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REGIME-CONDITIONED COVERAGE OF MONTE CARLO INTERVALS FOR TROPOMI-DERIVED SURFACE NO_2 DURING WINTER STAGNATION IN THE SOFIA BASIN

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Abstract Aggregate interval coverage can conceal systematic failure under winter stagnation. We propagate uncertainty in TROPOMI tropospheric NO_2, ERA5 boundary-layer height, 10 m wind and spatial representativeness through an explicit mixed-layer conversion. The central 90% interval is evaluated separately for stagnant and ventilated Sofia station-days, with Plovdiv as an out-of-basin control. In a synthetic January 2021 stress test, stagnant coverage is 63.9% versus 87.7% under ventilation; boundary-layer height contributes 61.4% versus 32.2% of first-order variance. These values verify the analysis pipeline and are not observational evidence.

1. Introduction

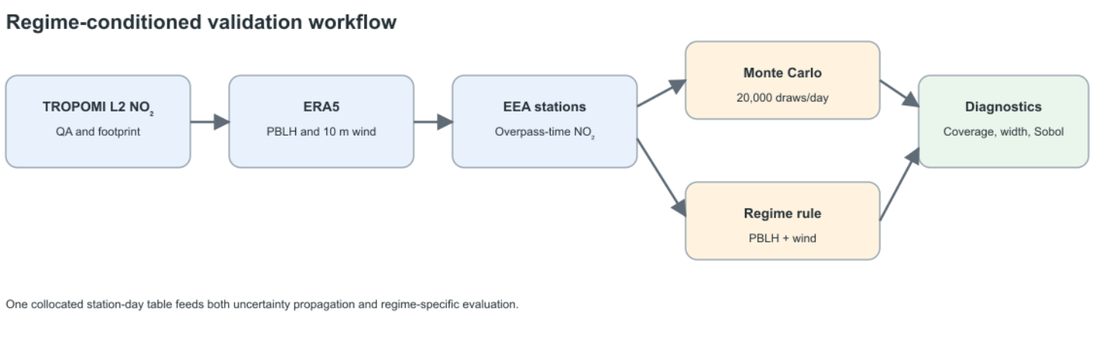
A satellite column is not a surface concentration. The conversion depends on the NO_2 profile, boundary-layer depth, chemistry, pixel–station representativeness and retrieval assumptions [3,4,7,8]. Those dependencies become most critical during Sofia winter stagnation, when weak winds and shallow mixing trap emissions near the surface.

H1: 90% interval coverage is lower under stagnation. H2: the first-order boundary-layer-height contribution is larger under stagnation.

2. Data and prespecified regimes

Inputs: TROPOMI Level-2 tropospheric NO_2 (qa_value ≥ 0.75) [3,4]; ERA5 boundary-layer height (H) and 10 m wind (u) [5,6]; overpass-time EEA station NO_2 (≥75% temporal completeness). Primary evaluation: three Sofia station aliases. Control: one Plovdiv alias.

Stagnant if $H < 350$ m and $u_{10} < 2.0$ m s^{-1}; ventilated otherwise. This is a prespecified stagnation proxy, not a direct observation of a temperature inversion.



3. Mixed-layer Monte Carlo model

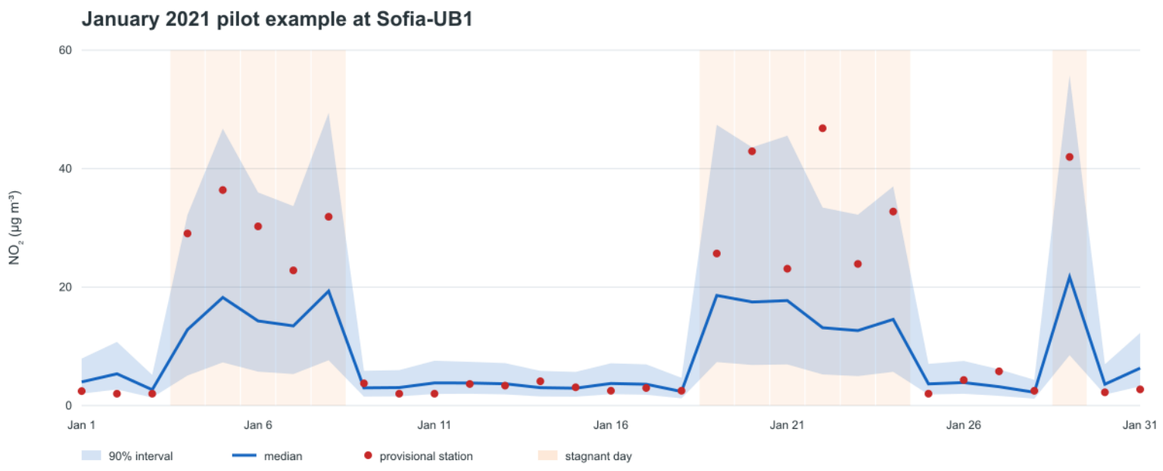
$$C^{(k)}_{d,s} = 10^6\, M(NO_2) \cdot \frac{\Omega^{(k)}(d,s)}{H^{(k)}(d,s)} \cdot R^{(k)}_{d,s} \cdot V^{(k)}_{d,s}$$

$$\text{Coverage: } \hat{p}_r = n_r^{-1} \Sigma\, \mathbb{1}(L \le y \le U) \qquad \text{Sobol: } S_i = Var[E(Y|X_i)] / Var(Y)$$

Ω is the screened tropospheric column; H is boundary-layer height; R is a station-day representativeness/local-enhancement factor; V is a bounded wind perturbation. Each station-day uses 20,000 draws. Coverage, width and interval score are evaluated jointly; day-block bootstrap intervals preserve within-day dependence [9,10]. The homogeneous-mixing equation is a transparent baseline, not a chemical-transport model.

4. Illustrative January 2021 pilot

SYNTHETIC PILOT — values demonstrate the pipeline only

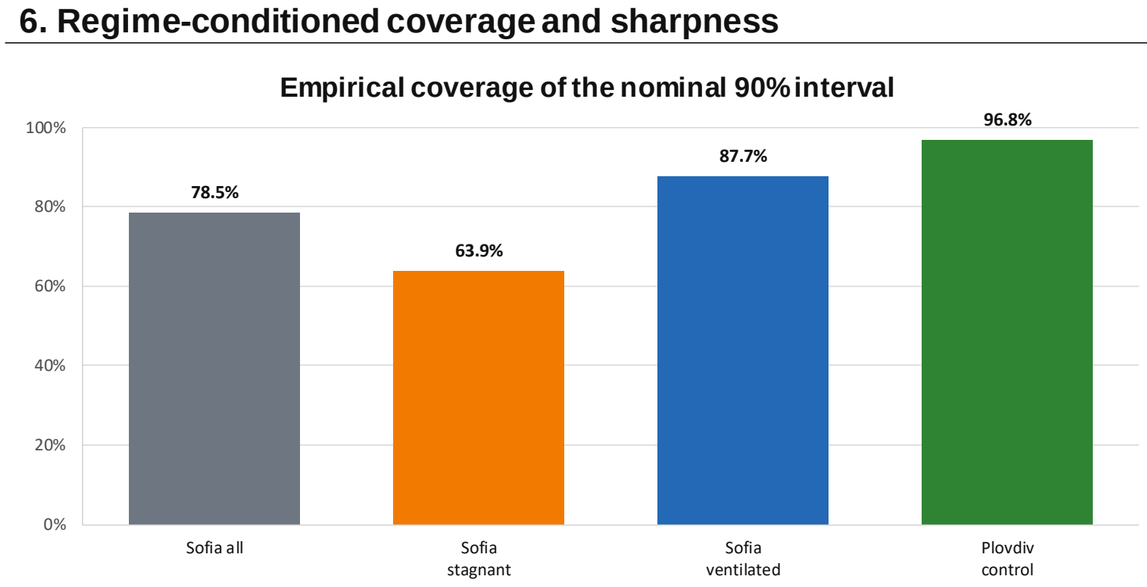


Stagnant episodes produce much wider intervals, yet several provisional station values still exceed the upper endpoint. The pattern motivates regime-specific calibration rather than a single pooled score.

5. Observational replacement and reporting

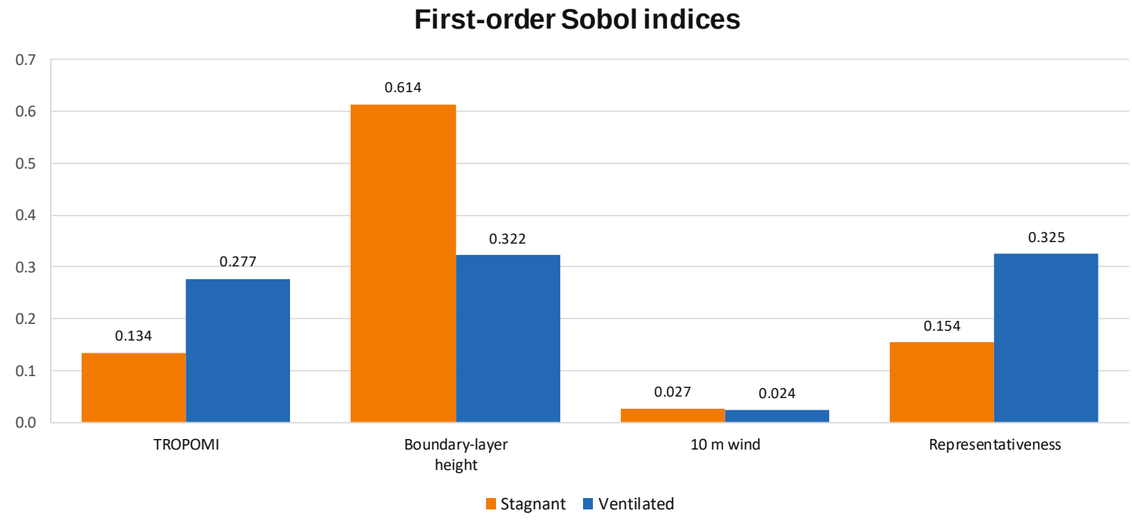
1. Collocate QA-screened TROPOMI footprints, ERA5 fields and station records at overpass time.
2. Preserve processor version, pixel footprint, QA, station metadata, exclusions and random seed.
3. Report regime counts, 90% coverage with day-block bootstrap intervals, median width and station-specific checks.
4. Estimate first-order Sobol indices with independent sample matrices; repeat threshold and input-range sensitivity analyses.
5. Keep Plovdiv separate from Sofia so the control cannot alter the primary basin estimate.

6. Regime-conditioned coverage and sharpness



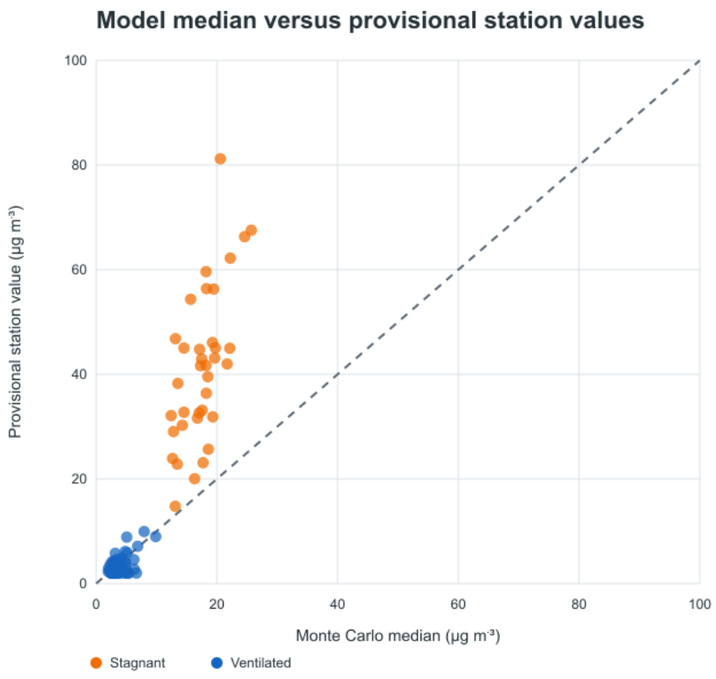
Sofia: 93 station-days on 31 days. Coverage is 63.9% under stagnation and 87.7% under ventilation: $\Delta\hat{p} = -23.8$ percentage points (95% day-block bootstrap: −39.2 to −7.7). Median width is 38.1 versus 5.1 µg m^{-3}; mean interval score is 100.2 versus 7.2. Plovdiv coverage is 96.8%. Wider stagnant intervals therefore do not restore nominal calibration in this stress test.

7. First-order sensitivity changes by regime



Boundary-layer height contributes 61.4% of first-order output variance under stagnation and 32.2% under ventilation. The result is conditional on the input distributions: it prioritises better vertical-structure information but does not prove that ERA5 height error alone causes the mismatch.

8. Surface-enhancement diagnostic



Ventilated points cluster near the 1:1 line, whereas stagnant Sofia points shift above it. This failure was deliberately embedded in the synthetic generator, so the figure verifies that the diagnostics recover a known mismatch; it does not establish the atmospheric hypothesis.

9. Conclusions

A pooled coverage score is not sufficient for an inversion-prone basin. The pilot verifies a reproducible analysis and defines a falsifiable observational test: persistent stagnant-regime undercoverage after data replacement would motivate explicit treatment of vertical structure and station representativeness. No atmospheric conclusion is drawn from the synthetic values.

References [1] Makariev & Trenchev, SES 2025. [2] Makariev & Trenchev, Aerospace Research in Bulgaria 38, 2026. [3] van Geffen et al., AMT 15, 2037–2060, 2022. [4] Verhoelst et al., AMT 14, 481–510, 2021. [5] Hersbach et al., QJRMS 146, 1999–2049, 2020. [6] Sinclair et al., AMT 15, 3075–3103, 2022.
[7] Horner et al., ACP 24, 13047–13064, 2024. [8] Kolev et al., Atmospheric Environment 34, 3223–3235, 2000. [9] Saltelli et al., CPC 181, 259–270, 2010. [10] Gneiting & Raftery, JASA 102, 359–378, 2007.