



Development and Evaluation of Online Gas-Phase Chemistry in the Global Variable-Resolution Atmospheric Model iAMAS (v2.5.1): Resolution-Dependent Surface Ozone over North China

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Abstract

Atmospheric composition is governed by multiscale processes spanning global transport to local chemistry. Simultaneously capturing these scales is essential, yet conventional modeling trades global coverage for regional detail restricted by artificial boundaries. Global variable-resolution (VR) modeling provides a unified alternative, yet online gas-
20 phase chemistry within nonhydrostatic VR frameworks remains limited, and how mesh refinement alters coupled physical–chemical responses is not fully understood. Here, we develop and evaluate an online gas-phase chemistry framework in the VR model iAMAS (v2.5.1). Operating on a unified unstructured mesh without lateral boundaries, the modular framework couples KPP-generated SAPRC-99 tropospheric chemistry, Linoz stratospheric ozone, Fast-J photolysis, emissions, transport, and deposition. Global baseline simulations at ~60 km resolution (U60km) for July 2019 validate large-scale tracer
25 distributions (O₃, NO₂, HCHO, CO) and surface ozone diurnal cycles across China. Regionally refined simulations at ~4 km over North China (V4km) demonstrate how online VR chemistry resolves cross-scale physical–chemical coupling over complex terrain. V4km recovers the observed ridge-high/valley-low nighttime ozone pattern, reversing spatial correlation from R=−0.40(U60km) to R=+0.46 by resolving slope circulations and heterogeneous NO_x emissions within a shallow nocturnal boundary layer. Refinement also reorganizes urban–rural and day–night ozone responses: higher urban NO_x suppresses
30 daytime ozone peak under VOC-limited conditions, whereas reduced coarse-grid NO_x dilution weakens rural nighttime titration and sustains higher ozone. These results demonstrate that mesh refinement in a global VR model alters the coupled dynamical–chemical state rather than merely sharpening concentration gradients, establishing iAMAS as a modular platform for seamless global-to-regional atmospheric-composition studies.



35 1 Introduction

Atmospheric composition emerges from tightly coupled physical and chemical processes that span global transport, synoptic and mesoscale circulations, boundary-layer turbulence, heterogeneous emissions, and nonlinear photochemistry (Akimoto, 2003; Monks et al., 2009; Brasseur & Jacob, 2017). A central modeling challenge is to retain these global chemical backgrounds while resolving the kilometer-scale local processes that govern regional air quality. Conventional global chemistry models such as GEOS-Chem and CAM-chem provide global coverage without lateral boundaries, but their coarse horizontal resolutions (~100–200 km) cannot resolve these localized features (Bey et al., 2001; Lamarque et al., 2012). Conversely, regional chemistry models such as WRF-Chem and CMAQ operate at convection-permitting scales, but their simulated chemical states depend on prescribed lateral chemical boundary conditions that often introduce dynamical and chemical inconsistencies (Grell et al., 2005; Byun & Schere, 2006; Tang et al., 2007). Bridging these disparate scales within a dynamically and chemically consistent atmosphere remains a fundamental modeling objective.

Global variable-resolution (VR) modeling offers a structural solution by using a smoothly varying mesh to maintain global coverage while concentrating computational resources over target regions (Ringler et al., 2011; Skamarock et al., 2018). The feasibility of comprehensive online chemistry within VR frameworks has been established by pioneering systems representing diverse model architectures and application priorities: the Multi-Scale Infrastructure for Chemistry and Aerosols version 0 (MUSICAv0) embeds tropospheric chemistry into a hydrostatic spectral-element framework (Schwantes et al., 2022; Tang et al., 2023); the ICOSahedral Nonhydrostatic model with Aerosols and Reactive Trace gases (ICON-ART) couples chemistry within a comprehensive Earth system infrastructure (Rieger et al., 2015; Schröter et al., 2018); and the Geophysical Fluid Dynamics Laboratory Atmospheric Model version 4 with Variable Resolution (GFDL AM4VR) utilizes a stretched-grid chemistry–climate design (Lin et al., 2024). While these systems demonstrate the power of multiscale chemistry modeling, a dedicated nonhydrostatic VR atmospheric chemistry model on unstructured meshes—combining convection-permitting dynamics with high computational efficiency independently of broader Earth system overhead—offers a distinct, complementary, and highly tractable architecture for multiscale atmospheric chemistry research. Within such a framework, the key scientific question is not simply whether mesh refinement sharpens spatial concentration fields, but how it fundamentally reorganizes the coupled pathways linking complex terrain, heterogeneous emissions, boundary-layer evolution, advective transport, and nonlinear chemical production and loss.

North China serves as an ideal natural laboratory to test these multiscale physical–chemical interactions. Dense and spatially heterogeneous anthropogenic emissions adjoin the complex Taihang–Yanshan mountain ranges, where terrain-driven circulations and mountain chimney effects (Chen et al., 2009; Miao et al., 2015), rapid boundary-layer transitions (Zhao et al., 2019), steep precursor gradients, and nonlinear ozone photochemistry (Li et al., 2020; Ma et al., 2021) interact over short spatial and temporal scales. The co-location of prominent topographic relief and intense precursor emissions makes this region an ideal test for evaluating cross-scale consistency and physical–chemical coupling in a global VR chemistry model.

To address this model-development need and investigate these scale-dependent processes, we extend the integrated Atmospheric Model Across Scales (iAMAS), a nonhydrostatic global VR model whose dynamical core is derived from MPAS-A and optimized for heterogeneous high-performance computing (Skamarock et al., 2012; Gu et al., 2022; Hao et al., 2023). Building upon previous iAMAS capabilities for natural aerosols (Feng et al., 2023), this study introduces a modular gas-phase chemistry framework. The kinetic preprocessor (KPP)-generated SAPRC-99 tropospheric chemistry and a simplified Linoz stratospheric ozone parameterization are fully coupled with Fast-J photolysis, emission processing, tracer transport, dry deposition, and wet scavenging on a unified unstructured mesh.

The objectives of this study are threefold. First, we describe the design and implementation of the online gas-phase chemistry framework in iAMAS v2.5.1. Second, we evaluate a global quasi-uniform 60 km configuration (U60km) against satellite retrievals, ozonesondes, and ground observations for July 2019 to characterize the global chemical state and baseline biases. Third, we utilize a variable-resolution configuration refined to ~4 km over North China (V4km) to examine how



regional mesh refinement alters the coupled response of surface ozone to resolved terrain, emission heterogeneity, boundary-layer dynamics, and photochemistry.

80 **2 Model Description and Experimental Design**

2.1 Overview of iAMAS

The integrated Atmospheric Model Across Scales (iAMAS v2.5.1) is a nonhydrostatic global variable-resolution physics-chemistry coupled atmospheric model. It employs a spherical centroidal Voronoi tessellation (SCVT) with C-grid staggering, supporting smoothly varying horizontal resolution through a single unified global mesh without requiring prescribed lateral
85 boundary conditions at the edge of a limited-area domain. Time integration uses a split-explicit scheme, in which a third-order Runge–Kutta method advances the slow meteorological modes while fast acoustic and gravity-wave modes are handled through acoustic substepping (Klemp et al., 2007; Wicker and Skamarock, 2002). Within each acoustic substep, horizontally propagating acoustic modes are integrated explicitly, whereas vertically propagating acoustic modes are integrated implicitly, since the vertical grid spacing is typically much finer than the horizontal spacing and would otherwise impose a severe
90 restriction on the acoustic time step. Its dynamical core is derived from the MPAS-A dycore (Skamarock et al., 2012), featuring specific optimizations and modifications for next-generation heterogeneous supercomputing platforms and the coupling of physical–chemical processes (Gu et al., 2022; Hao et al., 2023; Li et al., 2026).

The iAMAS incorporates diverse state-of-the-art and well-established physical schemes for microphysics (Thompson et al., 2008; Morrison et al., 2009; Morrison and Milbrandt, 2015), convection (Kain and Fritsch, 1993; Grell and Freitas, 2014;
95 Zheng et al., 2016; Wang, 2022), radiation (Iacono et al., 2008), surface-layer turbulence (Monin and Obukhov, 1954), land-surface processes (Chen and Dudhia, 2001), planetary boundary layer mixing (Hong et al., 2006; Nakanishi and Niino, 2009; Shin and Hong, 2015), and orographic gravity wave drag (Kim and Doyle, 2005; Choi and Hong, 2015). Of particular relevance for variable-resolution modeling, iAMAS offers several scale-aware convective and boundary-layer parameterization options — including the Grell-Freitas (Grell and Freitas, 2014), multi-scale Kain-Fritsch (Zheng et al., 2016), and new Tiedtke (Wang,
100 2022) convective schemes, alongside the Shin-Hong scale-aware boundary-layer scheme (Shin and Hong, 2015) — that support application across the wide range of horizontal resolutions spanned by variable-resolution configurations. Building on this physical framework, the iAMAS model has been applied to a range of weather and climate studies, demonstrating convection-permitting skill in reproducing the diurnal cycle of Mei-yu rainfall over East China (Xu et al., 2021), substantially improving typhoon track forecast skill for complex-track events (Gu et al., 2025a), revealing mechanisms underlying Indian
105 summer monsoon dry biases (Li et al., 2025), and attributing extreme rainfall over North China to fast warming over the Mongolian Plateau (Gu et al., 2025b).

Feng et al. (2023) further developed an online natural aerosol module within iAMAS, implementing dust emission, transport, and deposition processes coupled with aerosol–radiation interactions, enabling physically consistent simulation of mineral dust and sea-salt aerosols. This aerosol-enabled framework has been applied to investigate dust–climate interactions,
110 including dust impacts on the Indian summer monsoon (Feng et al., 2025), the simulation of long-range transported extreme dust storms over East Asia (Xue Y. et al., 2026), and global 3-km-resolution simulation of atmospheric responses to submarine volcanic eruptions on next-generation supercomputing platforms (Huang et al., 2023). The present study extends this framework with online tropospheric gas-phase chemistry, emission preprocessing and online injection, and a simplified representation of stratospheric ozone chemistry. The overall model architecture is illustrated in Figure 1.

115 **2.2 Gas-Phase Chemistry Framework in iAMAS**

The gas-phase chemistry framework includes chemical initialization, emission processing, photolysis, gas-phase chemistry, tracer transport, and dry and wet removal. At each model time step, these modules are called in sequence: photolysis



rates are computed from the current atmospheric state; emission fluxes are injected as lower-boundary tendencies; dry deposition and sub-grid turbulent mixing are applied; convective tracer transport redistributes species vertically; the gas-phase
120 ODE system is integrated in the troposphere by the KPP-generated Rosenbrock solver and in the stratosphere by the Linoz parameterization; and large-scale wet scavenging is applied for soluble species. Resolved-scale advection of all chemical tracers is handled by the dynamical core on the unified SCVT mesh.

2.2.1 Gas-Phase Chemistry Mechanism

iAMAS employs two chemical solvers partitioned at the dynamically diagnosed tropopause. In the troposphere, gas-phase
125 chemistry is solved using the SAPRC-99 mechanism (Carter, 2000), a lumped-structure mechanism comprising 82 species and 227 reactions in which non-methane organic compounds are grouped into reactivity-weighted surrogate classes rather than treated explicitly. The chemical ODE system at each grid cell is integrated by a second-order Rosenbrock solver with adaptive time-stepping, auto-generated by the Kinetic PreProcessor (KPP; Damian et al., 2002; Sandu & Sander, 2006) directly from the SAPRC-99 reaction list, ensuring numerical consistency between the mechanism specification and its solver. SAPRC-99
130 is selected for its established performance in regional ozone studies over East Asia (Kang et al., 2022); the modular KPP architecture allows alternative mechanisms to be substituted in future versions.

Above the tropopause, ozone chemistry is represented by the Linoz v2 parameterization (McLinden et al., 2000). The net photochemical production-minus-loss rate of ozone at each grid point is expressed as a first-order Taylor expansion linearized about a climatological reference state in local ozone, temperature, and overhead column ozone:

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$$P - L = PL_{\text{clim}} + (O_3 - O_{3 \text{ clim}}) \cdot \left(\frac{\partial PL}{\partial O_3} \right) + (T - T_{\text{clim}}) \cdot \left(\frac{\partial PL}{\partial T} \right) + (\Omega - \Omega_{\text{clim}}) \cdot \left(\frac{\partial PL}{\partial \Omega} \right)$$

where $O_{3 \text{ clim}}$, T_{clim} and Ω_{clim} are the climatological monthly mean ozone mixing ratio, temperature, and overhead column ozone, respectively; PL_{clim} is the climatological net production-minus-loss rate; and the three partial derivatives represent the
140 local sensitivity of production-minus-loss to ozone, temperature, and column ozone. The seven climatological coefficients are obtained from a precomputed monthly climatology and interpolated onto the iAMAS mesh. The tropopause boundary is diagnosed using a hybrid potential vorticity–potential temperature (PV– θ) method: the dynamical tropopause, defined by PV = 2 potential vorticity units (PVU; 1 PVU = $10^{-6} \text{ K m}^2 \text{ kg}^{-1} \text{ s}^{-1}$), is constrained from above by the $\theta = 380 \text{ K}$ isentropic surface in the tropics to avoid spuriously high PV-based placements at low latitudes (Highwood & Hoskins, 1998).

145 2.2.2 Chemical Initialization and Photolysis

Chemical species are initialized using a two-tier approach. Ozone profiles are derived from the TOST-v2 ozonesonde climatology (Zang et al., 2024; JJA 2019 seasonal mean, interpolated to the model levels), providing an observationally constrained initial distribution representative of summertime conditions. All remaining SAPRC-99 species are initialized from idealized background vertical profiles, in which long-lived species (e.g., NO_x , HNO_3 , CO, H_2O_2) are prescribed from a
150 reference tropospheric-stratospheric climatology, while short-lived radical species are initialized at photochemical steady state and subsequently renormalized to their parent lumped categories. These profiles are mapped to 49 SAPRC-99 surrogate species following the speciation and remapping approach of Grell et al. (2005) and Fast et al. (2006).

Photolysis rate coefficients are computed online using the Fast-J scheme (Wild et al., 2000), accounting for Rayleigh scattering, O_2 and O_3 absorption, and cloud attenuation via a relative-humidity-based liquid water path parameterization. J-
155 values are computed independently at each grid cell, allowing spatially varying solar zenith angles and terrain elevations to be resolved at native mesh resolution.



2.2.3 Emission Processing

Anthropogenic and fire emissions are processed through a two-stage offline-to-online workflow consistent with the Preprocessing / Model Integration architecture shown in Figure 1. In the preprocessing stage, emission fields are remapped from their native latitude–longitude grids onto the iAMAS SCVT mesh using a resolution-adaptive interpolation strategy. Relative to U60km, the V4km mesh preserves more of the spatial heterogeneity available in the native inventories instead of aggregating the emissions over approximately 60 km cells. The remapped fields are written to dedicated binary input files. During model integration, the emission driver reads these files online at each emission update interval, combines anthropogenic and fire contributions into a shared emission tendency, and adds this tendency to the chemical tracer array as a time-varying surface forcing.

Anthropogenic surface emissions follow the HTAP v3.2 global inventory (0.1° resolution; Guizzardi et al., 2025), with NMVOC species mapped to SAPRC-99 lumped surrogates using standard chemical speciation profiles (Grell et al., 2005; Fast et al., 2006) and temporally disaggregated to hourly rates via sector-specific diurnal and weekly activity profiles. Fire emissions are prescribed from FINN v2.5 (0.1° resolution; Wiedinmyer et al., 2023) and processed through the same workflow. Most anthropogenic emission species are injected into the lowest model layer; NO_x and SO₂, which disproportionately originate from elevated industrial and power-plant sources, are instead distributed across the lowest six model layers using a fixed, mass-conserving vertical weighting profile that places approximately half the emission in the surface layer with the remainder decaying with height. Fire emissions are distributed uniformly across the lowest 10 layers.

2.2.4 Tracer Transport, Dry Deposition, and Wet Scavenging

Resolved-scale advection uses the TVD-FFSL hybrid scheme (Li et al., 2026), ensuring mass conservation and monotonicity on the SCVT mesh. Sub-grid convective transport redistributes and scavenges tracers vertically using mass flux fields from the convective scheme (Zhao et al., 2009; 2013). Dry deposition follows the resistance-in-series framework of Wesely (1989), with aerodynamic, quasi-laminar, and surface resistances parameterized from model surface-layer diagnostics and land-use-specific lookup tables. Wet scavenging applies below-cloud washout for soluble species via Henry's Law (Sander, 2015); in-cloud gas-phase scavenging is not active in the current implementation, as cloud chemistry has not been implemented in the current iAMAS chemistry framework.

2.3 Numerical Experiments

Two simulations are conducted. U60km employs a globally quasi-uniform mesh (~60 km, 165,018 cells), providing a global baseline for evaluating iAMAS chemical performance against satellite column retrievals and surface observations. V4km employs a variable-resolution mesh that transitions from ~60 km globally to ~4 km over the North China refinement zone (245,783 cells), designed to investigate the impact of mesh refinement on surface ozone simulation over complex terrain while maintaining global coverage and two-way dynamical consistency. Both configurations use 55 vertical levels from the surface to 30,000 m; the complete parameterization suite is summarized in Table 1. The two mesh configurations and the regional refinement over North China are shown in Figure 2.

The two simulations use the same physical and chemical parameterizations but different dynamical time steps (300 s for U60km and 15 s for V4km) to satisfy their respective CFL constraints. Both simulations target July 2019, the peak of the North China ozone season under summertime photochemical conditions. This one-month period samples diurnal and synoptic variability relevant to the mechanisms examined in Section 3 while remaining computationally tractable at convection-permitting resolution; assessing seasonal and interannual robustness is left for future work.

To prevent meteorological drift over the month-long simulation while maintaining chemical-field continuity, both simulations employ an overlapping block-cycling reinitialization protocol. Each block spans 5 days, and consecutive blocks overlap on the final day of the preceding block. At the beginning of each new block, meteorological fields are reinitialized



from ERA5, whereas SAPRC-99 chemical concentrations are carried forward from the preceding block output. The overlapping first day of each new block serves as meteorological adjustment and is discarded; the following four days are retained. For example, after the 26–30 June spin-up block, the 30 June–4 July block retains 1–4 July, and the 4–8 July block retains 5–8 July. This procedure is repeated through the block beginning on 28 July, from which 29–31 July are retained, producing a continuous 31-day record for July 2019 without duplicated overlap days.

2.4 Observational Data for Model Evaluation

Model performance is evaluated against five observational datasets targeting both the global chemical climatology (U60km) and the regional North China ozone environment (V4km).

2.4.1 TOST-v2 Ozonesonde Climatology

TOST-v2 (Zang et al., 2024) provides a global ozone climatology from trajectory-mapped ozonesonde profiles on a $5^\circ \times 5^\circ \times 1$ km grid. The JJA 2019 seasonal mean is used both to initialize model ozone fields (Section 2.2.1) and as an observationally based reference for evaluating the simulated vertical ozone structure.

2.4.2 OMI/MLS Tropospheric Column Ozone

Tropospheric column ozone (TCO) is evaluated against the NASA Goddard OMI/MLS monthly mean product v2 (Ziemke et al., 2019; $1^\circ \times 1^\circ$), derived using the tropospheric ozone residual method. Model TCO is computed by integrating simulated ozone from the surface to the WMO thermal lapse-rate tropopause, consistent with the product definition.

2.4.3 TROPOMI NO₂ and HCHO Column Retrievals

Tropospheric NO₂ columns are obtained from the ESA CCI+ TROPOMI Level-3 monthly NO₂ product (v fv1.0; Glissenaar et al., 2025; $0.5^\circ \times 0.5^\circ$). HCHO columns are from the ESA CCI+ TROPOMI HCHO Level-3 monthly product (v2; De Smedt et al., 2021; $0.125^\circ \times 0.125^\circ$). Both products include averaging kernels; model columns are convolved with the averaging kernels prior to comparison following Eskes & Boersma (2003). Both are based on Sentinel-5P observations at ~13:30 local solar time, and model output is sampled at the corresponding overpass hour.

2.4.4 MOPITT CO Column Retrievals

CO total columns are obtained from the MOPITT Version 9 Joint Level-3 monthly mean product (Deeter et al., 2022; daytime; $1^\circ \times 1^\circ$). Model output is sampled at 10:30 local solar time, consistent with the Terra satellite overpass, and convolved with MOPITT averaging kernels and a priori profiles.

2.4.5 CNEMC Surface Ozone Observations

Surface ozone concentrations are obtained from China's National Ambient Air Quality Monitoring Network (CNEMC), which provides hourly near-surface O₃ mixing ratios at 1,354 stations nationwide. The dataset serves as the primary benchmark for the China-wide diurnal-cycle evaluation (U60km; all 1,354 stations) and the regional spatial and temporal analyses (234 stations within the North China refinement zone with valid July 2019 records). Model values are sampled from the lowest model layer of the horizontal grid cell nearest to each station. Regional stations are classified as complex terrain (station elevation ≥ 200 m; N = 59) or plain terrain (elevation < 200 m). Urban and rural subsets are defined as the highest and lowest 20% of the 234 stations, respectively, according to their observed July-mean NO₂ concentrations (N = 46 for each subset). The station distribution is shown in Figure S1. For spatial evaluations, observed and colocated model fields are first averaged over the relevant July daytime or nighttime hours at each station, and R, MB, NMB, and RMSE are then calculated across the station-level means. For diurnal-cycle evaluations, hourly observations and colocated model values are averaged by hour of



235 day over July and across the applicable station subset; the reported statistics are calculated from the resulting 24-point mean diurnal cycles. Because near-surface NO measurements are unavailable at these stations, NO₂ is used as the representative NO_x diagnostic in the following analyses; its longer lifetime provides a more stable spatial indicator of NO_x accumulation and permits direct comparison with observations.

3 Results and Discussion

240 3.1 Evaluation of the Online Chemistry Framework at Global Scale

The global-scale chemical performance of iAMAS is evaluated using the U60km simulation against multiple observational datasets for July 2019. The evaluated species span key dimensions of tropospheric ozone chemistry: ozone itself as the primary scientific target; NO₂ and HCHO as proxies for tropospheric NO_x loading and VOC oxidation activity, respectively; and CO as a long-lived transport tracer. Together, these diagnostics characterize the global chemical state and its principal biases before the variable-resolution application described in Sections 3.2 and 3.3.

255 **Tropospheric ozone.** Figure 3 presents the evaluation of tropospheric column ozone (TCO) against the OMI/MLS monthly mean product and the vertical structure against the TOST-v2 ozonesonde climatology. iAMAS reproduces the large-scale TCO spatial pattern with reasonable fidelity ($R = 0.70$, $MB = -0.9$ DU, $NMB = -2.7\%$, $RMSE = 5.5$ DU), capturing the Northern Hemisphere midlatitude enhancement over industrialized source regions and the depleted columns over the tropical oceans. Positive biases over southern and central Africa are spatially colocated with strong FINN fire emissions during the austral dry-season burning period (Figure S2). Negative biases over northern extratropical continents are consistent with the absence of biogenic emissions in the current implementation.

The zonal-mean vertical structure is evaluated against the TOST-v2 JJA 2019 seasonal mean, the closest available reference because monthly July fields are unavailable. iAMAS achieves a high spatial correlation of $R = 0.99$ and reproduces the characteristic tropical lower-tropospheric ozone minimum and the increase toward the upper troposphere and stratosphere. Because this comparison uses a seasonal climatological product while the simulation covers July 2019, it is interpreted primarily as an assessment of large-scale vertical structure rather than as a strict month-specific validation. The simulated tropopause, overlaid in Figure 3e, exhibits a meridionally coherent structure consistent with climatological expectations and supports the plausibility of the partitioning between the SAPRC-99 tropospheric and Linoz stratospheric chemical regimes.

260 The global positive bias ($NMB = +11.0\%$) is dominated by the tropical lower-tropospheric overestimation over biomass-burning regions identified in the TCO comparison; in the lower troposphere below ~8 km across most extratropical latitudes, relative biases are generally within $\pm 30\%$.

The mean diurnal cycle of surface ozone, evaluated against 1,354 CNEMC stations across China, is shown in Figure 4. iAMAS reproduces the observed temporal evolution ($R = 0.946$), including the nocturnal minimum associated with NO titration, the daytime photochemical buildup, and the afternoon maximum. The model exhibits a positive mean bias of +5.82 ppb ($NMB = +14.7\%$, $RMSE = 8.55$ ppb) that appears as an approximately uniform upward displacement of the mean diurnal curve. This behavior is consistent with an elevated ozone background, although other systematic errors in chemistry, emissions, deposition, and mixing may also contribute.

270 **Tropospheric NO₂ and HCHO columns.** Evaluation against TROPOMI/S5P monthly mean retrievals is shown in Figure 5. For NO₂, iAMAS achieves $R = 0.81$ ($NMB = -22.5\%$, $RMSE = 0.31 \times 10^{15}$ molecules cm⁻²), reproducing the major enhancements over East Asia, northern India, and central Africa. Negative biases over Europe and the eastern United States may reflect a combination of emission-inventory uncertainty and dilution of subgrid emission heterogeneity at 60 km resolution. Positive biases over central Africa and Mongolia/south-central Siberia are spatially associated with strong FINN fire emissions. For HCHO, iAMAS achieves $R = 0.78$ ($NMB = +11.3\%$), with overestimation over fire regions broadly matching the NO₂



275 pattern. The substantial underestimation over the Amazon, eastern United States, and Europe likely reflects the absence of biogenic VOC emissions in the current implementation.

CO total columns. Evaluation against MOPITT Version 9 is shown in Figure 6. iAMAS achieves $R = 0.74$ with a near-zero global mean bias ($NMB = +0.4\%$) and reproduces the dominant CO enhancements over central Africa and Mongolia/south-central Siberia associated with biomass burning, although both regions exhibit modest positive biases. The 280 large-scale agreement supports the overall plausibility of the combined emission processing, chemical loss, and dynamical transport.

Taken together, the multi-species evaluation shows that iAMAS U60km captures major large-scale spatial and temporal features of tropospheric chemistry sufficiently well to provide a baseline for the refinement analysis. For qualitative context, Figures S3–S6 present a quasi-global WRF-Chem simulation at 0.5° resolution (configuration in Supplementary Text S1). The 285 comparison indicates that the magnitude of the iAMAS skill and biases falls within a reasonable range relative to an established community chemistry model operating under broadly comparable conditions. Shared regional signatures also place several iAMAS biases in the context of uncertainties that can arise from common inventories or incompletely represented processes, including fire emissions and biogenic VOC chemistry, rather than uniquely model-specific deficiencies.

3.2 Nighttime Ozone over Complex Terrain: Coupled Effects of Terrain Resolution and Emission Heterogeneity

290 Having characterized the large-scale chemical performance of U60km, we now turn to the effect of mesh refinement on surface O_3 over the complex terrain of North China. Figure 7 presents the daytime and nighttime surface O_3 spatial distributions simulated by U60km and V4km, together with the V4km–U60km difference fields and station-based statistical metrics. During daytime, the two simulations exhibit similar spatial patterns (Figure 7a–b), with no systematic directional bias in the difference field (Figure 7c); their statistical metrics are also comparable, with $R = 0.42$ and 0.53 at all sites and $R = 0.52$ at both 295 configurations for complex terrain sites, indicating that horizontal resolution has limited impact on daytime O_3 model skill.

In contrast, nighttime performance shows marked divergence. V4km produces a pronounced high- O_3 band along the Taihang–Yanshan mountains and resolves localized low- O_3 pockets, while U60km yields a spatially uniform field that fails to capture this terrain-related O_3 heterogeneity (Figure 7d–e). The simulated nocturnal O_3 enhancement over ridges and slopes is consistent with observational evidence from the Taihang Mountains (Zhao et al., 2019). The difference field shows V4km 300 systematically exceeding U60km over the mountain region (Figure 7f). The improvement is most pronounced at complex-terrain sites: R changes from -0.40 in U60km to $+0.46$ in V4km, while the all-site R increases from 0.12 to 0.43 . V4km also reduces the all-site nighttime NMB from -13.1% to 2.1% , and RMSE decreases by ~ 2 ppb for both the complex-terrain and all-site samples. The sign reversal at complex-terrain sites indicates that refinement changes the simulated direction of the nighttime spatial gradient, whose dynamical and chemical context is examined below. The U60km bias here remains within 305 the error envelope of the coarse-resolution simulation (Figure S7).

Figure 8 presents vertical cross-sections along a SE ($114.52^\circ E$, $37.79^\circ N$) to NW ($112.02^\circ E$, $39.54^\circ N$) transect, revealing differences between the two configurations in the representation of nocturnal terrain structure and atmospheric processes. Originating from the plains east of Shijiazhuang and extending northwestward across the Taihang Mountains to the vicinity of Shuozhou, the transect traverses the plain and mountain foothills (0 – 60 km), slopes and ridges (60 – 180 km), a natural valley 310 (~ 195 km), and an urban valley (~ 250 km; Shuozhou). The geographic track and annotated zones are provided in Figure S8. In U60km, the ~ 60 km grid represents the Taihang terrain as a series of smooth steps and produces comparatively uniform wind and layered O_3 structures (Figure 8a). V4km better represents the alternating ridge–valley terrain and is accompanied by distinct dynamical and chemical responses (Figure 8b).

Regarding the dynamical response, V4km represents prominent slope circulations over the mountain foothills and ridge 315 zones (0 – 30 km and 60 – 180 km along the section). The simulated flow transports O_3 -rich residual-layer air toward the near-surface and is consistent with sustained nighttime O_3 over these zones. In the valley at ~ 195 km, the response is reversed:



simulated downslope drainage favors cold-air accumulation at the valley floor, where stable stratification limits exchange with the overlying residual layer and O_3 is depleted. The ΔO_3 field (Figure 8c) supports this interpretation, with V4km exceeding U60km over ridges and slopes and showing the opposite response in valleys. The white dashed line in Figure 8b marks the U60km terrain profile and shows that coarse-grid elevations at the sampled valley locations are 400–600 m higher than in V4km, substantially reducing the represented ridge–valley contrast and the associated circulation structure.

Regarding the chemical response, mapping the native 0.1° anthropogenic inventory to the V4km mesh preserves more urban–rural emission heterogeneity than mapping it to U60km; the corresponding nighttime NO_2 distributions are shown in Figure S9. The ΔNO_2 field (Figure 8d) illustrates contrasting responses along the transect. Near the origin (0–30 km; mountain foothills southwest of Shijiazhuang), V4km separates the foothill grid cells more clearly from the adjacent urban center and simulates lower local NO_2 than U60km, which aggregates emissions over a much larger area. The lower NO_2 in V4km weakens nocturnal NO titration and is spatially consistent with positive ΔO_3 near ~30 km in Figure 8c. Near the terminus (~250 km; the Shuozhou urban valley), V4km produces higher NO_2 than U60km, consistent with resolved higher emissions and stronger local accumulation. The associated increase in NO titration is consistent with the negative ΔO_3 feature near ~250 km. Thus, the cross-section supports a coupled interpretation in which terrain-related transport and the spatial distribution of NO_x jointly shape the nighttime O_3 response. The simulated sensitivity of nocturnal O_3 to urban NO_x is also consistent with recent multi-city observational evidence that urban cores in the North China Plain remain strongly NO_x influenced as regional emissions decline (Xue L. et al., 2026).

Together, these dynamical and chemical mechanisms demonstrate that V4km reproduces the nocturnal complex terrain O_3 pattern — elevated over ridges and slopes, depleted in valleys — through both resolved terrain circulations and more realistic emission spatial distributions, while U60km systematically underestimates ridge O_3 and overestimates valley O_3 , inverting the true spatial gradient. To provide observational support for the mechanisms identified above, Figure 9 examines the relationship between nighttime surface O_3 and NO_2 concentrations and the Topographic Position Index (TPI) at complex terrain sites ($N = 59$). TPI is defined as the elevation difference between a site and the mean elevation within a 30 km radius; positive values indicate ridge positions and negative values indicate valley positions, providing a quantitative, observation-independent characterization of local terrain context.

Figure 9a evaluates whether the model meshes represent the terrain-position contrasts needed for terrain-related circulation differences. V4km-resolved TPI correlates with the reference TPI derived from the 1 km DEM ($R = +0.75$, $p < 0.05$; slope = 0.56), indicating that V4km distinguishes ridge and valley positions, although the relief amplitude remains underestimated. U60km-resolved TPI is zero across the sampled sites and therefore contains little information about local ridge–valley position. Figure 9b shows the nighttime NO_2 –TPI relationship. Observed NO_2 decreases with TPI ($R = -0.47$, $p < 0.05$), indicating higher concentrations at valley than ridge sites. This pattern is consistent with reduced mixing and cold-pool trapping in valleys and may also reflect the locations of urban and industrial emissions within the sampled terrain. V4km captures a negative NO_2 –TPI relationship ($R = -0.39$, $p < 0.05$), whereas U60km yields a weak positive relationship ($R = +0.20$). Figure 9c shows the corresponding nighttime O_3 –TPI relationship. Observed O_3 increases with TPI ($R = +0.54$, $p < 0.05$), demonstrating a ridge-high, valley-low spatial pattern. V4km captures this positive relationship ($R = +0.46$, $p < 0.05$), whereas U60km produces a negative relationship ($R = -0.35$, $p < 0.05$). Together, these results are consistent with two coupled consequences of refinement: improved representation of ridge–valley terrain and associated transport, and preservation of more emission heterogeneity from the native 0.1° inventory. In the refined simulation, these changes favor greater residual-layer influence at elevated sites and stronger local titration where NO_x accumulates in populated valleys.

The preceding mechanisms — terrain-resolved circulations and emission redistribution — operate predominantly at night rather than during the day, a contrast governed by boundary layer state and illustrated in Figure S10. Daytime convective boundary layers reach 800–1800 m (Figure S10a–b), and strong turbulent mixing substantially weakens the local O_3 and NO_x gradients generated by terrain circulations and concentrated emissions; additionally, daytime O_3 budgets are dominated by



photochemical production, which is less sensitive to the spatial distribution of emissions than nighttime physical and chemical depletion processes. Although V4km's daytime PBLH is 10–20% lower than U60km's over complex terrain (Figure S10c–d), this difference manifests as a comparatively modest O₃ spatial divergence against a background of vigorous convective mixing, consistent with the smaller gap in daytime statistical metrics between U60km and V4km. At night, the stable boundary layer contracts to 100–400 m, with V4km producing PBLH values 20–40% lower than U60km over complex terrain (Figure S10g–h), suppressing vertical mixing and amplifying both the terrain-circulation O₃ transport and the emission-concentration NO_x titration effects, consistent with the pronounced spatial divergence documented in Figure 7. This PBLH-modulated contrast between daytime and nighttime resolution sensitivity is consistent with broader findings on the role of boundary-layer structure in controlling pollutant vertical distributions over North China (Li et al., 2021).

3.3 Resolution-Dependent Day–Night and Urban–Rural Ozone Responses

Section 3.2 established that mesh refinement primarily improves nighttime surface O₃ simulation over complex terrain through resolved terrain circulations and emission redistribution. We now turn to the diurnal cycle of surface O₃ across the full North China refinement zone, examining how the same resolution increase (~60 km to ~4 km) modifies the photochemical and boundary layer processes that govern the daily O₃ evolution.

Figure 10 presents the mean diurnal cycles of surface O₃ for all sites, urban sites (top 20% by observed NO₂, 46 sites), and rural sites (bottom 20% by observed NO₂, 46 sites), alongside the hourly resolution effect ($\Delta O_3 = V4km - U60km$). Observations exhibit a characteristic single-peak diurnal cycle, reaching a minimum at 05:00–07:00 BJT and a maximum at 14:00–16:00 BJT. Both U60km and V4km capture this pattern with high temporal correlation ($R > 0.90$), but U60km systematically overestimates daytime peak O₃ and underestimates nighttime O₃. V4km reduces RMSE across all site categories: from 10.5, 11.2, and 10.9 ppb (U60km) to 9.0, 9.4, and 8.6 ppb (V4km) for all, urban, and rural sites respectively. The ΔO_3 time series ($\Delta O_3 = V4km - U60km$, Figure 10d–f) reveals a characteristic dual-phase diurnal adjustment. A daytime reduction effect occurs from 09:00 to 17:00 BJT, where ΔO_3 is negative and most pronounced at urban sites (maximum –6 ppb, Figure 10e), effectively alleviating U60km's overestimation of the afternoon O₃ peak. A nighttime enhancement effect operates from 18:00 to 08:00 BJT, where ΔO_3 is positive and most prominent at rural sites (+8 to +10 ppb, Figure 10f), substantially correcting U60km's systematic underestimation of rural nocturnal O₃. At urban sites, the nighttime ΔO_3 signal shows a finer temporal structure: V4km closely tracks observations from 19:00 to 00:00 BJT, but then exceeds observations during 00:00–05:00 BJT as V4km O₃ declines more slowly than observed; this overestimation is addressed in the boundary layer analysis below.

Figure 11 presents the NO₂ diurnal cycles and the HCHO/NO₂ column formaldehyde-to-nitrogen dioxide ratio (FNR, $FNR < 1.0$ for VOC-limited conditions, $FNR > 2.0$ for NO_x-limited conditions, and intermediate values for a transitional regime), which is used as a qualitative proxy for the O₃ photochemical production regime (Ren et al., 2022). For urban sites (Figure 11b), V4km simulates substantially higher daytime NO₂ concentrations than U60km because the refined mesh avoids the substantial aggregation of native 0.1° emission fields that occurs on the ~60 km mesh. The FNR diagnostic (Figure 11e) indicates that urban sites in V4km remain in the VOC-limited regime throughout the day and are displaced further into this regime relative to U60km, which enters the transitional range during midday. Under this diagnostic framework, the higher urban NO_x in V4km is consistent with stronger VOC-limited suppression of O₃ production and contributes to the reduced daytime O₃ peak. For rural sites (Figure 11c), V4km simulates lower nighttime NO₂ concentrations than U60km, in closer agreement with observations. This response is consistent with reduced numerical dilution of high-NO_x urban air into surrounding rural grid cells. The associated weakening of nocturnal NO titration helps sustain higher rural nighttime O₃. The limited daytime V4km–U60km difference in rural FNR (Figure 11f) suggests that the rural response is dominated by nighttime NO_x and titration changes rather than a pronounced regime shift.

Figure 12 illustrates the vertical–diurnal evolution of the vertical turbulent mixing coefficient K_{zh} at urban sites, providing boundary-layer context for the urban O₃ response. During daytime (09:00–17:00 BJT), U60km produces a deeper



boundary layer (~1,750 m) than V4km (~1,600 m), and V4km Kzh is 10%–50% weaker in the mid-to-upper boundary layer (>300 m AGL; Figure 12d). This weaker mixing is consistent with greater retention of NO_x near the surface and the higher near-surface NO₂ shown in Figure 11b; together with the VOC-limited sensitivity indicated by FNR, it supports the diagnosed daytime O₃ reduction. At night (18:00–08:00 BJT), the urban-site subset in V4km has substantially larger near-surface Kzh (<300 m AGL) than U60km, with relative differences exceeding 100% (Figure 12d). The enhanced near-surface turbulence is consistent with stronger representation of urban land-surface heterogeneity in V4km. It provides a plausible pathway for more efficient downward mixing of residual-layer O₃, partially offsetting nocturnal titration. Consequently, V4km remains closer to observations during 19:00–00:00 BJT but sustains a higher O₃ floor than observed during 00:00–05:00 BJT, contributing to the overestimation identified in Figure 10b.

In summary, the resolution-dependent changes in the O₃ diurnal cycle are consistent with coordinated chemical and dynamical responses. At urban sites, the preservation of finer emission heterogeneity and a shallower daytime boundary layer increase near-surface NO_x; within the VOC-limited regime indicated by FNR, these changes support a reduction of the daytime O₃ peak. At night, stronger near-surface mixing in the urban-site subset provides a pathway for downward transport of residual-layer O₃, partly offsetting titration. At rural sites, reduced numerical dilution of urban NO_x into surrounding coarse cells lowers nighttime NO₂, weakens titration, and increases surface O₃.

4 Conclusions

This study presents the development and evaluation of a modular online gas-phase chemistry capability within the global nonhydrostatic variable-resolution model (the integrated Atmospheric Model Across Scales, iAMAS v2.5.1). By coupling KPP-generated SAPRC-99 tropospheric chemistry, Linoz stratospheric ozone parameterization, Fast-J photolysis, emissions processing, tracer transport, dry deposition, and wet scavenging on a unified unstructured SCVT mesh, the framework establishes a seamless multiscale physics–chemistry platform that operates without prescribed lateral boundary conditions.

Global baseline evaluations at quasi-uniform ~60 km resolution (U60km) for July 2019 confirm the model's fidelity in representing large-scale spatial patterns of tropospheric O₃, NO₂, HCHO, and CO, alongside the observed phase of the surface ozone diurnal cycle across China. High-resolution experiments refined to ~4 km over North China (V4km) demonstrate the cross-scale capability of the framework under complex environmental conditions. Refinement successfully recovers the observed ridge-high/valley-low nighttime surface ozone pattern over the Taihang–Yanshan mountain complex, reversing the spatial correlation from R = -0.40 (U60km) to R = +0.46 (V4km). Process diagnostics attribute this correction to the joint representation of resolved slope circulations and preserved NO_x emission heterogeneity interacting within a shallow nocturnal boundary layer. Furthermore, refinement reorganizes day–night and urban–rural ozone responses: higher near-surface urban NO_x suppresses the daytime ozone peak under stronger VOC-limited conditions, whereas reduced coarse-grid NO_x dilution weakens rural nighttime titration and sustains higher ozone levels.

The overarching scientific implication of this work is that mesh refinement in an online global VR chemistry model does not merely sharpen spatial concentration gradients. By modifying resolved terrain, the spatial co-location of emissions, boundary-layer depth and turbulence, numerical dilution, and local transport pathways, refinement fundamentally reorganizes the coupled dynamical–chemical state and shifts the governing chemical regimes across terrain positions, source environments, and times of day.

While this study establishes a foundation for seamless global-to-regional atmospheric composition modeling, several priorities remain for future development. The present single-month evaluation diagnoses an integrated response; dedicated factor-separation experiments are needed to isolate the individual contributions of terrain resolution, emission remapping, and boundary-layer physics. Model capabilities should be expanded to incorporate biogenic VOC emissions, comprehensive stratospheric chemistry, and online aerosol–gas and cloud–chemistry interactions. Furthermore, long-term multi-season



evaluations across diverse geographical regions will establish climate-scale robustness. By coupling nonhydrostatic physics and online chemistry on a scalable, parallelized SCVT mesh, iAMAS provides a flexible and computationally tractable global VR platform. This architecture establishes a foundation for seamless global-to-regional air quality modeling, simultaneous multi-region refinement over pollution hotspots, and future investigations into regional air quality and global climate interactions.

Code and data availability

The iAMAS source code used in this study is archived at Zenodo at <https://doi.org/10.5281/zenodo.20743487> (Xia and Zhao, 2026). ERA5 reanalysis data are available from the Copernicus Climate Data Store (<https://cds.climate.copernicus.eu/datasets/reanalysis-era5-pressure-levels> and <https://cds.climate.copernicus.eu/datasets/reanalysis-era5-single-levels>). Anthropogenic emissions are from the HTAP v3.2 inventory (https://edgar.jrc.ec.europa.eu/dataset_htap_v32), and fire emissions are from FINN v2.5 (<https://gdex.ucar.edu/datasets/d312009/dataaccess/>). The TOST-v2 ozonesonde climatology is available at <https://doi.org/10.5281/zenodo.13984482>. OMI/MLS tropospheric column ozone data are available from https://acd-ext.gsfc.nasa.gov/Data_services/cloud_slice/. TROPOMI tropospheric NO₂ and HCHO column products are available from <https://www.temis.nl/airpollution/no2col/cci-no2-tropomi.php> and <https://distributions.aeronomie.be/32ddd2e-3a37-4ca6-9b1e-762e09ebe4bb>, respectively. MOPITT CO total-column data are available from https://cmr.earthdata.nasa.gov/virtual-directory/collections/C3442474658-LARC_CLOUD/temporal/2019. CNEMC surface observations were obtained from the Ministry of Ecology and Environment of China through its data service (<https://air.cnemc.cn:18007/>).

Author contributions

ZX developed the model, designed the experiments, conducted the simulations, performed the analysis, and wrote the manuscript. CZ supervised the model development, experimental design, analysis, and manuscript writing. CJ contributed to model development. All other authors contributed to discussions and commented on the manuscript.

Competing interests

The authors declare that they have no conflict of interest.

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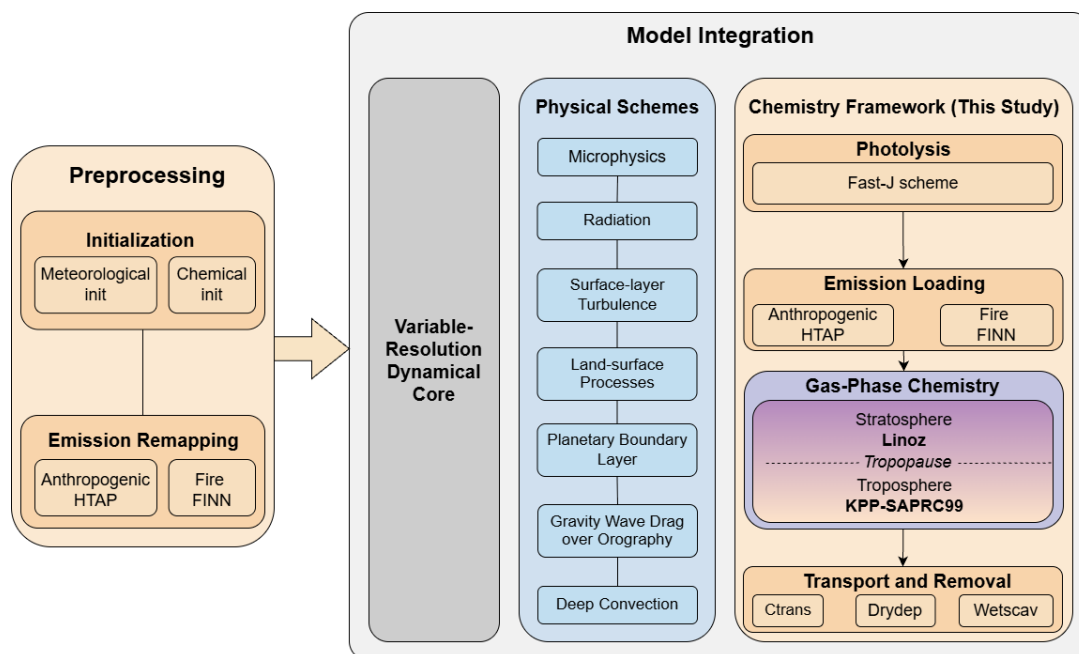


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Table 1. Configuration summary of the two iAMAS simulations conducted in this study.

Type	Parameter	U60km	V4km
General settings	Mesh resolution	~60 km (global)	~60 km (Outside)→~4 km (North China refinement zone)
	Dt	300 s	15 s
	Chemdt	1800 s	
	Model top	30,000 m	
	Vertical levels	55	
	Spin-up period	26–30 June 2019	
	Analysis period	1–31 July 2019	
Physics	Microphysics	Thompson (Thompson et al., 2008)	
	Radiation	RRTMG for longwave and short wave (Iacono et al., 2008)	
	Surface-layer turbulence	Monin_obukhov (Monin and Obukhov, 1954)	
	Land-surface	Noah (Chen and Dudhia, 2001)	
	Planetary boundary layer	YSU (Hong et al., 2006)	
	Gravity wave drag over orography	YSU_GWDO (Kim and Doyle, 2005; Choi and Hong, 2015)	
	Convection	Grell–Freitas (Grell and Freitas, 2014)	
Chemistry	Emission	HTAPv3.2 (Guizzardi et al., 2025) for anthropogenic; FINNv2.5 (Wiedinmyer et al., 2023) for fire	
	Photolysis	Fast-J (Wild et al., 2000); calculation interval: 1800 s	
	Convective tracer transport	Grell–Freitas (Grell and Freitas, 2014)	
	Dry deposition	Wesely (Wesely, 1989)	
	Wet scavenging	Below-cloud washout via Henry's Law (Sander, 2015)	
	Chemical mechanism	SAPRC-99 (Carter, 2000) in troposphere; Linoz (McLinden et al., 2000) in stratosphere	



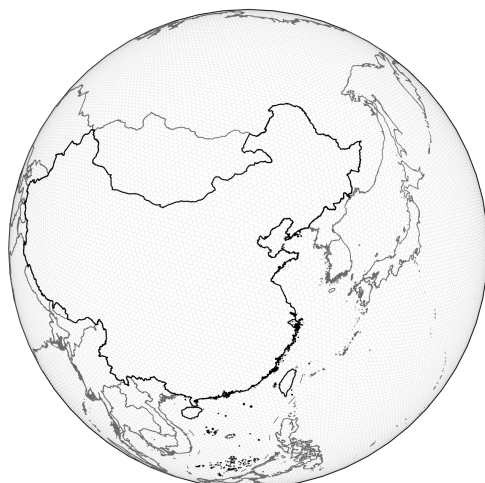
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Figure 1. Schematic of the iAMAS model architecture, illustrating the two-stage workflow from preprocessing to model integration. In the preprocessing stage, meteorological and chemical initial conditions are generated, and anthropogenic (HTAP) and fire (FINN) emission inventories are remapped onto the variable-resolution mesh. During model integration, the variable-resolution dynamical core couples a suite of physical schemes (microphysics, radiation, surface-layer turbulence, land-surface processes, planetary boundary layer, gravity wave drag over orography, and deep convection) with the chemistry framework developed in this study. The chemistry framework comprises online photolysis (Fast-J scheme), online emission loading (anthropogenic, fire), gas-phase chemistry partitioned at the diagnosed tropopause into stratospheric (Linoz) and tropospheric (KPP-SAPRC99) chemical regimes, and subsequent chemical transport, dry deposition, and wet scavenging.

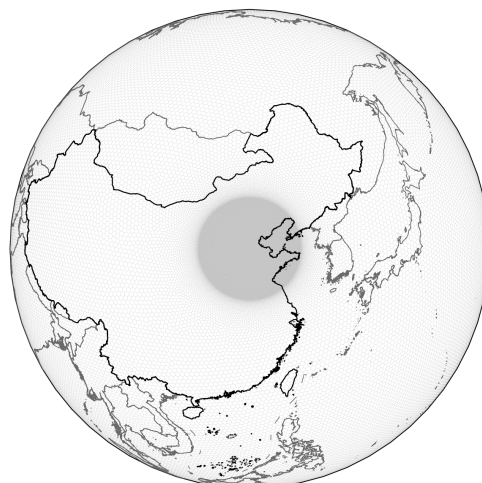
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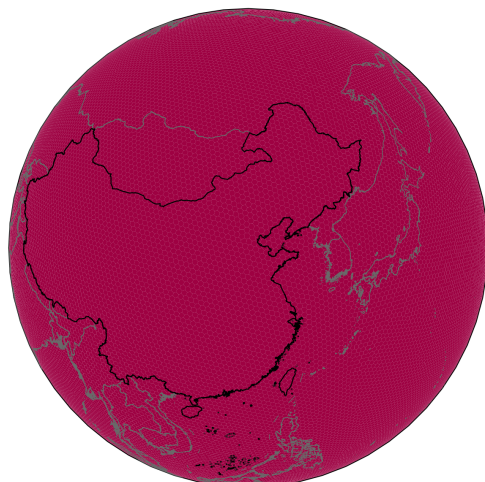
(a) U60km Mesh Topology



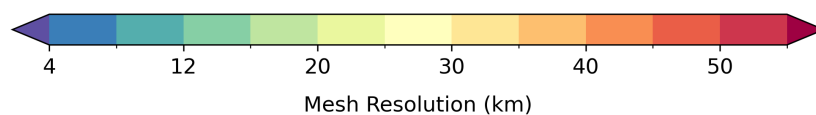
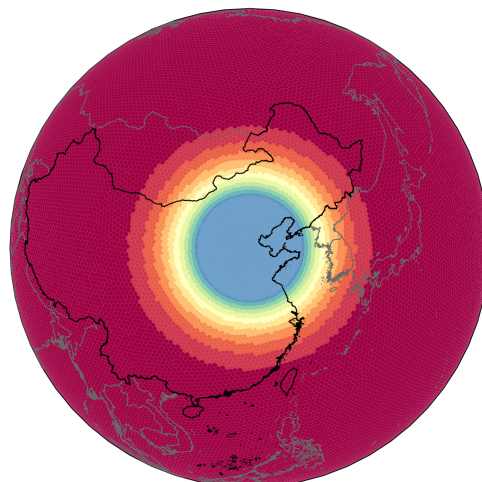
(b) V4km Mesh Topology



(c) U60km Resolution



(d) V4km Resolution



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Figure 2. Schematic of the iAMAS multiresolution unstructured meshes. Panels (a) and (b) show the mesh topology for the U60km (quasi-uniform 60 km) and V4km (variable-resolution 4 km) configurations, respectively. Panels (c) and (d) display the corresponding horizontal grid spacing (km). The V4km mesh contains a high-resolution region centered over North China (116.5°E, 38.0°N), with a refinement radius of 5°, within which the grid spacing is approximately 4 km before gradually increasing toward ~60 km outside the refinement region.

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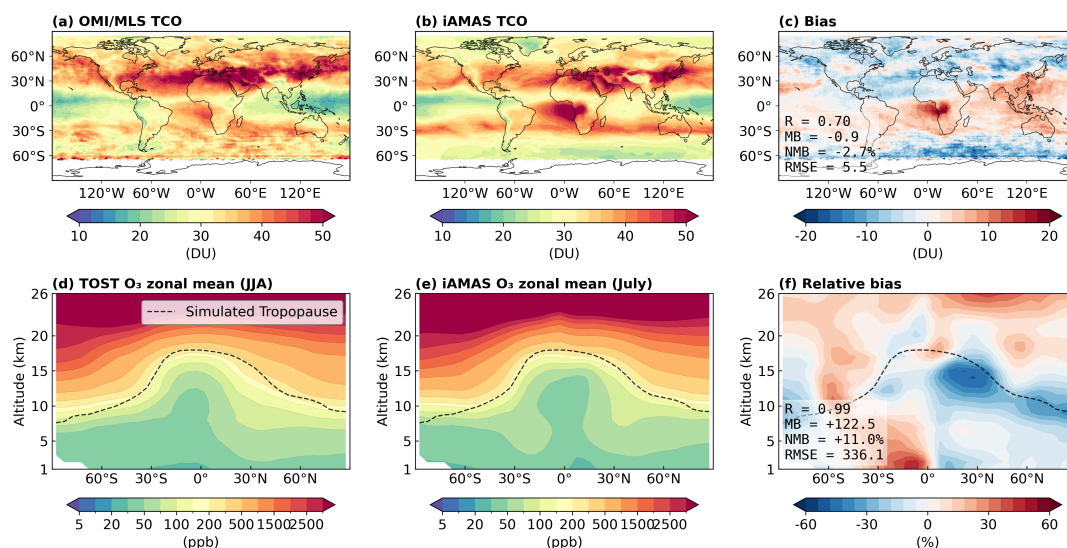
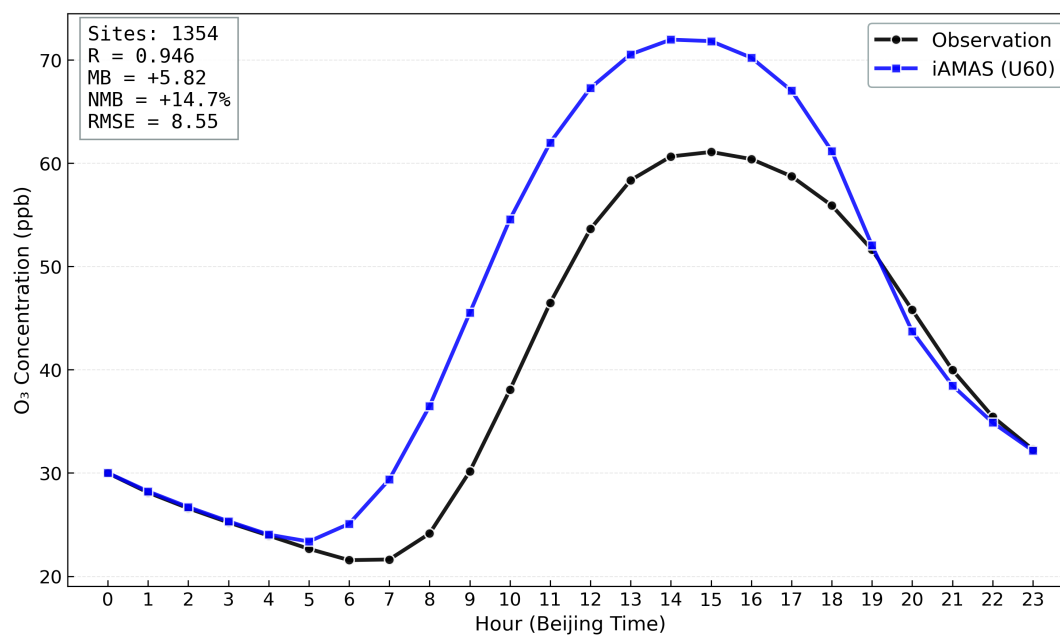


Figure 3. Evaluation of iAMAS U60km tropospheric ozone for July 2019. (a) OMI/MLS tropospheric column ozone (TCO; DU). (b) iAMAS-simulated TCO computed by vertically integrating ozone from the surface to the WMO thermal lapse-rate tropopause. (c) Bias (iAMAS – OMI/MLS; DU); global statistics (R, MB, NMB, RMSE) are shown in the lower-left inset. (d) TOST-v2 JJA 2019 zonal-mean ozone mixing ratio (ppb) as a function of altitude and latitude. (e) iAMAS July 2019 zonal-mean ozone mixing ratio (ppb); the dashed line indicates the simulated tropopause. (f) Relative bias of the iAMAS zonal-mean ozone with respect to TOST-v2 (%); global statistics are shown in the lower-left inset.



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Figure 4. Mean diurnal cycle of surface ozone (ppb) averaged over all 1,354 CNEMC monitoring stations across China for July 2019. Black circles indicate the observed hourly mean, and blue squares indicate the iAMAS U60km simulation sampled from the lowest layer of the nearest model grid cell. Statistics (R, MB, NMB, RMSE) are calculated from the 24 hourly values of the mean diurnal cycles and shown in the upper-left inset. Time is expressed in Beijing Time (BJT = UTC + 8).

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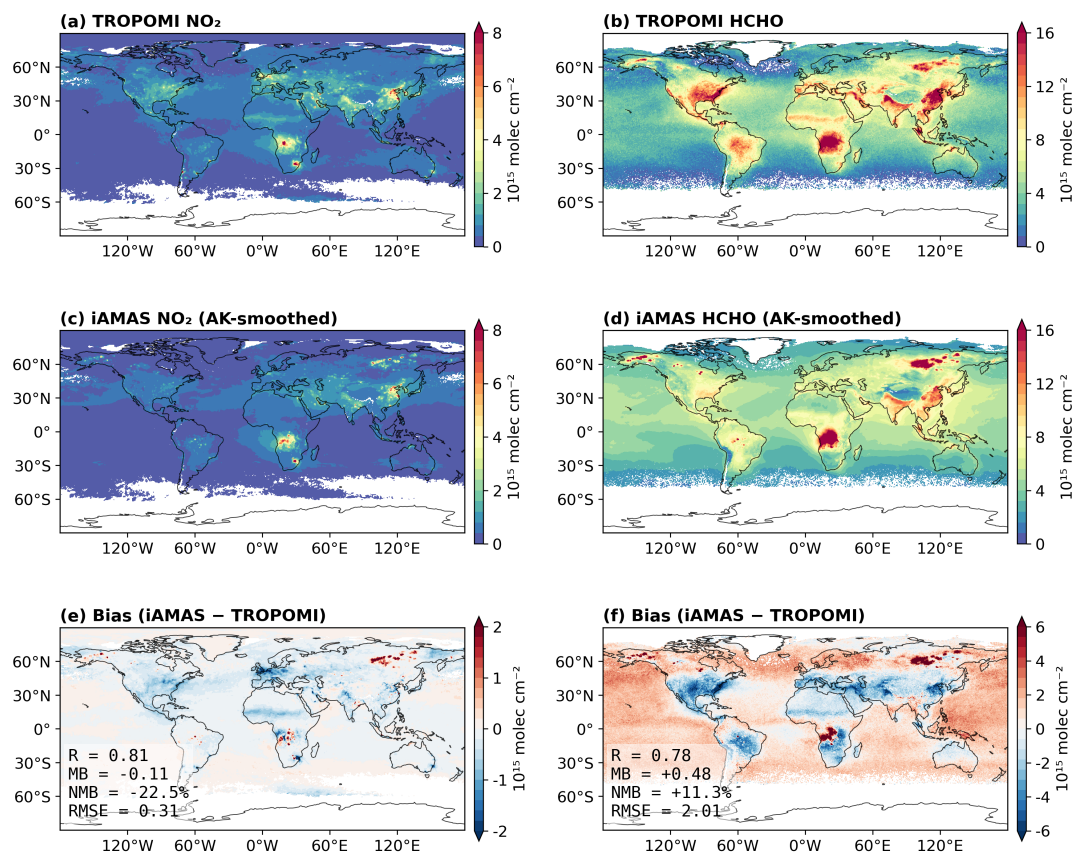


Figure 5. Evaluation of iAMAS U60km tropospheric column NO₂ (left column) and HCHO (right column) against TROPOMI/S5P for July 2019. (a, b) TROPOMI observed tropospheric columns (10^{15} molecules cm⁻²). (c, d) iAMAS simulated columns after application of TROPOMI averaging kernels, sampled at 13:30 local solar time. (e, f) Bias fields (iAMAS – TROPOMI; 10^{15} molecules cm⁻²); global statistics are shown in the lower-left inset of each panel.

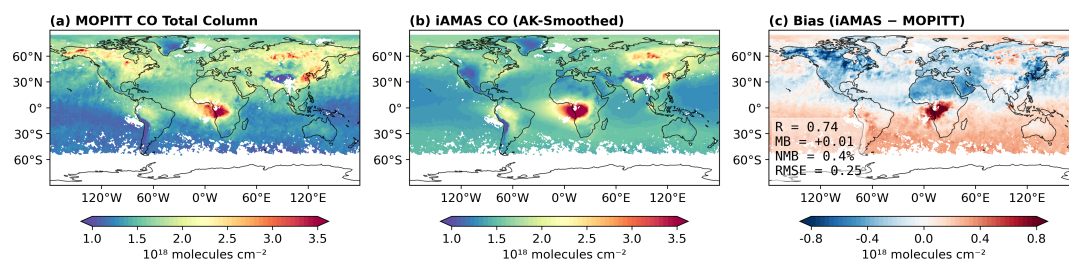


Figure 6. Evaluation of iAMAS U60km CO total columns against MOPITT Version 9 daytime retrievals for July 2019. (a) MOPITT observed CO total column (10^{18} molecules cm^{-2}). (b) iAMAS simulated CO total column after application of MOPITT averaging kernels and a priori profiles, sampled at 10:30 local solar time. (c) Bias field (iAMAS – MOPITT; 10^{18} molecules cm^{-2}); global statistics are shown in the lower-left inset.

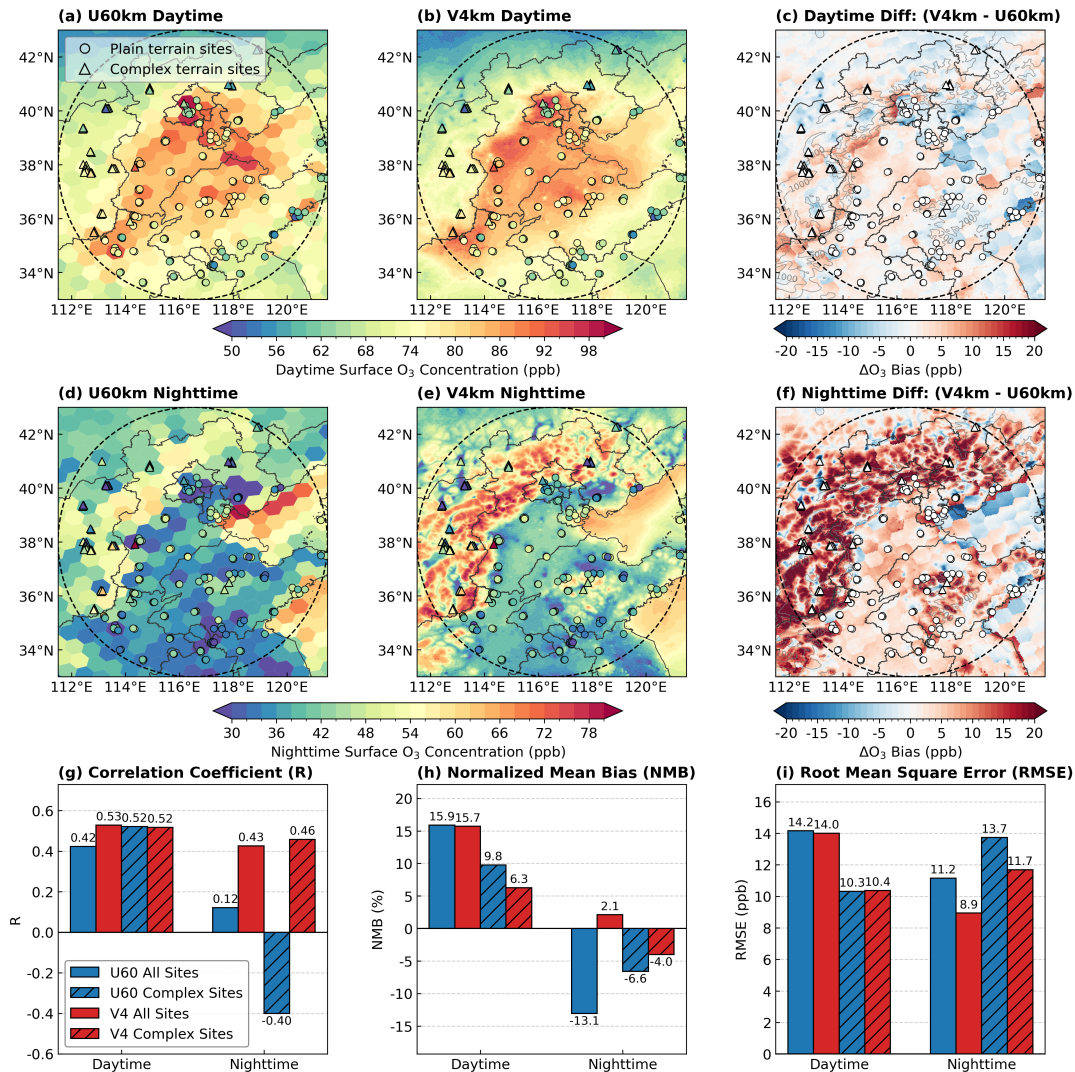


Figure 7. Daytime (08:00–19:00 BJT) and nighttime (20:00–07:00 BJT) surface O₃ spatial distributions and model evaluation statistics over the North China refinement zone for July 2019. (a, b) U60km- and V4km-simulated daytime surface O₃ concentrations (background shading, ppb); (c) daytime V4km – U60km difference (ΔO₃, ppb); (d, e) U60km- and V4km-simulated nighttime surface O₃ concentrations; (f) nighttime V4km – U60km difference. Observed station concentrations are overlaid as filled symbols using the same color scale: circles denote plain-terrain sites (elevation < 200 m) and triangles denote complex-terrain sites (elevation ≥ 200 m). (g–i) Correlation coefficient (R), normalized mean bias (NMB), and root-mean-square error (RMSE), calculated across station-level July daytime or nighttime mean concentrations, for all sites and complex-terrain sites; solid bars denote U60km and hatched bars denote V4km. An asterisk denotes $p < 0.05$ based on a two-sided Pearson correlation test.

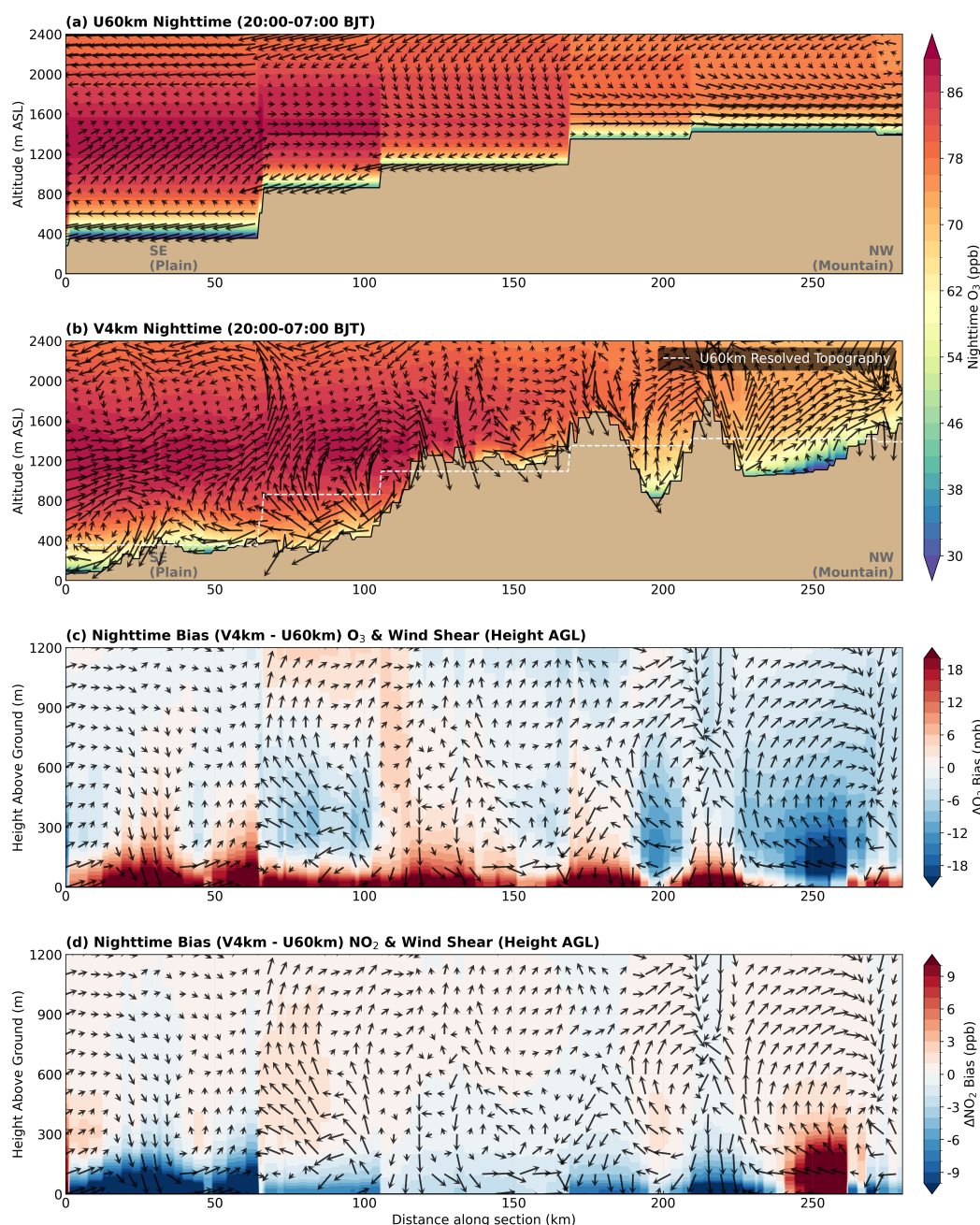


Figure 8. Nighttime (20:00–07:00 BJT) vertical cross-sections of O₃ concentration and wind vectors along the SE (114.52°E, 37.79°N) to NW (112.02°E, 39.54°N) transect for July 2019. (a) U60km O₃ mixing ratio (color shading, ppb) and along-section wind vectors (arrows); arrow lengths are rescaled by wind-speed percentile for visibility and indicate flow direction and relative strength rather than absolute wind speed. (b) V4km, as in (a); the white dashed line indicates the U60km terrain profile for comparison. (c) V4km – U60km nighttime O₃ difference (ΔO₃, ppb) and wind-vector difference (arrows), plotted as height above ground level (AGL). (d) V4km – U60km nighttime NO₂ difference (ΔNO₂, ppb) and wind-vector difference. The transect extends from the North China Plain through the Taihang Mountain foothills, ridges, and valleys to the Shuozhou urban basin. Key terrain zones are annotated in Figure S8.

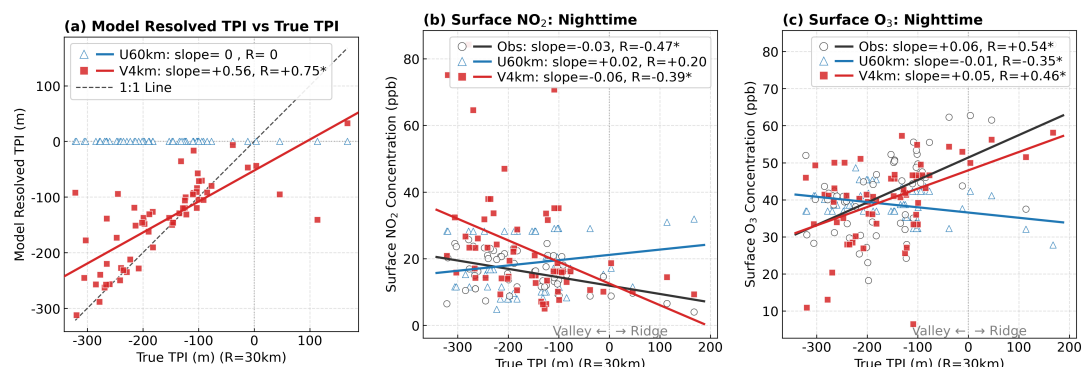


Figure 9. Topographic dependence of nighttime surface O₃ and NO₂ at complex-terrain sites (N = 59). (a) Model-resolved Topographic Position Index (TPI, m) versus reference TPI computed with a 30 km radius from 1 km DEM terrain data; the dashed line is the 1:1 reference. (b) Nighttime (20:00–07:00 BJT) surface NO₂ concentration versus reference TPI. (c) Nighttime surface O₃ concentration versus reference TPI. In (b) and (c), open circles denote observations, blue triangles denote U60km, and red squares denote V4km; solid lines are linear regression fits. Positive TPI values indicate ridge positions, and negative values indicate valley positions. An asterisk denotes $p < 0.05$ based on a two-sided Pearson correlation test.

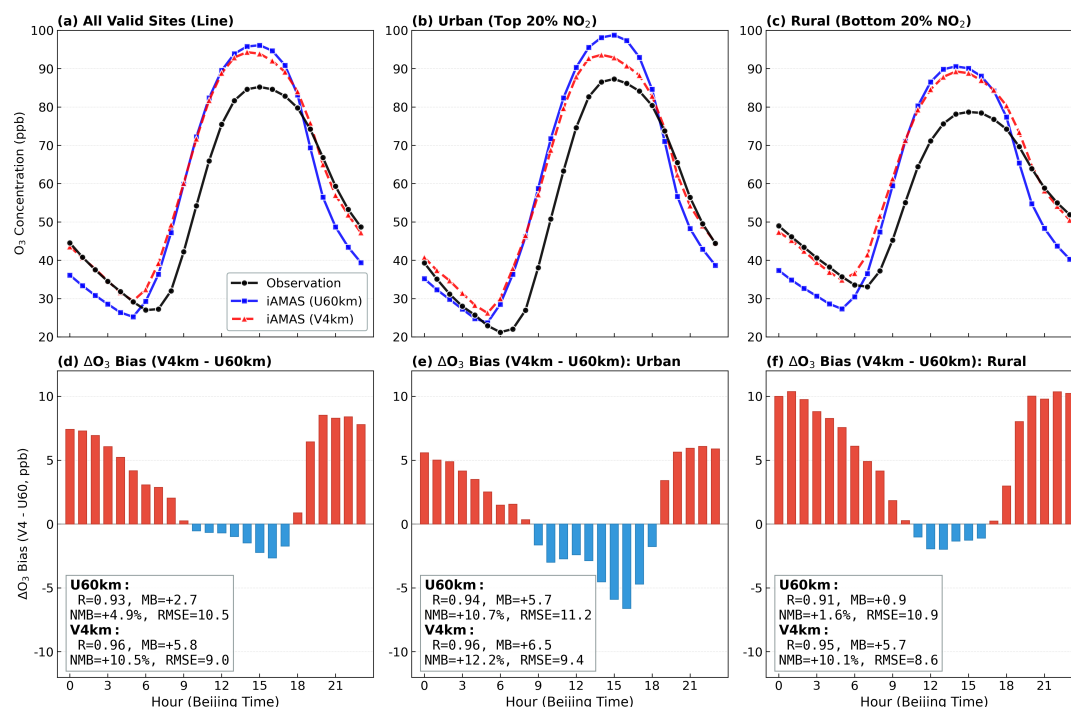


Figure 10. Mean diurnal cycles of surface O₃ concentration (ppb) and hourly resolution effect ($\Delta O_3 = V4km - U60km$, ppb) over the North China refinement zone for July 2019. Top row (a–c): observed (black circles), U60km-simulated (blue squares), and V4km-simulated (red triangles) diurnal O₃ cycles averaged over (a) all valid sites (N = 234), (b) urban sites (highest 20% by observed July-mean NO₂; N = 46), and (c) rural sites (lowest 20%; N = 46). Statistical metrics (R, MB, NMB, RMSE), calculated from the 24 hourly values of each mean diurnal cycle, are annotated in each panel. Bottom row (d–f): hourly ΔO_3 bar charts for the corresponding site categories; red bars indicate V4km > U60km, and blue bars indicate V4km < U60km. All times are in BJT.

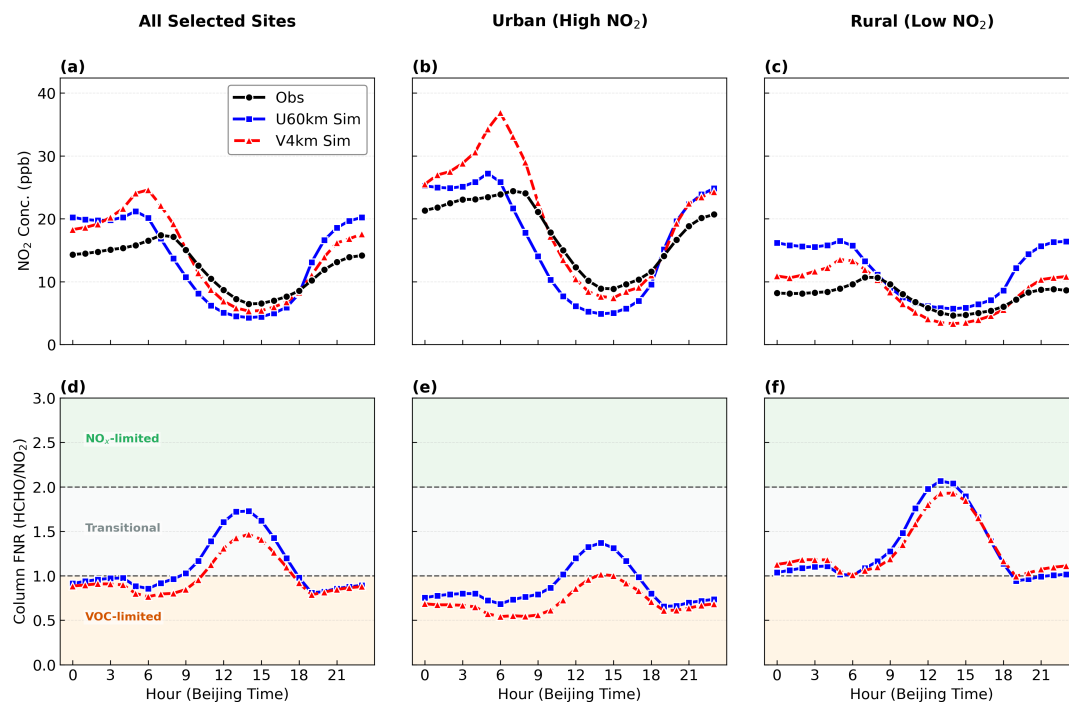


Figure 11. Diurnal cycles of surface NO_2 concentration (ppb; top row) and HCHO/NO_2 column ratio FNR (bottom row) for U60km (blue squares), V4km (red triangles), and observations (black circles, NO_2 only), averaged over (a, d) all valid sites, (b, e) urban sites, and (c, f) rural sites. Horizontal dashed lines in FNR panels indicate the VOC-limited (FNR < 1.0) and NO_x -limited (FNR > 2.0) regime boundaries; the shaded region between 1.0 and 2.0 denotes the transitional regime. All times are in BJT.

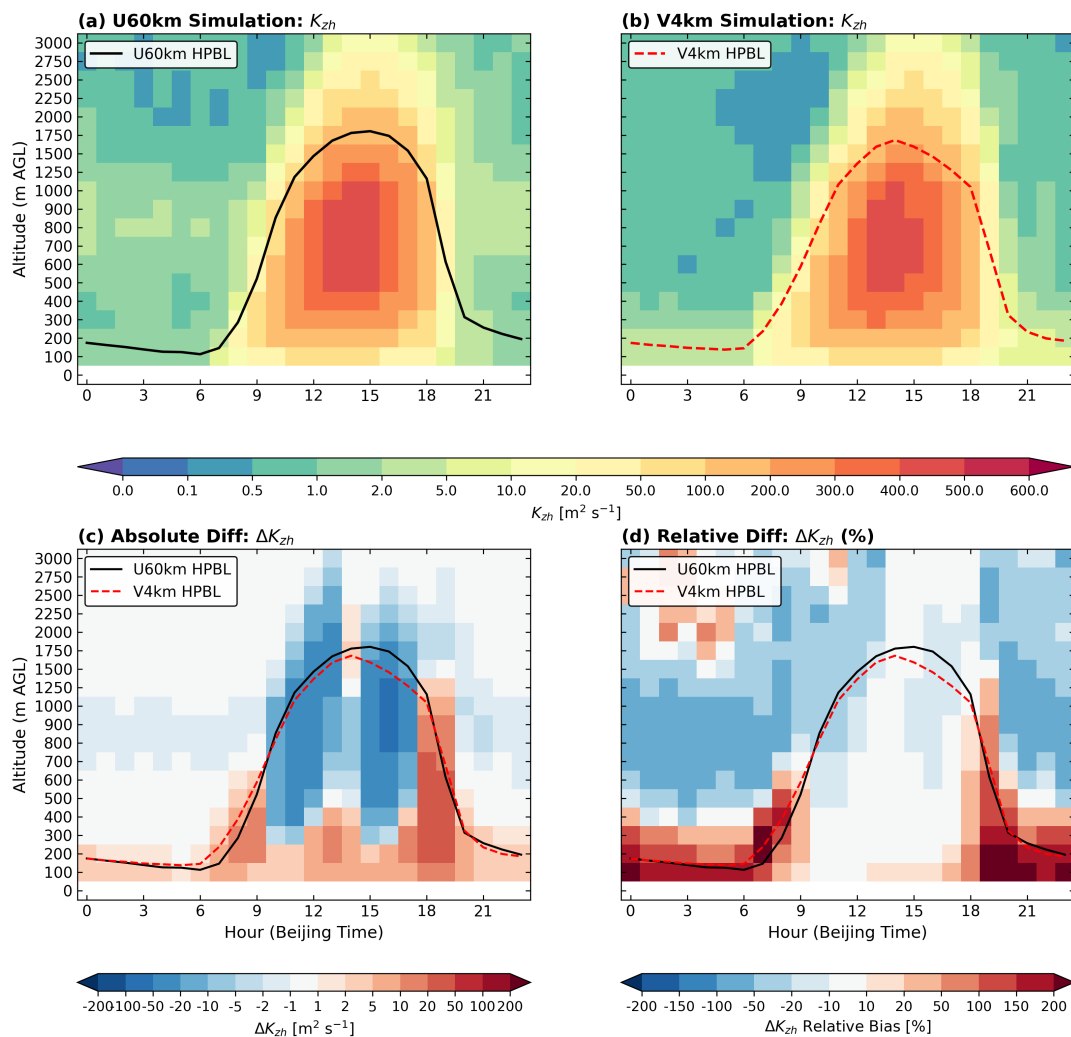


Figure 12. Vertical–diurnal evolution of boundary-layer structure averaged over urban sites within the North China refinement zone for July 2019. (a, b) Vertical turbulent mixing coefficient K_{zh} (m² s⁻¹) for U60km and V4km, respectively, with planetary boundary layer height (PBLH) overlaid as solid (U60km) and dashed (V4km) lines. (c) K_{zh} difference (V4km – U60km, m² s⁻¹) with both PBLH profiles overlaid. (d) Relative K_{zh} difference [(V4km – U60km)/U60km × 100%]. All times are in BJT.