Review

Journal of the Brazilian Chemical Society

https://dx.doi.org/10.21577/0103-5053.20240042

J. Braz. Chem. Soc. **2024**, *35*, 9, e-20240042, 1-19

A Systematic Review of Tropospheric Ozone Modeling Using Community Multiscale Air Quality Model (CMAQ)

Thiago F. da Costa, [a] *Josie B. B. Carvalho,* [a] *Rizzieri Pedruzzi,* [a] *Taciana T. A. Albuquerque* [b,c] *and Eduardo M. Martins* [a]

[a]*Departamento de Engenharia Ambiental e Sanitária, Universidade do Estado do Rio de Janeiro, 20950-000 Rio de Janeiro-RJ, Brazil*

[b]*Departamento de Engenharia Ambiental e Sanitária, Universidade Federal de Minas Gerais, 31270-901 Belo Horizonte-MG, Brazil*

[c]*Programa de Pós-Graduação em Engenharia Ambiental, Universidade Federal do Espírito Santo, 29075-710 Vitória-ES, Brazil*

Ozone (O_3) is a secondary pollutant, and modeling studies used to assess its behavior play a role in facilitating regulatory and decision-making processes in public policies. Thus, the Community Multiscale Air Quality (CMAQ), a chemical transport model, was specifically designed to simulate and forecast O_3 concentrations. This critical review includes publications between 2016 and 2023 showing the most used configurations. The research was carried out in the Scopus and Web of Science databases, and the articles were filtered using determined criteria. With this, it was observed that the most used model arrangements are Weather Research and Forecasting as a meteorological model, carbon bond 2005 as the chemical mechanism, 36 × 36 km with 35 vertical layers as grid resolution, CMAQ standard profiles as a boundary condition, Multi-resolution Emission Inventory for China, due to the high number of publications by Chinese researchers, and Model of Emissions of Gases and Aerosols from Nature as inventory and processor of biogenic emissions, respectively. It is concluded that this arrangement of configurations is the most widespread in the literature but shows that nowadays the publications predominantly lie over China and with greater prominence of this country in studies of influence on ozone simulation.

Keywords: CMAQ, review, state-of-art, secondary pollutants

1. Introduction

Ozone is a gaseous compound with the capacity to absorb UV-B and UV-C radiation. Its presence in the stratosphere is necessary for sustaining life on Earth, as it is a natural barrier filtering the radiation, diminishing the harmful effects on the ecosystem, including humans. Nevertheless, ozone undergoes a potent photochemical oxidant within the troposphere. Upon its formation, it instigates deleterious impacts on biotic entities, the environment, human health, and even human-built structures.[1,2]

Ground-level ozone formation results from many complex reactions involving various precursor species and solar radiation. The main factor in these reactions is the photo-stationary state between the nitrogen oxides (NO_X) family and ozone. However, this state consists of a null cycle where the formation and destruction of ozone and NO_X compounds are constant. Ozone accumulation occurs due to volatile organic compounds (VOCs), compounds that, because of the generation of hydroperoxyl radicals (HO_2), react with NO to form NO_2. When photolyzed, it will start the reactions for generating a new ozone molecule outside the photo-stationary state, thus causing the gas to accumulate. Therefore, the formation and accumulation of tropospheric ozone occur in a competition regime between the NO_X and HO_X families, where both will always be present in the troposphere but in different quantities. These two families will originate from nitrogen oxides (NO_X) and volatile organic compounds (HO_X). These two compounds will have non-linear influences, creating limiting regimes dictating ozone concentrations.[3]

Therefore, controlling ozone formation in the troposphere requires an in-depth study of the dynamics

*e-mail: tfc0sta20@gmail.com
Editor handled this article: Eduardo Carasek

of its processes and precursors. Part of this study lies in constructing a robust emissions inventory with as many cataloged emissions as possible. After this, a tool is needed that can determine their concentrations and interlink which processes will lead to this and how. This can be achieved by using computational models to simulate various real-world conditions in different scenarios and locations.[4,5]

Chemical transport models (CTMs) are employed to assess physical and chemical parameters and their interconnectedness in air quality. They constitute the foundational framework for air quality investigations, future scenario assessments, emissions reduction strategies, and the formulation of environmental policies and legislative measures to enhance the national air quality.[6] The Community Multiscale Air Quality (CMAQ) photochemical model was created to simulate complex interactions between the surface and the atmosphere, connecting secondary pollutants production, such as ozone particulate matter below 2.5 micrometers ($PM_{2.5}$), transport, and chemical reactions of trace pollutants to dry and wet deposition. The United States Environmental Protection Agency (USEPA) developed it in 1990 for regulatory purposes and to study the complicated relationships of the atmosphere. Its three-dimensional modeling solves advection and diffusion mechanisms horizontally in each grid cell and vertically by a specified number of layers. The model can simulate tropospheric ozone, particulate matter, visibility, acidification, toxic pollutants, multiplication of atmospheric pollutants, and mercury. Pollutants are mathematically resolved in relation to their movement in the atmosphere and in a way that all processes influencing them, such as emissions and meteorology, are coupled to the calculation.[7]

Since air quality involves complex interactions and chemical reactions, and secondary pollutants have been a problem worldwide, applying a well-developed chemical transport model is crucial to assess pollution levels and investigate mitigation strategies. Nonetheless, the CTM requires input data, parameterizations, and specific configurations, which may vary for different locations. Therefore, the objective of this work is to conduct a systematic review of the most commonly used configurations for modeling tropospheric ozone using the CMAQ.

2. Methodology

2.1. Exploratory methodology

This exploratory research systematically investigates the state of the art of ozone modeling in the troposphere using the CMAQ model. The methodology stages consist of the main steps of systematic review: planning, identification, selection, and extraction. These stages were performed using the START 3.3 Beta 03 software,[8,9] along with the creation of the review protocol and extraction form.

START (State of the Art through Systematic Review) is a program developed by researchers at the Federal University of São Carlos (UFSCAR), Brazil, to assist in constructing a systematic review compliant with internationally required parameters. The tool was designed to organize and detail the stages of the systematic review, enabling the researcher to filter, track, and select each study gathered by their survey process. The software offers a user-friendly interface, undergoes regular updates, features forums on its official website, and provides community support. Moreover, the constructed systematic review can be shared, allowing other researchers in the community to evaluate and audit it.[9]

The divisions were made following the software model as *per* Hernandes *et al*.[8]

2.1.1. Planning

The planning stage involves constructing the protocol to present the research question, keywords, databases, selection criteria, inclusion and exclusion factors, and the extraction form.

The protocol is the name given to the form constructed in the systematic review, containing all the questions and inclusion and exclusion criteria that will be presented in the following stages.

The planning stage aims to bring together all participants in the systematic review to discuss the best keywords for search engines, determine the most effective search string, and identify which databases will encompass the desired articles.[8]

In this study, the selected keywords for the search string were "CMAQ" and "ozone" because any synonym would attract works outside the scope of the research.

The problematic question was chosen based on the need to identify the best in settings of CMAQ to perform tropospheric ozone simulations that represent reality. It is necessary to seek studies that only consider the CMAQ model, only the ozone pollutant, and thus present the description of the main settings in their structure. Therefore, when formulating the main question, selecting the essential information for the paper gathering is mandatory. Based on this, the central research question for this study is: (*i*) What configurations are used in the modeling of tropospheric ozone in CMAQ?

Two secondary questions were also considered:

(*ii*) What factors influence ozone modeling in CMAQ?

(*iii*) What are the most commonly used configurations for real-case modeling?

2.1.2. Identification

The identification stage gathers articles using specified descriptors. Data were collected from two databases, Scopus and Web of Science, from 2016 to 2023. The period from 2016 to 2023 was chosen to assess the evolution of configurations, determining whether there are significant changes over the years or if the conditions for ozone modeling remain the same. These two databases were chosen due to their extensive collection of publications from various countries and the ability of Scopus, in particular, to search for related studies. Thus, if the string search did not retrieve all relevant studies, related ones could be manually added.

The prospected strings were:

"(TITLE-ABS-KEY (cmaq) AND TITLE-ABS-KEY (ozone)) AND PUBYEAR > 2015 AND PUBYEAR < 2023" for SCOPUS and "CMAQ (All fields) AND ozone (All fields) FROM 2016-01-01 TO 2023-12-31" for Web of Science, respectively.

The selection criteria are scientific articles only, articles in English, and primary studies. This pre-selection was made prior to the application of inclusion and exclusion factors.

2.1.3. Selection

Subsequently, articles were selected only by reading the title, keywords and abstract and based on the following criteria: the CMAQ being the model used in the study, ozone being the modeled pollutant, statistical studies involving CMAQ as the model with ozone as the pollutant, and other articles studying factors influencing ozone modeling in the model. Exclusion criteria include model comparisons, validation articles for extensions and updates, articles not using CMAQ to model ozone, articles without ozone as one of the simulated pollutants, and secondary studies. Only the title, abstract, and keywords from the articles were read during the selection phase.

2.1.4. Extraction

During the extraction phase, articles were read in their entirety to gather the information necessary for this review. The posed questions were: (*i*) What were the boundary conditions presented? (*ii*) What meteorological model was used? (*iii*) What was the chemical mechanism present in the study? (*iv*) What were the horizontal and vertical grid resolutions? (*v*) Which emissions inventory was used? (*vi*) What biogenic emissions processor was employed? (*vii*) Were there statistical data on the modeled ozone results? (*viii*) What was the theme studied? and (*ix*) which country was the study conducted?

Besides that, more criteria were added to refine the final articles to be included in this review. The elimination criteria for complete works were established: approved articles from the previous stage should describe all requested data, with only three data points being allowed to be absent; other publication types like book chapters and conference papers were not allowed; studies were removed if the complete publication could not be found; publications in journals with an impact factor lower than five and a Journal Citation Index (JCI) less than one were also rejected.

The responses were compiled in a documentation spreadsheet with all the publication data for creating the presented graphs and understanding the general overview. The percentage of configuration mentioned for each topic was calculated concerning the total number of publications (n = 188).

2.2. PRISMA diagram

The PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) diagram is a verification and auditing tool for systematic reviews, presenting a conceptual flowchart showcasing the stages, the number of exclusions and duplicates, and the rationales for removing each article from the study.[10] The diagram was designed to ease evaluation and systematic review tracking. This is done by documenting the requisites at each study stage. Both the author and reader can assess how many articles were reviewed at each phase, which were approved, and the reasons for both approval and rejection. This makes the work more accessible to audit, focusing on observing the data and how it was chosen.

The PRISMA diagram is available on the PRISMA website.[10] This diagram has three phases: identification, observation, and inclusion. Each phase shows the approved, rejected, and duplicate articles. In the second phase, exclusion reasons are displayed, detailing how many articles were excluded for each reason. In this study, the diagram was slightly modified, with three additional exclusion factors added in the last observation phase, as previously mentioned.

3. Model Approximations and Limitations

This section presents general insights from the review study before addressing the primary data focus. As such, we will address limitations and certain approximations in CMAQ modeling for tropospheric ozone.

In general, ozone simulation using CMAQ has shown statistically closer results to observed data, especially for coarse grid resolutions (36 × 36 km and 27 × 27 km). This suggests that the model performs well in capturing regional atmospheric dynamics.[11-15]

Typically, simulated ozone is overestimated in the summer and underestimated in winter. This is mainly due to the photochemical cycle of the NO_X family in the summer. The kinetic formation and destruction of the NO_X family due to solar incidence and emissions, mainly from mobile sources, reduce the available NO_2, thus producing less ozone in monitored data compared to the simulated ones. In winter, the nighttime chemistry of the NOy family produces many unstable forms, such as NO_3 and N_2O_5, which accumulate a significant amount of NO_2 in the boundary layer, making this compound available in higher concentrations than predicted in the software.[16-22]

Regarding its precursors, there is still difficulty in reproducing VOCs in the model, mainly due to source characteristics, chemical speciation, biogenic sources, and very sharp diurnal and nocturnal variations. Given that the origin of VOCs in urban environments varies geographically, but with population density, industrial parks, and urbanization, the model has difficulty allocating certain variations of these compounds and their reactivity. This compromises the simulated ozone concentration value. For instance, tropical countries with metropolitan regions having higher green area densities will emit more and a greater variety of biogenic volatile organic compounds than countries in the northern hemisphere, even in summer. These variations challenge the simulation.[16-22]

Simulated ozone data generally achieve values with higher concordances when refined by high-efficiency statistical tools such as DDM (Decoupled Direct Method), deep learning, and neural networks. These statistical approaches better fill in missing data, identify patterns or abrupt changes in data, and pinpoint significantly deviant points from the expected. Hence, they are capable of addressing gaps in the modeling such as missing emissions inventory data, ozone concentration peaks in heat episodes, diurnal and nocturnal variations, as well as local atmospheric movements The use of these tools enables the CMAQ model to approximate its simulated data to real-world data better. The application of these statistical methods is primarily focused on data approximation and outlier smoothing. The Decoupled Direct Method (DDM) is an exciting example incorporated into CMAQ. This method is present in a distinct version of the standard CMAQ model and is also available for download.[23] However, CMAQ-DDM stands out for its sensitivity study application. Sensitivity studies are routinely conducted in the model, where patterns are applied by modifying one or multiple variables within the system, such as emissions, meteorological data, and wildfires, to observe the resulting changes in simulation outcomes. DDM conducts this analysis internally by calculating standard concentrations and deposition velocities. Consequently, it can be applied in studies examining different boundary conditions, reaction kinetics, and deposition rates. Furthermore, other tools included in the new versions of CMAQ are the ISAM (Integrated Source Apportionment Method), a method used for ozone and $PM_{2.5}$, which assigns precursor information to emission sources. Also present is the STM (Sulfur Track Method), which associates information about sulfate production, both in particulate and gaseous phases, with emission sources, as well as initial and boundary conditions.[24-28]

Extreme weather events like typhoons, hurricanes, monsoons, and significant wildfires are not well-reproduced by the model, mainly due to underestimations of wind direction and speed, precipitation, and atmospheric pressure derived from WRF (Weather Research and Forecasting).[29-32]

One notable limitation highlighted is the difficulty of the model in representing concentration peaks or data in general. The model struggles to describe concentration points significantly deviating from the modeled pattern. Ozone episodes with high peaks cannot be well represented in the model, leading to underestimations. This might be due to both emissions inventory and underestimated meteorological variables. For instance, heatwave episodes often result from significant solar incidences, causing temperature spikes, both known to elevate ozone concentrations.[33-36]

4. Results

4.1. Studies identification

4.1.1. Databases and journals

Figure 1 presents the number of articles compiled according to the database. These data represent the number of papers found without applying prior criteria. Web of Science showed a significantly higher contribution, with 113 more articles. This disparity can be attributed to the implemented database "research string" being more generic on the Web of Science, leading to a broader search. Subsequently, we will demonstrate that specific keywords identified in the studies have little relevance to the scope of the current research, which can also be associated with the generic nature of this search string.

When observing Figure 2, it is crucial to keep in mind that these are the articles accepted, meaning those selected in the last extraction phase, not all downloaded from the

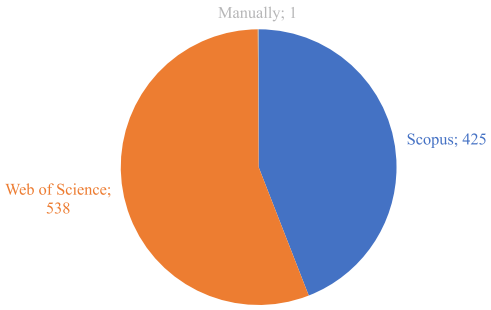


Figure 1. Number of studies found on the identification phase *per* database without any apllied criteria.

databases, as shown in the previous graph. This choice was made because the focus of the analysis of journal relevance for this review lies in the articles accepted. In this context, it can be observed that journals with higher impact factors are included in this category. "Atmospheric Environment" stands out as the journal with the highest number of publications, attributed to its scope covering a specialized topic in computational models, as well as emission inventory studies, both conducive to being conducted by studies utilizing the CMAQ model.

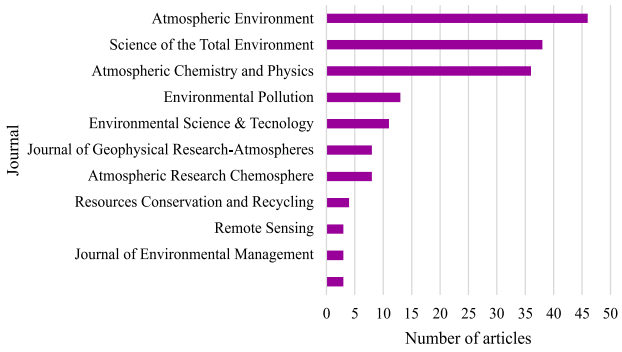


Figure 2. Number of articles accepted in this review *per* journal after the extraction phase.

4.1.2. Keyword analysis

The analysis of keywords was conducted after searching through the chosen databases. These keywords were the most frequently mentioned among the total articles gathered when applying the search strings. It reveals that the most frequent ones are those effectively employed in the search strings, notably "CMAQ" and "ozone." However, certain keywords with limited relevance to the proposed scope were identified, such as "WRF," "particulate matter," and "PM2.5" as shown in Figure 3.

The presence of "particulate matter" and "PM2.5" can be attributed to the similarity of studies, given that the literature encompasses numerous researches involving CMAQ, ozone, and particulate matter. Another contributing factor to including these keywords may be the absence of Boolean operators, such as "NOT" or "OR," in formulating

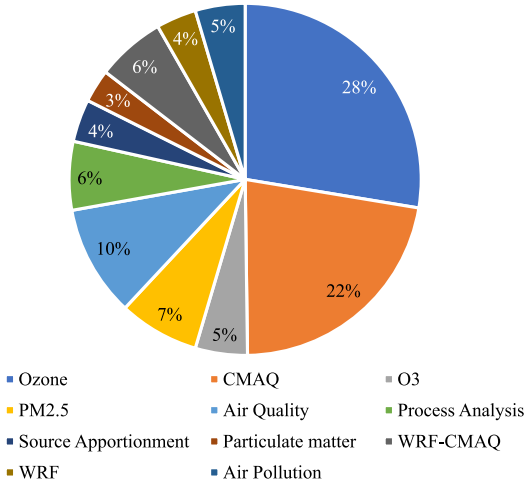


Figure 3. Most mention keywords in the identification step.

the search strings. The "NOT" operator would have helped exclude undesirable terms like "particulate matter" or "secondary pollutants," which would encompass all secondary pollutants, extending beyond the scope of the study. Conversely, the "OR" operator could have been employed to find other keywords associated with ozone, such as "O3." The presence of Boolean operators is described in the literature as a way to strengthen the search string and focus more centrally on the study objectives. The absence of few or no Boolean operators makes the search less representative.[37]

As for "WRF," its inclusion can be elucidated by the recurrence of this meteorological model in the majority of studies related to CMAQ, a point that will be addressed later.

On the other hand, the keywords "source apportionment" and "process analysis" are intrinsically linked to CMAQ, referring to processes embedded in the model script, which are applicable in simulations. The section on themes, titled "Utilization of the model and enhancements," extensively explores this topic, presenting a significant volume of studies in this area. Consequently, the presence of these keywords aligns consistently with the treatment of these themes in the literature.

4.1.3. Preliminary analysis of articles

While the studied area and scale are not within the scope of the analysis of this review, they provide valuable insights that aid in understanding the results shown about configurations. Figure 4 presents the number of studies *per* country. The most frequently mentioned is China, ranking first, followed by the United States of America. Together, these two nations account for the majority of publications.

China stands out due to the surge in scientific publications from the country, especially on topics related

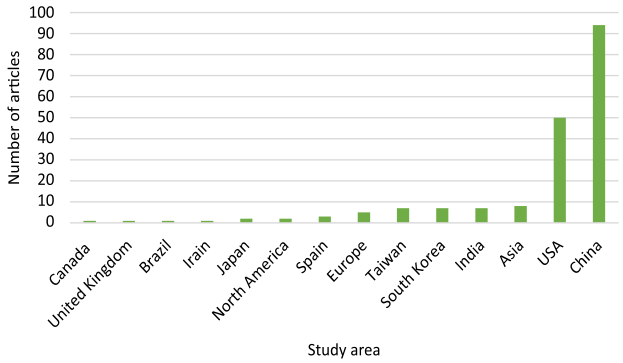


Figure 4. Number of studies published with the designated keywords by area.

to atmospheric pollution. The high number of publications from these countries will influence configurations like horizontal domains and emission inventories, which are specific configurations of each study, impacting the most frequently mentioned settings for these items.[38-42] Additionally, China and the United States have their own emissions inventory, which helps the application of CMAQ model since the emissions inventory is a must in air quality modeling

Regarding the annual publications, as illustrated in Figure 5, a rising trend is observed, with exceptions in the years 2017, 2020, and 2023. The decline in 2020 can be attributed to the onset of the coronavirus (COVID-19) pandemic, which prompted lockdown measures and led to a global decrease in scientific production. This downturn is particularly notable in China, a key contributor to studies related to CMAQ and air quality. Considering that the articles accounted for in the graph are only those found in the last phase of extraction and selected for this review.

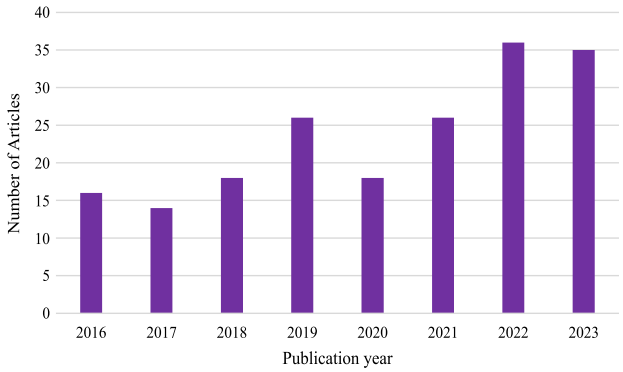


Figure 5. Number of studies published with the designated keywords by year.

Regarding 2017, the evident reduction is directly linked to the scope and exclusion criteria adopted in this systematic review. In 2023, there is one less publication compared to 2022 for the same reasons mentioned earlier. Despite the increase in publication volume that year, the exclusion criteria resulted in the removal of a significant number of studies, particularly concerning the impact factor of journals.

Figure 6 displays the primary themes explored in the assembled literature. The predominant subjects discussed among the main topic, which is anthropogenic emissions, are: emission evolution projections, projections of reduction due to the progression of mitigating measures and laws, analyses of global warming scenarios, evaluation of different categories of anthropogenic emissions (cars, industries, household), new emissions in a country, etc. This topic is highlighted due to the need to understand how emissions impact the ozone simulated in the model.[43-46]

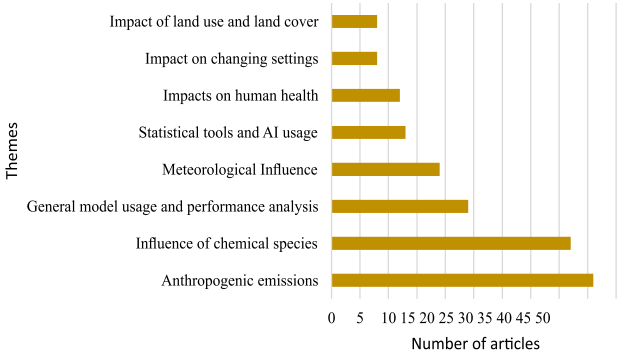


Figure 6. Number of mentions of the main themes presented in the articles.

Emissions are one of the primary success factors for simulations when compared with measured pollutants. Therefore, the higher concentration of studies on this topic arises from the need to understand emissions and accurately reproduce them within CMAQ. It is worth mentioning the influences of chemical origin that follow closely behind. These include the analysis of reactions in NO_x-limited or VOC-limited regimes, studies of mixed regimes, and the influence of various compounds on ozone formation, such as biogenic compounds, black carbon, halogens, and secondary organic aerosol. Since ozone is a secondary pollutant, it interacts with various other pollutants and atmospheric compounds. There is a significant focus on studies concerning the synergy between ozone and particulate matter 2.5 μm, both of which are secondary pollutants and are of great concern to the scientific community.

4.2. PRISMA diagram

The results from PRISMA diagram are in Figure 7. The survey shows the highest number of rejected articles during the selection stage because they are not simulating ozone. This fact may be primarily due to a broad search string. Hence, the reason for employing a new search string

for the Web of Science database. In total, 963 articles were found. Since two databases with similar strings were used, duplicate works were expected. START removed duplicate files whenever data from one database was downloaded. However, duplicate files were still manually checked during the following stages. In the initial stage, 61 duplicates were found. In the subsequent stages, duplicated works were still identified, mainly due to software malfunction in the initial eliminations. Consequently, 145 and 128 duplicates were further removed in the second and third stages, respectively.

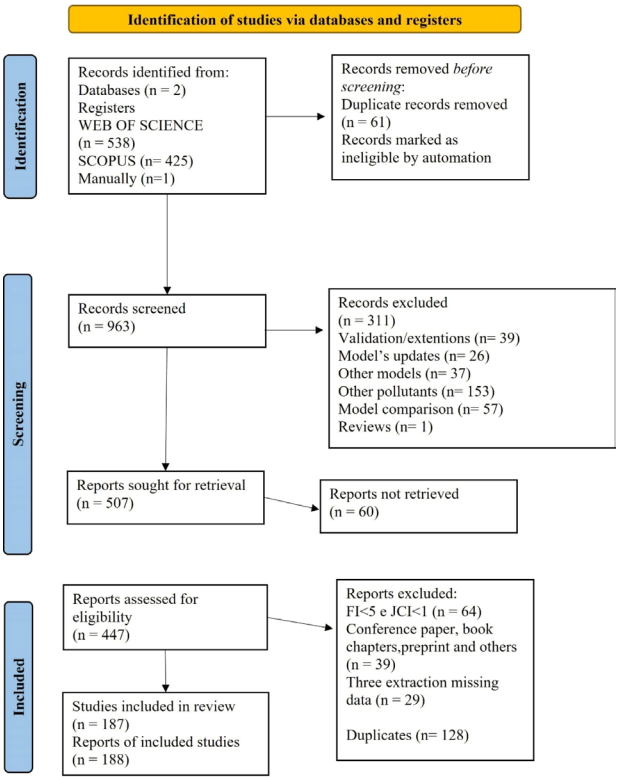


Figure 7. START 3.3, Beta 03 software, PRISMA diagram of this review (adapted from reference 10).

It is clear that after the election, the primary inclusion factor was "CMAQ as the photochemical model" followed by "ozone as the modeled pollutant", two factors which, according to the search tools and the search string, should naturally be implicit in the gathered studies. Therefore, these two inclusion criteria were necessary to eliminate these search errors. Another critical point is the studies on factors influencing simulated ozone. As CMAQ is a well-known model in the scientific community, many studies focus on various atmospheric mechanics that still need to be described by the model.

One event observed was that many studies passed to the extraction phase but when the full text was analyzed there were exclusionary factors from the selection phase that were noticed, in this case, the software counted the articles excluded for the screening phase. That is why there are still articles excluded from the diagram after the screening phase.

The most common justification was studies published in journal with lower impact factors and/or lower JCI, followed by studies outside the format. These last two justifications were created mainly for the richness and reliability of the data. In the end, a total of 188 studies, all scientific articles, were used for the systematic review in the English language.

4.3. Systematic analysis

4.3.1. Meteorological model

During the research, various uses of meteorological models were observed, from just the description of local meteorological fields to models established in the literature.

The most frequently used model was the Weather Research and Forecasting (WRF), a highly respected mesoscale model endorsed by the US EPA for integration with CMAQ. The WRF is a meteorological model developed by several environmental agencies and research groups to simulate atmospheric conditions for various applications, from weather forecasting and scientific studies of high and low atmospheric dynamics to accurate and ideal case simulations and support for other models, like chemical models. Its outputs generate several meteorological fields, covering wind direction, atmospheric pressure, relative humidity, and solar incidence.

Launched in 2000 and open-source, the WRF model came to substitute the Pennsylvania State University and National Center for Atmospheric Research Mesoscale Model (MM5) model and has been continuously improved since its launch.[47] It appeared in 93.09% of the publications as shown in Figure 8, showing that research modeling tropospheric ozone with CMAQ predominantly uses WRF as their meteorological field provider. The popularity of this model arises mainly from WRF being an official coupling

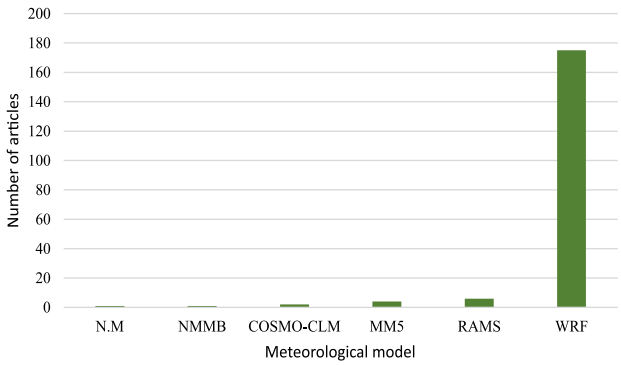


Figure 8. Number of mentions *per* meteorological model used in the simulation with CMAQ.

for CMAQ recognized by the developers of the model, leading to online coupling and automatic grid adjustments between WRF-CMAQ in the latest CMAQ versions.

The key findings include improving meteorological data through data assimilation or combining multiple models/tools. These tools consist of grouping two or more models or one model with different initial conditions to use a mean value for meteorological conditions. These values are used as input data for CTMs.

In the case of meteorological models, WRF can be used with fusion tools to enhance meteorological data for CMAQ. Another way to enhance meteorological input for CMAQ is the combination of WRF with CMAQ, where both models utilize data from each other online.[48,49] Therefore, the two-way online coupling with CMAQ was also presenting when the researchers improved the simulated ozone performance thanks to the incorporation of the direct effect of aerosols. For this type of effect involving chemical species, such as aerosols, and meteorological variables, such as cloud cover and solar radiation, it is advisable to employ an online model. This model allows for continuous feedback of meteorological data, with modifications being made by the species in the atmosphere. This approach can be implemented through meteorological models with chemical couplings, such as WRF-Chem, or by creating a bidirectional coupling between meteorological and chemical models, exemplified by WRF-CMAQ.

Both techniques, WRF and CMAQ offline and WRF-CMAQ online, are great tools. The first option helps to understand the separate process of meteorology and emissions. Thus, you can validate and point out individual mistakes one by one. The online includes advanced computational techniques for data analysis in both the meteorological and chemical model scripts, including kinetics, deposition, advection, and others in the chemical model, giving feedback on air pollutants concentration to meteorology. Consequently, CMAQ can collaborate with the meteorological model, using the concentration of species in the atmosphere to adjust cloud formations or irradiation rates through the radiative scattering of specific species.[50-52]

WRF can also model the influence of cyclonic regimes trapping ozone in the marine atmosphere in Japanese and Korean cities[53] and the evaluation of changes for more refined grids, as they generate uncertainties because the model cannot accurately predict certain meteorological phenomena.[54] Furthermore, meteorological conditions such as wind speed, higher temperatures, lower relative humidity, and low cloud fraction influence ozone concentration peaks.[55]

The tools that are part of the WRF responsible for generating input data are also subjects of studies. For the simulation of nighttime ozone, it is essential to consider the planetary boundary layer (PBL) height and land use, as they influence dry deposition rates of ozone and reaction rates.[56] This poorer representation of the nocturnal dynamics is also described by Yang *et al*.[57] and in a study in Madrid.[58] Another study on land use also shows better results when more recent satellite data describe land use.[59] An important factor is also the influence of solar radiation incidence with cloud cover and the effect of aerosols.[50] Soil moisture also proves to be a factor influencing the emission of VOCs, and ozone precursors, and needs to be analyzed both in WRF and Model of Emissions of Gases and Aerosols from Nature (MEGAN).[60] The discretization of the PBL is also a significant factor in simulations. In the study, the authors describe overestimation of ozone as mainly caused by temperature. Thus, they changed the PBL setting to Pleim-Xiu, which led to an improvement mainly because the setting better describes the conversion of sensible heat to latent due to vegetation.[61]

4.3.2. Grid resolution

Grid resolutions are responsible for accommodating the simulated phenomena within a specific space where mechanisms will work collectively in a uniform atmosphere. As the name suggests, a grid comprises a set of cells with equal sides. The measurement of these cells, which will occupy a particular domain, is called grid resolution.[62]

Unlike meteorological models, grid resolutions have seen more variations, mainly because studies diversify across scales, aiming to study different processes.

The most highlighted resolution in Table 1 was 36 × 36 km, which was used in 18.09% of the assessed works. This prominence is primarily due to regional domains not requiring significant computational performance. Another influencing factor is the large concentration of publications focusing on ozone-influencing factors in the United States and China, two continent-sized countries.[14,57,63]

Table 1. Number of mentions in studies of horizontal grid

Horizontal grid resolution / km	Number of mentions in horizontal grid resolution
36 × 36	34
27 × 9 × 3	21
12 × 12	20
36 × 12 × 4	18
36 × 12	12
4 × 4	9
27 × 27	9
12 × 4	8
27 × 9	7

The second most observed grid resolution in this review was 27 km × 9 km × 3 km, which was present in 11.17% of the works. This grid size is also relevant because publications focus on relieving the effects of boundary conditions utilizing nested domains, which is also very common in studies on China, the country with more publications.[37,43,64-69]

While the results show a higher number of publications at coarser resolutions, mainly due to the density of publications in the two leading countries, it is essential to understand that this review found many instances where finer resolutions are ideal for ozone simulation studies. Pan *et al*.[36] found that a resolution of 12 km is ideal for ozone production efficiency simulations. However, 4 km or smaller resolutions are needed to identify NO_X inhibition points.

Furthermore, meteorological events on a smaller scale, like vertical transports up to 900 m, are only observed at 1 km, and 4 km resolutions. Also, a more detailed mapping of local emission sources is only visible in 1 km grids, with an appropriate emission inventory being essential. These urban source influences are also found in the study by Karl *et al*.,[70] who recommend a shift to a 1 km grid for better representation, especially for coastal sources. However, these must be linked to a consistent emission inventory. Liu *et al*.[71] also found that when simulating premature deaths related to tropospheric ozone, finer resolutions (1 km in the study) presented a statistical sensitivity of 20% compared to coarser resolutions.

Although the study did not find a statistical difference between coarse and fine resolutions, the authors suggest that this could be due to the emission inventory, which had a resolution of 25 km. In contrast, the finer grids had 4 km, indicating potential differences. However, the study could not reproduce them due to a lack of suitable inventories.[72] Kota *et al*.[73] also highlighted this, showing that in megacities in India, finer grid resolutions are necessary for ozone modeling due to many distinct local emissions. In events like wildfires, grid resolutions are also crucial. In this case, resolutions smaller than 4 km are necessary, so these are not underestimated.[74]

Regarding vertical layers, the number of layers determines the accuracy of vertical diffusion and advection phenomena, the distribution of ozone across layers, possible regional transport, and its relationship with the planetary boundary layer. According to the works, the number of layers ranges from 15 to 45.

The most utilized number of layers was 35, found in 10.11% of the studies. The vast number of works employing 35 layers is due to best practices outlined in the WRF manual; consequently, in CMAQ, this can be observed in Table 2. However, pollutant concentrations are underestimated if there is production and transport above 10 km altitude. Therefore, resolutions with more than 40 layers are more suitable for studying such phenomena.[75] Still, there is a higher computational cost with the increase in vertical layers, resulting in a likely exclusion of this option, with more than 40 layers, by most studies.

Table 2. Number of mentions in studies of vertical layers

No. vertical layers	Number of mentions of vertical resolution
NM	63
35	19
30	12
15	10
14	10
23	7
25	7
27	6
18	6

NM: not mentioned.

For this topic, studies applied the process analysis tool in CMAQ, observing ozone peaks in China in layers at 500 m and 2 km above ground;[76] CMAQ tends to place higher ozone concentrations in layers closer to the ground and in the higher layers of the PBL, thus causing overestimation. Therefore, a more significant number of layers is needed to prevent this overloading tendency of the model. In the study, 34 layers produced the best concentration values, likely due to this mechanism.[33]

However, it is essential to mention the vast number of studies that did not mention this configuration. Describing the number of vertical layers is crucial for future studies in similar locations or new studies in the same place. This ensures that vertical movements are accurately described and that there are influences on simulated ozone results.

4.3.3. Chemical mechanism

CTMs require chemical mechanisms to describe reactions, their products, and their formation and consumption rates in the atmosphere. These mechanisms aim to gather chemical species and describe their behavior in the atmosphere.

The programs can have mechanisms ranging from simple species sets with 7 compounds to more complex sets with over 4000 species. Based on reactivity or chemical structure, these mechanisms can represent chemical species in grouped forms. The chemical reactions and constants are

from scientific literature, including field and bench studies (chambers). Regarding the chemical reactions, the CMAQ uses several chemical species, and usually, the emissions inventory is developed as single species, such as NO_2, VOC and $PM_{2.5}$. Consequently, there is the need to specify, for example, the VOC as different species, such as benzene, acetaldehyde, toluene, and others. This speciation will allow the model to use different chemical reactions and constants to simulate the air pollutant concentration. Another example is NO_X, which will be converted into NO and NO_2 for the model. The model first converts these pollutants into species that can be speciated, meaning a pollutant is divided into groups like the NO_X family mentioned earlier, or it can be aggregated, as different ketone chains are converted into the acyl (RCO) radicals.

Additionally, the model divides emissions into mass data and mole data. Chemical mechanisms use mole data, so mass data is used only for reporting. CMAQ works with three distinct programs regarding chemical mechanisms: Statewide Air Pollution Research Center (SAPRC), Carbon Bond (CB), and Regional Acid Deposition Model (RADM). CMAQ includes a chemical equation processor and two solvers to operate with various chemical mechanisms.[5]

Briefly described, the RADM is a grouped species mechanism that uses a reactivity-based weighting scheme to account for and group chemical compounds. For example, this mechanism explicitly treats alcohols and features a more detailed analysis of radical transport processes, less reactive VOCs, and biogenics. The Statewide Air Pollution Research Center, a chemical mechanism included in CMAQ, is a variable parameter version that is detailed and condensed. This means detailed species are condensed based on the variation of a certain parameters, especially its reactivity, particularly with the OH radical. For example, alkanes, except for methane, are divided into five different species within the mechanism, categorized based on their reactivity to OH. Unlike SAPRC, the Carbon Bond mechanism categorizes species based on bonds, regardless of the molecule type. It started with just two types of bond, and as updates were implemented, more species were added. Today, it includes reactions with radicals, NO_3, halogens, isoprene chemistry, and winter reactions. These few groupings make it lighter, facilitating its performance in models. Each of these mechanisms will perform speciation differently, and CMAQ will adjust the CMAQ Chemistry-Transport Model (CCTM) for its chemical calculations.[7,77,78]

Among the various chemical mechanisms used, the most cited was the Carbon Bond version 5 (CB05), appearing in 41.49% of the analyzed publications, followed by Carbon Bond version 6 (CB06) with 22.87%, and the 2007 version of the State Air Pollution Research Center (SAPRC-07) at 11.17%, alongside the newer SAPRC-11 at 7.98%.

The Carbon Bond mechanism (04) was created in 1989 and was one of the first chemical mechanisms created for third-generation models. This mechanism underwent multiple updates, adding chemical species and reactions. The Carbon Bond (05) is an update to Carbon bond version 4 (CB04) created in 2005, adding more chemical species and reactions and ten more organic species to better represent stable atmospheric organic species and radical formation.[78,79] The Carbon Bond (06) updates CB05 to correct photolysis rates, quantum yield, scattering effect, surface radiative effect, and albedo, meaning a version with a more comprehensive package of physical parameters.[80]

Although these mechanisms differ, the chemical approach does not show significant statistical differences in ozone simulation using different chemical mechanisms.[78] The widespread use of Carbon Bond as a mechanism in publications is because they are present in most of the default CMAQ program databases upon installation and because of their simplicity for chemical speciation. Figure 9 displays the publications that used a particular chemical mechanism in modeling to express the numbers concerning chemical mechanisms better.

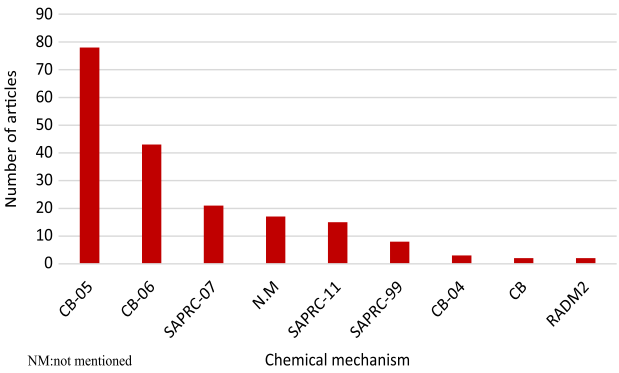


Figure 9. Number of articles mentioning the type of chemical mechanism used in the chemical speciation of the simulation.

The study of chemical compounds, kinetics, and reactions influencing simulated ozone was one of the main themes discovered in this review, making the chemical mechanism one of the most researched configurations in CMAQ today. Some standout studies include Hong *et al.*,[81] who observed that a higher simulated ozone concentration is generated by applying a more detailed chloride reaction mechanism in conjunction with the heterogeneous phase. Baker *et al.*[74] highlighted the need for a better understanding of the chemistry of NOy family compounds and peroxyacetyl nitrate (PAN) in chemical mechanisms for an improved simulation of ozone arising from wildfire events.

An essential factor observed was the chemistry of sulfur compounds and secondary organic aerosol. By integrating dimethyl sulfide (DMS) into a chemical mechanism, the ozone concentration decreased by 0.5 ppb along the coastline and between 0.25-0.40 ppb in urban areas in China.[82] Gantt *et al*.[83] studied the influence of iodide and bromide on ozone formation in coastal regions and their transport inland. They found an improvement in the underestimation and overestimation of ozone values. By applying halogen chemistry under boundary conditions, ozone decreased in the upper layers, leading them to believe that this regional transport is impacted by deposition over the ocean. In a study similar to the one above, researchers found that by employing more detailed halogen chemistry in the mechanism, there was a reduction in the ozone concentration between 2 and 5 ppb, primarily due to sea spray compounds and iodide that react with ozone.[84] The chemistry of nitrous acid (HONO) and its derived compounds was also explored, revealing that by implementing these reactions in the chemical mechanism, instances of underestimating ozone also decreased.[85] Liu and Wang[86] further updated the chemical mechanism by adding new heterogeneous mechanisms to the secondary aerosol through new reactions and new compounds from the NOy family. They found values closer to the observed ones for both ozone and nitrogen dioxide.

4.3.4. Initial and boundary conditions

Initial and boundary conditions are two modules that dictate the progress of the simulation in CMAQ. These preprocessors will apply the initial input data of the model for the start and continuation of the simulation. The initial conditions module will be responsible for the first hour of the simulation, where physical and chemical parameters will be implemented for the beginning of the atmosphere in the studied domain. In contrast, the boundary conditions module will be in charge of conditions at the borders of the simulation of the set grid. Boundary processes can be static or dynamic and can be continually updated during the simulation or have just a single input data set.[7,87]

In the collection of papers studied, there were descriptions of initial and boundary conditions for either the meteorological model for CMAQ only or for both. Since initial and boundary conditions for meteorological models are beyond the scope of this article, they will be disregarded. In this work, initial and boundary conditions were considered together since they originate from similar processes within the model, and in most studies, they are not mentioned separately.

For boundary conditions, Figure 10 shows that the use of the internal data of the model was the most common, being used by 15.96% of the evaluated works. The global Model for Ozone and Related Chemical Tracers (MOZART) was utilized by 13.30% of the evaluated works.

In the models, boundary conditions mitigate errors from external contributions to the domain of the model. Internal profiles are typical because they do not require a lot of input data or couplings in the model and processes that demand higher machine performance. However, these models do not demonstrate significant sensitivity.[88] For a better simulation, the ideal is that global models or nested grids continuously feed CMAQ with constant data and grid updates. Nevertheless, this scenario is not possible in all studies, primarily due to the high computational cost, which is why the default processes of the model are the most used.

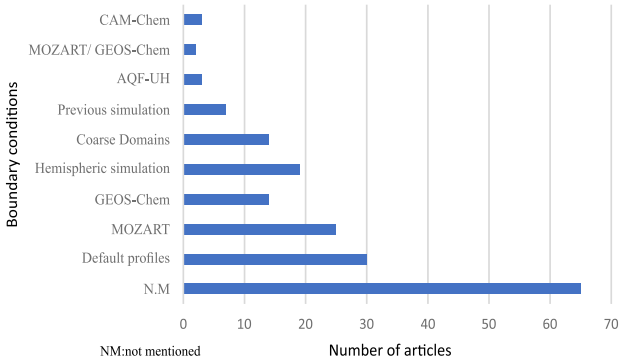


Figure 10. Number of articles mentioned by configuration type for boundary conditions used in the simulation.

What has been widely studied and applied are global models and dynamic conditions. Notable studies include: Li and Rappenglueck[56] observed that having well-defined boundary conditions from global models or statistical model outputs is crucial, especially for modeling nighttime ozone.

Another study indicated that dynamic boundary conditions help reduce modeled bias, while static conditions tend to overestimate ozone.[48] Chen *et al*.[76] tested MOZART, noting a significant increase in upper tropospheric to tropopause ozone concentrations, possibly due to stratospheric ozone intrusion caused by the HaiKui typhoon.

Nested domains have also proven significant. Li *et al*.[35] applied an observational nesting to measure the improvement in ozone simulation linked to meteorology. The nesting influences wind speed and direction and boundary layer height. Observational nested domains showed better ozone modeling and the two meteorological data points compared to the base case. However, the ozone peak case indicated a change in wind direction that neither the nested domain nor the base case observed, necessitating further study.

4.3.5. Emission inventory

Simulations require the provision of extensive data in order to construct the modeled environment. Many countries lack complete data and broad monitoring networks to provide consistent model input data. In this sense, emissions inventories processors were created for a more practical approach in transforming input data to files ready for the models.[7] Therefore, for emission inventories in this study accounted any form of pollutant emissions cataloging shown in the articles, be the database, global inventories, probe files, campaign data, official emissions inventories from the countries.[89]

As such, MEIC (Multi-resolution Emission Inventory for China) at 28.72%, followed by the NEI (National Emissions Inventory), accounting for 21.28%, were the two most-used inventories among the researched works. China and other Asian countries published several studies using CMAQ simulations in the investigated time frame, making up many of the articles obtained for this review. Both inventories predominate because both countries are the most significant contributors to the topic in published articles.

As illustrated in Figure 11, the MEIC inventory stands out as the most referenced, primarily due to the substantial number of publications originating from China. As indicated in the analysis of study locations, China dominates publications involving CMAQ, representing the highest number of studies overall. Consequently, the inclusion of the emission inventory of the country is evident. This also underscores the potential of the country to adapt CMAQ configurations for different nations beyond the United States. Another implication of this graph is the demonstrated necessity for a national emissions inventory or one tailored to the specific locale to achieve more accurate simulation outcomes.

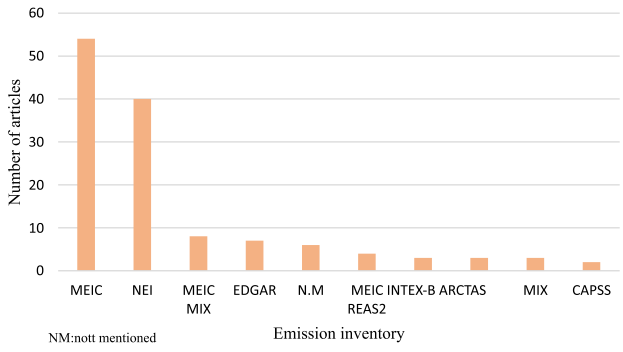


Figure 11. Number of mentions of articles by type of predominant emission inventory used in the simulation.

In terms of the studies, notable highlights include Ring *et al.*[90] findings that there is a need to improve the detailing of ship emissions and conditions in port areas in emission inventories. Karl *et al.*[70] also studied ships and indicated a need for better detailing of non-metallic volatile organic compound emissions from ships.

Shankar *et al.*[91] researched specific fire inventories in the United States. They observed that while there is no statistical difference between them, the specific fire inventories provided better results compared to the American NEI inventory.

Matichuk *et al.*[19] showed that the North American inventory is not comprehensive enough to cover all industries in the oil and gas sector, affecting the concentration of ozone precursors in the simulation.

Jeon *et al.*[92] modified the Fire Inventory from NCAR (FINN) by adjusting the fire plume height to 4.4 km, yielding good CMAQ-simulated ozone results. Without this modification, the data performed poorly.

Regarding other inventories, the Emissions Database for Global Atmospheric Research (EDGAR), although it appeared alone in only 3.72% of the publications, is frequently used in combination with other inventories in many studies. Its extensive use is because it draws data from global monitoring investigations, making it popular among countries lacking inventories or monitoring data for pollutant modeling. However, the quality of results from the EDGAR can vary based on the region and the level of detail used in the inventory.

The emission inventory proves to be one of the most critical factors in a simulation. According to the studies, having a good emission inventory with all sources determined in the study domain and a complete chemical mechanism with the speciation of all possible chemical species in a given area produces simulated data with much more minor errors when compared to real data. Most studies point out uncertainties and significant discrepancies concerning measured data, underscoring the need for better-implemented emission inventories.

4.3.6. Biogenic emissions processor

In modeling tropospheric ozone and anthropogenic emission inventories, it is essential to characterize biogenic emissions. This is because they are responsible for VOCs emissions that also contribute to ozone accumulation. These classes of programs function similarly to anthropogenic emissions processors. Indeed, some simulations use the very processors for anthropogenic emissions to characterize biogenic VOCs.[93]

The MEGAN was the most frequently mentioned biogenic emissions program in 56.38% of the articles. It is the latest model concerning the estimation of biogenic emissions, offering global emissions estimates based on land-use variables such as emission factors, leaf area

index, and plant types. MEGAN is a global model offering resolutions between 1 and 100 km. Thus, it is suitable for both global and regional models.[94]

It was introduced as a successor to the previous biogenic emissions model, BEIS (Biogenic Emissions Inventory System). A distinctive feature of MEGAN is its canopy-scale calculation of biogenic compound emissions. Emission rates of reactive species are determined using deviations from the standard conditions of the leaves, losses, and production from the leaf layer and branches. This is then extrapolated to the tree canopy scale. In this canopy environment, the model considers meteorological factors for compound dispersion, losses to plant consumption, and other biological processes, reactions between them, and gas/particle phase transformations. Another crucial aspect of the canopy scale is that the program categorizes emissions concerning foliar types, which are then extrapolated to plant species within the catalog of the program. All of this, coupled with geographical information used as input data for the simulation, allows the estimation of the characteristics of the emitting ecosystem within the domain.[94]

As shown in Figure 12, the use of the MEGAN model stands out in publications mainly because it is the most recent version of biogenic emissions. It offers a broader range of data on the natural ecosystemsof the world, more detailed chemistry of biogenic aerosols and gases (especially isoprenes), and its canopy scale calculation aligned with geographical information, which reduces underestimation errors. Figure 12 displays the primary biogenic processors found in the study.

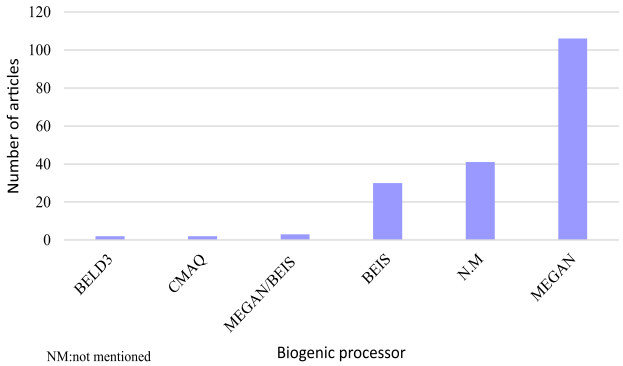


Figure 12. Number of mentions by type of biogenic emissions processor used in the CMAQ simulation.

Regarding the studies, highlights include that Wu *et al.*[60] studied the influence of biogenic VOCs in China and found that soil humidity significantly influences the model when simulating biogenic VOCs.

Wang *et al.*[95] used a drought scenario in MEGAN, revealing that both ozone and secondary organic aerosol concentrations were reduced with this setup.

Liu *et al.*[96] projected biogenic VOC emissions in China and their influence on 2050 ozone concentrations using IPCC's (Intergovernmental Panel on Climate Change) projected scenarios. Results indicate that higher biogenic emissions will be generated with the rise in global temperature.

Liu *et al.*[97] estimated the contribution of biogenic VOCs to ozone formation in China's Pearl River Delta. Remote sensing was used to refine the MEGAN data, improving the agreement index for ozone concentration values and meteorological parameters.

A series of studies use MEGAN solely as a biogenic source inventory, adding specific regional biogenic VOC emissions and reducing both underestimation and overestimation biases of simulated ozone due to including an additional source not as accurately simulated by SMOKE or EDGAR.[76,95,96,98-106]

5. Recent Studies

This section addresses the representation of the most recent findings in the literature discussed in this review, aiming to determine whether the configurations depicted by the data from the entire study period reflect the most recent settings used in studies over the past year. Table 3 provides a summary of the data from the latest articles compiled in this review.

6. Conclusion

The main highlights of the review are: ozone modeling shows promising results in regional domains; ozone is overestimated in the summer but underestimated in the winter; ozone peaks, maximum concentration events, and extreme meteorological events are not well-reproduced by CMAQ; boundary conditions derived from global models are the most recommended regarding computational cost and results; the most worked themes in the gathered articles were modifications, studies on emission inventories, and the analysis of chemical factors in ozone simulation; the most mentioned countries were China and the United States; the substantial number of publications from China significantly influenced this review, as the country leads in terms of publications given that a considerable portion of the configurations represented here were applied within its territory. This underscores the applicability of CMAQ beyond the United States. The most common configurations were WRF as the meteorological model, horizontal grid resolution of 36 × 36 km, vertical resolution of 35 layers, boundary conditions from CMAQ's internal profiles, CB05 chemical mechanism, MEIC emission inventory, and

Table 3. Most mention configures from the recent year, 2023

Configuration	Most mention	Advantages	Disadvantages	Most mention country	Reference
Meteorological model	Weather Research and Forecast	WRF meteorological model was created to be coupled to CMAQ; currently, it even features online functionality together with CMAQ to exchange information from meteorological fields with chemical fields	–	China	38-43,46,65,66,68,69, 107-128
Horizontal grid resolution	27 × 9 × 3 km	nested domains alleviate boundary effects and make the simulation more reliable; resolution with multiples of 3 is widely used in Asian studies and studies of countries outside the United States; more refined resolutions make the assimilation of fonts and relief easier	higher computational cost, longer simulation time	China	38,42,46,65, 66,68,69,111
Vertical grid resolution	14 / 30 / 35 layers	fewer vertical layers bring faster simulations and better understandings of the PBL and near-ground regions when concentrated in the lower layers of the troposphere; 30 to 35 layers are closer to ideal and are capable of representing the dynamics of the troposphere, both the PBL and the free troposphere	few layers do not reproduce well the evolution and transport of pollutants, such as mixtures with eddies, and heat exchange with the soil and relief; high reliefs end up becoming obstacles to good reproduction when you have this configuration; for 30 to 35 layers, higher computational cost and simulation time	China	68,109-111,113, 121,122,126,127
Boundary conditions	Nested/MOZART	nested models are used to smooth model boundary conditions placing grids with coarser resolutions before the grid targeted by the study means that concentrations of species outside the domain, when entering the domain, have less associated error	higher computational cost	China	38,39,41,65, 113,125,129
Chemical mechanism	Carbon Bond 06	as it is a mechanism that has a reduced size compared to other mechanisms and high precision when aggregating species by structure, this mechanism becomes attractive for simulations[77]	the chemistry of RO_2 radicals is very rudimentary according to Liu *et al.*[77]	China	39,66,68,69,107, 111,112,117,119-122, 124,127
Emission inventory	MEIC	Chinese government emissions inventory. Created for the territory with a wealth of sources, covering emissions of the main pollutants and greenhouse gases; With spatial detail, this inventory makes the detail of the emissions contribution to the emissions processor more effective, thus enabling CMAQ to project the reactions of primary pollutants with greater accuracy	–	China	39,66,68,69,107, 109,110,113,114, 118,125-127
Biogenic processor	MEGAN	global model with leaf area calculation, capable of extrapolating emission values more adequately than its predecessor based on different uses of soil and vegetation; it makes biogenic VOC emissions more suitable for the emissions processor and consequently for CMAQ kinetics calculations	most countries do not have sufficient data on vegetation cover and land use and occupation there are no LAI data for all types of vegetation and furthermore, there are still no emission factors for all biomes[94]	China	38-43,46,65,66, 68,69,109-116,118, 119,125,128,129

WRF: Weather Research and Forecast; CMAQ: Community Multi Scale Air Quality Model; PBL: Planetary Boundry Layer; MOZART: Model for Ozone and Related Chemical Tracers; RO_2: alkyl peroxyl radical; MEI: Multi-resolution Emission Inventory for China; MEGAN: Model of Emissions of Gases and Aerosols from Nature; VOC: volatile organic compound; CMAQ: Community Multi Scale Air Quality Model; LAI: leaf area index.

MEGAN as the biogenic processor. The least mentioned configurations were vertical layers, boundary conditions, and biogenic processors.

An important conclusion drawn from the literature survey was that the emission inventory is the most necessary configuration and causes the most concern within the CMAQ ozone modeling studies, which is also the most mentioned theme in the collected studies.

The importance of emission inventories arises because they allocate all emission sources in the studied domain, the temporal interval of the simulation, and all chemical species and reactions involved in the atmosphere domain. Emission inventories are complex and labor-intensive tools that most countries lack detailed enough, resulting in few sources or insufficient information for a model. Moreover, this data collection is crucial in the simulation because ozone, being a secondary pollutant, depends not only on emissions but also on a detailed atmosphere chemistry for better prediction. Therefore, the most significant error was found, and this review concludes that future ozone simulation studies should focus on detailing emission sources, encompassing the most significant possible number of sources within the domain. This would then also discretize their emissions and study appropriate chemical speciation along with local geography.

Another important observation is the chemical mechanisms, which need further detailing in reactions, especially involving the NO_y family, biogenic compounds, and secondary organic aerosol. These greatly influence ozone formation and, therefore, its simulation. Detailed understanding is needed to reduce underestimations and overestimations of the CMAQ.

For future reviews, it is suggested to include a topic on the WRF processors for microphysics, planetary boundary layer, and cumulus parameterization.

Acknowledgments

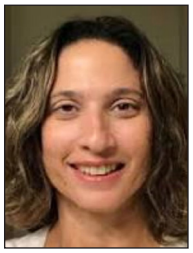
This work was carried out with the support of the Coordination for the Improvement of Higher Education Personnel-Brazil (CAPES)-Financing Code 001 and the FAPERJ project- apq1 e-26/211.921/2021.

Thiago F. da Costa *is a doctoral student at the State University of Rio de Janeiro (UERJ) in the postgraduate program in environmental engineering. Their undergraduate degree is in environmental engineering, with a master's degree in environmental technology. He has expertise in Python and R programming languages, as well as the QGIS software. Currently, during the doctoral program, he is working with the CMAQ model, the subject of the systematic review, to simulate the occurrence of episodes with high concentrations of tropospheric ozone in the metropolitan region of Rio de Janeiro.*

Josie B. B. Carvalho *is a doctoral student and holds a Master's degree in Environmental Engineering from the State University of Rio de Janeiro (UERJ). She is also an Environmental Chemistry Specialist from UERJ, with a Bachelor's degree in Chemistry Education from the University of Grande Rio (UNIGRANRIO) and a technical degree in Chemistry from the Federal Institute of Rio de Janeiro (IFRJ). As an educator, she is a faculty member of the Specialization Course in Sanitary and Environmental Engineering (CESA UERJ). Additionally, she serves as a reviewer for the Brazilian Journal of Environment (RVBMA) and evaluates programs such as PIBIEX, PROEXTENSÃO, PIBICT, and PROCIÊNCIA at IFRJ and IFBaiano.*

Rizzieri Pedruzzi *holds a degree in environmental engineering from Espírito Santenses Integrated Colleges (FAESA-ES), a Master's degree in environmental engineering from Federal University of Espírito Santo (UFES), and a PhD in Sanitation, Environment, and Water Resources from UFMG. Currently, he works as an associate professor at UERJ in the Department of Sanitary and Environmental Engineering at the School of Engineering. He has extensive experience in computational modeling, working with dispersion models such as CALLPUFF and AERMOD, as well as air quality models like CMAQ, as presented in the study. Additionally, he is involved in editing and processing emission inventories for the SMOKE model, meteorological modeling using the Weather Research and Forecasting (WRF) model, air quality modeling using Community Multiscale Air Quality (CMAQ), and assessment and validation of meteorological and air quality modeling using the Python language.*

Taciana T. A. Albuquerque *holds a degree in Meteorology from the Federal University of Alagoas (2003). She obtained her Master's degree (2005) and PhD (2010) in Atmospheric Sciences with an emphasis*



on Atmospheric Pollution from the Institute of Astronomy, Geophysics, and Atmospheric Sciences (IAG) at the University of São Paulo. She is an Associate Professor at the Federal University of Minas Gerais (UFMG) in the Department of Sanitary and Environmental Engineering. Albuquerque is a research professor affiliated with two postgraduate programs as a permanent member: the Postgraduate Program in Sanitation, Environment, and Water Resources (SMARH) at UFMG and the Postgraduate Program in Environmental Engineering (PPGEA) at the Federal University of Espírito Santo (UFES). Her expertise lies in Atmospheric Sciences, with a focus on air pollution. She engages in research related to Air Quality, Diagnosis and Assessment of Air Pollution, Air Pollution Control, Atmospheric Monitoring, Quantification and Characterization of Atmospheric Particles in Urban Environments, Emission Control Plans, Atmospheric Dispersion Studies (EDA), and the application of regional models for assessing air quality, the formation of secondary pollutants, and local meteorological conditions.

Eduardo M. Martins *holds a degree in Chemistry from the Federal University of Rio de Janeiro (1998), a master's degree in Physical Chemistry from the Federal University of Rio de Janeiro (2001), and a PhD in Physical Chemistry from the Federal University of Rio de Janeiro (2005). He conducted postdoctoral research at the University of California Irvine (UCI) in 2017. Currently, he is an associate professor at the Faculty of Technology at the State University of Rio de Janeiro. Monteiro has been involved in research in the field of urban atmospheric pollution, air quality management, kinetic processes of tropospheric ozone formation, emissions of gases from soils, and greenhouse gas emissions in landfills. He conducts experimental work monitoring non-regulated pollutants using chromatographic techniques and simulation work on the dispersion of atmospheric pollutants and chemical models. He is a professor in the Environmental Engineering Graduate Program (PEAMB/UERJ-Professional Master's), the Environmental Engineering Doctorate Program (DEAMB/UERJ), and the Chemistry Graduate Program (PPGQ/UERJ-Master's and PhD). Monteiro was awarded the Young Scientist of Our State by FAPERJ in 2015 and is a research productivity grantee from PROCIÊNCIA-UERJ.*

References

1. da Silveira, V. R.; de Oliveira Jr., J. F.; da Silva, M. S.; Silva, C.; Alves, A. R.; Pontes, A. S.; Pimentel, L. C. G.; Rotunno Filho, O. C.; *Land Use Policy* **2021**, *101*, 105148. [Crossref]
2. Wang, T.; Xue, L.; Brimblecombe, P.; Lam, Y. F.; Li, L.; Zhang, L.; *Sci. Total Environ.* **2017**, *575*, 1582. [Crossref]
3. Karlsson, P. E.; Klingberg, J.; Engardt, M.; Andersson, C.; Langner, J.; Karlsson, G. P.; Pleijel, H.; *Sci. Total Environ.* **2017**, *576*, 22. [Crossref]
4. Kwok, R. H. F.; Baker, K. R.; Napelenok, S. L.; Tonnesen, G. S.; *Geosci. Model Dev.* **2015**, *8*, 99. [Crossref]
5. Luecken, D. J.; Napelenok, S. L.; Strum, M.; Scheffe, R.; Phillips, S.; *Environ. Sci. Technol.* **2018**, *52*, 4668. [Crossref]
6. Shi, C.; Fernando, H. J. S.; Hyde, P.; *Sci. Total Environ.* **2012**, *416*, 374. [Crossref]
7. Byun, D.; Schere, K. L.; *Appl. Mech. Rev.* **2006**, *59*, 51. [Crossref]
8. Hernandes, E.; Zamboni A.; Fabbri, S.; *CLEI Electronic J.* **2012**, *15*, 3. [Crossref]
9. Hernandes, E.; Zamboni, A.; Fabbri, S.; *Start*, version 3.03 Beta; Universidade Federal de São Carlos, Brasil, 2012.
10. Page, M. J.; McKenzie, J. E.; Bossuyt, P. M.; Boutron, I.; Hoffmann, T. C.; Mulrow, C. D.; Shamseer, L.; Tetzlaff, J. M.; Akl, E. A.; Brennan, S. E.; Chou, R.; Glanville, J.; Grimshaw, J. M.; Hróbjartsson, A.; Lalu, M. M.; Li, T.; Loder, E. W.; Mayo-Wilson, E.; McDonald, S.; McGuinness, L. A.; Stewart, L. A.; Thomas, J.; Tricco, A. C.; Welch, V. A.; Whiting, P.; Moher, D.; *BMJ* **2021**, *372*, 71. [Crossref]
11. Liu, H.; Liu, S.; Xue, B.; Lv, Z.; Meng, Z.; Yang, X.; Xue, T.; Yu, Q.; He, K.; *Atmos. Environ.* **2018**, *173*, 223. [Crossref]
12. Liu, J.; Wang, L.; Li, M.; Liao, Z.; Sun, Y.; Song, T.; Gao, W.; Wang, Y.; Li, Y.; Ji, D.; Hu, B.; Wang, Y.; Kulmala, M.; *Atmos. Chem. Phys.* **2019**, *19*, 14477. [Crossref]
13. Moniruzzaman, C. G.; Bowden, J.; Arunachalam, S.; *Atmos. Environ.* **2020**, *243*, 117859. [Crossref]
14. Yang, X.; Wu, K.; Wang, H.; Liu, Y.; Gu, S.; Lu, Y.; Zhang, X.; Hu, Y.; Ou, Y.; Wang, S.; Wang, Z.; *Atmos. Environ.* **2020**, *226*, 117392. [Crossref]
15. Zhang, M.; Katiyar, A.; Zhu, S.; Shen, J.; Xia, M.; Ma, J.; Harsha Kota, S.; Wang, P.; Zhang, H.; *Atmos. Chem. Phys.* **2021**, *21*, 4025. [Crossref]
16. Chen, K.; Guo, H.; Hu, J.; Kota, S.; Deng, W.; Ying, Q.; Myllyvirta, L.; Dahiya, S.; Zhang, H.; *Resour., Conserv. Recycl.* **2019**, *142*, 232. [Crossref]
17. He, H.; Liang, X. Z.; Sun, C.; Tao, Z.; Tong, D. Q.; *Atmos. Chem. Phys.* **2020**, *20*, 3191. [Crossref]
18. Kang, D.; Mathur, R.; Pouliot, G. A.; Gilliam, R. C.; Wong, D. C.; *npj Clim. Atmos. Sci.* **2020**, *3*, 6. [Crossref]
19. Matichuk, R.; Tonnesen, G.; Luecken, D.; Gilliam, R.; Napelenok, S. L.; Baker, K. R.; Schwede, D.; Murphy, B.;

Helmig, D.; Lyman, S. N.; Roselle, S.; *J. Geophys. Res.: Atmos.* **2017**, *122*, 13545. [Crossref]
20. Qin, M.; Yu, H.; Hu, Y.; Russell, A. G.; Odman, M. T.; Doty, K.; Pour-Biazar, A.; McNider, R. T.; Knipping, E.; *Atmos. Environ.* **2019**, *202*, 167. [Crossref]
21. Vijayaraghavan, K.; Cho, S.; Morris, R.; Spink, D.; Jung, J.; Pauls, R.; Duffett, K.; *Atmos. Environ.* **2016**, *141*, 209. [Crossref]
22. Wang, P.; Chen, Y.; Hu, J.; Zhang, H.; Ying, Q.; *Environ. Sci. Technol.* **2019**, *53*, 1404. [Crossref]
23. Hakami, A.; Henze, D. K.; Seinfeld, J. H.; Singh, K.; Sandu, A.; Kim, S.; Byun, D.; Li, Q.; *Environ. Sci. Technol.* **2007**, *41*, 7807. [Crossref]
24. Cheng, X.; Hao, Z.; Zang, Z.; Liu, Z.; Xu, X.; Wang, S.; Liu, Y.; Hu, Y.; Ma, X.; *Atmos. Chem. Phys.* **2021**, *21*, 13747. [Crossref]
25. Park, S. Y.; Park, C.; You, J. W.; Lee, S. H.; Lee, H. W.; *Atmos. Environ.* **2018**, *192*, 104. [Crossref]
26. Penn, S. L.; Boone, S. T.; Harvey, B. C.; Heiger-Bernays, W.; Tripodis, Y.; Arunachalam, S.; Levy, J. I.; *Environ. Res.* **2017**, *156*, 791. [Crossref]
27. Sun, H.; Fung, J. C. H.; Chen, Y.; Chen, W.; Li, Z.; Huang, Y.; Lin, C.; Hu, M.; Lu, X.; *Sustainable Cities Soc.* **2021**, *75*, 103372. [Crossref]
28. Wang, M. Y.; Yim, S. H. L.; Wong, D. C.; Ho, K. F.; *Sci. Total Environ.* **2019**, *662*, 385. [Crossref]
29. Baker, K. R.; Woody, M. C.; Tonnesen, G. S.; Hutzell, W.; Pye, H. O. T.; Beaver, M. R.; Pouliot, G.; Pierce, T.; *Atmos. Environ.* **2016**, *140*, 539. [Crossref]
30. Qu, K.; Wang, X.; Yan, Y.; Shen, J.; Xiao, T.; Dong, H.; Zeng, L.; Zhang, Y.; *Atmos. Chem. Phys. Discussions* **2021**, 1. [Crossref]
31. Sharma, S.; Sharma, P.; Khare, M.; *Atmos. Environ.* **2017**, *159*, 34. [Crossref]
32. Shu, L.; Xie, M.; Wang, T.; Gao, D.; Chen, P.; Han, Y.; Li, S.; Zhuang, B.; Li, M.; *Atmos. Chem. Phys.* **2016**, *16*, 15801. [Crossref]
33. Flynn, C. M.; Pickering, K. E.; Crawford, J. H.; Weinheimer, A. J.; Diskin, G.; Thornhill, K. L.; Loughner, C.; Lee, P.; Strode, S. A.; *Atmos. Environ.* **2016**, *147*, 133. [Crossref]
34. Jaén, C.; Udina, M.; Bech, J.; *Atmos. Environ.* **2021**, *246*, 118037. [Crossref]
35. Li, X.; Choi, Y.; Czader, B.; Roy, A.; Kim, H.; Lefer, B.; Pan, S.; *Atmos. Chem. Phys.* **2016**, *16*, 3127. [Crossref]
36. Pan, S.; Choi, Y.; Roy, A.; Jeon, W.; *Atmos. Environ.* **2017**, *164*, 398. [Crossref]
37. Faggion Jr., C. M.; Hagenfeld, D.; *J. Dent.* **2019**, *86*, 89. [Crossref]
38. Xu, Y.; Shen, A.; Jin, Y.; Liu, Y.; Lu, X.; Fan, S.; Hong, Y.; Fan, Q.; *Atmos. Environ.* **2023**, *303*, 119757. [Crossref]
39. Yi, X.; Sarwar, G.; Bian, J.; Huang, L.; Li, Q.; Jiang, S.; Liu, H.; Wang, Y.; Chen, H.; Wang, T.; Chen, J.; Saiz-Lopez, A.; Wong, D. C.; Li, L.; *J. Geophys. Res.: Atmos.* **2023**, *128*, e2023JD038898. [Crossref]
40. Qi, Q.; Wang, S.; Zhao, H.; Kota, S. H.; Zhang, H.; *J. Cleaner Prod.* **2023**, *401*, 136801. [Crossref]
41. Qu, K.; Wang, X.; Cai, X.; Yan, Y.; Jin, X.; Vrekoussis, M.; Kanakidou, M.; Brasseur, G. P.; Shen, J.; Xiao, T.; Zeng, L.; Zhang, Y.; *Atmos. Chem. Phys.* **2023**, *23*, 7653. [Crossref]
42. Lou, C.; Jiang, F.; Tian, X.; Zou, Q.; Zheng, Y.; Shen, Y.; Feng, S.; Chen, J.; Zhang, L.; Jia, M.; Xu, J.; *Sci. Total Environ.* **2023**, *865*, 161212. [Crossref]
43. Zhu, S.; Wang, P.; Wang, S.; Geng, G.; Zhao, H.; Wang, Y.; Zhang, H.; *Engineering* **2023**, *28*, 130. [Crossref]
44. Su, F.; Xu, Q.; Yin, S.; Wang, K.; Liu, G.; Wang, P.; Kang, M.; Zhang, R.; Ying, Q.; *J. Environ. Manage.* **2023**, *338*, 117778. [Crossref]
45. Mathur, R.; Kang, D.; Napelenok, S. L.; Xing, J.; Hogrefe, C.; Sarwar, G.; Itahashi, S.; Henderson, B. H.; *J. Geophys. Res.: Atmos.* **2022**, *127*, e2022JD036926. [Crossref]
46. Kim, T.; Choi, D.; Ko, W.; Kim, Y.; Kim, J.; Kwak, K. H.; Kang, Y. H.; Kim, S.; *Atmos. Environ.* **2023**, *314*, 120071. [Crossref]
47. Skamarock, W. C.; Klemp, J. B.; Dudhia, J.; Gill, D. O.; Barker, D. M.; Wang, W.; Powers, J. G.; *NCAR Technical Note* **2008**, *475*, 113. [Crossref]
48. Skipper, T. N.; Hu, Y.; Odman, M. T.; Henderson, B. H.; Hogrefe, C.; Mathur, R.; Russell, A. G.; *Environ. Sci. Technol.* **2021**, *55*, 4504. [Crossref]
49. Bates, J. T.; Pennington, A. F.; Zhai, X.; Friberg, M. D.; Metcalf, F.; Darrow, L.; Strickland, M.; Mulholland, J.; Russell, A.; *Environ. Modell. Software* **2018**, *109*, 182. [Crossref]
50. Nguyen, G. T. H.; Shimadera, H.; Sekiguchi, A.; Matsuo, T.; Kondo, A.; *Atmos. Environ.* **2019**, *207*, 182. [Crossref]
51. Yu, S.; Mathur, R.; Pleim, J.; Wong, D.; Gilliam, R.; Alapaty, K.; Zhao, C.; Liu, X.; *Atmos. Chem. Phys.* **2014**, *14*, 11247. [Crossref]
52. Nguyen, G. T. H.; Shimadera, H.; Uranishi, K.; Matsuo, T.; Kondo, A.; *Atmos. Environ.* **2020**, *226*, 117398. [Crossref]
53. Zheng, Y.; Jiang, F.; Feng, S.; Cai, Z.; Shen, Y.; Ying, C.; Wang, X.; Liu, Q.; *Sci. Total Environ.* **2021**, *768*, 144520. [Crossref]
54. Rooney, B.; Zhao, R.; Wang, Y.; Bates, K. H.; Pillarisetti, A.; Sharma, S.; Kundu, S.; Bond, T. C.; Lam, N. L.; Ozaltun, B.; Xu, L.; Goel, V.; Fleming, L. T.; Weltman, R.; Meinardi, S.; Blake, D. R.; Nizkorodov, S. A.; Edwards, R. D.; Yadav, A.; Arora, N. K.; Smith, K. R.; Seinfeld, J. H.; *Atmos. Chem. Phys.* **2019**, *19*, 7719. [Crossref]
55. Baker, K. R.; Nguyen, T. K. V.; Sareen, N.; Henderson, B. H.; *Atmos. Environ.* **2020**, *234*, 117543. [Crossref]
56. Li, X.; Rappenglueck, B.; *Atmos. Environ.* **2018**, *195*, 210. [Crossref]
57. Yang, Y.; Zhao, Y.; Zhang, L.; Zhang, J.; Huang, X.; Zhao, X.; Zhang, Y.; Xi, M.; Lu, Y.; *Atmos. Chem. Phys.* **2021**, *21*, 1191. [Crossref]
58. Valverde, V.; Pay, M. T.; Baldasano, J. M.; *Sci. Total Environ.* **2016**, *543*, 670. [Crossref]

59. Tao, H.; Xing, J.; Zhou, H.; Chang, X.; Li, G.; Chen, L.; Li, J.; *Atmos. Environ.* **2018**, *189*, 9. [Crossref]
60. Wu, K.; Yang, X.; Chen, D.; Gu, S.; Lu, Y.; Jiang, Q.; Wang, K.; Ou, Y.; Qian, Y.; Shao, P.; Lu, S.; *Atmos. Res.* **2020**, *231*, 104656. [Crossref]
61. Zhang, Y.; Bash, J. O.; Roselle, S. J.; Shatas, A.; Repinsky, A.; Mathur, R.; Hogrefe, C.; Piziali, J.; Jacobs, T.; Gilliland, A.; *Sci. Total Environ.* **2020**, *744*, 140960. [Crossref]
62. Russell, A.; Dennis, R.; *Atmos. Environ.* **2000**, *34*, 2283. [Crossref]
63. Yao, S.; Wei, W.; Cheng, S.; Niu, Y.; Guan, P.; *Atmosphere* **2021**, *12*, 619. [Crossref]
64. Wu, K.; Wang, Y.; Qiao, Y.; Liu, Y.; Wang, S.; Yang, X.; Wang, H.; Lu, Y.; Zhang, X.; Lei, Y.; *Environ. Pollut.* **2022**, *300*, 118914. [Crossref]
65. Wang, R.; Wang, L.; Sun, J.; Zhang, L.; Li, Y.; Li, K.; Liu, B.; Zhang, J.; Wang, Y.; *Sci. Total Environ.* **2023**, *905*, 166987. [Crossref]
66. Fan, S.; Li, Y.; *Sci. Total Environ.* **2023**, *860*, 160456. [Crossref]
67. Wu, R.; Zhao, Y.; Xia, S.; Hu, W.; Xie, F.; Zhang, Y.; Sun, J.; Yu, H.; An, J.; Wang, Y.; *Sci. Total Environ.* **2022**, *812*, 152447. [Crossref]
68. Lei, Y.; Wu, K.; Zhang, X.; Kang, P.; Du, Y.; Yang, F.; Fan, J.; Hou, J.; *Atmos. Res.* **2023**, *285*, 106619. [Crossref]
69. He, G.; He, C.; Wang, H.; Lu, X.; Pei, C.; Qiu, X.; Liu, C.; Wang, Y.; Liu, N.; Zhang, J.; Lei, L.; Liu, Y.; Wang, H.; Deng, T.; Fan, Q.; Fan, S.; *Atmos. Chem. Phys.* **2023**, *23*, 13107. [Crossref]
70. Karl, M.; Bieser, J.; Geyer, B.; Matthias, V.; Jalkanen, J. P.; Johansson, L.; Fridell, E.; *Atmos. Chem. Phys.* **2019**, *19*, 1721. [Crossref]
71. Liu, T.; Lau, A. K. H.; Sandbrink, K.; Fung, J. C. H.; *J. Geophys. Res.: Atmos.* **2018**, *123*, 4175. [Crossref]
72. Wang, X.; Li, L.; Gong, K.; Mao, J.; Hu, J.; Li, J.; Liu, Z.; Liao, H.; Qiu, W.; Yu, Y.; Dong, H.; Guo, S.; Hu, M.; Zeng, L.; Zhang, Y.; *Atmos. Environ.* **2021**, *246*, 118131. [Crossref]
73. Kota, S. H.; Guo, H.; Myllyvirta, L.; Hu, J.; Sahu, S. K.; Garaga, R.; Ying, Q.; Gao, A.; Dahiya, S.; Wang, Y.; Zhang, H.; *Atmos. Environ.* **2018**, *180*, 244. [Crossref]
74. Baker, K. R.; Woody, M. C.; Valin, L.; Szykman, J.; Yates, E. L.; Iraci, L. T.; Choi, H. D.; Soja, A. J.; Koplitz, S. N.; Zhou, L.; Campuzano-Jost, P.; Jimenez, J. L.; Hair, J. W.; *Sci. Total Environ.* **2018**, *637-638*, 1137. [Crossref]
75. Mathur, R.; Xing, J.; Gilliam, R.; Sarwar, G.; Hogrefe, C.; Pleim, J.; Pouliot, G.; Roselle, S.; Spero, T. L.; Wong, D. C.; Young, J.; *Atmos. Chem. Phys.* **2017**, *17*, 12449. [Crossref]
76. Chen, X.; Liu, Y.; Lai, A.; Han, S.; Fan, Q.; Wang, X.; Ling, Z.; Huang, F.; Fan, S.; *Environ. Pollut.* **2018**, *232*, 55. [Crossref]
77. Liu, Y.; Li, J.; Ma, Y.; Zhou, M.; Tan, Z.; Zeng, L.; Lu, K.; Zhang, Y.; *J. Environ. Sci.* **2023**, *123*, 522. [Crossref]
78. Kitayama, K.; Morino, Y.; Yamaji, K.; Chatani, S.; *Atmos. Environ.* **2019**, *198*, 448. [Crossref]
79. Luecken, D. J.; Phillips, S.; Sarwar, G.; Jang, C.; *Atmos. Environ.* **2008**, *42*, 5805. [Crossref]
80. Emery, C.; Jung, J.; Koo, B.; Yarwood, G.*; Improvements to CAMx Snow Cover Treatments and Carbon Bond Chemical Mechanism for Winter Ozone*; Utah Department of Environmental Quality: USA, 2015. [Link] accessed in March 2024
81. Hong, Y.; Liu, Y.; Chen, X.; Fan, Q.; Chen, C.; Chen, X.; Wang, M.; *Sci. Total Environ.* **2020**, *723*, 137697. [Crossref]
82. Li, S.; Zhang, Y.; Zhao, J.; Sarwar, G.; Zhou, S.; Chen, Y.; Yang, G.; Saiz-Lopez, A.; *Atmosphere* **2020**, *11*, 849. [Crossref]
83. Gantt, B.; Sarwar, G.; Xing, J.; Simon, H.; Schwede, D.; Hutzell, W. T.; Mathur, R.; Saiz-Lopez, A.; *Environ. Sci. Technol.* **2017**, *51*, 1458. [Crossref]
84. Muñiz-Unamunzaga, M.; Borge, R.; Sarwar, G.; Gantt, B.; de la Paz, D.; Cuevas, C. A.; Saiz-Lopez, A.; *Sci. Total Environ.* **2018**, *610-611*, 1536. [Crossref]
85. Fu, X.; Wang, T.; Zhang, L.; Li, Q.; Wang, Z.; Xia, M.; Yun, H.; Wang, W.; Yu, C.; Yue, D.; Zhou, Y.; Zheng, J.; Han, R.; *Atmos. Chem. Phys.* **2019**, *19*, 1. [Crossref]
86. Liu, Y.; Wang, T.; *Atmos. Chem. Phys.* **2020**, *20*, 6323. [Crossref]
87. Tang, Y.; Bian, H.; Tao, Z.; Oman, L. D.; Tong, D.; Lee, P.; Campbell, P. C.; Baker, B.; Lu, C. H.; Pan, L.; Wang, J.; McQueen, J.; Stajner, I.; *Atmos. Chem. Phys.* **2021**, *21*, 2527. [Crossref]
88. Sharma, S.; Khare, M.; *Atmos. Environ.* **2017**, *151*, 117. [Crossref]
89. Bieser, J.; Aulinger, A.; Matthias, V.; Quante, M.; Builtjes, P.; *Geosci. Model. Dev.* **2011**, *4*, 47. [Crossref]
90. Ring, A. M.; Canty, T. P.; Anderson, D. C.; Vinciguerra, T. P.; He, H.; Goldberg, D. L.; Ehrman, S. H.; Dickerson, R. R.; Salawitch, R. J.; *Atmos. Environ.* **2018**, *173*, 96. [Crossref]
91. Shankar, U.; McKenzie, D.; Prestemon, J. P.; Haeng Baek, B.; Omary, M.; Yang, D.; Xiu, A.; Talgo, K.; Vizuete, W.; *Atmos. Chem. Phys.* **2019**, *19*, 15157. [Crossref]
92. Jeon, W.; Choi, Y.; Souri, A. H.; Roy, A.; Diao, L.; Pan, S.; Lee, H. W.; Lee, S. H.; *Sci. Total Environ.* **2018**, *613-614*, 820. [Crossref]
93. Guenther, A.; Nicholas, C.; Fall, R.; Klinger, L.; Mckay, W. A.; Scholes, B.; *J. Geophys. Res.* **1995**, *100*, 8873. [Crossref]
94. Guenther, A.; Karl, T.; Harley, P.; Weidinmyer, C.; Palmer, P. I.; Geron, C.; *Atmos. Chem. Phys.* **2006**, *6*, 3181. [Crossref]
95. Wang, P.; Liu, Y.; Dai, J.; Fu, X.; Wang, X.; Guenther, A.; Wang, T.; *J. Geophys. Res.: Atmos.* **2021**, *126*, e2020JD033263. [Crossref]
96. Liu, S.; Xing, J.; Zhang, H.; Ding, D.; Zhang, F.; Zhao, B.; Sahu, S. K.; Wang, S.; *Atmos. Environ.* **2019**, *218*, 117020. [Crossref]
97. Liu, Y.; Fan, Q.; Chen, X.; Zhao, J.; Ling, Z.; Hong, Y.; Li, W.; Chen, X.; Wang, M.; Wei, X.; *Atmos. Chem. Phys.* **2018**, *18*, 2709. [Crossref]
98. Abel, D. W.; Holloway, T.; Harkey, M.; Meier, P.; Ahl, D.; Limaye, V. S.; Patz, J. A.; *PLoS Med.* **2018**, *15*, e1002599. [Crossref]

99. Abel, D. W.; Holloway, T.; Martínez-Santos, J.; Harkey, M.; Tao, M.; Kubes, C.; Hayes, S.; *Environ. Sci. Technol.* **2019**, *53*, 3987. [Crossref]
100. Han, B. S.; Baik, J. J.; Kwak, K. H.; *Atmos. Environ.* **2019**, *218*, 117012. [Crossref]
101. Hata, H.; Hata, H.; Inoue, K.; Kokuryo, K.; Tonokura, K.; *Environ. Sci. Technol.* **2020**, *54*, 5947. [Crossref]
102. Huang, C.; Wang, T.; Niu, T.; Li, M.; Liu, H.; Ma, C.; *Atmos. Environ.* **2021**, *251*, 118276. [Crossref]
103. Liu, Y.; Li, L.; An, J.; Huang, L.; Yan, R.; Huang, C.; Wang, H.; Wang, Q.; Wang, M.; Zhang, W.; *Atmos. Environ.* **2018**, *186*, 113. [Crossref]
104. Wang, N.; Lyu, X. P.; Deng, X. J.; Guo, H.; Deng, T.; Li, Y.; Yin, C. Q.; Li, F.; Wang, S. Q.; *Sci. Total Environ.* **2016**, *573*, 1554. [Crossref]
105. Yu, M.; Zhu, Y.; Lin, C. J.; Wang, S.; Xing, J.; Jang, C.; Huang, J.; Huang, J.; Jin, J.; Yu, L.; *J. Environ. Manage.* **2019**, *244*, 127. [Crossref]
106. Zhang, J.; Choi, M.; Ji, Y.; Zhang, R.; Zhang, R.; Ying, Q.; *ACS Earth Space Chem.* **2021**, *5*, 1958. [Crossref]
107. Huang, C.; Niu, T.; Wu, H.; Qu, Y.; Wang, T.; Li, M.; Li, R.; Liu, H.; *Remote Sens* **2023**, *15*, 1711. [Crossref]
108. Skipper, T. N.; Lawal, A. S.; Hu, Y.; Russell, A. G.; *Atmos. Environ.* **2023**, *294*, 119492. [Crossref]
109. Yaluk, E. A.; Wang, Y.; Jiang, S.; Huang, L.; Lu, G.; Zhu, A.; Bian, J.; Xue, J.; Du, Y.; Chen, N.; Manomaiphiboon, K.; Chen, H.; Zhang, K.; Li, L.; *Atmos. Environ.* **2023**, *309*, 119931. [Crossref]
110. Wang, Y.; Jiang, S.; Huang, L.; Lu, G.; Kasemsan, M.; Yaluk, E. A.; Liu, H.; Liao, J.; Bian, J.; Zhang, K.; Chen, H.; Li, L.; *Sci. Total Environ.* **2023**, *872*, 162118. [Crossref]
111. Cho, S. Bin; Song, S.-K.; Shon, Z.-H.; Moon, S.-H.; *Sci. Total Environ.* **2023**, *882*, 163021. [Crossref]
112. Chang, J. H. W.; Griffith, S. M.; Kong, S. S. K.; Chuang, M. T.; Lin, N. H.; *Atmos. Chem. Phys.* **2023**, *23*, 6357. [Crossref]
113. Ouyang, S.; Deng, T.; Liu, R.; Chen, J.; He, G.; Leung, J. C. H.; Wang, N.; Liu, S. C.; *Atmos. Chem. Phys.* **2022**, *22*, 10751. [Crossref]
114. Ma, J.; Zhu, S.; Wang, S.; Wang, P.; Chen, J.; Zhang, H.; *Atmos. Chem. Phys.* **2023**, *23*, 4311. [Crossref]
115. Xiong, K.; Xie, X.; Mao, J.; Wang, K.; Huang, L.; Li, J.; Hu, J.; *Environ. Pollut.* **2023**, *319*, 120926. [Crossref]
116. Shen, Y.; Jiang, F.; Feng, S.; Xia, Z.; Zheng, Y.; Lyu, X.; Zhang, L. Y.; Lou, C.; *Sci. Total Environ.* **2023**, *858*, 159767. [Crossref]
117. Wang, R.; Duan, W.; Cheng, S.; Wang, X.; *Sci. Total Environ.* **2023**, *887*, 164113. [Crossref]
118. Qi, H.; Duan, W.; Cheng, S.; Cai, B.; *Chemosphere* **2023**, *337*, 139258. [Crossref]
119. Jung, D.; Soler, R.; de la Paz, D.; Notario, A.; Muñoz, A.; Ródenas, M.; Vera, T.; Borrás, E.; Borge, R.; *Chemosphere* **2023**, *341*, 139919. [Crossref]
120. Kuo, C. P.; Fu, J. S.; *Environ. Int.* **2023**, *176*, 107969. [Crossref]
121. Baker, K. R.; Valin, L.; Szykman, J.; Judd, L.; Shu, Q.; Hutzell, B.; Napelenok, S.; Murphy, B.; Connors, V.; *Sci. Total Environ.* **2023**, *903*, 166606. [Crossref]
122. Baker, K. R.; Liljegren, J.; Valin, L.; Judd, L.; Szykman, J.; Millet, D. B.; Czarnetzki, A.; Whitehill, A.; Murphy, B.; Stanier, C.; *Atmos. Environ.* **2023**, *293*, 119465. [Crossref]
123. Chuang, M. T.; Chou, C. C. K.; Lin, C. Y.; Lee, J. H.; Lin, W. C.; Chen, W. N.; Liu, C. Y.; Chang, C. C.; *Atmos. Res.* **2023**, *287*, 106713. [Crossref]
124. Wan, Z.; Cai, Z.; Zhao, R.; Zhang, Q.; Chen, J.; Wang, Z.; *Mar. Pollut. Bull.* **2023**, *193*, 115169. [Crossref]
125. Wu, Y.; Chen, W.; You, Y.; Xie, Q.; Jia, S.; Wang, X.; *Atmos. Chem. Phys.* **2023**, *23*, 453. [Crossref]
126. Cao, J.; Pan, G.; Zheng, B.; Liu, Y.; Zhang, G.; Liu, Y.; *Environ. Pollut.* **2023**, *335*, 122290. [Crossref]
127. Fu, X.; Chen, D.; Wang, X.; Li, Y.; Lang, J.; Zhou, Y.; Guo, X.; *Sci. Total Environ.* **2023**, *903*, 166252. [Crossref]
128. Wang, K.; Xie, F.; Sulaymon, I. D.; Gong, K.; Li, N.; Li, J.; Hu, J.; *Sci. Total Environ.* **2023**, *859*, 160211. [Crossref]
129. Li, W.; Han, X.; Li, J.; Lun, X.; Zhang, M.; *Sci. Total Environ.* **2023**, *905*, 166602. [Crossref]

Submitted: December 13, 2023
Published online: March 28, 2024