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Feasibility of robust estimates of ozone production rates using a synergy of satellite observations, ground-based remote sensing, and models

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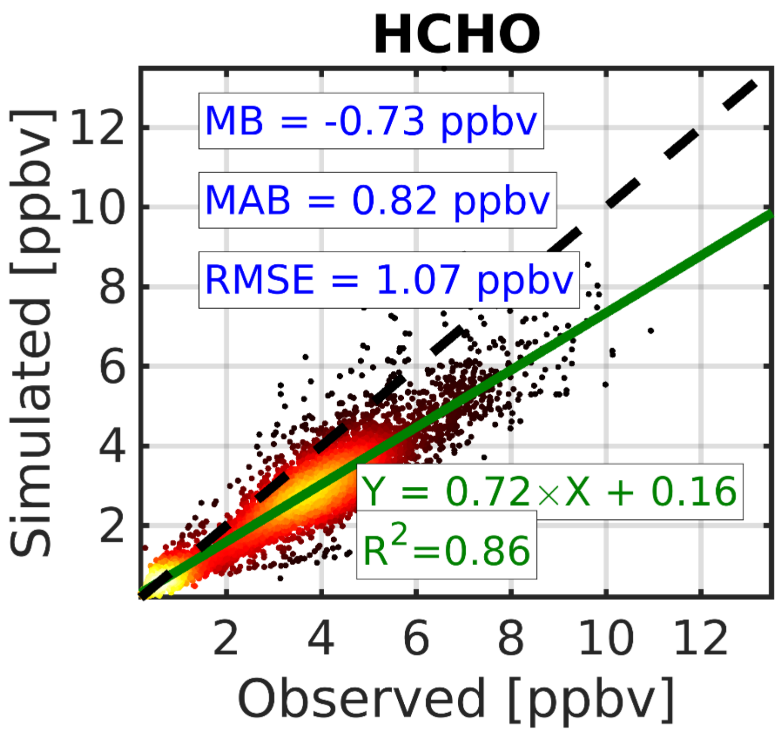

Figure S1. F0AM HCHO validation against observations during SENEX aircraft campaign.

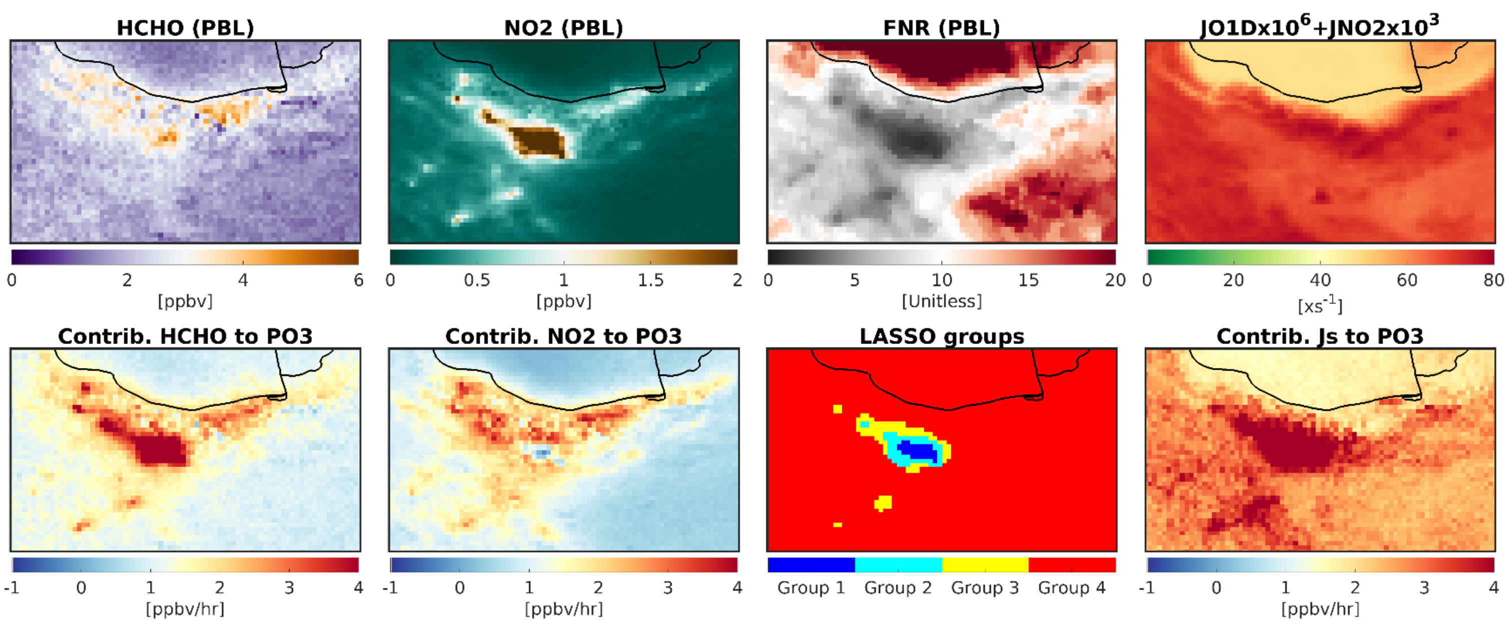

Figure S2. (first row) PBL concentrations of HCHO, NO2, FNR and sum of scaled jO1D and jNO2 derived from TROPOMI and models in July 2019; (second row) the contributions of HCHO, NO2, and photolysis rates to PO3, along with the defined LASSO ozone production sensitivity regimes for PO3 estimates. The location is Tehran, Iran.

Table S1. Characteristics of selected atmospheric composition aircraft campaigns used in this study.

Campaign	When	Where	Why
DISCOVER-AQ-TX	September 2013	Houston-Galveston-Brazoria in Texas	To understand a complex urban photochemical environment with abundant petrochemical facilities and elevated mobile sources
DISCOVER-AQ-DC	June–July 2011	Washington D.C. and Maryland	To study urban-focused photochemical environment experiencing extreme hot and sunny days
DISCOVER-AQ-CO	July–August 2014	Denver-Boulder-Fort Collins in Colorado	To understand urban air quality in a complex meteorological environment due to topography
KORUS-AQ	May-June 2016	South Korea	To study the effect of local and external sources of ozone in an extremely complex chemical environment
ATOMs	August 2016 – May 2018	Pacific and Atlantic Ocean	To enhance our understanding of ozone pollution in remote areas
INTEX-B	March – May 2006	Gulf of Mexico and Pacific	To study the effect of background pollution
SENEX	May–July 2013	Southeast U.S.	To understand the interplay role of biogenic and anthropogenic emissions in shaping air pollution

Table S2. The box model configurations and inputs.

Temporal resolution of samples	10 or 30 sec
Time steps	30 minutes
Number of solar cycles	5
Dilution constant	1/86400 (s^{-1}) (=24-hr lifetime)
Meteorological Inputs	Observed Pressure, Temperature, and Relative Humidity
Photolysis frequencies initial guess	LUT based on the NCAR TUV model calculations
Photolysis frequencies corrections (campaign#†)	Measured jNO_2 (1-8), jO^1D (4-8), jHCHO (4-5 and 8), and jH_2O_2 (4-5 and 8)
Compounds (campaign#†) used for constraining the box model	CO (1-8), NO_x (1-8), O_3 (1-8), SO_2 (4 , 7) , CH_4 (1-8), HNO_3 (1-8), H_2O_2 (4-5 and 7-8), Isoprene (1-4 and 6-7), Monoterpenes (1-4 and 7), Acetone (1-8), Ethyne (4-8), Ethane (4-8), Ethene (4-8), Methanol (1-8), Propane (4-8), Benzene (2-8), Xylene (1 and 4 and 7), Toluene (1-4 and 7), Glyoxal (4), Glycolaldehyde (4), Acetaldehyde (1-8), Ketone (1-4, 6 and 8)
Unconstrained compounds (campaign#†) used for validation	HO_2 (4-5 and 8), OH (4-5 and 8), NO (1-8), NO_2 (1-8), PAN (1-8), HCHO (1-8)
Chemical Mechanism	CB06

† (1) DISCOVER-Baltimore-Washington, (2) DISCOVER-Texas-Houston, (3) DISCOVER-Colorado, (4) KORUS-AQ, (5) INTEX-B, (6) SENEX, (7) SEAC4RS, and (8) ATOMs