

Supplement of

Technical Note: DACNO₂ – A Multi-Constraint Deep Learning Framework for High-Resolution 3D NO₂ Field Estimation

Wenfu Sun^{1,2}, Frederik Tack¹, Lieven Clarisse², Michel Van Roozendael¹

¹ Royal Belgian Institute for Space Aeronomy (BIRA-IASB), Brussels, Belgium.

² Université libre de Bruxelles (ULB), Spectroscopy, Quantum Chemistry and Atmospheric Remote Sensing (SQUARES), Brussels, Belgium.

Correspondence to: Wenfu Sun (wenfu.sun@aeronomie.be)

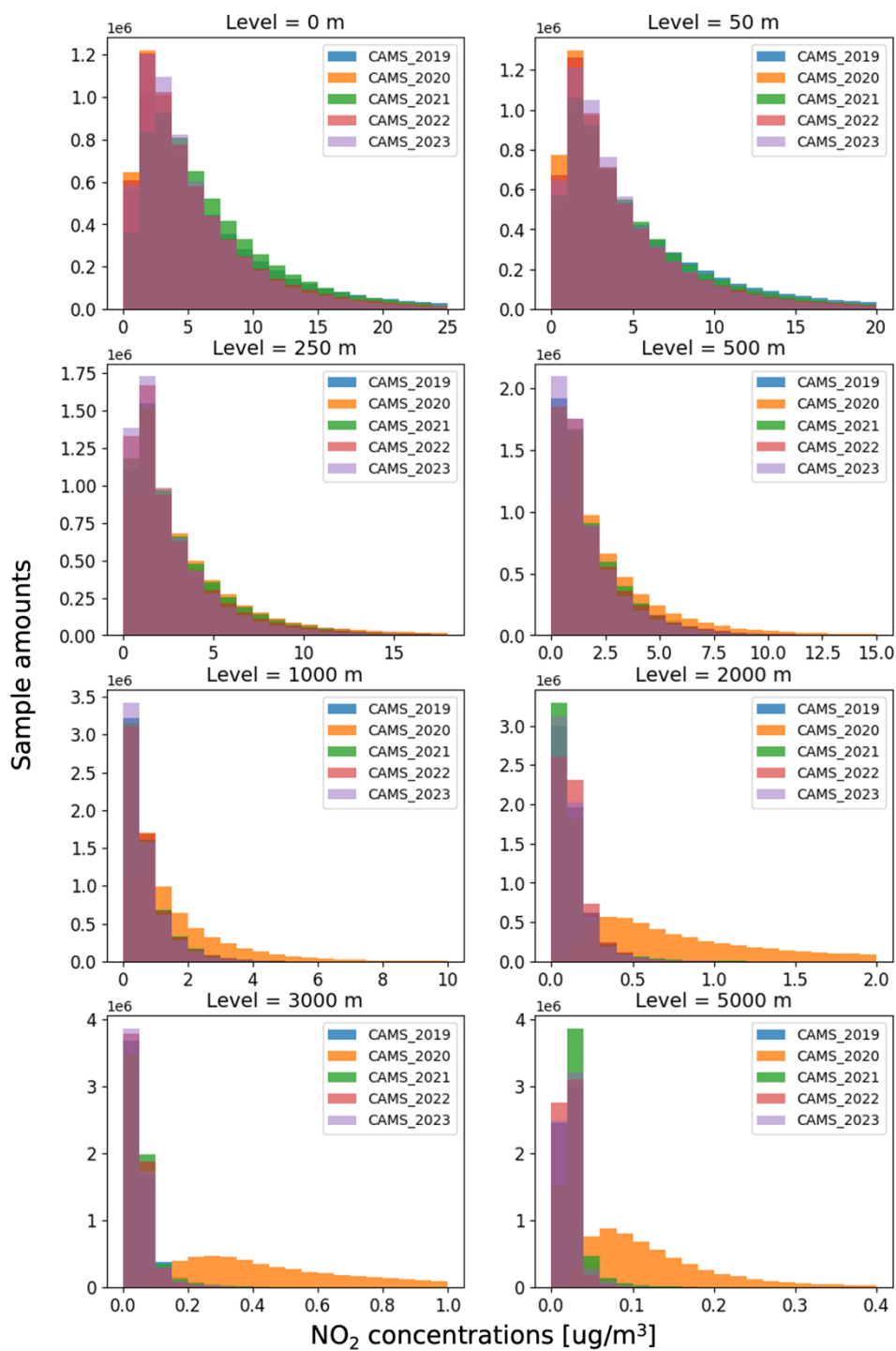


Figure S1. Distributions of CAMS NO₂ concentrations for 2019–2023 at each vertical level. Each panel displays the frequency histogram of daily grid cell NO₂ values (µg/m³) at various heights (0, 50, 250, 500, 1000, 2000, 3000, and 5000 m) for each year. Notably, 2020 exhibits a marked shift toward higher NO₂ values above 1000 m compared to other years, indicating anomalies in the data for that year.

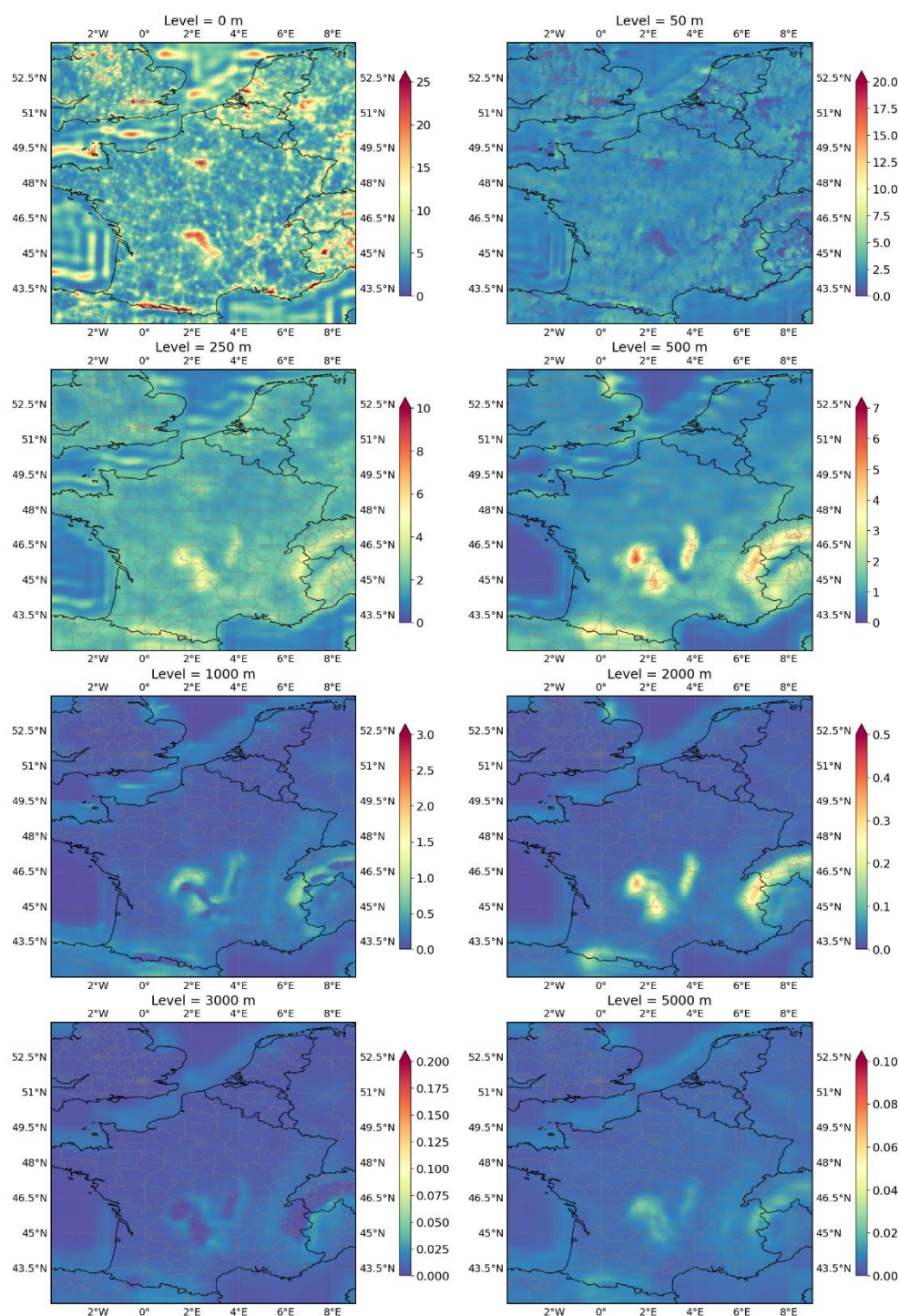


Figure S2. Annual mean NO₂ fields for 2023 from the DACNO₂-onlyobs model at eight vertical levels (0, 50, 250, 500, 1000, 2000, 3000, and 5000 m). This test model was trained exclusively with EEA surface NO₂ measurements, following a similar Phase-2 and Phase-3 process but without CAMS NO₂ constraints. Results show that effective NO₂ estimates are produced primarily near the land surface, while artifacts appear at higher levels and over the ocean, highlighting the need for physically consistent simulated data to support spatial and vertical constraints in high-resolution 3D NO₂ modeling.

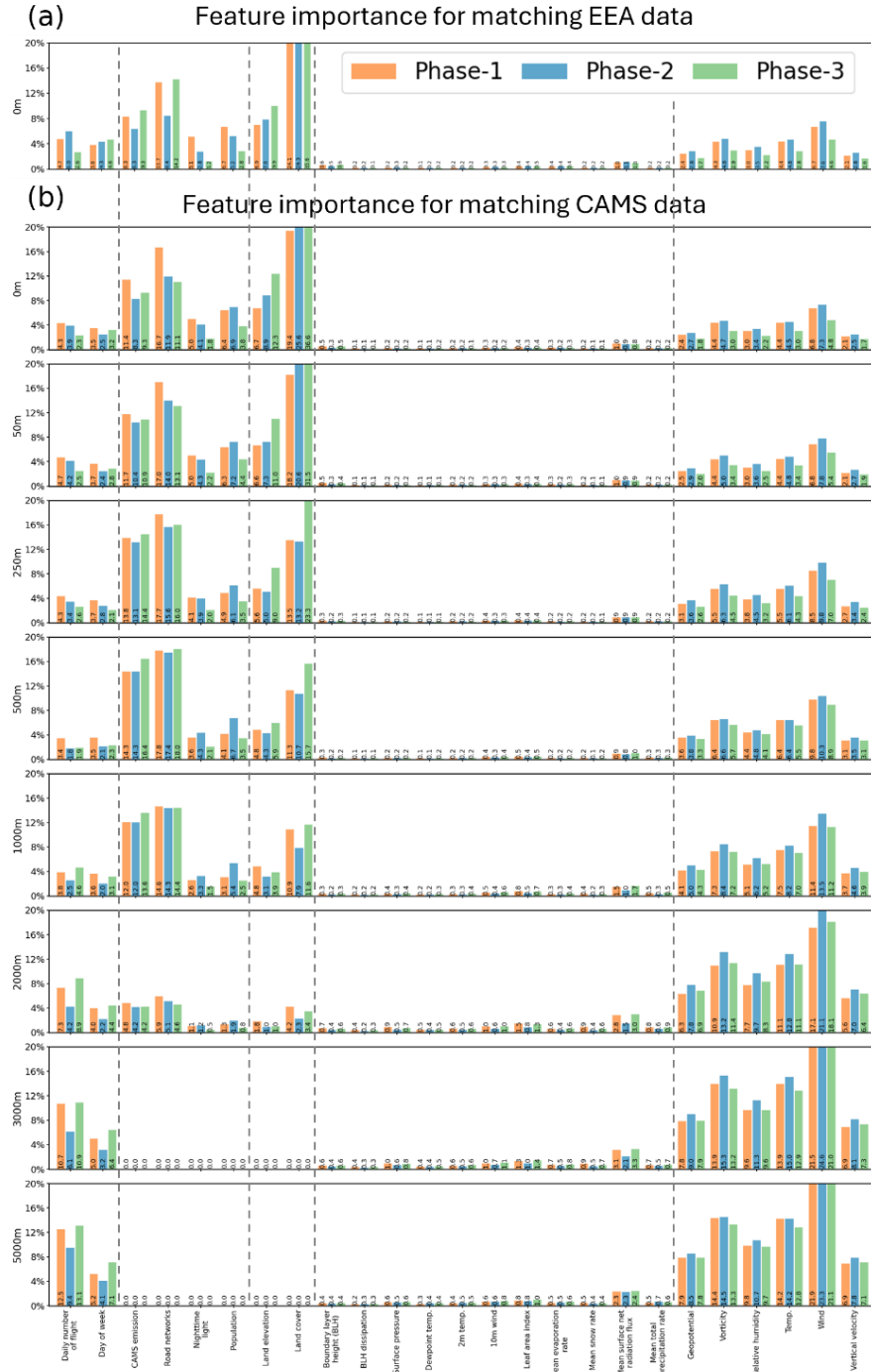


Figure S3. Relative importance of each individual input feature for DACNO₂ model predictions, evaluated using the integrated gradients (IG) method. (a) Feature contributions to RMSE between DACNO₂ surface NO₂ estimates and EEA ground-based measurements for 2023. (b) Feature contributions to RMSE between DACNO₂ and CAMS NO₂ estimates at different vertical levels for 2023. Features are grouped (separated by dashed lines) into temporal indicators, emission inventories and proxies, geography, ERA5 single-level meteorology, and ERA5 multi-level meteorology. Results are shown for each model training phase (i.e., Phase-1, Phase-2, and Phase-3), illustrating how the relative influence of individual input features varies with training constraints and altitude. Feature definitions and sources are provided in Table 1.

10

Table S1. Evaluation performance of DACNO₂-S5P

Year 2023								
UTC11-13								
DACNO ₂ -S5P					CAMS-S5P-2km			
EEA-S5P	RMSE (ug/m ³)	r	R ²	Bias (ug/m ³)	RMSE (ug/m ³)	R	R ²	Bias (ug/m ³)
Total	5.07	0.77	0.59	0.05	5.27	0.76	0.55	-0.94
Urban	5.41	0.74	0.54	-0.63	5.60	0.76	0.51	-1.98
Suburban	5.08	0.79	0.62	0.63	5.24	0.78	0.60	-0.67
Rural	4.08	0.80	0.61	1.01	4.40	0.78	0.55	1.27
DACNO ₂ -S5P-10km								
Total levels	0.98	0.94	0.88	0.03	CAMS-S5P (10 km)			
L0	1.82	0.91	0.82	0.06				
L50	1.52	0.92	0.85	-0.06				
L250	1.11	0.92	0.84	0.14				
L500	0.78	0.89	0.80	0.06				
L1000	0.36	0.83	0.68	0.03				
L2000	0.08	0.70	0.49	-0.01				
L3000	0.03	0.63	0.39	0.00				
L5000	0.01	0.53	0.22	0.00				

Note: This table is similar to Tables 2 and 3. The DACNO₂-S5P model is a Phase-3 model developed for the TROPOMI overpass time, predicting a 3-hour average NO₂ (11:00–13:00 UTC) using the three-phase strategy. CAMS-S5P and EEA-S5P represent process-based and measured NO₂ data during overpass time. CAMS-S5P-2km is derived by bilinearly interpolating the CAMS-S5P data.