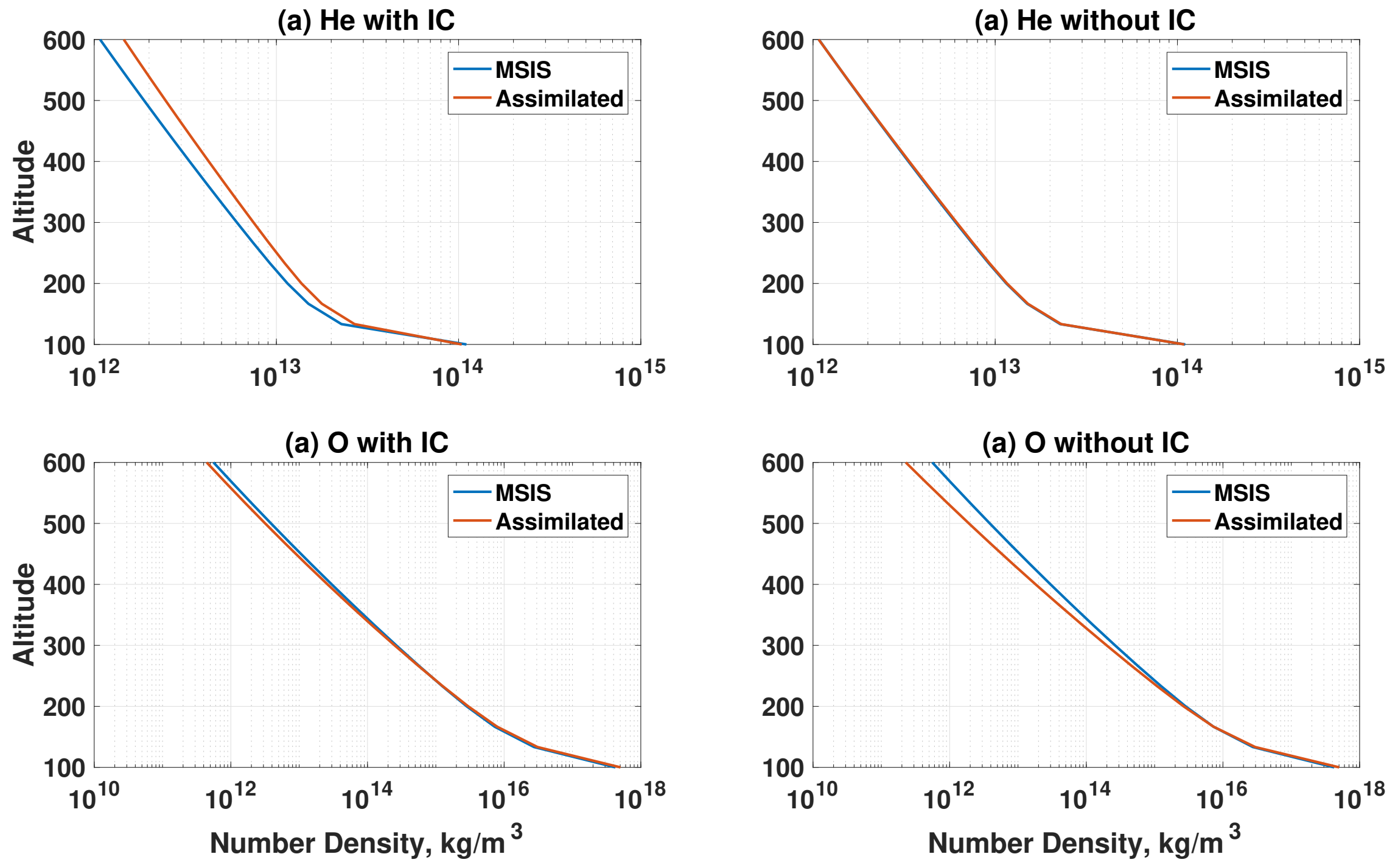

Figure: He and O vertical profile on 2007034.

Table: Contribution of composition and temperature variations

	125 km		500 km				
	(m^{-3}) *MSIS*	(m^{-3}) *Assimilated*	(m^{-3}) *MSIS*	(m^{-3}) *Assimilated*	*Total % Overprediction*	*from Comp*	*from Temp*
w/ IC							
Oxygen	1.27e17	1.49e17	3.87e12	3.18e12	21.7	-21.1	42.8
Helium	4.47e13	4.61e13	1.88e12	2.46e12	-23.6	-2.4	-21.2
w/o IC							
Oxygen	1.27e17	1.48e17	3.87e12	1.91e12	102.6	-33.5	136.1
Helium	4.47e13	4.45e13	1.88e12	1.89e12	-0.5	0.5	-1.0

Storm-time Calibration

We also perform storm-time calibration to show that the methodology works effectively even during periods of high variability; we perform assimilation on a 3-hourly time-scale.

Table: RMS values with and without IC (Intercalibration)

	w/ IC		w/o IC	
	MSIS	*Assimilated*	*MSIS*	*Assimilated*
AGU Storm, Days 348-350, 2006				
CHAMP	49.1%	16.7%	60.5%	16.9%
GRACE	81.8%	15.2%	105.1%	14.5%

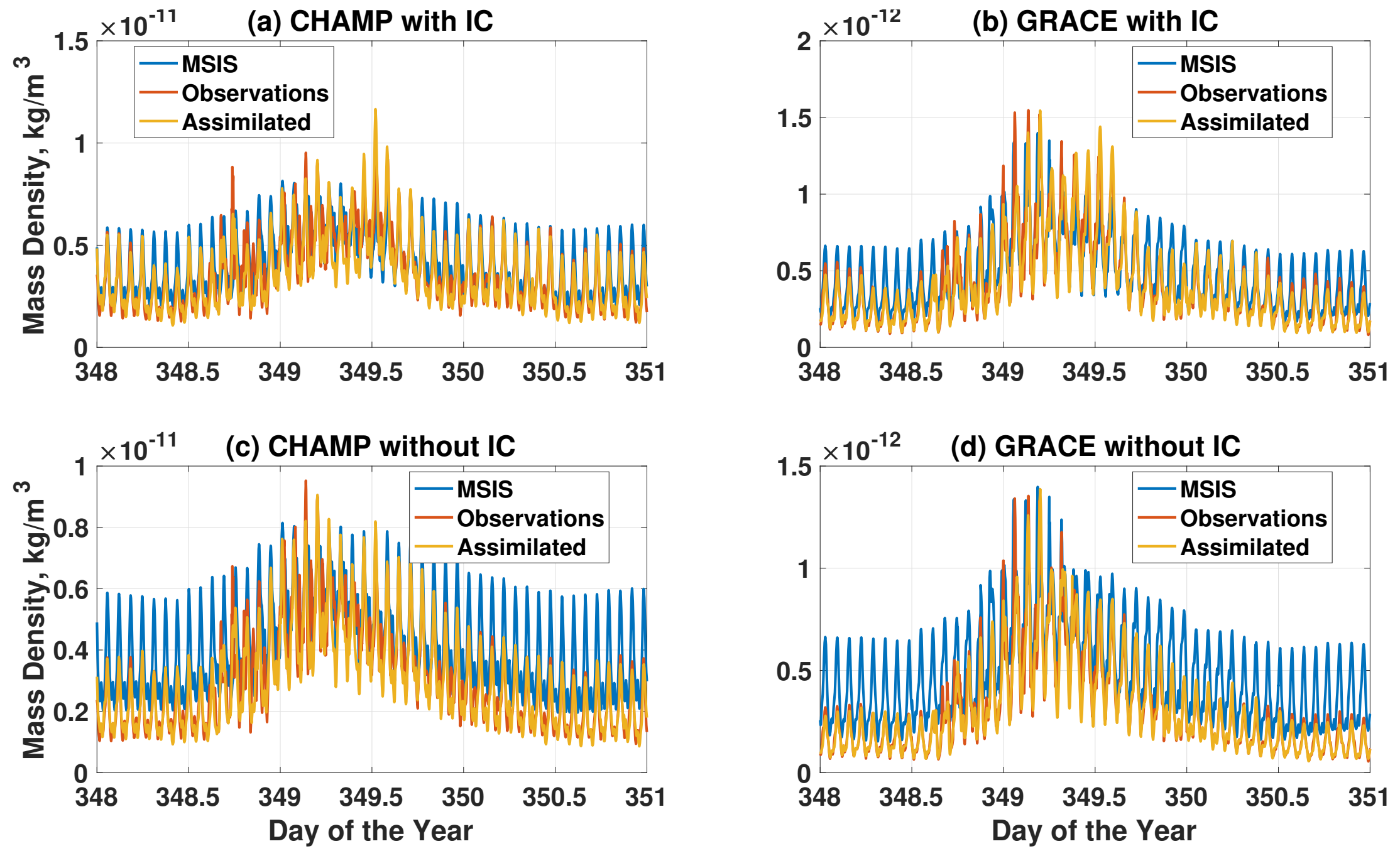

Figure: Calibration during the AGU storm, days 348-350, 2006

Conclusion

The developed method can be used for investigation and inference of thermosphere dynamics and variations and calibration of empirical models.

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