Photo Credit: NASA

ΨJ

TEMPO (hourly)

Sentinel-4 (hourly)

GEMS (hourly)

How well can assimilation of geostationary trace-gas observations constrain NOx emissions in the US?

Chia-Hua Hsu^{1,3}, Arthur P. Mizzi^{2,1}, Daven K. Henze¹ and Brian C. McDonald³ ¹Department of Mechanical Engineering, University of Colorado, Boulder, CO, USA ²NASA Ames Research Center/BAERI, Moffett Field, CA, USA ³NOAA Chemical Sciences Laboratory, Boulder, CO



Equator

Introduction & Objective

- NOx is precursor to Ozone (O₃) & PM_{2.5} which leads to 50,000 80,000 premature death per year (Dedoussi et al, 2020)
- LEO satellite NO₂ observations (e.g., OMI, TROPOMI) are widely used in constraining/accessing NOx emissions (Li et al, 2021, Miyazaki et al., 2017, Qu et al., 2019)
- The geostationary instrument such as (TEMPO, GEO-XO) will provide *high spatial-temporal resolution NO₂ measurement* over North America in near future.

• Objectives:

- 1. Exploring the potential benefit of assimilating high spatial-temporal resolution NO₂ measurement from a geostationary instrument such as TEMPO, or NOAA's potential GEO-XO mission.
- 2. How well can GEO satellite observations constraint the NOx emissions compared to LEO satellite?

Experimental design : OSSEs

- Synthetic tropospheric TEMPO and TROPOMI NO₂ slant column density (SCD):
- \rightarrow Nature Run (true atmosphere): WRF-Chem simulation with COVID-19 period emissions
- → Instrument sensitivity (scattering weight, SW): TEMPO NO2 SW LUTs (from Harvard SAO)
- \rightarrow Accuracy (SNR, $\sigma/_{SCD}$): Predicted equation based on regression analysis of TEMPO proxy and TROPOMI data
- \rightarrow Cloud screening: WRF maximum cloud fraction < 0.5



TEMPO NO₂ vs. TROPOMI NO₂

	Synthetic TEMPO NO ₂	Synthetic TROPOMI NO ₂
Pixel resolution	2.0x 4.5 km ²	3.5 x 5.5 km ²
Spatial coverage	North America	Part of North America
Temporal coverage	Hourly (8-17 LST)	Midday (~13:30 LST)
#OBS	10 ⁷ /hour	10 ⁶ /day
Accuracy (SNR, $\sigma/_{SCD}$)	< 0.2	> 0.2
SW vertical resolution	47	34





60[°] W

Experimental design: Modeling configuration

- Modeling system (forward run) : WRF-Chem/DART (Mizzi et al. 2016)
- Data assimilation configurations:
- → Independent data assimilation: TEMPO & TROPOMI NO₂ OBS only updated NOx concentration and NOx emissions
- → Multi-model ensemble: Different physics options for each ensemble member (e.g., PBL, cumulus and land surface model).
- \rightarrow NOx emissions were adjusted in each DA cycle and the emissions scaling factors were propagated with time.
- \rightarrow Assimilating super-observation (12x12 km) of TEMPO and TROPOMI NO₂ raw data (inverse-variance weighting)
- Simulation time periods: 2020/04/01 2020/04/06 (6 days)

Experiments	Descriptions	
TEMPO	Assimilating synthetic TEMPO NO ₂	
TROPOMI	Assimilating synthetic TROPOMI NO ₂	

Mod	del Configurations	
Model version	WRF-Chem v4.2.2	
Emissions (BAU)	Forward run	
Emissions (COVID-19)	True emissions (Harkins et al., 2021)	
Biogenic emissions	MEGAN2.1	
Fire emissions	FINN1.5	
IC/BC	MET: NAM, CHEM: RAQMS	
Gas phase chemistry	RACM_ESRL	
Aerosol module	MADE/SORGAM	
Resolutions	12 km with 51 vertical layers	
Data ass	imilation configurations	
Filter type	EAKF (Anderson, 2003)	
Ensemble members	10	
DA cycle	3-hours	
DA window	± 1.5 hours	
Horizontal (vertical) localization	ⁿ 300km (off)	



Result- NOx emissions adjustment





Result- NOx emissions adjustment





Result- NOx Emissions Relative Error



Conclusion and Future Works

- TEMPO experiment can retrieve true NOx emissions much faster than TROPOMI experiment.
- The NOx emissions in most of the urban region are also better constrained in the TEMPO NO₂ experiment.
- The estimated NOx emissions in TEMPO experiment are biased low (under investigation)

• We expect that future geostationary satellite observations could improve the skill of top-down emission estimates and our ability to track the impact of specific emissions regulations on changes in air quality.



References:

- Anderson, J. L., (2003). A local least squares framework for ensemble filtering, Mon. Weather Rev., 131, 634–642.
- Dedoussi, et al. (2020). Premature mortality related to United States cross-state air pollution. Nature, 578, 261–265
- Harkins, et al. (2021). A fuel-based method for updating mobile source emissions during the COVID-19 pandemic. Environmental Research Letters, 16, 065018.
- Li, et al. (2021). Assessment of updated fuel-based emissions inventories over the contiguous United States using TROPOMI NO2 retrievals. Journal of Geophysical Research: Atmospheres, 126, e2021JD035484.
- Mizzi, A. P., Arellano Jr., A. F., Edwards, D. P., Anderson, J. L., and Pfister, G. G., (2016). Assimilating compact phase space retrievals of atmospheric composition with WRF-Chem/DART: a regional chemical transport/ensemble Kalman filter data assimilation system, Geosci. Model Dev., 9, 965–978.
- Miyazaki et al. (2017). Decadal changes in global surface NOx emissions from multi-constituent satellite data assimilation, Atmos. Chem. Phys., 17, 807–837.
- Qu et al. (2019). Hybrid mass balance/4D-Var joint inversion of NOx and SO2 emissions in East Asia. Journal of Geophysical Research: Atmospheres, 124, 8203–8224.

Q & A