

Evaluation of the WRF-Chem Performance for the air pollutants over the United Arab Emirates

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Abstract

This study presents a comprehensive evaluation of the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem) in simulating meteorological parameters and concentrations of air pollutants across the United Arab Emirates (UAE) for June and December 2022, representing the contrasting summer and winter climatic conditions. The assessment of WRF-Chem performance involves comparisons with ground-based observations for meteorological parameters and satellite retrievals from the Tropospheric Monitoring Instrument (TROPOMI) for gaseous pollutants and the Moderate Resolution Imaging Spectroradiometer (MODIS) for aerosols. The comparison with TROPOMI column concentrations demonstrates that WRF-Chem performs well in simulating the spatio-temporal patterns of total column CO and tropospheric column NO₂, O₃, despite certain deficiencies in modeling tropospheric NO₂ column concentrations. In particular, WRF-Chem shows a strong correlation with TROPOMI retrievals, with correlation coefficients ranging from 0.53 to 0.82 during summer and 0.40 to 0.69 during winter for these gaseous pollutants. The model tends to overestimate NO₂ levels, with a higher discrepancy observed in summer (0.50×10^{15} molecules/cm²) compared to winter (0.18×10^{15} molecules/cm²). In comparison with TROPOMI-CO data, the discrepancies are more pronounced in winter, with an underestimation of 0.12×10^{18} molecules/cm². Additionally, WRF-Chem consistently overestimates ozone levels in both seasons. WRF-Chem also exhibits a moderate correlation with both AERONET and MODIS AOD measurements. The correlation at Mezaira is 0.60, while a correlation of 0.65 is observed with MODIS AOD. However, the model tends to overestimate AOD, with a bias of 0.46 at Mezaira and 0.35 compared to MODIS AOD.

30 Meteorological evaluations reveal that the model generally overestimated T2m in summer
31 ($\leq 0.2^{\circ}\text{C}$) and underestimated it in winter ($\sim 3^{\circ}\text{C}$) with correlation coefficients between 0.7 and
32 0.85. Temperature biases are linked to surface property representation and model physics. For
33 WS10m, biases were within ± 0.5 m/s, indicating good agreement, although overestimations
34 suggest deficiencies in surface drag parameterization. The dry bias observed was consistent
35 with other studies due to dry soil, inaccurate mesoscale circulation representation, and bias in
36 forcing data. The model also overestimated incoming shortwave radiation by ~ 30 W/m² in
37 December due to reduced cloud cover. Night-time cold and dry biases were observed due to
38 more substantial wind speeds and cooler air advection. Comparisons with ERA5 reanalysis
39 showed regional T2m variations with high correlation coefficients (0.97 in summer, 0.92 in
40 winter). Both WRF-Chem and ERA5 displayed consistent seasonal patterns in the planetary
41 boundary layer, correlating with temperature changes and indicating good overall model
42 performance.

43 **Keywords:** Air quality modeling, air pollutants, TROPOMI satellite retrievals, MODIS, WRF-
44 Chem, UAE.

45 **Key points:**

- 46 ● First high-resolution WRF-Chem air quality modeling study over the United Arab
47 Emirates (UAE)
- 48 ● WRF-Chem's ability to simulate meteorological parameters and pollutant levels over
49 the UAE is assessed during summer and winter in 2022.
- 50 ● The model strongly correlated with TROPOMI satellite data, achieving correlation
51 coefficients of 0.53-0.82 in summer and 0.40-0.69 in winter for gaseous pollutants.
- 52 ● Lower model skill in simulating tropospheric NO₂ columns, in contrast to the more
53 accurate modeling of total CO and tropospheric O₃ columns, particularly in summer.
- 54 ● WRF-Chem demonstrated a moderate correlation with AERONET and MODIS for
55 AOD during the summer, with correlation coefficients of 0.60 and 0.65, respectively.
- 56 ● Meteorological analysis revealed a tendency to overestimate surface temperature by 0.2
57 °C in summer and underestimate it by 3 °C in winter across land regions. Surface wind
58 speed is overestimated by 0.1-0.5 m/s in both seasons across various regimes.

59

60 **1. Introduction**

61 The United Arab Emirates (UAE), a federation of seven emirates, has undergone rapid
62 urbanization and industrialization over the last five decades, which has had a profound impact
63 on its air quality (Ramadan, 2015). The major factors affecting air quality in the UAE include
64 emissions from industrial activities, vehicular traffic, construction projects (Teixido et al.,
65 2021), and occasionally, natural phenomena such as dust storms, which are quite prevalent in
66 the region due to its desert climate (Environment Agency – Abu Dhabi, 2018; Francis et al.,
67 2020; 2022b; Karagulian et al., 2019). The rapid economic growth of the UAE, especially in
68 cities like Dubai and Abu Dhabi, has led to a surge in energy demand and water, the latter
69 obtained from desalination and cloud seeding activities (Wehbe et al., 2023), largely met
70 through the burning of fossil fuels (Shahbaz et al., 2014). This has resulted in increased
71 emissions of pollutants like oxides of nitrogen (NO_x), sulfur dioxide (SO₂), particulate matter
72 (PM), and volatile organic compounds (VOCs). Moreover, the heavy traffic in urban areas
73 contributes to the elevated levels of ground-level ozone and particulate pollution (Abuelgasim
74 & Farahat, 2020; Li et al., 2010). Understanding the dynamics of air quality in the UAE
75 involves considering both the environmental challenges posed by rapid development and the
76 steps being taken to mitigate these impacts. The pursuit of balancing economic growth with
77 environmental sustainability is central to this discourse. This area of study is not only vital for
78 ensuring the health and well-being of the population but also plays a crucial role in the UAE's
79 vision for a sustainable future.

80

81 The swift urban expansion in the UAE, which is expected to continue in the coming decades,
82 could intensify air pollution sources. With surface observations sparse in this region, satellite
83 remote sensing becomes a crucial method for air quality monitoring (Chudnovsky et al., 2014;
84 Fonseca et al., 2023; Francis et al., 2023). What is more, satellite measurements themselves
85 fall short in clarifying the different atmospheric processes responsible for peak pollution levels.
86 Consequently, integrating chemistry transport models with satellite-derived and ground-based
87 observations can significantly improve our understanding of pollutant emissions, distribution,
88 transport, and transformation in the targeted regions (Eltahan et al., 2018; Li et al., 2018;
89 Yarragunta et al., 2020; Yin et al., 2021). Air quality (AQ) modelling is dedicated to
90 unravelling the complicated aspects of atmospheric chemistry and transport across both global
91 and regional levels, as explored in numerous studies conducted around the world (Emmons et
92 al., 2010; Kumar et al., 2011, 2018; Tie et al., 2001; Yarragunta et al., 2019, 2020, 2021).

93 Despite facing limitations due to the often low spatial and temporal resolution of observational
94 data, AQ models effectively generate detailed air quality information for remote regions (e.g.,
95 Guo et al., 2024a). They predict the formation and removal of air pollutants and facilitate a
96 thorough examination of the transport and photo-chemical transformation of trace gases
97 following their emission into the atmosphere (Archer-Nicholls et al., 2015; Georgiou et al.,
98 2018; Nhu et al., 2021; Sicard et al., 2021). They are also employed globally for operational
99 air quality forecasting (Jena et al., 2021; Koo et al., 2012; Kumar et al., 2012, 2021; Srinivas
100 et al., 2016; Zhang et al., 2012). Air quality models are categorized into two types: 'fully
101 coupled' models, which integrate interactions between chemistry and meteorology, and 'offline'
102 models, where chemistry and meteorology simulations are conducted independently (Gao &
103 Zhou, 2024). Some of state of the art AQ models include the Weather Research and
104 Forecasting (WRF) model coupled with chemistry (WRF-Chem; Grell et al., 2005; Skamarock
105 et al., 2008), WRF-Chem-MADRID (Model of Aerosol Dynamics, Reaction, Ionization and
106 Dissolution; Zhang et al., 2010), CESM2 (Community Earth System Model version 2; Emmons
107 et al., 2020), CHIMERE (Menut et al., 2021), LOTOS-EUROS(v2.0) (Long Term Ozone
108 Simulation European Operational Smog; Manders et al., 2017) and COSMO/MESSy
109 (Consortium for Small Scale Modelling/ Modular Earth Submodel System; Kerkweg & Jöckel,
110 2012). However, before using these AQ models for operational or research applications, it is
111 crucial to conduct thorough evaluations to assess the quality of their predictions. The AQ model
112 chosen for the current study is WRF-Chem with its foundational meteorological component,
113 WRF. WRF-Chem has been used for research studies in the Arabian Peninsula (Parajuli et al.
114 2019, 2023, 2024), with the meteorological component optimized for simulations over the
115 region (Chaouch et al., 2017; Nelli et al., 2020; Abida et al., 2022; Fonseca et al. 2020, 2021,
116 2022a).

117
118 The majority of studies conducted in the UAE and similar arid regions have primarily
119 focused on evaluation of meteorological parameter including temperature, humidity, wind, and
120 solar radiation (Parajuli et al., 2019; Nelli et al., 2020; Fonseca et al., 2020, 2021) with a few
121 others investigating the particulate matter (PM) dynamics, especially mineral dust. For
122 instance, Ukhov et al., (2021) noted inaccuracies in the WRF-Chem model related to the
123 commonly used bulk Goddard Chemistry Aerosol Radiation and Transport (GOCART; Chin
124 et al., 2022) aerosol module, affecting PM_{2.5} and PM₁₀ diagnostics. Karagulian et al. (2019)
125 highlighted the effectiveness of integrating WRF-Chem model simulations with satellite and
126 ground observations to understand and predict the impact of severe dust storms on air quality.

127 Karumuri et al., (2022) reported significant air quality changes due to COVID-19 lockdown
128 measures, with reduced trace gas concentrations but increased particulate matter from dust
129 activities, the latter stressed by Francis et al. (2022a) who attributed it to changes in the
130 atmospheric circulation. Moreover, Parajuli et al. (2022, 2023) utilized high-resolution WRF-
131 Chem simulations and advanced aerosol schemes to analyse the dust and rainfall dynamics,
132 providing insights into the direct and indirect effects of dust on rainfall, which aids in better
133 regional water resource planning through accurate rainfall predictions. In particular, while
134 through the indirect effects dust promotes precipitation provided there is sufficient moisture
135 for both normal and extreme rainfall events, the dust direct effects on precipitation shift from
136 negative for normal rainfall events (weaker sea-breeze arising from surface cooling) to positive
137 in extreme events (smaller effects on the sea breeze). Zhang et al. (2024) stressed the two-way
138 interaction between dust aerosols and the Planetary Boundary Layer (PBL) dynamics: aerosols
139 directly impact the PBL structure through direct and indirect effects, while the the modified
140 PBL characteristics and low-level circulation modulate aerosol processes. All the
141 aforementioned studies focus on dust aerosols, there is no assessment to date of the model
142 performance for the simulation of gaseous pollutants over the region. This is crucial, given the
143 complex dynamics between anthropogenic and natural factors in air quality management and
144 the necessity of tailored model configurations for accurate environmental assessments in arid
145 regions.

146

147 This study represents the first comprehensive evaluation of the WRF-Chem model in the
148 Arabian Peninsula, with a focus on the UAE, a country that is representative of those in the
149 region, specifically examining concentrations of air pollutants along with crucial
150 meteorological parameters relevant to air quality studies. The primary objective of this study
151 is twofold:

152

- 153 ● Evaluate the WRF-Chem's ability to replicate meteorological conditions. This involves
154 comparing the model's simulation of temperature, wind speed, relative humidity,
155 downward short-wave radiation and boundary layer height against ground-based
156 observations and data from the European Centre for Medium-Range Weather
157 Forecasting (ECMWF) fifth reanalysis product, ERA5 (Hersbach et al., 2020);
- 158 ● Assess the model's performance in simulating concentrations of key gaseous pollutants,
159 specifically NO₂, O₃, and CO, which are prevalent in the region (Teixido et al., 2021),
160 against data from the TROPOspheric Monitoring Instrument (TROPOMI; Veefkind et

161 al., 2012) onboard the Sentinel-5 Precursor (S5P) satellite. Additionally, aerosol optical
162 depth (AOD) at 550 nm from AERONET and MODIS satellite observations are used
163 to evaluate the model's skill in simulating aerosol concentrations.

164

165 The structure of the paper is as follows. Section 2 describes the configuration of the WRF-
166 Chem considered in this work. Section 3 elaborates on the methodology and datasets used in
167 this study. Section 4 provides a comprehensive assessment of the model's simulated data
168 against observational datasets, reanalysis and satellite-derived products. Section 5 concludes
169 by outlining the main findings.

170 **2. WRF-Chem configuration**

171 WRF-Chem version 4.3.1 is employed to simulate the atmospheric conditions and transport
172 of pollutants in the UAE. WRF-Chem is a mesoscale regional chemistry transport model,
173 developed by the National Oceanic and Atmospheric Administration (NOAA) Earth System
174 Research Laboratory (ESRL), with contributions from the global science community. In WRF-
175 Chem, the air quality and meteorological components are predicted simultaneously using the
176 same grid, transport, timestep, and sub-grid scale physics. A detailed description of the model
177 is found in Grell et al., (2005), Skamarock et al., (2008) and Powers et al., (2017). The physics
178 schemes employed in the simulations are the Rapid Radiative Transfer Model for Global
179 Circulations Models (RRTMG) for radiation parametrization of both short and long wave
180 radiation (Iacono et al., 2008), the cloud microphysics is represented by the Morrison 2-
181 moment (Morrison et al., 2009), and the Kain-Fritsch scheme is used for convective
182 parameterisation (Kain, J.S, 2004) with the subgrid-scale cloud feedback to radiation switched
183 on (Alapaty et al., 2012). The Unified Noah model is used to represent the land surface model
184 (Tewari et al., 2004), with an improved representation of soil texture and land use/land cover
185 (LULC) over the UAE (Temimi et al., 2020). The boundary layer dynamics are represented by
186 the Yonsei University (YSU) scheme (Hong, 2010). The chosen physics schemes are listed in
187 Table 1. The simulated mesoscale meteorology is kept in line with the analysed meteorology
188 through spectral nudging to the National Centre for Environmental Prediction (NCEP) Global
189 Forecast System (GFS) analyses used to drive the model, in an attempt to limit errors in the
190 mesoscale transport. During the simulations, horizontal and vertical wind, potential
191 temperature and water vapour mixing ratio are nudged to GFS analyses in all model layers

192 above the planetary boundary layer on a time-scale of 6 hours for scales above ~1000 km.
193 Meteorological conditions were initialised by NCEP GFS 6-hourly analyses at 0.25° resolution.

194 This study utilised the Model for Ozone and Related Chemical Tracers, version 4
195 (MOZART-4) chemical mechanism for calculating gas-phase chemistry, which includes 81
196 chemical species with 159 gas-phase reactions and 38 photolysis processes (Emmons et al.,
197 2010). Aerosol chemistry is represented by the GOCART (Chin et al., 2002) module, along
198 with the Tropospheric, Ultraviolet and Visible (TUV) full photolysis scheme (Madronich,
199 1987; Tie, 2003), which deploys climatological O₃ and O₂ columns. Dry deposition is
200 calculated using Wesely (1989). Anthropogenic emissions are taken from the Emission
201 Database for Global Atmospheric Research (EDGAR) version 8.1 at a 0.1 × 0.1° horizontal
202 resolution for 2022 (Crippa et al., 2020), consistent with the simulation period. Emissions
203 include SO₂, NO_x, CO, Non-Methane Volatile Organic Compounds (NMVOC), NH₃, black
204 carbon (BC) and organic carbon (OC). Biogenic emissions are calculated online by the Model
205 of Emissions of Gases and Aerosol from Nature (MEGAN; Guenther et al., 2012). The
206 chemistry boundary conditions (BCs) used in domain D01 and the initial conditions (ICs) for
207 all domains in the WRF-Chem simulations are extracted from CAM-chem model forecasts
208 (Emmons et al., 2020). In this work, we run the WRF-Chem model on the three nested domains
209 with horizontal resolutions of 27-, 9-, and 3-km corresponding to 283×205, 271×193, and
210 256×178 grid points, respectively. In the vertical, there are 45 layers, with the lowest model
211 level at about 27 m above the surface. The outermost domain covers most of the Middle East
212 and the surrounding region, while the innermost domain covers the entire UAE (Fig. 1(a)). The
213 analysis in this research article exclusively utilizes results from the inner domain (D03). Fig.
214 1(b) shows the spatial distribution of UAE airport stations, the WISE-UAE observational site,
215 and AERONET locations for AOD measurements.

216

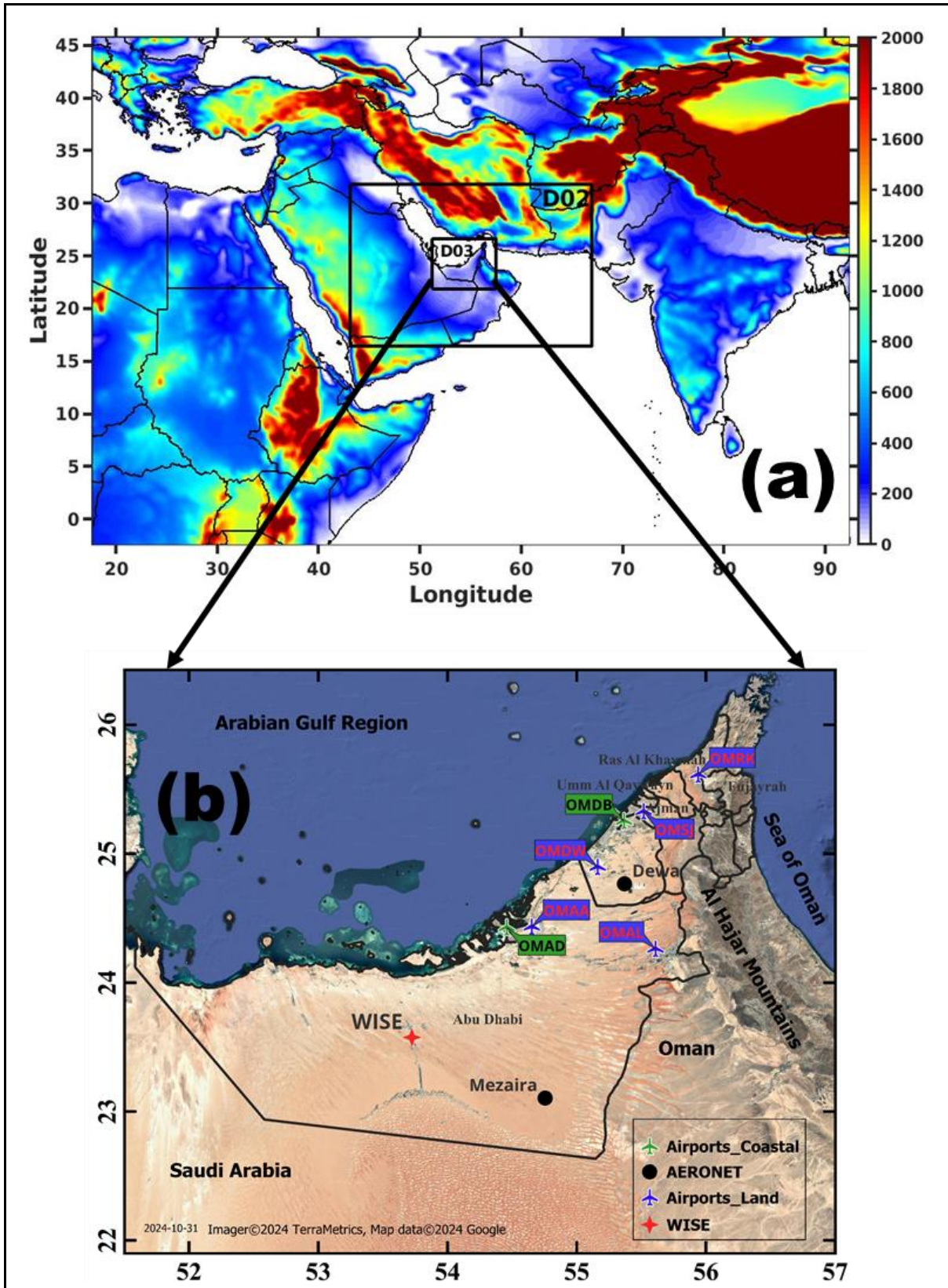


Figure 1: Model Configuration: (a) The WRF domain configuration consists of three telescoping nests, with the outermost boundaries denoting the parent grid (D01). D02 and D03 are the nested domains. Bottom panel (b) is a zoom of the innermost domain (D03)

showing the spatial distribution of the seven automatic weather stations operated in airports (land stations (5) are denoted by blue color, coastal stations (2) are represented by green color) along with Wind-blown Sand Experiment (WISE)-United Arab Emirates (UAE) Site by red color star and black dots represent two AERONET stations (Mezaira and Dewa). The shading in (a) represents the orography (m). Further details about the stations are given in Tables S1.

217

218 The WRF-Chem simulation is driven by anthropogenic emissions from the EDGAR
219 database, version 8.1, at a horizontal resolution of $0.1^\circ \times 0.1^\circ$ for the year 2022 (Crippa et al.,
220 2020). The EDGAR emission inventory accounts for day-to-day variability (e.g., weekday
221 versus weekend) and hourly fluctuations (diurnal cycle) of anthropogenic emissions, as
222 detailed by Crippa et al. (2020). For example, road transport emissions are generally lower at
223 night and higher during daytime hours, while agricultural emissions tend to peak during
224 specific months. To achieve an hourly resolution for the model, we scaled the coarsely resolved
225 emission data using predefined hourly, daily, and monthly scaling factors (temporal profiles).
226 The initial temporal profiles are derived from the work of Olivier et al. (2003) and have been
227 refined to place greater emphasis on the most relevant emission sectors for each pollutant
228 within the study region. According to the Environment Agency – Abu Dhabi (2018), the
229 primary sectors contributing to emissions include traffic, the power industry, energy used in
230 buildings, and the manufacturing industry. Using these optimised emission profiles, emissions
231 for NO_2 and CO were dynamically adjusted during the model simulations to better capture local
232 emission patterns and their variability. However, the results indicated that emissions for NO_2
233 and CO are underestimated by EDGAR. Although WRF-Chem simulations incorporate
234 temporal profiles of emissions, the impact of these emission estimates on daily variations could
235 not be fully assessed in this study due to the lack of ground-based measurements and the limited
236 temporal resolution of satellite data. MODIS and TROPOMI satellites each pass over the study
237 area only once per day, restricting the ability to capture daily variations comprehensively.
238 Consequently, this article is limited in its assessment of daily emission variability. Moreover,
239 WRF-Chem supports the vertical distribution of trace gas emissions, which is particularly
240 useful for capturing emissions released at elevated altitudes, such as those from combustion
241 stacks. Accurately representing the vertical distribution of emissions is important for
242 simulating atmospheric processes. However, incorporating this complexity would likely
243 provide minimal improvements in model accuracy for regions where surface emissions

244 dominate, and where observational constraints are largely limited to coarse vertical resolution
 245 or surface-level data. Therefore, in this study, all emissions were injected into the lowest model
 246 layer to align with the observational data characteristics and the typical conditions in the study
 247 area.

248 **Table 1: WRF-chem model setup**

249

Model set-up	Option
Model version	4.3.3
Domain	3 domains
Horizontal resolution	D01:27km, D02:9km and D03:3km
Simulation period	Monthly runs from June and December 2022
Model spin-up period	2 days in each month
Vertical resolution	45 eta levels up to 50 hPa.
Domain size	D01: 283×205 grids, D02: 271×193 grids and D03: 256×178 grids
Meteorological boundary	NCEP FNL reanalysis (0.25°, 6-hourly)
Chemical boundary	CAM-Chem (Emmons, Fasullo, et al., 2020)
Physical Process	Parameterization Scheme
Microphysics	Morrison double moment (Morrison et al., 2009)
Cumulus parameterization	Kain-Fritsch (Kain, 2004) with the subgrid-scale cloud-radiation feedbacks activated (Alapaty et al., 2012)
Shortwave radiation	Rapid Radiative Transfer Model for GCMs (RRTMG) (Iacono et al., 2008)
Longwave radiation	Rapid Radiative Transfer Model for GCMs (RRTMG) (Iacono et al., 2008)
Land surface	Unified Noah land surface model (Tewari et al., 2004)
Planetary boundary layer	Yonsei University scheme (Hong, 2010)
Chemistry option	Scheme used
Gas phase chemistry	MOZART-4 (Emmons et al., 2010)
Aerosol chemistry	GOCART (Chin et al., 2002)

Photolysis	Madronich F-TUV (Madronich, 1987; Tie, 2003)
Biogenic emissions	MEGAN (Guenther et al. 2012)
Dry deposition	Wesely (Wesely 1989)

250

251 **3. Data Sets and methodology**

252 **3.1 Meteorology observations**

253 In this study, meteorological data from 8 automatic weather stations (AWS) operated at
 254 UAE airports are utilized to assess the WRF-Chem air temperature at 2 meters above ground
 255 (T2m), wind speed at 10 meters (WS10m), and relative humidity at 2 meters above ground
 256 (RH2m) forecasts during June and December of 2022. The spatial distribution of the stations
 257 across the UAE is illustrated in Fig. 1(b) (refer to Table S1 for more details). These locations
 258 are categorically divided into two regions—land stations (station code L OMAA, OMDW,
 259 OMAL, OMSJ, OMRK) and coastal stations (station code: OMAD, OMDB)—following the
 260 criteria outlined in Branch et al., (2021). Subsequent analyses are based on these two primary
 261 categories, with the land region comprising 5 stations and the coastal region comprising 2
 262 stations (Fig. 1b). In addition to the UAE airports data, we utilized meteorological data from
 263 the WInd-Blown Sand Experiment (WISE)-UAE measurements. The WISE-UAE experiment
 264 started on 25 July 2022 at Madinat Zayed (23.5761°N, 53.7242°E; elevation: 119 m; Fig. 1b),
 265 located 120 km southwest of Abu Dhabi, UAE. An overview of the instrumentation and
 266 experiment site used during WISE-UAE is provided in Nelli et al. (2024(a, b)). This study uses
 267 WS10m T2m, RH2m, and downward shortwave radiation flux (SW) from these measurements
 268 to validate the WRF-Chem simulations for December 2022. The specifications and accuracies
 269 of the instruments used in WISE-UAE are outlined in detail, along with the stringent quality
 270 control procedures applied, as described in Nelli et al. (2024(a,b,c)).

271 **3.2 AERONET**

272 The Aerosol Robotic Network (AERONET) program is a global federation of ground-based
 273 sun photometers comprising more than 400 stations worldwide (Holben et al., 1998).
 274 AERONET utilizes multiple bands ranging from UV to near-IR wavelengths to measure
 275 spectral sun irradiance and sky radiances, from which Aerosol Optical Depth (AOD) at 550 nm
 276 and other aerosol properties are derived. A detailed description of the AERONET retrievals is

277 provided in Holben et al. (1998). This study uses Level 2.0 AOD data at 550 nm from Mezaira
278 for June and from Dewa for December 2022, with an hourly resolution. It is important to note
279 that AOD retrieved from AERONET is accurate to within 0.01 (Dubovik et al., 2000).

280 **3.3 ERA-5 Reanalysis data**

281 The fifth-generation ECMWF reanalysis, known as ERA-5 (Hersbach et al., 2020),
282 represents a significant advancement over its predecessor, ERA-Interim, introduced by Dee et
283 al. (2011). ERA-5 incorporates a sophisticated four-dimensional variational (4D-Var) data
284 assimilation method, utilizing the 41r2 cycle of the Integrated Forecast System (IFS). This
285 system is enhanced by integrating a soil and ocean wave models, offering a comprehensive
286 approach to climate data analysis. We accessed ERA-5 data through the Copernicus Climate
287 Change Service Climate Data Store (CDS) for this research. The dataset provides atmospheric
288 observations across 137 hybrid vertical levels, with raw model data interpolated onto 37
289 distinct pressure levels. These levels span from 1000 hPa, close to the Earth's surface, up to 1
290 hPa, reaching altitudes of approximately 80 km. Further details on the ERA-5 dataset are
291 available in Dee et al. (2011) and Hersbach et al. (2020). Our study utilizes explicitly hourly
292 data for a selection of meteorological parameters: T2m, WS10m, SW, and planetary boundary
293 layer height (PBL), for June and December 2022.

294 **3.4 Satellite-borne observations: TROPOMI**

295 Launched by the European Space Agency (ESA) on October 13, 2017, the TROPOMI
296 instrument is aboard the S5P satellite, operating in a near-polar sun-synchronous orbit.
297 Positioned at an altitude of 817 km, the S5P satellite crosses the equator at a local solar time of
298 13:30, boasting a wide swath of approximately 2600 km, and providing daily global coverage.
299 TROPOMI features four distinct spectrometers that measure the radiation in the ultraviolet
300 (UV) and UV-visible (UV-VIS) range (270 to 500 nm), near-infrared (NIR) range (675 to 775
301 nm), and short-wave infrared (SWIR) range (2305 to 2385 nm) spectral bands (Veefkind et al.,
302 2012). Notably, the last two spectral bands, NIR and SWIR, are newly introduced in
303 TROPOMI compared to its predecessor OMI (Ozone Monitoring Instrument). TROPOMI's
304 data products encompass daily observations of trace gases, including CO, O₃, NO₂, CH₄,
305 HCHO, aerosols, and cloud properties. This study utilized daily tropospheric NO₂, total CO
306 columns, and ozone profile level 2 products downloaded from the GES DISC website
307 (<https://disc.gsfc.nasa.gov/>) for the period of June and December 2022. The specific data sets

308 employed for the present study include S5P_OFFL_L2_O3_PR for O₃,
309 S5P_OFFL_L2_CO for CO, and S5P_OFFL_L2_NO₂ for NO₂, covering the study region
310 bounded by longitudes [51°,58°] and latitudes [21°,27°]. Further details on each product,
311 including the retrieval algorithms and validation results, are summarized in the following
312 section.

313

314 TROPOMI retrieval of NO₂ columns are derived using UV-VIS spectrometer backscattered
315 solar radiation measurements in the wavelength range of 405-465 nm and provides total and
316 tropospheric NO₂ vertical column density with a near-nadir resolution of 7 × 3.5 km. The total
317 NO₂ slant column density (SCD) is retrieved from the measured solar irradiance spectra using
318 the Differential Optical Absorption Spectroscopy (DOAS) method. Tropospheric and
319 stratospheric slant column densities are separated from SCD by a data assimilation system
320 based on the chemistry transport model V5 (TM5-MP). Afterwards, they are converted to
321 vertical column densities (VCDs) with the help of look-up table of altitude-dependent air-mass
322 factors (AMFs) and information on the vertical distribution of NO₂ from TM5-MP a priori
323 profile with a horizontal resolution of 1° x 1° and a time step of 30 min (Boersma et al., 2018;
324 Van Geffen et al., 2022). The TROPOMI NO₂ product has been extensively evaluated using
325 ground-based and aircraft observations and is found to have a high correlation and low bias of
326 less than 30% with respect to in-situ measurements (Griffin et al., 2019; Ialongo et al., 2020).
327 We used the both reprocessed (RPRO) and offline (OFFL) TROPOMI NO₂ data files from the
328 most recent processor versions depending on availability for a given day of observations.
329 Additionally, there is another NO₂ product available as near-real time (NRTI). NRTI data files
330 are generated using TM5-MP forecast data rather than analysis data as with REPO and OFFL
331 files (Van Geffen et al., 2022). The differences between the OFFL/REPO and NRTI NO₂
332 products are generally very small (Ialongo et al. (2020) and references therein).

333

334 The Shortwave Infrared Carbon Monoxide Retrieval (SICOR) algorithm is used to retrieve
335 CO total column densities from TROPOMI in the spectral range of 2305 to 2385 nm (Landgraf
336 et al., 2016). The SICOR algorithm accounts for a profile-scaling approach that scales retrieved
337 CO total column to the a priori reference profile. The a priori reference profiles are taken from
338 the global chemistry transport model simulations of TM5-MP, and vary based on the location,
339 month and year (Krol et al., 2005). The detailed outline of all settings and other auxiliary data
340 sets used for CO retrievals is given in Landgraf et al., (2016). This study limits the analysis to
341 CO pixels corresponding to clear-sky conditions and mid-level clouds by filtering the data

342 using the quality flag variable (qa_value). The scenes corresponding to qa_value > 0.5 are used
343 in this current analysis as suggested in the ATBD (algorithm theoretical baseline document;
344 Landgraf et al., 2016). In this present work, TROPOMI CO measurements for June and
345 December 2022 have been analysed. Moreover, we use either the reprocessed (RPRO) or
346 offline (OFFL) data files from most recent processor versions depending on availability for a
347 given day of observations. Wizenberg et al., (2021) compared global TROPOMI retrieved CO
348 total columns with corresponding ACE-FTS (Atmospheric Chemistry Experiment- Fourier
349 transform spectrometer) columns for the period from November 2017 to May 2020 and found
350 a small relative bias of -0.83% with a correlation coefficient of 0.93 between two data sets.
351 Similar results are also found between TROPOMI CO with corresponding CO fields from the
352 ECMWF assimilation system: Borsdorff et al. (2018) reported a small mean difference between
353 the two data sets of 3.2% with a correlation coefficient of 0.97.

354 TROPOMI also provides ozone profiles (5P_OFFL_L2__O3__PR) at 33 pressure levels
355 with a horizontal resolution of 28x28 km. It measures radiances and irradiances in the
356 ultraviolet wavelength of 270-330 nm and provides the ozone profile information. The Optimal
357 Estimation (OE) algorithm is used to retrieve the ozone profile data. Before this stage, various
358 pre-processing steps are applied to the measured spectra before the estimation of the ozone
359 profile. The main process of the algorithm is the OE method, which combines the information
360 from the measured spectra with the a-priori information. The latter is based on climatology as
361 described in Labow et al., (2015). The description of the various pre-processing steps
362 performed to retrieve ozone profiles is presented in the Algorithm Theoretical Basis Document
363 (Veefkind, et al., 2021). The validation of TROPOMI retrieved ozone profile data against the
364 ground-based measurements reported a median bias of 0.3% for OFFL/REPO products while
365 0.8% for NRTI ozone products (Lambert et al., 2023). Our focus is specifically on the
366 tropospheric ozone column due to its direct relevance to surface air quality. Total column ozone
367 measurements are primarily influenced by stratospheric ozone, which accounts for
368 approximately 90% of the total column, while tropospheric ozone comprises only around 10%.
369 Given this, we have used ozone profile data from the surface to 100 hPa., designated as
370 tropospheric ozone columns for this study and referred to as TROPOMI-O₃, expressed in
371 Dobson Units (DU), where 1 DU = 2.69x10¹⁶ molecules/cm².

372 **3.5 Satellite-borne observations: MODIS**

373 The Moderate Resolution Imaging Spectroradiometer (MODIS) sensor was launched into the
374 polar sun-synchronous orbit at an altitude of 705 km aboard NASA's two Earth Observing
375 System (EOS) satellites, Terra (Feb-2000) and Aqua (June-2002) [Kaufaman et al., 1997;
376 Remer et al., 2005] . The equator crossing times of two satellites were, Terra crossing at 1030
377 LST and Aqua crossing at 1330 LST. The MODIS sensor has a swath of ~2330 km and
378 provides near-global coverage with a temporal resolution of 1-2 days. The sensor measures the
379 reflected solar radiation from the Earth's atmosphere and the surface as well as emitted thermal
380 radiation at 36 spectral bands from 0.41 to 14 μm with three spatial resolutions: 250m, 500m,
381 and 1km. Seven of these bands operating in the spectral range of 0.415-2.155 μm can
382 effectively retrieve the AOD over land and ocean [Levy et al. 2013 ; Hsu et al. 2015 ; Sayer et
383 al., 2014a; 2014b; 2015] . The MODIS retrieval algorithm is based on the lookup table
384 approach with a pre-defined set of aerosol types, loadings and geometries [Floutsi et al. 2016].
385 A comprehensive description of retrieval algorithms and details of MODIS instrument are
386 found elsewhere [Remer et al. 2008; Levy et al. 2013]. MODIS AOD retrieval algorithms have
387 been substantially validated against in-situ and/or other remote sensing data sets from regional
388 to global scales and are updated periodically [Remer et al. 2008 ; Li et al. 2009]. The
389 uncertainty of AOD retrievals is estimated to be $\pm 0.05 \pm 0.20 \times \text{AOD}$ over land and $\pm 0.03 \pm 0.15$
390 $\times \text{AOD}$ over ocean [Remer et al., 2005; 2008]. The present study utilized Level 2 MODIS
391 aerosol products (Collection 6.1) obtained from the Atmosphere Archive and Distribution
392 System (LAADS DAAC). These products consist of 5-minute satellite swaths with a spatial
393 resolution of 10 km, covering the period of June and December 2022. (Devadiga, 2024).

394 **3.6 Satellite data processing**

395 In order to quantitatively compare the WRF-chem simulations with satellite measurements,
396 the model outputs must be processed using the appropriate method as described in the literature
397 (Kumar et al., 2012). Direct comparison between satellite retrievals and model outputs is not
398 recommended, as satellite measurements depend on column averaging kernels (AK) and a-
399 priori profiles. The AK vector represents the vertical sensitivity of the retrieved column relative
400 to the true vertical profile of the target variable in the atmosphere. It indicates how changes in
401 the true atmospheric profile at different vertical levels influence the retrieved column values,
402 allowing for a more accurate comparison between model simulations and TROPOMI data by

403 convolving the model outputs with the AK. The typical AK vectors are plotted over the WISE-
 404 UAE location to know the sensitivity of AK at different pressure levels (Figure S7)

405 The column density from the WRF-Chem model is re-gridded to match the TROPOMI
 406 instrument's grids and is vertically interpolated to the TROPOMI pressure levels before it is
 407 multiplied by the AK. This treatment of the WRF-Chem-simulated profile with the column
 408 averaging kernels allows for a comparison that is independent of the chemical transport model
 409 (CTM) a-priori assumptions and the vertical sensitivity of the retrieval process; therefore, it
 410 can be directly compared with the TROPOMI-derived tropospheric column of NO₂. The
 411 TROPOMI-NO₂ and TROPOMI-CO products also provide a column averaging kernel matrix.
 412 In this case the column AK averaging kernel accounts for the vertical distribution and
 413 sensitivity of the measurements, as classically done by Borsdorff et al., (2014) as:

$$414 \quad X_{ret} = X_{a\ prior} + AK \times (X_{true} - X_{a\ prior}) + e_x \text{-----}(1)$$

415 where X_{true} is model simulation profile of trace gas; X_{ret} is the retrieved profile or smoothed
 416 model profile; e_x represents the error on the retrieved trace gas profile; $X_{a\ prior}$ is the a-priori
 417 information provided in the TROPOMI data set. For TROPOMI-NO₂ data, the contribution of
 418 the a priori profile and error on the retrieved profile can be eliminated, as explained in Borsdorff
 419 et al., (2014). In particular, eq. (1) simplifies to

$$420 \quad X_{ret} = AK \times (X_{true}) \text{-----} (2)$$

421 where X_{true} represents WRF-Chem simulation profile for both NO₂ and CO, AK represents the
 422 averaging kernels information provided in the TROPOMI data set for NO₂ and CO and X_{ret}
 423 represents smoothed model profile for NO₂ and CO.

424 For validation of ozone, we have used the TROPOMI ozone profile level 2 data product
 425 S5P_OFFL_L2__O3__ that provides the ozone concentrations at 33 pressure levels. This data
 426 product also includes the a priori information and column averaging kernel for each pressure
 427 level. In order to compare our model profile with the one given by this dataset, the model output
 428 is horizontally and vertically interpolated to TROPOMI grids and vertical levels. The final
 429 model profile was calculated by the Eq. (3)

$$430 \quad X_{ret} = X_{a\ prior} + AK \times (X_{true} - X_{a\ prior}) \text{-----}(3)$$

431 where X_{true} represents WRF-Chem simulation profile for O₃, AK represents the averaging
 432 kernels information provided in the TROPOMI data, X_{ret} represents smoothed model profile
 433 for O₃ and $X_{a\ prior}$ is the a-priori information provided in the TROPOMI data. Since the highest
 434 vertical level in WRF-Chem-simulated trace gas concentration is 50 hPa, the remaining vertical

435 layers of ozone and CO are made equal to the a priori concentration of respective trace gases
 436 as described by ATBD (Landgraf et al., 2016).

437 **3.7 Evaluation methodology**

438 Meteorological parameters from the WRF-Chem model are extracted for the grid points
 439 closest to the surface observation sites of the AWS. As noted before, the meteorological
 440 parameters are categorized and averaged for land and marine regions separately for the regional
 441 analysis. To enable the comparison of atmospheric column data from the TROPOMI satellite
 442 retrievals with WRF-Chem outputs, the data must undergo smoothing through an appropriate
 443 method described in Section 3.4, as direct comparison between satellite retrievals and
 444 simulations is not feasible due to discrepancies highlighted in previous literature. Additionally,
 445 and owing to the spatial resolution differences between WRF-Chem and ERA5 datasets, it is
 446 necessary to remap the model data to the ERA5 grids for accurate comparison. A wide range
 447 of statistical parameters is available for evaluating model simulations. In this study, we
 448 employed statistical skill scores including the Pearson correlation coefficient (r), the Mean Bias
 449 (MB), the Root Mean Square Error (RMSE), and the Mean Absolute Error (MAE), which have
 450 been extensively discussed and applied in similar contexts (Fonseca et al., 2021; Ivatt & Evans,
 451 2020; Temimi et al., 2020b).

452 The following equations (eq. 4 to eq. 7) are used to calculate these statistical matrixes in the
 453 present study,

454

$$455 \quad r = \frac{\sum_{i=1}^N [(O_i - \underline{O_i})(M_i - \underline{M_i})]}{\sqrt{\sum_{i=1}^N (O_i - \underline{O_i})^2 \sum_{i=1}^N (M_i - \underline{M_i})^2}} \quad \text{-----(4)}$$

$$456 \quad \text{RMSE} = \left(\frac{1}{N} \sum_{i=1}^N (M_i - O_i)^2 \right)^{\frac{1}{2}} \quad \text{-----(5)}$$

$$457 \quad \text{MB} = \frac{1}{N} \sum_{i=1}^N (M_i - O_i) \quad \text{-----(6)}$$

$$458 \quad \text{MAE} = \frac{1}{N} \sum_{i=1}^N |M_i - O_i| \quad \text{-----(7)}$$

459

460 where O_i denotes the i -th observation, M_i represents the corresponding WRF-chem model
 461 simulated value, and N is the number of model and observation pairs. $\underline{M_i}$ and $\underline{O_i}$ are the model
 462 and observational means (i.e. average of 1-30 June and 1-31 December), respectively. The
 463 correlation coefficient (r) is an indication of the phase agreement between the modelled and

464 observed time-series. The RMSE measures the average error in the model predictions, while
465 the MAE determines the mean error between the model forecasts and observations regardless
466 of whether it is an under or overestimate. The MB is a measure of the systematic error and
467 gives information as to whether the model is over or underpredicting the corresponding
468 observed values.

469 **4. Results and Discussion**

470 **4.1 Model performance for key meteorological variables**

471 The capability of the WRF-Chem model to reproduce realistic spatiotemporal patterns of
472 key meteorological variables has been assessed by comparing the model outputs to
473 observational reanalysis data for June and December 2022, representing contrasting summer
474 and winter conditions over the UAE. Evaluating the accuracy of WRF-Chem’s meteorological
475 forecasts in the study area is essential before applying the model forecasts to air quality
476 assessments. Accordingly, we compared the model predictions for T2m, RH2m, WS10m, and
477 SW against ground-based observations at seven airport stations and *in-situ* measurements from
478 the WISE-UAE field campaign (details in Table S1). Additionally, the boundary layer height
479 is evaluated against ERA5 reanalysis data, which offers a spatial resolution of approximately
480 28 km, higher than the other currently available reanalysis datasets. Detailed results of this
481 analysis are presented in the supplementary material, with key findings summarized here to
482 support the paper’s discussion. The aforementioned meteorological parameters are selected,
483 given their critical role in influencing air pollutant behavior (Ritter et al., 2013).

484 **4.1.1 Evaluation against *In-Situ* Observations**

485 The WRF-Chem model evaluation against observations across the seven meteorological
486 stations (Table S1) at the UAE airports for T2m, RH2m, and WS10m during June and
487 December 2022 reveals a close agreement between the modeled and observed values (Table
488 S2). The cold bias reported by several studies, including Branch et al. (2021), Temimi et al.
489 (2020a), and Abida et al. (2022), which occurs primarily at night, is reduced in the WRF-Chem
490 simulations presented here. In fact, and for the June month, the air temperature bias is positive,
491 ~0.2 °C. This stresses the importance of properly simulating the observed aerosol loading in
492 this hyper arid region. Deficiencies in the land surface model and radiation schemes and in the
493 representation of the surface properties, particularly the surface emissivity that may be

494 overestimated in the model (Parajuli et al., 2023), can also account for this discrepancy. The
495 WRF-Chem model also exhibits a noteworthy dry bias in this region, linked to an incorrect
496 simulation of the soil moisture and the mesoscale land-sea breeze circulation, which is present
497 in both seasons. The strength of the near-surface wind speed tends to be overestimated in WRF-
498 Chem in the UAE by about 1-3 m/s, which has been attributed to an incorrect representation of
499 its subgrid-scale variability and deficiencies in the surface drag parameterization scheme (Nelli
500 et al., 2020; Fonseca et al., 2020; Temimi et al., 2020b). Here, the biases are much smaller,
501 within 0.5 m/s. This, together with the improved representation of the observed air temperature,
502 reflects an overall improved simulation of the boundary layer dynamics in the model.

503

504 The WRF-Chem model evaluation against WISE-UAE measurements (detailed in Table
505 S3 and Fig. S1) reveals a comparable performance to that seen concerning the seven airport
506 stations. SW observations are also available for this site. An evaluation against the WRF-Chem
507 values reveals the model overestimates the incoming shortwave radiation flux by about 30
508 W/m^2 for December, which can be attributed to reduced cloud cover, a known WRF deficiency
509 (Wehbe et al., 2019; Fonseca et al. 2020, 2022a). An inspection of the diurnal cycle revealed
510 the cold (typically by 2-3 °C) and dry (by about 20%) biases occur mostly at night, when the
511 wind speed in the model is higher than that observed, suggesting increased advection of cooler
512 and drier desert air into the site.

513 **4.1.2 Evaluation against ERA5 reanalysis data**

514 The WRF-Chem model predictions are also evaluated against ERA5 reanalysis data for
515 T2m, WS10m, SW, and PBL during June and December 2022. The air temperature biases are
516 within 1 °C, with a cold bias present in both months, more pronounced over inland areas, with
517 correlation coefficients 0.9 (Fig. S2). It is important to note that ERA5 overestimates the
518 temperature at night and underestimates it during the day typically by 1-2 °C in the country for
519 all seasons (Nelli et al., 2024a), meaning the cold bias shown by WRF-Chem does not
520 necessarily indicate a poorer performance. The skill scores for WS10m and SW are also similar
521 to those estimated concerning the station observations and the WISE-UAE field measurements.
522 For the PBL height, the model reproduces its spatial and seasonal variations (Fig. S3), largely
523 driven by the temperature seasonal cycle (cf. Figs. S2; Basha et al., 2019). The PBL height,
524 and over land areas, ranges from 2400-2500 m in the summer during the day to less than 500
525 m in winter at night. Over the Arabian Gulf, the PBL is deeper in the winter months in both

526 ERA-5 and WRF-Chem (800 m vs. 200 m), owing to stronger winds and enhanced turbulent
527 mixing (Dai, 2024).

528 This comprehensive evaluation of the predicted meteorological parameters against those
529 observed at seven UAE airport sites, the WISE-UAE experimental site, and ERA5 reanalysis
530 data demonstrates that WRF-Chem reliably captures them, including their spatial and seasonal
531 variations across the UAE. As WRF-Chem integrates meteorological and chemical processes,
532 precise meteorological simulations are essential to ensure accurate chemical computations
533 within the model domain.

534 **4.2 Model performance for the gaseous pollutants**

535 The study incorporates comparative assessments with satellite data from the TROPOMI
536 instrument, including evaluations of the tropospheric column of NO₂ (denoted as TROPOMI-
537 NO₂), total column CO (TROPOMI-CO), and tropospheric column ozone (TROPOMI-O₃) for
538 the corresponding periods within the UAE. The satellite overpass takes place daily at 13:30
539 local time; therefore, model simulations corresponding to this time are utilized here for
540 comparison over the study area. After smoothing the model concentrations using the a priori
541 and averaging kernel matrix, as detailed in Section 3.4, the results are compared with the
542 corresponding TROPOMI products.

543

544 In the troposphere, nitrogen oxides (NO_x = NO + NO₂) are vital for ozone production and
545 depletion processes in sunlight. Due to their relatively short lifespan, NO_x concentrations are
546 closely linked to emission sources, making them highly sensitive to inaccuracies in emission
547 estimates compared to other pollutants. In our model setup, we adopt the recommendation of
548 Emmons et al. (2010), assigning 10% of NO_x emissions as NO₂. As a result, the model tends
549 to underestimate TROPOMI NO₂ levels, particularly in regions with high emission sources,
550 such as urban centres. The Environment Agency – Abu Dhabi (2018) reported that oil and gas,
551 road transport, and electricity generation are the primary sectors contributing to NO_x total
552 emissions, accounting for 42%, 34%, and 13%, respectively, for the base year of 2015 in the
553 Emirate of Abu Dhabi. Fig. 2 presents the average spatial distributions of absolute differences
554 between the model-simulated and the TROPOMI-retrieved tropospheric column NO₂, scatter
555 plots, and histograms of relative frequency. The satellite retrievals indicate elevated levels of
556 NO₂ columns, exceeding 5x10¹⁵ molecules/cm², in densely populated industrial areas adjacent
557 to the major cities of Dubai and Abu Dhabi in both summer and winter (Fig. S4). Conversely,

558 lower NO₂ values, less than 1.5×10^{15} molecules/cm², are observed over the less urbanized
559 areas. The higher columns are associated with significant economic development driven by a
560 high demand in power generation and water desalination projects, which primarily depends on
561 the combustion of fossil fuels (Abuelgasim & Farahat, 2020; Li et al., 2010). The model
562 effectively reproduces the spatial distributions of NO₂ during the summer and winter of 2022
563 as depicted in Fig. 2. Even though the biases are positive in rural areas, the observed column
564 NO₂ concentration is underestimated by up to 2×10^{15} molecules/cm² in the heavily populated
565 north-eastern UAE, in particular around Ras Al Khaimah and Dubai (Fig. 2a) the sixth-largest
566 city by population in the country and home to a global ceramic manufacturing company. This
567 discrepancy suggests that anthropogenic and industrial emissions might be improperly
568 represented in the EDGAR emission inventory, at least for the UAE. Challenges range from
569 the incomplete characterization of emissions in source regions to the impact of model
570 resolution on capturing sub-grid emission sources. Besides deficiencies in the emission
571 sources, other reasons may explain the model's underperformance in this region. Hoshyaripour
572 et al. (2016) found that the PBL is shallower and more stable at night when simulated with the
573 YSU boundary layer scheme used in the WRF-Chem runs, resulting in a higher accumulation
574 of NO_x in the surface layers. As the evaluation conducted here against satellite observations is
575 daily, an incorrect representation of the atmospheric dynamics will be reflected in the WRF-
576 Chem predictions. Additionally, the existing model configuration does not include the
577 formation of secondary aerosols, indicating a potential area for improvement in future versions.
578 The absence of a vertical distribution of anthropogenic emissions in the model simulations also
579 plays a pivotal role in these model discrepancies. The satellite retrieved TROPOMI-NO₂
580 averaged for the d03 is 1.1×10^{15} molecules/cm² in summer and 1.03×10^{15} molecules/cm² in
581 winter, with the corresponding model simulated column concentration of 1.6×10^{15} and $1.2 \times$
582 10^{15} molecules/cm², respectively. The model demonstrated a moderate correlation with
583 satellite-derived NO₂ column measurements, achieving correlation coefficients of 0.59 for
584 summer and 0.58 for winter (refer to Table 2). It tended to overestimate NO₂ levels more in
585 summer, with a discrepancy of 0.5×10^{15} , compared to 0.2×10^{15} molecules/cm² in winter.
586 Moreover, the evaluation shows RMSE values of 0.2×10^{15} to 0.1×10^{15} molecules/cm² and
587 MAE values of 0.7×10^{15} to 0.5×10^{15} molecules/cm² during the seasons. The frequency
588 distributions in Fig 2(c) and (f) illustrate the differences in NO₂ concentrations between the
589 WRF-Chem model and TROPOMI observations during summer and winter, respectively. In
590 panel 2(c), the distribution of differences is entirely positive, indicating that the WRF-Chem
591 model consistently overestimates NO₂ concentrations compared to TROPOMI observations for

592 the summer of 2022. In contrast, Fig. 2(f) shows both positive and negative differences,
 593 indicating that the WRF-Chem model exhibits a mix of overestimations and underestimations
 594 of NO₂ concentrations in winter, although the majority of differences are still positive. This
 595 suggests a more variable alignment between WRF-Chem and TROPOMI-NO₂ in winter, with
 596 a general tendency toward overestimation but occasional instances of underestimation.
 597

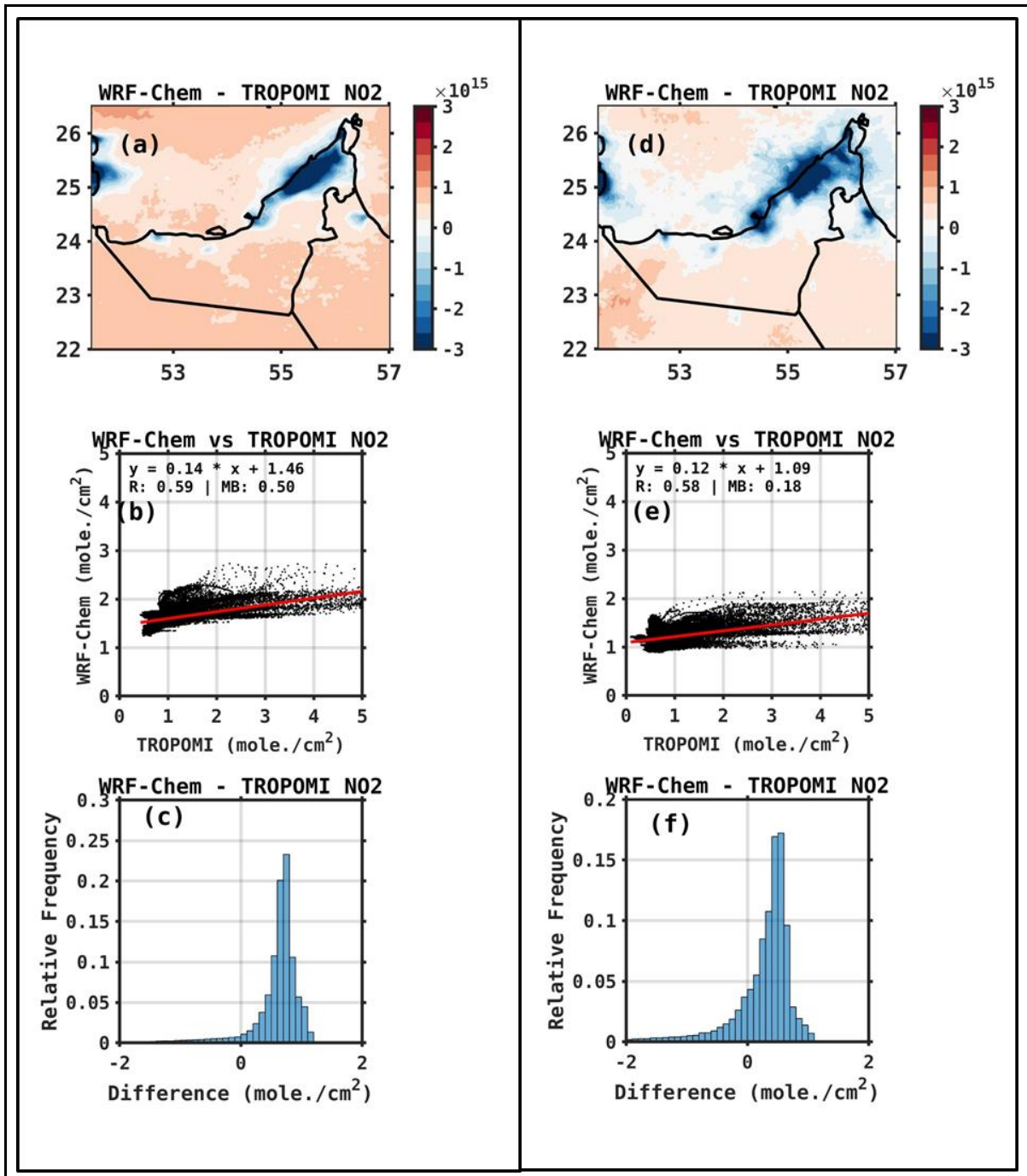


Figure 2: Evaluation of WRF-chem against satellite-derived NO₂: The average difference between tropospheric column NO₂ (mole/cm²) from the TROPOMI satellite and simulated by WRF-Chem, for (a) June and (d) December 2022. (b)-(e) and (c)-(f) are as (a) and (d) but showing scatter plots and histograms of the differences, respectively.

598

599 In Fig. 3, the assessment of the model-simulated total column CO and the corresponding
600 TROPOMI-retrieved values is presented. The statistical metrics comparing these datasets are
601 provided in Table 2. Fig. S5, shows the comparison of total column CO concentrations over
602 the domain as observed by the TROPOMI satellite and simulated by the WRF-Chem model (.
603 Panels (a) and (c) display TROPOMI-CO for summer and winter, showing spatial variations
604 in CO concentration across the region. High concentrations, particularly over the northern
605 areas, while lower concentrations found the southern areas. Panels (b) and (d) illustrate
606 corresponding WRF-Chem CO simulations for the same periods, providing a model-based
607 estimate of CO distribution. The WRF-Chem model appears to capture the general spatial
608 patterns observed by TROPOMI, though there may be some discrepancies in the intensity and
609 precise locations of high CO concentrations. This comparison highlights areas where the WRF-
610 Chem model aligns well with satellite observations and regions where further adjustments in
611 model parameters may be necessary to better replicate observed patterns. The TROPOMI-
612 retrieved CO columns display values of 1.92×10^{18} and 1.79×10^{18} molecules/cm² for summer
613 and winter, respectively. In contrast, the simulated column values are of 1.93×10^{18} for summer
614 and 1.91×10^{18} molecules/cm² for winter. Thus, comparing WRF-Chem and TROPOMI-CO
615 data reveals more pronounced discrepancies, with a minor overestimation of 0.02×10^{18}
616 molecules/cm² in summer and a significant underestimation of 0.12×10^{18} molecules/cm² in
617 winter. Shami et al. (2022) found that the EDGAR emissions inventory underestimates CO
618 emissions when compared to Lebanon's national emission inventory, identifying the road
619 transport sector as the primary source of CO emissions. Consequently, EDGAR's estimates for
620 CO emissions are lower than those provided by Waked et al. (2012) for the same region. The
621 Environment Agency – Abu Dhabi (2018) reported that the road transport sector is the primary
622 source of CO emissions in Abu Dhabi, accounting for 74% of the total CO emissions.
623 Additionally, the industrial sector contributes 21% to the total CO emissions. Kumar et al.
624 (2022) observed an underestimation of CO by the WRF-Chem model, attributing it to an
625 inaccurate representation of anthropogenic emissions on the vertical scale, not represented in
626 the current WRF-Chem simulations as noted for NO₂. This could result in a more rapid

627 deposition of CO molecules at the surface, thereby leading to the observed underestimation. In
628 the summer months, the underprediction of the column CO over coastal areas, in particular
629 around the major urban centers, and the overprediction over inland regions suggests
630 deficiencies in the representation of the atmospheric flow (e.g., a too strong onshore flow),
631 coupled with the aforementioned biases in the emission inventory. In contrast, in winter the
632 biases are positive, and probably more strongly linked to chemistry than to meteorological
633 dynamics.

634 The model output correlates reasonably well with TROPOMI-CO with a correlation coefficient
635 of 0.82 and 0.40 and an RMSE of 0.03×10^{18} and 0.04×10^{18} molecules/cm² in summer and
636 winter, respectively (Table 2). The frequency distribution in Fig. (c) shows most differences,
637 with a slight positive skew, suggesting a tendency for the WRF-Chem model to slightly
638 overestimate CO concentrations compared to TROPOMI observations for summer. In contrast,
639 Fig. (f) displays a broader distribution with a more pronounced positive skew, indicating larger
640 and more variable overestimations by WRF-Chem in winter. In winter seasons, the lower
641 correlation coefficients and higher biases for TROPOMI-CO as compared to TROPOMI-NO₂
642 might be attributed to the complexities inherent in modeling and observing CO distributions,
643 which local emission sources, atmospheric chemistry, and transport processes can influence.
644 These findings are consistent with research conducted in India, where Dekker et al. (2019)
645 reported a correlation of 0.81 between TROPOMI and WRF-Chem CO levels during a high
646 pollution episode in November 2017. Similarly, in East Asia, Zhang et al. (2016a) documented
647 correlations between WRF-Chem simulated and the Measurements of Pollution in the
648 Troposphere (MOPITT)-retrieved CO columns, with a r-value of 0.59 and RMSE of 4.6×10^{17}
649 molecules/cm² for summer, and 0.69 with RMSE of 5.2×10^{17} molecules/cm² for winter,
650 respectively.

651

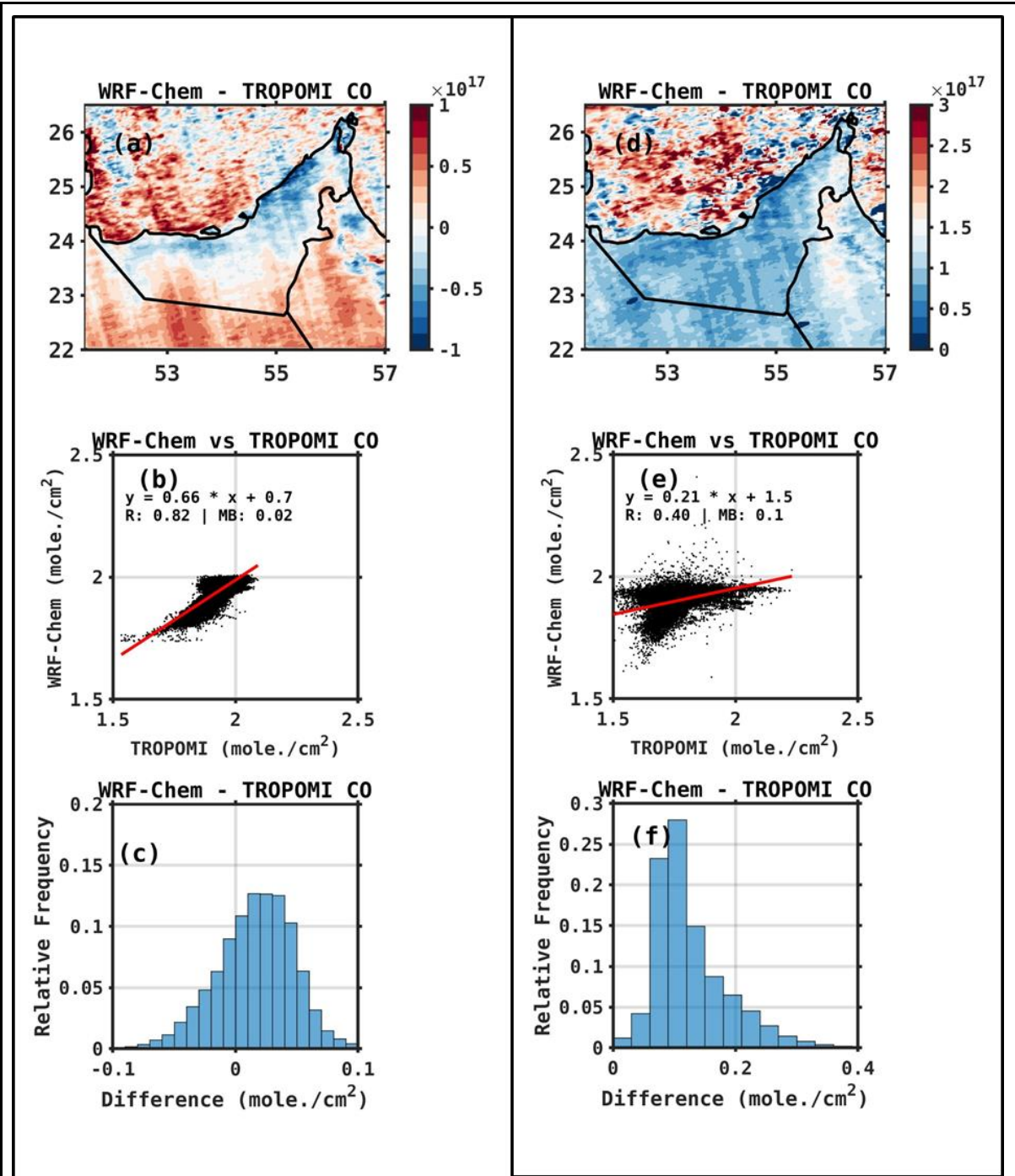


Figure 3: Evaluation of WRF-Chem against satellite-derived CO: Same as Fig. 2 but for the total column of CO.

652

653 Figure S6 presents the spatial distribution of tropospheric ozone concentrations over the
 654 UAE as observed by TROPOMI (TROPOMI-O₃) and simulated by the WRF-Chem model
 655 during the summer and winter of 2022. In Figures S5 (a) and (b), TROPOMI shows varying
 656 O₃ concentrations with higher values, particularly along the northern coastal regions, where

657 concentrations reach up to 20 DU. Similarly, WRF-Chem demonstrates a comparable spatial
658 pattern, with elevated O₃ concentrations in the same regions, reaching up to 40 DU, indicating
659 that the model captures the general distribution observed by TROPOMI. In Figure S5 (c),
660 representing winter, TROPOMI exhibits a different distribution pattern, with overall lower O₃
661 concentrations compared to summer. The WRF-Chem simulation in winter also shows a
662 broader distribution of O₃, with concentrations reaching up to 25 DU. While the WRF-Chem
663 model aligns reasonably well with TROPOMI observations, discrepancies in concentration
664 levels highlight both the model's ability to replicate seasonal variations and areas where
665 improvements may be needed, especially in the winter months. The comparison of the WRF-
666 Chem simulated tropospheric ozone columns with the TROPOMI-retrieved columns
667 (TROPOMI-O₃) is illustrated in Fig. 4, with the statistical comparisons detailed in Table 2. The
668 TROPOMI-O₃ columns show higher in summer, at 16.6 DU, and lower values in winter, at
669 13.4 DU, which is attributed to increased photochemical activity during the summer months
670 (Reddy et al., 2012; Coates et al., 2016; Badia & Jorba, 2015; Abdallah et al., 2018; Baldasano
671 et al., 2011) The WRF-Chem simulations show these variations, with values of 32.8 DU for
672 summer and 24.8 DU for winter, respectively. Therefore, model output is strongly correlated
673 to the TROPOMI-O₃ column concentration, with a correlation coefficient of 0.78 and 0.83 and
674 an RMSE (MAE) of 1.4 and 1.0 DU (15.9 and 11.2 DU) during summer and winter,
675 respectively. The WRF-Chem model systematically overestimates ozone levels by 15.9 and
676 11.2 DU in summer and winter, respectively. The frequency distribution in Fig. 4(c) represents
677 the differences between WRF-Chem and TROPOMI-O₃ concentrations during the summer,
678 showing that they are more pronounced with a positive skew. This indicates a consistent
679 tendency for the WRF-Chem model to overestimate O₃ concentrations compared to TROPOMI
680 observations in summer. Similarly, Fig. 4(f) displays a frequency distribution for winter with
681 a positive skew and narrower spread, highlighting that WRF-Chem also tends to overestimate
682 O₃ concentrations compared to TROPOMI during this season, although with less variability in
683 the overestimations. Therefore, the WRF-Chem model systematically overestimates O₃
684 concentrations throughout the year, with a slightly more consistent bias observed in winter. Hu
685 et al. (2021) highlighted the substantial influence of meteorological factors on ozone
686 production, noting that temperature, relative humidity, and sunshine duration play significant
687 roles in descending order of importance. Strong solar radiation and elevated temperatures
688 enhance photochemical reactions, increasing ozone formation. In comparison with ERA-5 data
689 (Fig. S1) and station data (Table S2), the colder temperatures observed in WRF-Chem,
690 particularly in winter months when tropospheric column O₃ biases are less positive (Table 2),

691 may explain the overestimation of O₃ concentrations in the model. Zhang et al. (2020) found
692 that low wind speeds and high atmospheric pressure can hinder pollutant dispersion, leading to
693 ozone accumulation, while Lu et al. (2019) observed that high humidity conditions can deplete
694 O₃ through interactions with water vapor and the production of OH radicals. WRF-Chem's
695 negative RH2m bias against in situ measurements in both summer and winter (Tables S2 and
696 S3), combined with temperature biases, may contribute to the model's overprediction of O₃.
697 Further exploration of these chemical interactions would require additional sensitivity analyses
698 beyond this study's scope. Future work should focus on refining model fidelity by improving
699 the representation of chemical processes and emissions to enhance air quality projections and
700 deepen our understanding of regional pollution patterns.

701 The disparities between WRF-Chem and TROPOMI data highlight the intrinsic challenges
702 in air quality monitoring and prediction. WRF-Chem's limitations may stem from its
703 dependency on emissions inventories, which, as noted above, can have significant
704 discrepancies compared to actual emissions, uncertainty in the meteorological forcing data, and
705 the representation of atmospheric chemistry. TROPOMI, while offering high-resolution
706 satellite observations, is subject to constraints related to retrieval algorithms and the influence
707 of atmospheric conditions on measurement accuracy. Liu et al. (2022) identified that
708 uncertainties in column observations arise from the challenges in differentiating between
709 stratospheric and tropospheric contributions and uncertainties in the tropospheric air mass
710 factor and its spectral fitting. Integrating model predictions with satellite observations,
711 alongside ground-based measurements, is crucial for enhancing our understanding of air
712 quality dynamics and improving predictive capabilities. This synergistic approach can help
713 mitigate biases, enhance accuracy, and provide a more comprehensive view of atmospheric
714 pollutants' distribution over this region.

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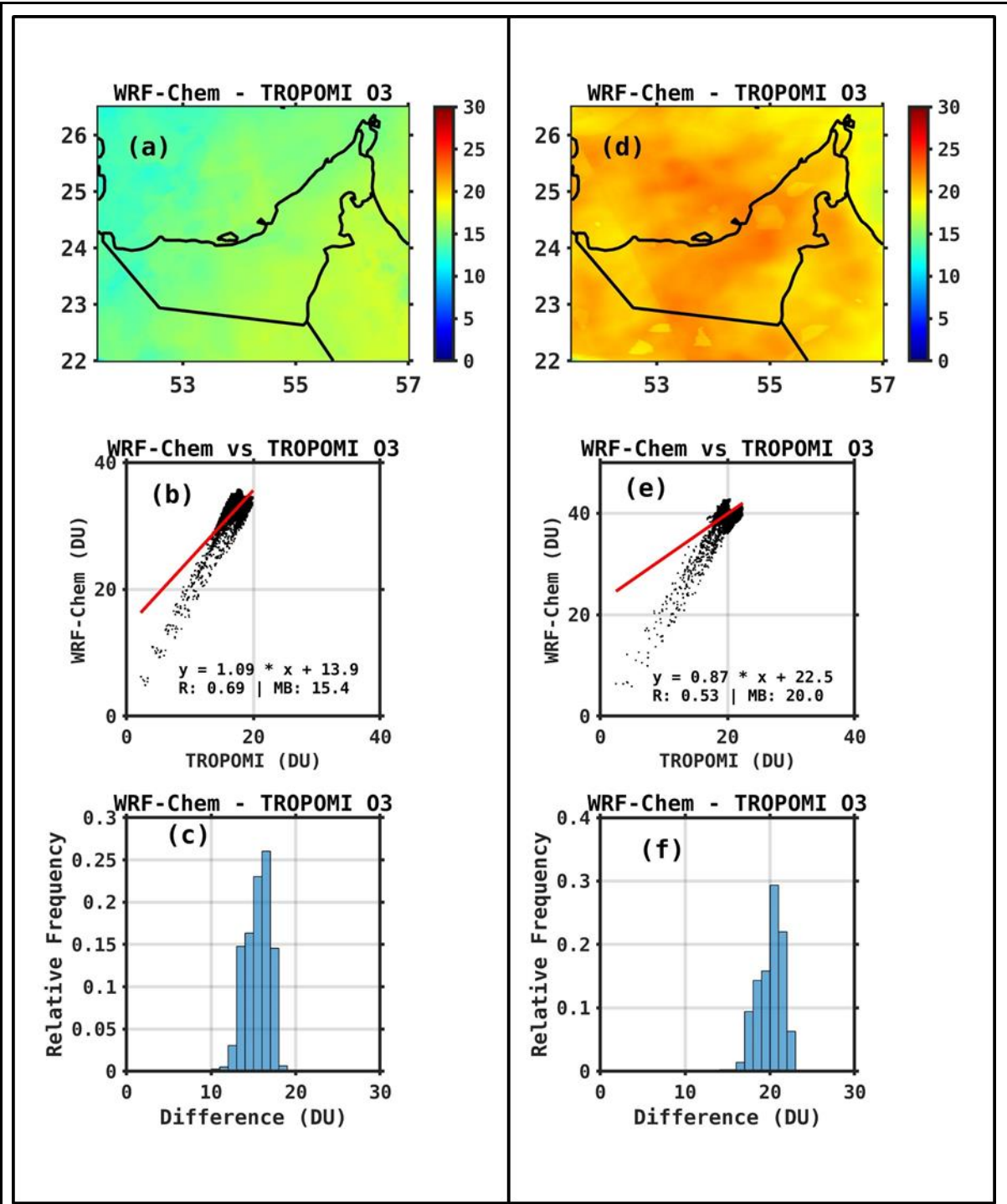


Figure 4: Evaluation of WRF-Chem against satellite-derived O₃: Same as Fig. 5 but for total column of ozone.

716

717 **Table 2: Statistical verification scores for evaluation against TROPOMI measurements:** skill
 718 scores between TROPOMI columns (mole. /cm²), tropospheric column NO₂ (TROPOMI-NO₂), total
 719 column carbon monoxide (TROPOMI-CO), tropospheric column ozone (TROPOMI-O₃) and MODIS
 720 AOD with corresponding WRF-chem simulated columns during June and December of 2022 over UAE.

721 The first two columns show the model and satellite monthly-mean values, with the other four giving
 722 the MB, MAE and RMSE in units of mole. / cm² for TROPOMI-NO₂ and CO and in DU for O₃
 723

Parameter	Month	MOD	SAT	MB	MAE	R	RMSE
NO ₂ (x10 ¹⁵)	June	1.6	1.1	0.50	0.74	0.59	0.16
	Dec	1.2	1.0	0.18	0.54	0.58	0.15
O ₃		39.6	19.3	20.0	20.0	0.53	1.70
		33.1	17.3	15.4	15.4	0.69	1.62
CO (x10 ¹⁸)		1.93	1.92	0.02	0.03	0.82	0.03
		1.91	1.79	0.12	0.12	0.40	0.04
AOD		0.85	0.54	0.3	0.32	0.65	0.22
		0.28	0.28	0.0	0.11	0.30	0.13

724

725 4.3 Model performance with respect to AOD

726 4.3.1 AERONET

727 The analysis of daily mean AOD at Mezaira for June 2022 (Fig. 5(a)) and DEWA for
 728 December 2022 (Fig. 5(b)) reveals the model tends to overestimate the observed AOD values,
 729 in particular in the summer month when it is the highest (Nelli et al. 2020, 2022). In June at
 730 Mezaira, the AERONET AOD shows a steady increase from around 0.5 to approximately 1.0
 731 by the end of the month, which is in line with the expected build-up of aerosols with the annual
 732 maxima typically occurring in July (Nelli et al., 2022). The WRF-Chem model captures this
 733 upward variation but consistently overestimates the observed AOD, especially toward the end
 734 of the month. This overestimation is highlighted by the MB of 0.46. The general overestimation
 735 of the observed wind speed concerning ground-based measurements (Tables S2 and S3; Fig.
 736 S1) can at least partially explain this bias, together with an incorrect representation of the
 737 particle size distribution and hence the sedimentation rates, leading to excessive amounts of
 738 suspended dust (Ukhov et al., 2021; Parajuli et al., 2023). The moderate correlation coefficient

739 ($r = 0.60$) suggests that the model's day-to-day variability reasonably follows that observed.
740 This is expected, as dust lifting in the warmer months is mainly associated with the Shamal
741 winds (Yu et al., 2016), which are fairly well represented in the model. Conversely, at DEWA
742 in December (Fig. 5(b)), the observed AODs are lower, fluctuating between 0.2 and 0.3,
743 indicative of the season's lower aerosol concentrations (Nelli et al., 2020). The WRF-Chem
744 model again follows the observed variation but shows occasional significant overestimations,
745 most notably on December 10th, where simulated AOD spikes to 1.6, far exceeding the
746 observed AODs. Dust lifting in the colder months is typically associated with the passage of
747 mid-latitude weather systems (Nelli et al., 2022), which the WRF model does not fully
748 reproduce, in particular with respect to its timing (Temimi et al., 2020b; Taraphdar et al., 2021).
749 This discrepancy is reflected in the weak correlation coefficient ($r = 0.16$) and the MB of 0.05.
750 The overestimation of the near-surface wind speed at the location of the airport stations (Table
751 S2) and the WISE-UAE site (Table S3) is also in line with the higher amounts of atmospheric
752 dust in the model. Fig. 5 shows that, while the WRF-Chem model demonstrates the ability to
753 capture seasonal variations in AOD, it tends to overestimate AOD levels in both summer and
754 winter months, suggesting a need for calibration of the aerosol parameterization scheme in the
755 model or the emissions input. This comparison highlights the model's potential and limitations
756 in simulating the UAE-specific aerosol conditions, as well as where research is needed to
757 optimize the model performance.
758

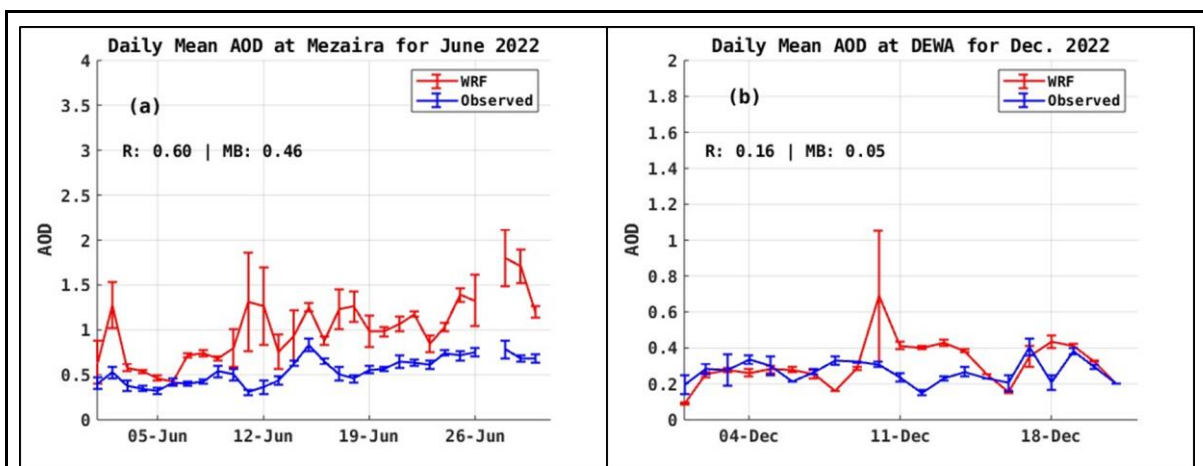


Figure 5: Evaluation of WRF-Chem against AERONET AOD: Daily mean Aerosol Optical Depth (AOD; dimensionless) from WRF-Chem simulations (red) and AERONET observations (blue) at Mezaira during June 2022 (a) and Dewa during December 2022 (b). The lines give the daily mean values and the error bars show one standard deviation from the

mean computed using the hourly values. The correlation (r) and mean bias (MB) are given in the plot.

759

760 **4.3.2 MODIS**

761 The comparison between WRF-Chem simulated and MODIS AOD (MOD-AOD) is
762 depicted in Fig. 6, with the statistical comparisons summarized in Table 2. The satellite-derived
763 MOD-AOD values follow the same seasonal cycle as the ground-based AERONET
764 observations: they are higher in the summer, averaging 0.54, and lower in winter, averaging
765 0.28, reflecting the annual cycle in aerosol loading in the region (Nelli et al., 2020). The WRF-
766 Chem simulations capture these seasonal variations, with corresponding AODs of 0.85 in
767 summer and 0.28 in winter. The model AOD demonstrates moderate correlation with MODIS
768 AOD, yielding correlation coefficients of 0.65 for summer and 0.30 for winter, similar to the
769 ones with respect to the AERONET AOD, indicating the satellite-derived and ground-based
770 AOD estimates are in close agreement, which has been noted by Nelli et al. (2020). The WRF-
771 Chem model systematically overestimates AOD by 0.31 in summer, a similar (albeit of a
772 smaller magnitude) bias with that respect to the AERONET station (Fig. 5(a)), while slightly
773 underestimating by 0.004 in winter.

774

775 For June, WRF-Chem generally overestimates AOD compared to the MODIS' estimates, in
776 particular over the southern and central UAE, as shown in the spatial distribution of the
777 difference between them (Figs. 6(a)-(c)). The frequency distribution shows most differences
778 clustering around zero, with a slight positive skew, reinforcing the model's overestimation
779 tendency for this month. Stronger wind speeds and an incorrect representation of the dust
780 physical and optical properties can explain the model bias. In contrast, in December there are
781 more balanced results, with WRF-Chem showing a closer alignment with MODIS AOD on
782 average. The spatial distribution of the model bias displays areas in the central and southern
783 UAE where the MODIS AOD exceeds the WRF-Chem values, with anomalies of the opposite
784 sign over the Arabian Gulf and parts of the Al Hajar mountains in Oman. Mostamandi et al.
785 (2023) showed that, over the Arabian Gulf and in the WRF-Chem model, the dust deposition
786 rates decrease away from the coastlines, with coastal UAE having lower deposition rates than
787 inland sites. Excessive dust deposition over the Rub Al Khali Desert is consistent with a clearer
788 atmosphere closer to the coastlines in the model when compared to the MODIS measurements.

789 The positive bias over the Arabian Gulf can be attributed to higher amounts of dust transported
 790 upstream by north-westerly winds and/or reduced dust deposition over the water in WRF-
 791 Chem. The frequency distribution in December shows a balanced spread around zero,
 792 suggesting a more accurate seasonal fit than in June. These findings, together with those in Fig.
 793 5 with respect to the AERONET station observations, underscore the influence of seasonal
 794 atmospheric conditions on WRF-Chem's performance and suggest the need for seasonal
 795 adjustments in the aerosol parameterization to improve model accuracy in capturing the UAE's
 796 unique aerosol dynamics.
 797

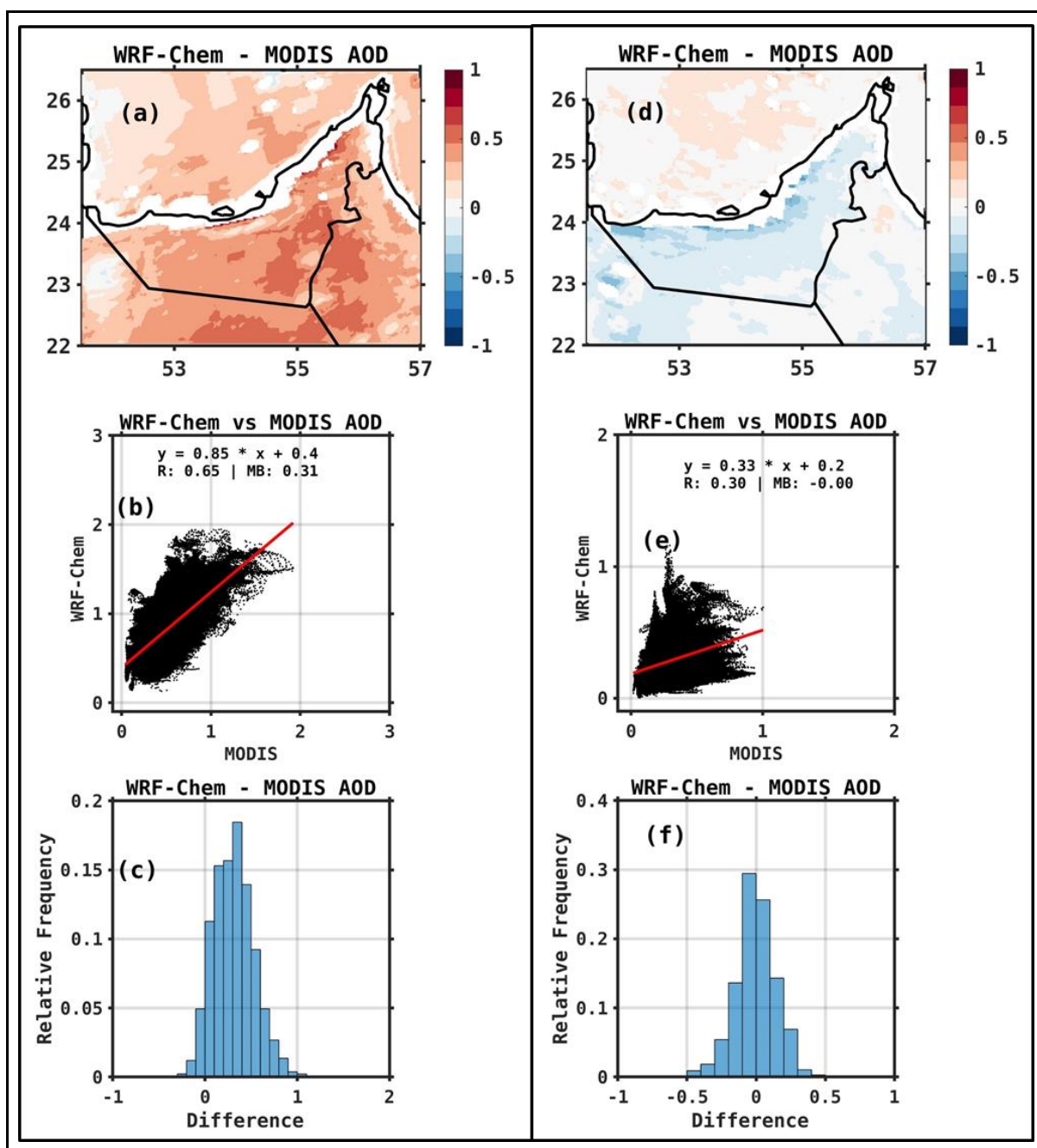


Figure 6: Evaluation of WRF-Chem against MODIS AOD : Same as Fig. 2 but for the MODIS AOD.

798

799 **4.4. Aerosol influence on Ozone**

800 Tropospheric or surface ozone (O_3) is one of the most significant greenhouse gases after
801 carbon dioxide (CO_2) and methane (CH_4) (Ehhalt and Prather, 2001). It plays a critical role in
802 the Earth's radiation budget, contributing to an increase in radiative forcing of up to 0.47 W/m^2
803 and accounting for 3-7% of global warming (Gauss, 2003; Ehhalt and Prather, 2001). Elevated
804 O_3 levels in the atmospheric boundary layer are toxic and can significantly impact human health
805 and vegetation (Adams et al., 1989). The interactions between reactive gaseous pollutants and
806 aerosols are a major focus in the development of air quality and climate models. Aerosols,
807 through scattering and absorption of solar radiation, influence photolysis rates and can either
808 increase or decrease the formation of O_3 and its precursors (He and Carmichael, 1999). Studies
809 have shown that aerosols impact ozone production and loss by altering photolysis frequencies
810 (Dickerson et al., 1997; Jacobson, 1998). For example, Li et al. (2011) used an air quality model
811 to evaluate the changes in photolysis frequencies caused by sulfate, nitrate, ammonium, and
812 mineral dust aerosols in central and eastern China, finding a 5.4% decrease in daily average
813 surface ozone concentrations. Similarly, Lou et al. (2014) found that aerosols reduced annual
814 mean photolysis frequencies, $j(O^1D)$ and $j(NO_2)$, by 6–18% in polluted eastern China, resulting
815 in reductions of up to 0.5 ppbv in O_3 during spring and summer, using a global chemical
816 transport model. Attributing ozone levels to a specific source region is particularly challenging,
817 as ozone concentrations are influenced by various processes, including stratosphere-
818 troposphere exchange, significant hemispheric background levels, dominant local emissions,
819 and complex photochemical reactions involving multiple trace gases (Fiore et al., 2003).
820 Therefore, it is crucial to understand the impact of aerosol feedback on surface ozone in the
821 UAE, a region with high aerosol loading in the Arabian Peninsula.

822 From Fig. 4 and the discussion in section 4.2, it is evident that ozone levels are higher during
823 the summer season, which coincides with a dominance of aerosols over the UAE. In order to
824 better understand the impact of aerosols on ozone concentrations, we conducted a simulation
825 in which all aerosol components in the WRF-Chem model are turned off (No aerosol + radiative
826 feedback on), simulating an aerosol-free atmosphere over the UAE. This simulation is

827 conducted alongside a control simulation (All aerosol + radiative feedback on) in which all
828 aerosol processes are included, both for June 2022. The results of these simulations, comparing
829 the scenarios with and without aerosols, are presented in Fig. 7 and highlight the influence of
830 aerosols on ozone formation and spatial distribution in the region. This analysis focuses on
831 daytime hours (04-12 UTC) and non-daytime hours (13-03 UTC) to delve deeper into ozone
832 dynamics, as ozone production predominantly occurs during the daytime compared to non-
833 daytime hours. Figs. 7 (a)-(b) shows the ozone distribution with and without aerosols during
834 the daytime hours (04-12 UTC; 08-16 LT). Both panels depict higher ozone concentrations over
835 the northern regions, with a clear gradient decreasing towards the south-eastern areas during
836 daytime hours. The influence of aerosols on ozone production is evident in areas where the
837 ozone levels are slightly elevated, suggesting that aerosols contribute to ozone production/loss
838 under daytime conditions based on the nature of the aerosols. Fig. 7 (c) highlights the difference
839 in ozone concentrations between simulations with and without aerosols for daytime hours. The
840 difference shows localized areas of positive and negative changes, indicating regions where
841 aerosols either enhance or suppress ozone levels. Notably, over the northern areas, particularly
842 in oceanic regions where the ozone concentrations are the highest, the differences are generally
843 positive, reflecting a positive feedback of aerosols on ozone production, particularly over the
844 Arabian Gulf. On the other hand, over land areas, where the ozone is lower, the lower
845 photolysis rates may limit ozone production. Therefore, the impact of aerosols on ozone varies
846 based on their origin, such as dust events. These aerosols can have anthropogenic, natural, or
847 marine origins (Filioglou et al., 2020; Nelli et al., 2021). Aerosols significantly influence
848 surface ozone through atmospheric chemical and physical processes. Depending on their
849 nature, aerosols can either increase or decrease ozone levels, as observed in various studies
850 (Gao et al., 2023; Shi et al., 2022). As noted in studies such as Wang et al. (2019), Mukherjee
851 et al. (2020), and Qu et al. (2021), the reduction in the incoming shortwave radiation flux will
852 hinder the generation of ozone, as well as an increase in the NO/NO₂ ratio, which can happen
853 when the pollutants' concentration increases in a shallower boundary layer. On the other hand,
854 higher amounts of CO and NO₂ will promote the production of ozone.

855 Fig. 7 (d) and (e) illustrate ozone concentrations with and without aerosols for the remaining
856 hours (non-daytime). The patterns are largely similar to those observed during the daytime,
857 except over urban areas where the ozone concentration is much reduced owing to the lack of
858 *in situ* generation due to the absence of sunlight and underestimation of ozone precursor
859 concentration. Fig. 7(d) shows slightly higher concentrations than Fig. 7(e), suggesting that

860 aerosols continue to have an impact on ozone production, albeit less pronounced, during non-
861 daytime periods. Fig. 7(f) presents the difference in ozone concentrations between simulations
862 with and without aerosols for the non-daytime hours. The spatial distribution of positive and
863 negative differences follows a similar pattern to that observed during the daytime hours, though
864 the magnitudes are generally larger. This suggests that ozone advection from upstream sources
865 may play a role. Additionally, marine aerosols can contribute to ozone production through their
866 nature.

867

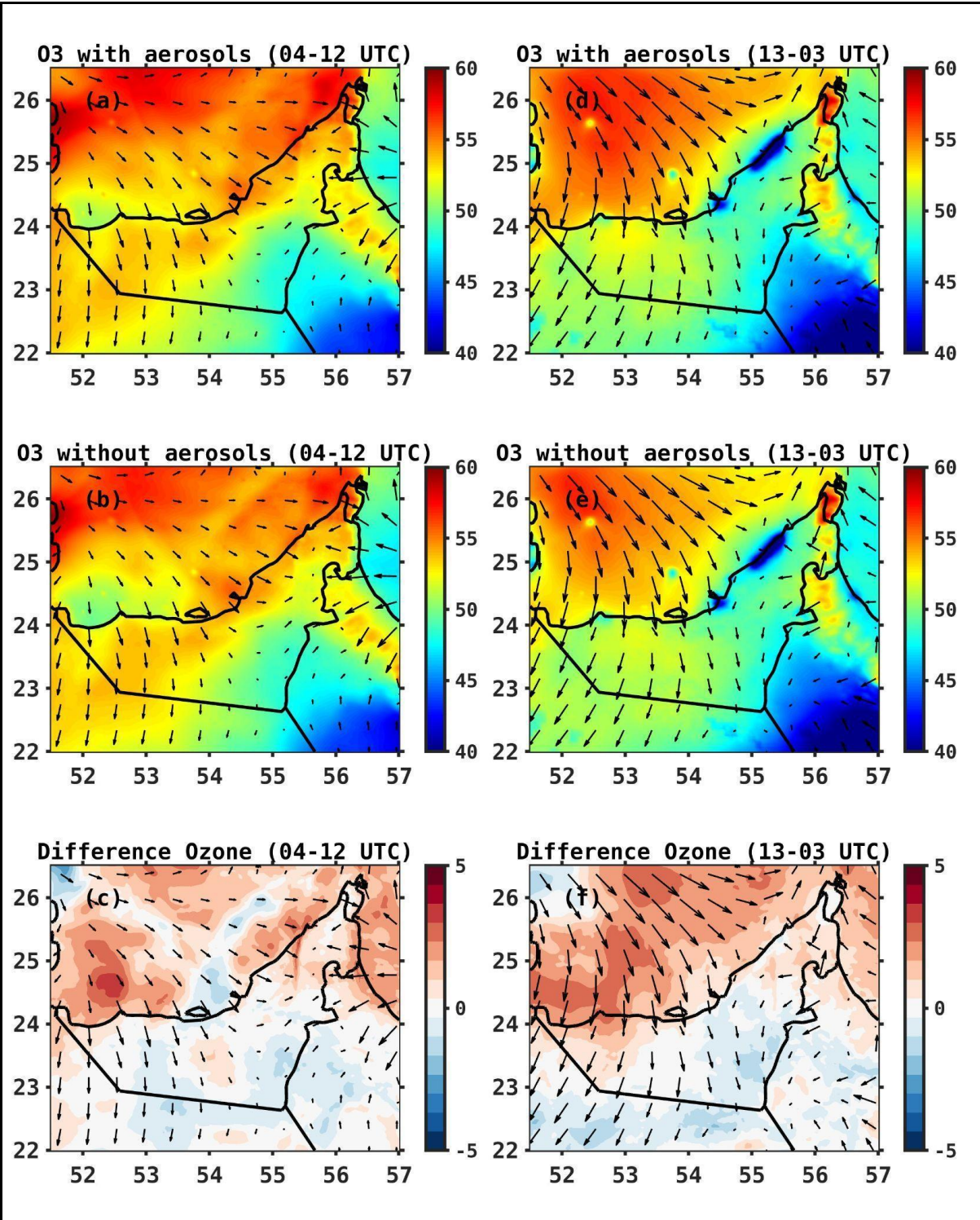


Figure 7: Ozone (O_3) Sensitivity Simulations: Spatial distribution of surface ozone concentrations (ppb) simulated by the WRF-Chem model with (a) and without (b) aerosols over the UAE for specified daytime hours during June 2022. (d)-(e) are as (a)-(b) for the remaining hours. Panels (c) and (f) illustrate the difference (%) in ozone concentrations (with aerosols minus without aerosols) during daytime hours and the remaining hours, respectively. The 10-m wind vectors (m/s) are overlaid on each plot, indicating the wind

patterns influencing the ozone distribution.

868

869 **5. Conclusions**

870 This study rigorously evaluates the performance of the Weather Research and Forecasting
871 model coupled with chemistry (WRF-Chem) in simulating meteorological parameters and air
872 pollutants over the United Arab Emirates (UAE) during June and December 2022, representing
873 contrasting summer and winter conditions. The model's performance is assessed through
874 comparisons with ground-based observations and ERA-5 reanalysis data for meteorological
875 parameters, as well as AERONET, TROPOMI, and MODIS satellite observations for air
876 pollutants.

877

878 We evaluated WRF-Chem model's accuracy in simulating meteorological parameters, in
879 particularly 2-meter temperature (T2m), 10-meter wind speed (WS10m), and 2-meter relative
880 humidity (RH2m) across 7 locations in the UAE. The model generally overestimates T2m in
881 summer by less than 0.2 °C and underestimates it in winter by 3°C, with correlation coefficients
882 ranging from 0.7 to 0.85 among the stations. This is comparable performance with compared
883 to that reported studies (e.g., Branch et al., 2021; Temimi et al., 2020b), reflecting the added
884 value of explicitly predicting chemistry fields in this aerosol-rich region. An incorrect
885 representation of surface properties, such as the albedo and surface emissivity, and deficiencies
886 in the model physics and dynamics, may explain the referred temperature biases. For WS10m,
887 the model's bias is within ± 0.5 m/s, indicating good agreement for both land and marine areas.
888 The tendency for the model to overestimate the observed wind speed may arise from
889 deficiencies in the surface drag parameterization scheme and an underrepresentation of its
890 subgrid-scale variability (Nelli et al., 2020). In any case, and as for air temperature, the
891 magnitude of the biases is much smaller than that reported in other studies, for which the wind
892 speed biases exceed 3 m/s (Branch et al., 2021; Fonseca et al., 2020; Temimi et al., 2020b).
893 The dry bias noted in these studies, however, is also seen in the WRF-Chem simulations,
894 possibly arising from a drier soil, an incorrect representation of the mesoscale (sea-/land-
895 breeze) circulations, and a dry bias in the forcing data. The WRF-Chem model evaluation
896 against WISE-UAE measurements reveals a comparable performance to that seen with respect
897 to the airport stations w.r.t T2m, WS10m and RH2m. An evaluation against the WRF-Chem
898 values reveals the model overestimates the incoming shortwave radiation flux (SW) by about

899 30 W/m² for December, which can be attributed to reduced cloud cover, a known WRF
900 deficiency (Wehbe et al., 2019; Fonseca et al. 2020, 2022a). An inspection of the diurnal cycle
901 revealed the cold (typically by 2-3 °C) and dry (by about 20%) biases occur mostly at night,
902 when the wind speed in the model is higher than that observed, suggesting increased advection
903 of cooler and drier desert air into the site.

904 The comparison of ERA5 reanalysis data with WRF-Chem simulations revealed regional
905 variations in T2m, specifically underestimation in the UAE's southern region and
906 overestimation in the north-western region. Statistical metrics for summer show an
907 underestimation of 1 °C and a correlation coefficient (r) of 0.97. In comparison, for winter a
908 similar pattern is seen with an underestimation of 1 °C and a r value of 0.92 over the domain.
909 The fact that WRF-Chem performs well against in-situ data and ERA5 reanalysis with respect
910 to air temperature is also an indication that the reanalysis dataset performs well in this region,
911 as noted by Fonseca et al. (2022b) and Nelli et al. (2024a). The mean PBL from ERA5 is largely
912 consistent with that from the WRF-Chem outputs, with both data sets displaying a clear
913 seasonal variation—increased PBL during summer and decreased in winter, correlating with
914 temperature changes.

915 Regarding gaseous pollutants, both WRF-Chem and satellite data show higher TROPOMI-
916 NO₂ columns greater than 5x10¹⁵ molecules/cm² in urban and industrial regions such as Dubai,
917 Abu Dhabi, and Ras Al Khaimah, reflecting emissions from economic activities like power
918 generation, water desalination, and industries. Lower concentrations (<1.5x10¹⁵
919 molecules/cm²) are noted in less urbanized areas. The WRF-Chem model closely reproduces
920 the TROPOMI-NO₂ spatial patterns, even though it tends to underestimate the observed
921 concentrations in the Abu Dhabi region and underestimate the north-eastern UAE, which has
922 been tied to deficiencies in the emission inventory. Moderate correlation coefficients (0.59 in
923 summer and 0.58 in winter) confirm the model's effectiveness in capturing NO₂'s day-to-day
924 variability. WRF-Chem overestimates the observed TROPOMI-O₃ column, as indicated by
925 positive MB values of around 11-16 DU, yet maintains high correlation coefficients (0.78 in
926 summer and 0.83 in winter), suggesting accurate ozone concentration simulations. Colder and
927 drier conditions, along with deficiencies in the representation of the observed chemistry,
928 particularly concerning the NO_x emissions linked to the O₃ concentration, can explain the
929 WRF-Chem biases. TROPOMI-CO column simulations, on the other hand, exhibit significant
930 discrepancies in winter and lower correlation coefficients, highlighting challenges in accurately

931 modelling CO levels. Besides an incorrect emission inventory, discrepancies in the
932 representation of the atmospheric flow and its effect on the pollutant's dispersion, can explain
933 the model performance. In summer, the analysis conducted here stresses the WRF-Chem
934 model's strengths in simulating CO, NO₂ and O₃ columns with high fidelity with respect to the
935 TROPOMI's observations, but also points out its limitations in estimating CO columns
936 accurately in winter.

937 Regarding aerosol optical depth (AOD) observed by AERONET stations and the MODIS
938 satellite, the WRF-Chem model generally tends to overestimate AOD, particularly during the
939 summer months. At Mezaira in June, AERONET data showed a steady increase in AOD, which
940 the WRF-Chem model captured but consistently overpredicted due to factors such as
941 overestimated wind speeds and inaccuracies in particle size distribution. In December at
942 DEWA, observed AOD levels were lower, and while the model followed the observed trends,
943 it occasionally produced large spikes, reflecting challenges in accurately capturing the effects
944 of mid-latitude weather systems. Correlation coefficients for AOD comparisons reveal
945 moderate (0.60) to weak model performance depending on the season, influenced by dust
946 transport mechanisms. Comparisons with MODIS satellite-derived AOD similarly indicated
947 seasonal overestimations during the summer, with a closer alignment observed in winter.
948 Spatially, overestimations in southern and central UAE in June were linked to strong winds
949 and dust properties, while December results were more balanced. Biases over the Arabian Gulf
950 were attributed to dust transport and deposition dynamics. Overall, the findings indicate that
951 while the WRF-Chem model captures seasonal AOD variations, adjustments to aerosol
952 parameterization and dust representation are necessary to improve model accuracy.

953 This study also explores the impact of aerosols on surface ozone (O₃) in the UAE by altering
954 photolysis rates through the scattering and absorption of solar radiation. Using WRF-Chem
955 model simulations for June 2022, we compared scenarios with and without aerosols to assess
956 their influence. The results show higher ozone concentrations during daytime in northern
957 regions, with aerosols contributing to localized increases or decreases. Marine aerosols notably
958 enhance O₃ production over the Arabian Gulf, while lower photolysis rates limit ozone
959 formation over land areas. During non-daytime hours, aerosol influence continues but is less
960 significant, with urban areas experiencing reduced ozone levels due to limited photochemical
961 activity. Additional sensitivity simulations and in-situ observations are needed to validate these
962 findings further.

963 The WRF-Chem model exhibits enhanced capability in simulating key meteorological
964 parameters and satisfactory performance in air pollutants over the UAE, showcasing significant
965 improvements in regional-scale dynamics. This is evidenced by high skill scores with respect
966 to observational data, with a clear improvement over previous research outcomes, particularly
967 during summer. This comprehensive assessment validates the model's effectiveness and
968 identifies potential areas for improvement in simulating air pollutant concentrations across the
969 hyper-arid and aerosol-rich UAE. The discrepancies between model simulations and various
970 observational data sets likely arise from improper emission inventories, particularly
971 anthropogenic emissions, which must be optimized based on existing country-specific datasets.
972 Other sources of uncertainty are model parameterization schemes and the quality of the
973 meteorological and chemistry input data. Integrating model predictions with satellite
974 observations and ground-based measurements is crucial for advancing air quality monitoring
975 and enhancing the predictive accuracy of atmospheric pollutant distributions in the UAE. This
976 collective approach aids in addressing biases and improving the overall understanding of
977 regional air quality dynamics.

978

979 **Code and Data Availability**

980 The authors would like to acknowledge that the products used in this study are freely accessible
981 online: (i) ERA-5 reanalysis data is extracted from the Copernicus Climate Change Service
982 Climate Data Store (Hersbach et al. 2023a,b); (ii) Nitrogen Dioxide (NO₂), Ozone (O₃) and
983 Carbon Monoxide (CO) column concentrations estimated from the measurements collected by
984 the Tropospheric Monitoring Instrument (TROPOMI) onboard the Sentinel 5-P satellite are
985 extracted from the National Aeronautics and Space Administration's (NASA's) website; (iii)
986 Aerosol Optical Depth from Moderate Resolution Imaging Spectroradiometer (MODIS) (iv)
987 National Centers for Environmental Prediction (NCEP) Final (FNL) Operational Global
988 Analysis meteorological data used to drive the WRF-chem simulations is downloaded from the
989 National Center for Atmospheric Research (NCAR) Research Data Archive website
990 (NCEP/NWS/NOAA/USDC, 2000), with the chemistry data used to force WRF-Chem, the
991 output of the Community Atmosphere Model with Chemistry (CAM-chem) model, extracted
992 from NCAR's website (Bucholz et al., 2019); (iv) the WRF-Chem model used, version 4.3.1,
993 is freely available from the developers' website (WRF, 2023), with the pre-processor tools

994 available at NCAR's website (NCAR, 2023). All figures displayed in this manuscript were
995 generated with the Matrix Laboratory (MATLAB) software version 2023 (Mathworks, 2023).

996 **Acknowledgment**

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1010 quality of this work.

1011 **Conflict of interest**

1012 The authors declare they do not have any conflict of interest.

1013 **Author contribution**

1014 Conceptualisation and methodology: D.F. and Y.Y.; Data curation and visualization: Y.Y.; formal
1015 analysis and interpretation: Y.Y., R.F., N.N., and D.F.; project administration and supervision: D.F.;
1016 writing—original draft: Y.Y.; review and editing: all authors.

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