Simulation of the Air Quality in Southern California, USA in July and October of the Year 2018

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Abstract: A numerical investigation of the air quality in Southern California, USA in the year 2018 is presented using the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem). In July, a heat wave occurred, and in October, Santa Ana conditions prevailed; these conditions and their impact on air quality are the scope of the present numerical study. The high spatial resolution in the simulation includes two nested domains of 1 km and 3 km, respectively. Local climate zones land use categories are combined with the complex urban model building effect parameterization coupled with the building energy model (BEP+BEM) and the detailed MOZART-T1 chemical reaction mechanism, which is the MOZART-T1 mechanism for trace gases with GOCART aerosols. Thus, the model is suitable to compare simulation results to in situ and satellite measurements of O₃, NO₂, CH₄, and CO. The meteorology is captured well by the model. Comparison of simulation results with observations shows a good agreement of NO₂ and ozone, whereas CO mixing ratios are generally underestimated. This hints at missing emissions in the 2017 National Emissions Inventory (NEI) dataset. Both the heat wave and the Santa Ana winds increase the air pollution with gas-phase species in Los Angeles. In both cases, nighttime boundary layer heights are small, which causes emissions to reside near the ground. During Santa Ana winds, NOₓ removal on aerosols is reduced. Methane mixing ratios are modeled very well at most stations in Los Angeles, but predictions of low emissions near the University of California cause inaccuracies at that location. Modeled and observed PM2.5 agree well on low-pollution days, but high-pollution events are generally missed by the model. During the heat wave, both modeled and observed PM2.5 concentrations exceed the recommended NAAQS National Ambient Air Quality Standards value of 12.5 g/m³. The present modeling approach serves as a base for the study and prediction of special weather events and their impact on air pollution.

Keywords: air quality; high resolution; Los Angeles; WRF-Chem; heat wave; Santa Ana winds; Southern California

1. Introduction

The Los Angeles (LA) basin, including the megacity, is known to be a highly polluted area. The highest reading of the ozone mixing ratio since 1994 was 185 ppb in central LA, observed in September 2020 [1]. The Ozone National Ambient Air Quality Standards of 70 ppb for an eight-hour averaging time (8 h) is exceeded frequently in the LA basin. High levels of ozone may cause respiratory problems, chest pains, and inflammation of the airways and lungs, and the high levels of ozone are especially dangerous for people with lung diseases such as asthma [2].

Emission reduction policies for PM2.5, NOₓ, and VOC mixing ratios have lead to a considerably improved air quality in the LA basin. For example, NOₓ concentrations decreased by 80% from 1999 to 2019 in an ongoing linear trend [3]. Concentrations of nitrogen dioxide exceeding 0.2 ppm may cause irritations of the airways and aggravate...
respiratory diseases such as asthma, leading to coughing and wheezing [4]. Long exposure to high NO\textsubscript{2} concentrations may contribute to the development of asthma and respiratory infections. Additionally, NO\textsubscript{x} plays a major role in the formation of ozone, acid rain, and nitrite particles, which may degrade visibility as haze.

The U.S. Environmental Protection Agency (EPA) has set the annual and 24 h standards for the PM2.5 concentration to 12 µg/m\textsuperscript{3} and 35 µg/m\textsuperscript{3}, respectively. Prolonged exposure to high concentrations of fine particulate can lead to health issues such as increased hospital admissions for heart or lung causes, acute and chronic bronchitis, strokes, and increased cardiovascular mortality [5].

While NO\textsubscript{x} and VOC mixing ratios in the LA basin keep decreasing every year, pollution caused by PM2.5 [6] and ozone [3] is persistent. During the daytime, ozone is mostly produced by the NO\textsubscript{2} photolysis:

\[
\text{NO}_2 + h\nu \rightarrow O(^3\text{P}) + \text{NO} \quad (1)
\]

\[
O(^3\text{P}) + O_2 + M \rightarrow O_3 + M \quad (2)
\]

The NO\textsubscript{2} mixing ratio is strongly affected by emissions of NO and volatile organic compounds (VOCs) and can be produced by reactions of NO with HO\textsubscript{2}:

\[
\text{NO} + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH} \quad (3)
\]

or VOCs such as methyldioxyd (CH\textsubscript{3}O\textsubscript{2}) in a reaction cycle involving methane and the OH radical:

\[
\text{OH} + \text{CH}_4 \rightarrow \text{CH}_3 + \text{H}_2\text{O} \quad (4)
\]

\[
\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{O}_2 \quad (5)
\]

\[
\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{O} + \text{NO}_2 \quad (6)
\]

The methoxy radical CH\textsubscript{3}O further reacts with oxygen to form the hydroperoxy radical

\[
\text{CH}_3\text{O} + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{HO}_2 \quad (7)
\]

which can further convert NO to NO\textsubscript{2} and thus increase the ozone concentration. During nighttime, ozone is removed by depositions and by reactions with NO\textsubscript{x}:

\[
\text{O}_3 + \text{NO} \rightarrow \text{O}_2 + \text{NO}_2 \quad (8)
\]

\[
\text{O}_3 + \text{NO}_2 \rightarrow \text{O}_2 + \text{NO}_3 \quad (9)
\]

and may even be fully depleted in areas with high NO\textsubscript{x} pollution. During the daytime, NO\textsubscript{3} mixing ratios typically are low due to the rapid photolysis reactions:

\[
\text{NO}_2 + h\nu \rightarrow \text{O} + \text{NO} \quad (10)
\]

\[
\text{NO}_3 + h\nu \rightarrow \text{O} + \text{NO}_2 \quad (11)
\]

With the elevated NO\textsubscript{3} mixing ratio at nighttime, N\textsubscript{2}O\textsubscript{5} can be produced in large quantities through

\[
\text{NO}_2 + \text{NO}_3 + \text{M} \rightarrow \text{N}_2\text{O}_5 + \text{M} \quad (12)
\]

A heterogeneous sink of NO\textsubscript{x} is a reaction of N\textsubscript{2}O\textsubscript{5} with water on aerosols or other surfaces:

\[
\text{N}_2\text{O}_5(g) + \text{H}_2\text{O}(l) \rightarrow 2\text{HNO}_3(g) \quad (13)
\]

LA is also the largest emitter of carbon in the USA [7], including the toxic CO as well as greenhouse gases such as CO\textsubscript{2} and methane. Methane is a major driver to climate change, right after CO\textsubscript{2}. The Intergovernmental Panel on Climate Change (IPCC) estimates
the global warming potential of one ton of methane to be 84 and 28 times stronger than one ton of CO$_2$ over a period of 20 and 100 years, respectively [8]. Even though the methane concentration is approximately 200 times smaller than the CO$_2$ concentration, manmade methane drives 25% of global warming due to its larger global warming potential. Methane has a relatively short atmospheric lifetime of approximately 12 years, which allows mitigation efforts to have near-term climate effects. Surface and remote sensing observations of CO$_2$ and methane in LA were conducted as part of the Megacity Carbon Project and the California Methane Survey [9–15] for the years 2015 through 2018, showing that the major emitters of methane are landfills, dairies, and the oil and gas sectors.

High air pollution in the LA basin is strongly correlated to high outside temperatures [5]. On warm days with temperatures of 30 °C and higher, air quality standards are exceeded almost every day. For this reason, heat waves or other meteorological events, such as Santa Ana winds, can have profound effects on the air quality in cities. Santa Ana winds are warm, dry winds which come from the Mojave Desert and are blown over the mountains into Southern California. Santa Ana winds occur most commonly during the cold season from October through March.

Several studies have investigated air quality in Los Angeles, focusing on the historical improvements to air quality and how it can be applied to other cities [16], estimating the effect of air quality modeled with computer simulations on health [17] or case studies for particular events such as the COVID-19 crisis [18,19]. Regional air quality models are well suited to study the air pollution in the LA basin, since they allow for a high spatial resolution needed in order to model that complex terrain.

In the present study, version 4.3 of the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem) [20–22] is used to model the air quality in the LA basin during a heat wave in July 2018 and a Santa Ana winds event in October 2018. The goal is to study two different weather events with the same modeling approach to develop a general tool for the simulation and investigation of particular weather events without adjustment of the sub-models incorporated in the code. For this purpose, the open-source code WRF-Chem has been modified and improved, and the numerical simulations of the two specified events above are studied and discussed in the present investigation.

Various observations are available for the year 2018, including greenhouse gas measurements performed during the Megacity Carbon Project [9,23], TROPOspheric Monitoring Instrument (TROPOMI) observations [24,25], and in situ measurements of NO$_2$, PM2.5, O$_3$, and CO at several stations throughout Southern California [26]. The new, highly detailed MOZART-T1 chemistry mechanism [27] suited to model tropospheric air quality is used in combination with the local climate zones [28] land use categories and the BEP+BEM urban model [29,30]. The study aims to validate the complex simulation approach with novel sub-models for particularly challenging weather events and creates a base for more predictive simulations of the impact of these events on air pollution.

The next sections concern the model and the configuration before the results will be presented and compared to the observations.

2. Configuration and Methods

In this section, the configuration of WRF-Chem [20,22] and the models as well as boundary and initial conditions of the simulations are presented.

The software WRF-Chem version 4.3 is employed. WRF-Chem [20,22] is a state-of-the-art regional numerical weather prediction system with online computation of chemistry. The standard configuration is extended by the new, highly sophisticated MOZART-T1 chemistry mechanism [27] suited to model tropospheric air quality is used in combination with the local climate zones [28] land use categories and the BEP+BEM urban model [29,30]. This new combination is suitable to include the chemical reactions and land use categories to account for the complex processes occurring simultaneously. The model configuration is summarized in Table 1.
Table 1. Configuration of WRF-Chem.

| Parameter                      | Setting                                      |
|--------------------------------|----------------------------------------------|
| Longwave radiation             | LW RRTMG scheme [31]                         |
| Shortwave radiation            | SW RRTMG scheme [31]                         |
| Microphysics                   | WSM 6-class graupel scheme [32]              |
| Land-surface model             | Noah Land-Surface Model [33]                 |
| Surface-layer model            | Monin–Obukhov Similarity scheme [34]        |
| Boundary-layer model           | Bougeault and Lacarrere (BouLac) [35]        |
| Cumulus parameterization       | Not needed due to high model resolution      |
| Urban parameterization         | BEP+BEM [29,30]                              |
| Initial and boundary data      | ERA-5 [36], CAM-CHEM [37]                    |
| Sea surface temperature data   | Optimum Interpolation SST v2.1 [38]          |
| Time step                      | 15 and 5 s (domain 1 and 2)                 |
| Simulated time range           | 30 June 2018–13 July 2018                    |
| Nudging                        | 8 October 2018–22 October 2018               |
| Horizontal resolution          | 3 and 1 km (domain 1 and 2)                  |
| Longitude and latitude         | 268 × 325 horizontal grid cells (both domains) |
| Vertical grid size             | 60 levels                                    |
| Vertical size of the first cell| ≈5 m                                         |
| Pressure at top boundary       | 50 hPa                                       |
| Chemistry mechanism            | MOZART-T1 [27]                               |
| Aerosols                       | GOCART [39]                                  |
| Photolysis scheme              | Updated TUV [40]                              |
| Emissions                      | 2017 National Emissions Inventory [41]       |
| Bioemissions                   | MEGAN [42]                                   |
| Wildfire emissions             | FINN [43]                                    |

The simulation domain is centered northeast of Los Angeles using the Lambert Conformal projection with a reference latitude of 34.12°, a reference and standard longitude of −117°, and true latitudes of 33.12° and 35.12°; see Figure 1. In order to refine the grid near Los Angeles and San Diego, two domains are used with the one-way nesting method. Domain 1 with a coarser resolution of 3 km serves as the boundary conditions for domain 2 with a 1 km resolution. Both domains have 268 × 325 horizontal grid cells and thus cover an area of 804 × 975 km² and 268 × 325 km², respectively. ERA-5 [36] and CAM-CHEM [37] data serve as initial conditions for both domains and as boundary conditions for domain 1.

In the vertical direction, 60 non-equidistant grid cells with a finer resolution near the ground are used, starting with approximately 5 m at the ground level. The high resolution near the ground is needed in order to fully utilize the building effect parameterization (BEP) coupled with the building energy model (BEM) urban model [29,30]. Local climate zones (LCZ) categories [28] allow for universal representation of urban land use (LU). Urban surfaces are differentiated by ten categories, which differ in height and spacing of buildings and in surface imperviousness. The LCZ data used in the present work were created by Demuzere et al. [44], who classified the whole USA and used training data from experts for the Los Angeles basin. Figure 1b,c shows the LCZ categories, where category 11 means rocky or paved ground (LCZ E). Categories 6 (open arrangement of low-rise building) and 8 (open arrangement of large low-rise building) are dominant in LA. A few grid cells are categorized as LCZ 2 (dense mid-rise buildings). A more detailed explanation of the LCZ categories is given by Stewart and Oke [28]. For grid cells classified as LCZ A–D, F, and G (lightly wooded landscapes, heavy wooded landscapes, bushes and shrubs, grass, soil and sand, and water), and E, rocky or paved ground, the MODIS LU categories are used, which offer a more accurate representation with 15 MODIS categories as opposed to 6 LCZ categories.
Regarding chemistry, the new Model for Ozone and Related chemical Tracers (MOZART) T1 mechanism [27] with GOCART aerosols [39] is used. MOZART-T1 contains 151 gas-phase species with 65 photolysis and 287 kinetic reactions and is suited for detailed tropospheric air quality modeling. The Model of Emissions of Gases and Aerosols from Nature (MEGAN) [42], 2017 National Emissions Inventory (NEI) [41], and the 2018 Fire INventory from NCAR (FINN) [43] are used as biogenic, anthropogenic, and wildfire emissions, respectively. NEI anthropogenic emissions are produced only every three years so that the 2017 data are adapted for the year 2018 and are staggered by one day, since the weekdays shift by one within a week. The NEI 2017 and FINN emissions are year- and day-specific. Fossil fuel emissions are based on continuous emission monitoring systems. Soil–NO$_x$ emissions, even though they are biogenic, are included in the NEI 2017 emissions and thus are also year- and day-specific. The MEGAN bioemissions are not year- and day-specific; they only include monthly variations.

Meteorological time steps of 15 s and 5 s for domains 1 and 2, respectively, are chosen to fulfill the Courant criterion. Chemistry is updated between every meteorology time step, and radiative transfer is updated every tenth meteorological time step.

The time periods of 30 June 2018–13 July 2018 and 8 October 2018–22 October 2018 are simulated with WRF-Chem, which coincide with a heat wave and strong Santa Ana winds in Southern California, respectively. The first modeled five days should be seen as the model spin-up time. Meteorological nudging with a nudging timescale of one hour is active during the first week. The nudging is inactive inside the boundary layer. After the first week, nudging is turned off so that the model is freely running during the second week.

Some changes have been made to the standard WRF-Chem model and the preprocessing software. The Wesely dry deposition module [45] has been updated to support LCZ categories by classifying the LCZ categories as “urban and built-up land” in the subroutine module_dep_simple.F. The mozbc software for adapting the CAM-Chem chemistry data to WRF-Chem has been modified to support the hybrid sigma coordinate introduced in WRF V3.9, which is used in the present model. A bug occurring for high-resolution simulations with the anthropogenic emissions preprocessing software epa_anthro_emiss, provided by NCAR, caused by a wrong interpolation from the emission grid to the model grid, is corrected. Additionally, in the standard version of the code, methane emissions are not considered and the MOZART lower boundary conditions for methane are active, which causes the methane mixing ratios in the lowest grid cell to be constant and equal.
to their initial values. Therefore, in the present study, methane emissions are added and the standard MOZART lower boundary conditions for methane are turned off, so that the methane mixing ratio is freely running.

3. Results and Discussion

In this section, simulation results are presented and discussed in a comparison to observations. First, the meteorology of the heat wave in July 2018 and the Santa Ana winds in October 2018 is shown. Then, a comparison of modeled and observed O₃, CO, and NO₂ mixing ratios at several monitoring sites in the South Coast Air Quality Monitoring District [26] is presented. For comparison to in situ data, results of the high-resolution domain 2 are used. NO₂ and CO total vertical column densities (VCDs) are available from TROPOMI level 2 data, which are also compared with the simulation results. Moreover, modeled and observed methane mixing ratios and PM2.5 concentrations as part of the LA Megacity Carbon Project are presented and discussed.

3.1. Meteorology

Modeled 10 m wind speed and 2 m temperature at 3 p.m. on 5–8 July 2018 are shown in Figure 2. The hottest day is 6 July (see Figure 2b), with a temperature of more than 40 °C in Los Angeles. The temperature decreases by approximately three degrees on both of the following days. The modeled 10 m wind speed and relative humidity on 14 October, 2 p.m., 15 October, 3 a.m., 15 October, 12 a.m., and 16 October, 4 p.m. are shown in Figure 3. As can be seen, dry air from the Mojave Desert is transported from the northeast over the mountains towards Los Angeles. On October 15 and 16 (Figure 3c,d), the relative humidity is near zero over a large area, including LA. There are inaccuracies in the wind direction at southwest Los Angeles (see Figure 4), which cause slightly humid air from the ocean to be transported to LA. The daytime temperatures during the Santa Ana winds in LA are in the range of 25 to 30 °C.

Figure 2. Modeled 10 m wind speed and 2 m temperature on 5 July, 3 p.m. (a), 6 July, 3 p.m. (b), 7 July, 3 p.m. (c), and 8 July, 3 p.m. (d).
3.2. Comparison of Simulated $O_3$, CO, and NO$_2$ Mixing Ratios with Observations

In this section, modeled NO$_2$, $O_3$, and CO mixing ratios are compared to observations from monitoring sites in the South Coast Air Quality Monitoring District [26]. NO$_2$ is measured with the chemiluminescence method at all stations discussed in this work. An overview of the stations and sites is given in Table 2, and the locations of the stations is shown in Figure 5. Mean bias, RMSE, and the correlation coefficient of observed and simulated mixing ratios are shown in Tables 3 and 4 for 30 June–13 July and 8–22 October 2018, respectively. Figure 6 shows a comparison of the modeled mixing ratios as well as 2 m temperature at the nearest grid cell in comparison to data from the station at LA North Main Street from 30 June–13 July 2018. The night before the hottest day (6 July), the NO$_2$ and CO mixing ratios have very large maximum values, which is likely caused by the low nocturnal boundary layer height of tens of meters. Both the NO$_2$ mixing ratio and the ozone maximum on the following day are somewhat underestimated. On 9–11 July, observed nighttime ozone levels are near zero whereas simulated ozone levels are between 20 ppb and 40 ppb. The simulated nighttime boundary layer height is several hundred meters, whereas the real height is probably tens of meters, as suggested by the lower nocturnal observed temperature and large mixing ratios of observed NO$_2$ and CO. The discrepancies are most likely due to the generally overestimated 2 m temperature. Otherwise, simulation
and observations agree very well, as shown by the correlations of around 0.7. Due to the high nocturnal temperature, the mixing ratios of NO$_3$ and N$_2$O$_5$ are small during the night, resulting in a fast decay of N$_2$O$_5$ through the reaction N$_2$O$_5$ + M $\rightarrow$ NO$_2$ + NO$_3$ + M, and the NO concentration is high, resulting in a fast reaction NO + NO$_3$ $\rightarrow$ 2 NO$_2$.

### Table 2. Overview of the stations used for the comparison of model results and observations.

| County     | Station Number | Station Name          |
|------------|----------------|-----------------------|
| Los Angeles| 0002           | Azusa                 |
| Los Angeles| 1103           | North Main Street     |
| Los Angeles| 1201           | Reseda                |
| Los Angeles| 1302           | Compton               |
| Los Angeles| 6012           | Santa Clarita         |
| San Diego  | 1008           | Camp Pendleton        |
| San Diego  | 1014           | Donovan               |
| San Diego  | 1016           | Kearny Villa Road     |
| San Diego  | 1022           | Lexington Elementary School |

### Table 3. Statistics of observed and simulated concentrations of O$_3$, NO$_2$, and CO from 30 June–13 July 2018.

| Station                   | Species | Correlation R | Mean Bias | RMSE   |
|---------------------------|---------|---------------|-----------|--------|
| LA Azusa                  | O$_3$   | 0.85          | 0.0047 ppm | 0.014 ppm |
| LA Azusa                  | NO$_2$  | 0.62          | –5.2 ppb  | 7.4 ppb |
| LA Azusa                  | CO      | 0.60          | –0.11 ppm | 0.16 ppm |
| LA North Main Street      | O$_3$   | 0.77          | 0.0024 ppm | 0.012 ppm |
| LA North Main Street      | NO$_2$  | 0.65          | –0.27 ppb | 7.3 ppb |
| LA North Main Street      | CO      | 0.76          | –0.022 ppm| 0.11 ppm |
| LA Reseda                 | O$_3$   | 0.8           | 0.00049 ppm| 0.012 ppm |
| LA Reseda                 | NO$_2$  | 0.63          | –1.9 ppb  | 5.0 ppb |
| LA Reseda                 | CO      | 0.45          | 0.024 ppm | 0.13 ppm |
| LA Compton                | O$_3$   | 0.6           | 0.0068 ppm | 0.013 ppm |
| LA Compton                | NO$_2$  | 0.64          | 0.080 ppb | 4.5 ppb |
| LA Compton                | CO      | 0.63          | –0.026 ppm| 0.10 ppm |
| SD Donovan                | O$_3$   | 0.74          | –0.0074 ppm| 0.013 ppm |
| SD Donovan                | NO$_2$  | 0.35          | 13 ppb    | 16 ppb |
| SD Kearny Villa Road      | O$_3$   | 0.68          | 0.0035 ppm | 0.012 ppm |
| SD Kearny Villa Road      | NO$_2$  | 0.37          | –0.057 ppb| 4.9 ppb |
| SD Lexington Elementary School | O$_3$  | 0.79          | 0.0023 ppm | 0.011 ppm |
| SD Lexington Elementary School | NO$_2$ | 0.56          | 1.3 ppb   | 3.7 ppb |
| SD Lexington Elementary School | CO   | 0.71          | –0.076 ppm | 0.10 ppm |

Figure 7 displays mixing ratios of ozone, NO$_2$, and CO for three stations in LA, i.e., Azusa (Station 0002), Reseda (Station 1201), and Compton (Station 1302) during early July 2018. At Azusa (Figure 7a–c), modeled and observed ozone mixing ratios agree well (correlation R = 0.85). There are several days, for example 4 and 6 July, for which NO$_2$ mixing ratios are underestimated by the model, so that the nighttime ozone depletion is not found. CO is below the detection limit of 0.2 ppm for many days. The model does generally underpredict CO mixing ratios at Azusa. At Reseda (Figure 7d–f), again, model and observations generally agree very well for both ozone (R = 0.80) and NO$_2$ (R = 0.63). NO$_3$, however, is underestimated by the model from 7–9 July. CO is overestimated by the model the first days of July and underestimated for 7 and 9 July, but agrees well with the observations on the other days. At Compton (Figure 7g–i), the nighttime ozone depletion occurs more often than for the other stations and is underestimated for the days after 7 July, even though NO$_2$ is underestimated for only three days by the model. Modeled and observed CO agree very well (R = 0.63), with the exception of 9 July.
Figure 5. Map of the location of the stations for domain 2.

Figure 6. Comparison of in situ measurements with modeled variables at the ground at LA North Main Street in July 2018. No measurements for NO and the planetary boundary layer height are available.

Figure 8 shows mixing ratios of ozone and NO\textsubscript{2} as well as 2 m temperature at two stations in San Diego, i.e., Donovan (Station 1014) and Kearny Villa Road (Station 1106), during early July 2018. At station Donovan in San Diego (Figure 8a–c), which is very close to the Mexican border, the model strongly overrepresents NO\textsubscript{2}, with a mean bias of 13 ppb, which also leads to an underestimation of nighttime ozone. The model overestimates NO\textsubscript{2} emissions coming from Tijuana. At Kearny Villa Road (Figure 8d–f), NO\textsubscript{2} is overestimated by the model in the first week of July and underestimated thereafter, resulting in a small mean bias of 1.3 ppb, most likely again due to errors in the emission dataset. Ozone generally agrees well with the observations (R = 0.68).
Figure 7. Comparison of in situ measurements with modeled ozone, NO$_2$, and CO at the ground at Los Angeles, i.e., Azusa (a–c), Reseda (d–f), and Compton (g–i) in early July 2018.

Figure 9 shows a comparison of modeled NO$_2$, O$_3$, and CO mixing ratios as well as relative humidity at 2 m at the nearest grid cell in comparison to data from the station at LA North Main Street from 8–22 October 2018. As can be seen, modeled and observed NO$_2$ mixing ratios agree very well (R = 0.76). Beginning with the Santa Ana winds on 15 October, NO$_2$ mixing ratios increase strongly. The nocturnal PBL height is near zero after 15 October, so that nighttime emissions of NO$_x$ stay close to the ground, increasing the mixing ratios. Additionally, due to the low humidity, the heterogeneous loss of N$_2$O$_5$ (see reaction (13)) is slowed down. The rate of reaction (13) of the MOZART-T1 mechanism increases with larger relative humidity, with increases of approximately 96% and 380% for RH of 50% and 100% in comparison to the rate at 0% RH. As a consequence, the mixing ratio of N$_2$O$_5$ is much larger on October 16 in comparison to the other days.

Figure 10 shows mixing ratios of ozone, NO$_2$, and CO for three stations in LA, i.e., Azusa (Station 0002), Reseda (Station 1201), and Compton (Station 1302), and two stations in San Diego, i.e., Donovan (Station 1014) and Kearny Villa Road (Station 1106), from 8–22 October 2018. During October, NO$_2$ mixing ratios are more frequently underestimated by the model in comparison with early July, which is also reflected in the underestimation of nighttime ozone depletion by the model. CO is also underestimated, so that the explanation might be of meteorological nature, most likely an overestimation of the vertical mixing
by the model. At Reseda (Figure 10d–f), modeled and observed NO₂ agree well (R = 0.61), albeit with underestimations of NO₂ for a few days. Air pollution at Compton (Figure 10g–i) is underestimated during October, with a mean bias of −6.9 ppb and −0.33 ppm for NO₂ and CO, respectively. Nighttime boundary layer heights are relatively large during these overestimations, around 200 m instead of near zero heights, which is likely the reason for the underestimation. The overestimation of the boundary layer may in turn be caused by an overestimation of the nighttime temperature. It might be worthwhile to optimize the simulation of the boundary layer in future studies.

Figure 8. Comparison of in situ measurements with modeled ozone, NO₂, and T₂ at the ground at San Diego, i.e., Donovan (a–c) and Kearny Villa Road (d–f) in early July 2018.

Figure 11 shows a comparison of modeled NO₂, O₃, and CO mixing ratios as well as relative humidity at 2 m at the nearest grid cell in comparison to data from the station at San Diego, El Cajon, Lexington Elementary School from 8–22 October 2018. Nighttime NO₂ is underestimated on several days, resulting in an overestimation of ozone. During these days, air is coming from the south, which implies that the emission data for Tijuana, Mexico are incomplete. CO is also likely to be underestimated during these days for the same reason. The effects of the Santa Ana winds are also apparent at San Diego but are overrepresented in the simulation.

Figure 12 displays mixing ratios of ozone and NO₂ as well as 2 m temperature at two stations in San Diego, i.e., Donovan (Station 1014) and Kearny Villa Road (Station 1106) from 8–22 October 2018. At station Donovan in San Diego (Figure 12a–c) NO₂ is overrepresented during 8–15 October, with the agreement to observations improving for 16–22 October, resulting in a relatively low overall correlation of 0.4. The NEI 2017 emissions inventory for Mexico is based on the projected 2016 Mexico inventories provided by SEMARNAT with a monthly to annual time resolution, depending on the source of the emission, which may explain the discrepancies. Modeled and observed ozone mixing ratios agree moderately well for most of the modeled time ranges (R = 0.55). At Kearny Villa Road (Figure 12d–f), again there is a mix of over- and underestimations of the NO₂ mixing ratio and, consequently, nighttime ozone by the model, so that the correlations are approximately 0.5 for both species.
Table 4. Statistics of observed and simulated concentrations of O$_3$, NO$_2$, and CO from 8–22 October 2018.

| Station                      | Species | Correlation R | Mean Bias  | RMSE   |
|------------------------------|---------|---------------|------------|--------|
| LA Azusa                    | O$_3$   | 0.61          | 0.0061 ppm | 0.012 ppm |
| LA Azusa                    | NO$_2$  | 0.40          | −3.7 ppb   | 7.1 ppb |
| LA Azusa                    | CO      | 0.26          | −0.10 ppm  | 0.14 ppb |
| LA North Main Street        | O$_3$   | 0.71          | 0.0051 ppm | 0.013 ppm |
| LA North Main Street        | NO$_2$  | 0.76          | 2.0 ppb    | 8.8 ppb |
| LA North Main Street        | CO      | 0.59          | −0.091 ppm | 0.22 ppm |
| LA Reseda                   | O$_3$   | 0.75          | 0.0040 ppm | 0.012 ppm |
| LA Reseda                   | NO$_2$  | 0.61          | −2.0 ppb   | 7.8 ppb |
| LA Reseda                   | CO      | 0.54          | −0.026 ppm | 0.18 ppm |
| LA Compton                  | O$_3$   | 0.56          | 0.016 ppm  | 0.021 ppm |
| LA Compton                  | NO$_2$  | 0.55          | −6.9 ppb   | 12 ppb   |
| LA Compton                  | CO      | 0.31          | −0.33 ppm  | 0.59 ppm |
| SD Donovan                  | O$_3$   | 0.55          | −0.0043 ppm| 0.014 ppm |
| SD Donovan                  | NO$_2$  | 0.40          | 12 ppb     | 18 ppb   |
| SD Kearny Villa Road        | O$_3$   | 0.54          | 0.0079 ppm | 0.015 ppm |
| SD Kearny Villa Road        | NO$_2$  | 0.50          | −2.5 ppb   | 7.7 ppb  |
| SD Lexington Elementary School | O$_3$   | 0.037         | 0.0095 ppm | 0.015 ppm |
| SD Lexington Elementary School | NO$_2$  | 0.63          | −3.3 ppb   | 7.2 ppb  |
| SD Lexington Elementary School | CO      | 0.75          | −0.10 ppm  | 0.14 ppm |

Figure 9. Comparison of in situ measurements with modeled variables at the ground at LA North Main Street in October 2018. No measurements for N$_2$O$_5$ and the planetary boundary layer height are available.
CO is generally underestimated throughout the simulation domain, as can be seen by the negative mean bias at all stations. The main source of CO is direct emissions, so that an underprediction of the CO emissions by the model is the most likely cause of the inaccuracies. Meteorological inaccuracies such as a too-high boundary layer height or inaccurate wind directions cannot be ruled out. Emmons et al. [27] found, in their evaluation of the CAM-Chem model, which provides the initial and boundary conditions for this study, a strong low bias of approximately 40% for CO in the Northern Hemisphere, which may also contribute to low bias of CO found in the present study. However, the observed NO$_2$ mixing ratios generally agree well with the simulated results, so that meteorological inaccuracies are not likely the only reason for the underestimation of CO.
Figure 11. Comparison of in situ measurements with modeled variables at the ground at San Diego, El Cajon, Lexington Elementary School in October 2018. No measurements for the planetary boundary layer height are available.

Figure 12. Comparison of in situ measurements with modeled ozone and NO\textsubscript{2} as well as 2 m temperature at the ground at San Diego, i.e., Donovan (a–c) and Kearny Villa Road (d–f) in October 2018.

3.3. Comparison of Simulations and TROPOMI VCDs

Modeled total vertical column densities (VCDs) are calculated by vertically integrating from the ground to the top of the simulation domain at an altitude of 20 km, tropospheric
VCDs by integration from the ground to 10 km. Comparing the simulation results to the TROPOMI data (see Figure 13), some differences are obvious. Modeled tropospheric NO$_2$ VCDs at large cities such as Los Angeles, Las Vegas, and Tijuana are much larger in comparison to the observations. This is in contrast to the ground-level NO$_2$ mixing ratio, for which model and observations typically agree very well with underestimations by the model on a few days. The model might overestimate both the strength of the emissions and the vertical mixing, so that NO$_2$ mixing ratios outside of the lowest grid cell are larger. A large NO$_2$ VCD in Baja California, Mexico is found by both the model and the satellite. The modeled VCD is transported over a smaller range in comparison to the observation, which may mean that NO$_2$ sinks in the model are overestimated. A large source of NO$_2$ in the north of the model domain, near Lone Pine, is not at all present in the observations. The source of the emissions is the FINN wildfire data. The Georges Fire was reported on 8 July, three days after the date in the figure, and lasted approximately 10 days. The fire in the FINN data apparently starts approximately a week early, which is the cause of the error. For CO, large total VCDs are also found in Baja California, Mexico. Similar to NO$_2$, the modeled VCDs are only large close to the emission site, which is inconsistent with the observations. Due to the long lifetime of CO of approximately a hundred days, the discrepancy of the observations and the model may be of meteorological nature, such as an overestimation of the diffusion. Trends of CO, such as smaller CO VCDs over mountains, are visible in both the model and the observations, but they are stronger in the observations.

Figure 13. Observed (a) and modeled (b) NO$_2$ VCD on 5 July 2018 (8 p.m.). Observed (c) and modeled (d) CO VCD on 6 July 2018 (9 p.m.).

### 3.4. Comparison of Modeled and Observed Methane Mixing Ratios

The comparison of observed [9,23] and modeled methane mixing ratios is shown in Figure 14 during early July 2018. Table 5 shows the statistics of observed and simulated concentrations. Results at CaNoga Park (CNP), FULlerton (FUL), and University of Southern California (USC) in Los Angeles are shown. For several days, there are substantial deviations from the typical CH$_4$ mixing ratio of 1.9 to 2 ppm in both the model and the measurements. At CNP and FUL (Figure 14a,b), the high-methane episodes are mostly well represented by the model, with correlations of more than 0.81 and small mean biases and relatively small RMSE, but are underestimated on multiple days, including 7 and 8 July. The high-methane episodes occur with the onset of the heat wave and during the nighttime with very small boundary layer heights, consistent with the high NO$_2$ and CO episodes. The observations sites for methane are at large heights (e.g., 260 m for CNP), but still the low nighttime vertical mixing confines the emissions to a smaller space, enhancing the methane concentration. At USC, the high-methane episodes are mostly missed by the model, as shown by the relatively negative mean bias of −75 ppb. The model does show
higher methane concentrations on 7 July, but still underrepresents them. The EPA methane emissions at and near USC are relatively low, approximately three to five times lower than the emissions near CNP and FUL; therefore, it is likely that methane sources near USC are misrepresented by the model.

Table 5. Statistics of observed and simulated methane concentrations from 30 June–13 July 2018.

| Station | Correlation R | Mean Bias | RMSE  |
|---------|---------------|-----------|-------|
| CNP     | 0.62          | 3.3 ppb   | 70 ppb|
| FUL     | 0.81          | 2.3 ppb   | 63 ppb|
| USC     | 0.76          | −75 ppb   | 129 ppb|

Figure 14. Modeled and observed CH$_4$ mixing ratio at Canoga Park (a), Fullerton (b), and University of South California (c) in Los Angeles, in early July 2018.

3.5. Comparison of Simulated and Observed PM2.5 Concentrations

PM2.5 concentrations at six stations in the Los Angeles and San Diego counties are shown in Figures 15 and 16 during July and October, respectively. Modeled dust aerosols are not considered in the modeled PM2.5 concentration, since the GOCART module overestimates dust aerosol production in the San Diego and Tijuana regions. In the model, dust aerosols are advected to LA on 7 and 11 July, and 13 and 16 October, and lead to concentrations of more than 100 µg/m$^3$ not seen in the observations, and, therefore, the dust aerosols are neglected in the simulations. Low-pollution episodes agree well with the model; however, high-pollution episodes, such as on 5 July in the LA region, are generally not represented by the model. The heat wave leads to a clear increase in both modeled and observed PM2.5 concentrations over the recommended National Ambient Air Quality Standards value of 12.5 µg/m$^3$, which confirms the results of Nussbaumer and Cohen [6], who found a positive correlation of particulate mass with temperature, which is mostly associated with an increase in the number density of organic aerosols. The beginning of the Santa Ana winds on 16 October reduces the PM2.5 concentrations for most stations. PM2.5 concentrations generally increase with lower humidity due to slower losses due to deposition, so this is behavior is unusual. The smaller concentration might be due to fast losses of PM2.5 due to advection caused by the large Santa Ana wind speeds or due to the low humidity reducing condensation of water vapor onto the particles.
Figure 15. Comparison of in situ measurements with modeled PM2.5 at the ground at Los Angeles North Main Street (a), Reseda (b), Santa Clarita (c), Camp Pendleton (d), Donovan (e), and El Cajon, Lexington Elementary School (f) in July 2018.

Figure 16. Comparison of in situ measurements with modeled PM2.5 at the ground at Los Angeles North Main Street (a), Reseda (b), Santa Clarita (c), Camp Pendleton (d), Donovan (e), and El Cajon, Lexington Elementary School (f) in October 2018.
4. Summary and Conclusions

The air quality in the LA basin was simulated with a modified version of WRF-Chem V4.3 during 30 June–13 July 2018 and 8–22 October 2018. A heat wave occurred on around July 6, and Santa Ana winds prevailed on October 15 and 16. Modeled O$_3$, NO$_2$, and CO mixing ratios, as well as PM2.5 concentrations, were compared to in situ measurements. A high-resolution simulation, 1 km in the horizontal and 5 m at lowest level in the vertical direction, together with the 2017 NEI Data emission inventory, LCZ land use categories, and the BEP+BEM model, as well as the implementation of methane as a free-running species, allow for a state-of-the-art simulation of the meteorology and chemistry occurring in the LA basin. The agreement of observed and modeled NO$_2$, O$_3$, and CH$_4$ mixing ratios is generally good. High-pollution episodes coincide with low nocturnal boundary layer heights. The model underestimates NO$_2$ mixing ratios on several days for most stations, which may be correlated to an overestimation of vertical mixing. This, in turn, also causes errors in the simulation of ozone, since ozone depletes due to high nocturnal NO$_2$, which occurs less frequently in the model. The NO$_2$ mixing ratio is generally higher after the heat wave and when Santa Ana winds begin.

The CO mixing ratio is generally underestimated by the model, which might be due to inaccuracies in the emission dataset. At San Diego, NO$_2$ is generally overestimated by the model, especially at Donovan near the Mexican border. The emission dataset is likely to overestimate the emissions coming from Tijuana, Mexico. Episodes with low PM2.5 are captured well by the model; however, high PM2.5 events are strongly underestimated. The heat wave leads to a clear increase in PM2.5 concentrations. PM2.5 concentrations are lowered during the Santa Ana winds event.

There are significant deviations of from the typical CH$_4$ mixing ratio of 1.9 to 2 ppm in both the model and the observations. The methane mixing ratio is modeled very well at Fullerton and Canoga Park, but high-methane events at the University of California are not found by the model. The methane mixing ratio is 3–5 times lower at USC than for the other two mentioned locations, which hints to a possible incompleteness of the emission dataset. NO$_2$ and CO VCDs are transported over smaller distances by the model, likely due to an overestimation of transport-based sinks in the case of NO$_2$. NO$_2$ VCDs over cities are larger in the model than in the observations. Model discrepancies are mostly due to inaccuracies in the emission dataset and the boundary layer model, which should be improved in future investigations. Overall, both the heat wave and Santa Ana winds had negative effects on the air quality with the exception of lower PM2.5 concentrations during the Santa Ana winds. Thus, the present model is suitable to provide valuable insight into the influence of special weather conditions on the air quality.

In a future study, it is worthwhile to improve the model of the planetary boundary layer, since in the present study, high-pollution episodes are highly correlated with small nocturnal boundary layer heights. In particular, a parameter study of the planetary boundary layer model with LCZ land use categories and the urban model BEP+BEM could improve future air quality modeling.

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References

1. South Coast Air Quality Management District Ozone Season and Wildfire Impacts. 2020. Available online: http://www.aqmd.gov/docs/default-source/Agendas/Governing-Board/2020/2020-nov-025.pdf?sfvrsn=2 (accessed on 21 February 2022).
2. Nuvolone, D.; Petri, D.; Voller, F. The effects of ozone on human health. Environ. Sci. Pollut. Res. 2018, 25, 8074–8088. [CrossRef]
3. Nussbaumer, C.M.; Cohen, R.C. The Role of Temperature and NOx in Ozone Trends in the Los Angeles Basin. Environ. Sci. Technol. 2020, 54, 15652–15659. [CrossRef]
4. Hesterberg, T.W.; Bunn, W.B.; McClellan, R.O.; Hamade, A.K.; Long, C.M.; Valberg, P.A. Critical review of the human data on short-term nitrogen dioxide (NO2) exposures: Evidence for NO2 no-effect levels. Crit. Rev. Toxicol. 2009, 39, 743–781. [CrossRef]
5. Pope, C.A., III; Dockery, D.W. Health effects of fine particulate air pollution: lines that connect. J. Air Waste Manag. Assoc. 2006, 56, 709–742. [CrossRef]
6. Nussbaumer, C.M.; Cohen, R.C. Impact of OA on the Temperature Dependence of PM2.5 in the Los Angeles Basin. Environ. Sci. Technol. 2021, 55, 3549–3558. [CrossRef]
7. Moran, D.; Kanemoto, K.; Jiborn, M.; Wood, R.; Többen, J.; Seto, K.C. Carbon footprints of 13,000 cities. Environ. Res. Lett. 2018, 13, 064041. [CrossRef]
8. Pachauri, R.K.; Allen, M.R.; Barros, V.R.; Broome, J.; Cramer, W.; Christ, R.; Church, J.A.; Clarke, L.; Dahe, Q.; Dasgupta, P.; et al. Climate Change 2014: Synthesis Report. Contribution of Working Groups I, II and III to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change; IPCC: Geneva, Switzerland, 2014.
9. Verhulst, K.; Karion, A.; Kim, J.; Salameh, P.; Sloop, C.; Keeling, R.; Weiss, R.; Duren, R.; Miller, J. In Situ Carbon Dioxide and Methane Measurements from the Los Angeles Megacity Carbon Project. Atmos. Chem. Phys. 2017, 17, 8313–8341. [CrossRef]
10. Hedelius, J.K.; Feng, S.; Roehl, C.M.; Wunch, D.; Hillyard, P.W.; Podolske, J.R.; Iraci, L.T.; Patarasuk, R.; Rao, P.; O’Keeffe, D.; et al. Emissions and topographic effects on column CO2 (XCO2) variations, with a focus on the Southern California Megacity. J. Geophys. Res. Atmos. 2017, 122, 7200–7215. [CrossRef]
11. Miller, J.B.; Lehman, S.J.; Verhulst, K.R.; Miller, C.E.; Duren, R.M.; Yadav, V.; Newman, S.; Sloop, C.D. Large and seasonally varying biospheric CO2 fluxes in the Los Angeles megacity revealed by atmospheric radiocarbon. Proc. Natl. Acad. Sci. USA 2020, 117, 26681–26687. [CrossRef]
12. Duren, R.M.; Thorpe, A.K.; Foster, K.T.; Rafiq, T.; Hopkins, F.M.; Yadav, V.; Bue, B.D.; Thompson, D.R.; Conley, S.; Colombi, N.K.; et al. California’s methane super- emitters. Nature 2019, 575, 180–184. [CrossRef]
13. Yadav, V.; Duren, R.; Mueller, K.; Verhulst, K.R.; Nehrkorn, T.; Kim, J.; Weiss, R.F.; Keeling, R.; Sander, S.; Fischer, M.L.; et al. Spatio-temporally Resolved Methane Fluxes From the Los Angeles Megacity. J. Geophys. Res. Atmos. 2019, 124, 5131–5148. [CrossRef]
14. Wäke, J.; Kort, E.A.; Duren, R.; Mueller, K.L.; Verhulst, K.; Yadav, V. Detecting Urban Emissions Changes and Events With a Near-Real-Time- Capable Inversion System. J. Geophys. Res. Atmos. 2019, 124, 5117–5130. [CrossRef]
15. Zeng, Z.C.; Wang, Y.; Pongetti, T.J.; Gong, F.Y.; Newman, S.; Li, Y.; Natraj, V.; Shia, R.L.; Yung, Y.L.; Sander, S.P. Tracking the atmospheric pulse of a North American megacity from a mountaintop remote sensing observatory. Remote Sens. Environ. 2020, 248, 112000. [CrossRef]
16. Parrish, D.D.; Xu, J.; Croes, B.; Shao, M. Air quality improvement in Los Angeles—Perspectives for developing cities. Front. Environ. Sci. Eng. 2016, 10, 11. [CrossRef]
17. Stewart, D.R.; Saunders, E.; Pereira, R.A.; Fitzgerald, R.; Campbell, D.E.; Stockwell, W.R. Linking air quality and human health effects models: An application to the Los Angeles air basin. Environ. Health Insights 2017, 11, 1178630217737551. [CrossRef]
18. Connerton, P.; Vicente de Assunção, J.; Maura de Miranda, R.; Dorothee Slovic, A.; José Pérez-Martínez, P.; Ribeiro, H. Air Quality during COVID-19 in Four Megacities: Lessons and Challenges for Public Health. Int. J. Environ. Res. Public Health 2020, 17, 5067. [CrossRef]
19. Pan, S.; Jung, J.; Li, Z.; Hou, X.; Roy, A.; Choi, Y.; Gao, H.O. Air Quality Implications of COVID-19 in California. Sustainability 2020, 12, 7067. [CrossRef]
20. Grell, G.A.; Peckham, S.E.; Schmitz, R.; McKeen, S.A.; Frost, G.; Skamarock, W.C.; Eder, B. Fully coupled “online” chemistry within the WRF model. *Atmos. Environ.* 2005, 39, 6957–6975. [CrossRef]

21. Fast, J.D.; Gustafsson, W.I.; Jr; Easter, R.C.; Zaveri, R.A.; Barnard, J.C.; Chapman, E.G.; Grell, G.A.; Peckham, S.E. Evolution of ozone, particulates, and aerosol direct radiative forcing in the vicinity of Houston using a fully coupled meteorology-chemistry-aerosol model. *J. Geophys. Res.* 2006, 111. [CrossRef]

22. Skamarock, W.C.; Klemp, J.B.; Dudhia, J.; Gill, D.O.; Barker, D.M.; Wang, W.; Powers, J.G. A Description of the Advanced Research WRF Version 3. NCAR Technical Note N-475+ STR; 2008; Available online: https://opensys.ucar.edu/islandora/object/technotes:500 (accessed on 18 January 2022).

23. Kim, J.; Verhulst, K.; Lukee, T.; Salameh, P.; Cox, A.; Walker, S.; Paplawsky, B.; Prinzivalli, S.; Fain, C.; Stock, M.; et al. *In Situ Carbon Dioxide, Methane, and Carbon Monoxide Mole Fractions from the Los Angeles Megacity Carbon Project*; Technical Report; National Institute of Standards and Technology: Gaithersburg, MD, USA, 2021. [CrossRef]

24. ESA; CSP. TROPOMI Level 2 Carbon Monoxide Total Column Products; Technical Report; European Space Agency: Paris, France, 2021. [CrossRef]

25. ESA; CSP. TROPOMI Level 2 Nitrogen Dioxide Tropospheric Column Products; Technical Report; European Space Agency: Paris, France, 2021. [CrossRef]

26. EPA. Pre-Generated Data Files. 2022. Available online: https://aqs.epa.gov/airnow/download_files.html (accessed on 18 January 2022).

27. Emmons, L.K.; Schwantes, R.H.; Orlando, J.J.; Tyndall, G.; Kinnison, D.; Lamarque, J.F.; Marsh, D.; Mills, M.J.; Tilmes, S.; Bardeen, C.; et al. The Chemistry Mechanism in the Community Earth System Model Version 2 (CESM2). *J. Adv. Model. Earth Syst.* 2020, 12, e2019MS001882. [CrossRef]

28. Stewart, I.D.; Oke, T.R. Local Climate Zones for Urban Temperature Studies. *Bull. Am. Meteorol. Soc.* 2012, 93, 1879–1900. [CrossRef]

29. Martilli, A.; Clappier, A.; Rotach, M.W. An urban surface exchange parameterisation for mesoscale models. *Bound.-Layer Meteorol.* 2002, 104, 261–304. [CrossRef]

30. Salamanca, F.; Martilli, A. A new Building Energy Model coupled with an Urban Canopy Parameterization for urban climate simulations-part II. Validation with one dimension off-line simulations. *Theoretical Appl. Climatol.* 2010, 99, 345–356. [CrossRef]

31. Iacono, M.J.; Delamere, J.S.; Mlawer, E.J.; Shephard, M.W.; Clough, S.A.; Collins, W.D. Radiative forcing by long-lived greenhouse gases: Calculations with the AER radiative transfer models. *J. Geophys. Res. Atmos.* 2008, 113. [CrossRef]

32. Hong, S.Y.; Lim, J.O.J. The WRF single-moment 6-class microphysics scheme (WSM6). *Asia-Pac. J. Atmos. Sci.* 2006, 42, 129–151.

33. Niu, G.Y.; Yang, Z.L.; Mitchell, K.E.; Chen, F.; Ek, M.B.; Barlage, M.; Kumar, A.; Manning, K.; Niyogi, D.; Rosero, E.; et al. The community Noah land surface model with multipparameterization options (Noah-MP): 1. Model description and evaluation with local-scale measurements. *J. Geophys. Res. Atmos.* 2011, 116. [CrossRef]

34. Janjić, Z. The surface layer in the NCEP Eta Model. In Proceedings of the Eleventh Conference on Numerical Weather Prediction, Norfolk, VA, USA, 19–23 August 1996; pp. 19–23.

35. Bougeault, P.; Lacarrere, P. Parameterization of orography-induced turbulence in a meso-beta—Scale model. *Mon. Weather Rev.* 1989, 117, 1872–1890. [CrossRef]

36. Hersbach, H.; Bell, B.; Berrisford, P.; Hirahara, S.; Horányi, A.; Muñoz-Sabater, J.; Nicolas, J.; Peubey, C.; Radu, R.; Schepers, D. The ERA5 global reanalysis. Q. J. R. Meteorol. Soc. 2020, 146, 1999–2049. [CrossRef]

37. Buchholz, R.R.; Emmons, L.K.; Tilmes, S.; TCD Team. CAM-Chem Output for Boundary Conditions. Technical Report. UCAR/NCAR Lat: 0 to 90. Lon: 0 to 360, February–May 2019. 2021. Available online: https://wiki.ucar.edu/pages/viewpage.action?pageId=372834733 (accessed on 18 January 2022).

38. Huang, B.; Liu, C.; Banzon, V.; Freeman, E.; Graham, G.; Hankins, B.; Smith, T.; Zhang, H.M. Improvements of the Daily Optimum Interpolation Sea Surface Temperature (DOISST) Version 2.1. *J. Clim.* 2021, 34, 2923–2939. [CrossRef]

39. Chin, M.; Ginoux, P.; Kinne, S.; Torres, O.; Holben, B.N.; Duncan, B.N.; Martin, R.V.; Logan, J.A.; Higurashi, A.; Nakajima, T. Tropospheric aerosol optical thickness from the GOCART model and its comparison with satellite and Sun photometer measurements. *J. Atmos. Sci.* 2002, 59, 461–483. [CrossRef]

40. Madronich, S.; Flocke, S.; Zeng, J.; Petropavlovskikh, I.; Lee-Taylor, J. Tropospheric Ultraviolet-Visible Model (TUV) version 4.1. *Nat. Cent. Atmos. Res. 2002.* 3000.

41. Janssens-Maenhout, G.; Dentener, F.; Van Aardenne, J.; Monni, S.; Pagliari, V.; Orlandini, L.; Klimont, Z.; Kurokawa, J.i.; Akimoto, H.; Ohara, T.; et al. EDGAR-HTAP: A Harmonized Gridded Air Pollution Emission Dataset Based on National Inventories; JRC68434, EUR Report No EUR; European Commission Publications Office: Ispra, Italy, 2012; Volume 25, 625–641. [CrossRef]
44. Demuzere, M.; Hankey, S.; Mills, G.; Zhang, W.; Lu, T.; Bechtel, B. Combining expert and crowd-sourced training data to map urban form and functions for the continental US. *Sci. Data* **2020**, *7*, 264. [CrossRef]

45. Wesely, M. Parameterization of surface resistances to gaseous dry deposition in regional-scale numerical models. *Atmos. Environ. (1967)* **1989**, *23*, 1293–1304. [CrossRef]