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Editorial

Editorial for the Special Issue "Atmospheric Dispersion and Chemistry Models: Advances and Applications" (Second Edition)

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Atmospheric dispersion and chemical transport models (CTMs) are indispensable tools for understanding the behavior of pollutants in the atmosphere and their link to anthropogenic emission sources. Collectively, these modeling systems provide critical scientific support for air quality management, environmental policy-making, and public health protection. As the field advances with higher-resolution simulations, improved emissions characterization, and more sophisticated chemistry–dynamics coupling, the need for dedicated forums to disseminate these methodological and applied developments becomes increasingly vital.

The first Special Issue, which was also published as a book, covered several developments and applications related to atmospheric dispersion and chemistry models that occurred between 2022 and 2023 [1]. Those studies demonstrated the profound benefits of such models for diverse scientific and technical applications in atmospheric chemistry and environmental sciences, ranging from the characterization of aerosols and chemical species in the atmosphere to risk analyses and decision-making for pollutant releases, nuclear accidents, and climate change. Building on that success, this second volume, which is a follow-up to the first edition published three years ago, aims to showcase the latest progress in the field. The scope of this Special Issue encompasses the development of atmospheric dispersion models and CTMs, such as the implementation of new physical and chemical schemes, online and offline coupling with meteorological models, application studies related to atmospheric transport and chemistry, urban air quality assessments, and model evaluation.

This Special Issue comprises 10 high-quality articles that advance our understanding of atmospheric processes and improve the tools we use to simulate them. The articles in this volume are summarized below, reflecting a broad spectrum of research in atmospheric modeling. Thus, the first published article in this Special Issue, by Chen et al. [2], uses atmospheric dispersion modeling to assist in the definition of minimum detection limits (MDLs) for Continuous Monitoring Systems (CMSs), composed of a network of fixed-point sensors, for methane emissions at oil and gas facilities. Based on these analyses, recommendations are made with regard to assessing the MDL and how dispersion models can be used to normalize the results to standard sets of meteorological conditions. The second article, by Besiktas et al. [3], employed the ALOHA atmospheric dispersion model to simulate a natural gas pipeline jet fire in Istanbul, Türkiye. Their study underscores how source release factors—such as pipe length and diameter—and both synoptic and local atmospheric conditions influence thermal radiation threat distances. These findings provide essential data for enhancing emergency intervention and safety protocols for natural gas infrastructure. In the third paper, Janicke [4] proposed a methodology to simplify the complex nitrogen oxide chemistry in airport environments by deriving effective NO-to-NO_2 conversion rates.

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By integrating these rates into the LASPORT dispersion model and applying it to the Los Angeles International Airport environment, the study achieved a high correlation with the observed NO_2 concentrations. Farhane and Souhar [5] introduced a generalized 3D model for predicting pollutant concentrations incorporating various parameterizations for wind speed profiles, turbulent diffusivity, and dry deposition processes within the atmospheric boundary layer. The analytical solutions obtained were validated against empirical data under particular environmental scenarios. Li et al. [6] compared the CALPUFF modeling system and CFD simulations for toxic high-sulfur gas dispersion in complex mountainous terrain. Their results showed consistent patterns between the models, suggesting that CALPUFF could be used to provide emergency response in microscale mountainous environments instead of CFD models. Given its significantly lower computational cost, CALPUFF may serve as a viable alternative to CFD models in emergency scenarios where time is a critical factor.

Laudan et al. [7], explored the use of high-resolution urban climate modeling to mitigate air pollution hotspots in urban areas. To this end, they coupled the responsive traffic and emission model MATSim with the PALM-4U CFD-LES dispersion model—which incorporates a chemistry module—to implement a feedback loop between traffic dynamics and air quality. Their simulation of a time-based traffic toll in Berlin demonstrated that adaptive management can effectively lower NO_2 concentration peaks during morning rush hours. Parra [8], on the other hand, investigated the high $PM_{2.5}$ levels observed in Quito, Ecuador, during New Year celebrations, where emissions from fireworks and combustion frequently exceed World Health Organization (WHO) guidelines. Through numerical experiments using WRF-Chem, $PM_{2.5}$ maps were developed to study the dispersion and distribution of $PM_{2.5}$. The planetary boundary layer height (PBLH)—which was significantly lower in the city's southern district—was found to play a critical role in modulating pollution severity, establishing a robust framework for future air quality forecasting and public health warnings. Zhou et al. [9] presented the first comprehensive evaluation of the CUACE/Haze-Fog chemical transport model, operated by the China Meteorological Administration (CMA). By comparing daily forecasts against Sentinel-5P TROPOMI satellite column retrievals and ground observations, the authors identified a systematic underestimation of NO_2 during winter. This bias was attributed to a failure in propagating the surface data assimilation to NO_2 columns under complex vertical stratification, highlighting the need to integrate satellite-based vertical constraints into operational forecasting to improve accuracy in complex atmospheric conditions. Olaguer and Vaerten [10] used the MicroFACT chemical transport model to simulate an ozone episode in Detroit when ozone reached 76 ppb during prevailing southwesterly wind. Their findings suggest that the entrainment of ozone from layers aloft is critical for explaining historical limit exceedances. Finally, Bezerra et al. [11] investigated wildfire-driven pyro-convective cloud development in the southern Amazon using the Meso-NH model. The results provide a basis for future developments related to understanding tropical pyro-convective clouds and indicate that background thermodynamic instability is the primary control in vertical plume development, modulating the role of fire intensity. Incorporating high-resolution thermodynamic profiles into coupled CTMs could improve the representation and characterization of such events.

The 10 papers that comprise this second Special Issue of "Atmospheric Dispersion and Chemistry Models: Advances and Applications" demonstrate the remarkable versatility of contemporary modeling frameworks. From optimizing methane detection networks to designing air quality-driven traffic policies, these studies underscore the essential role of atmospheric dispersion and chemical transport models in advancing atmospheric chemistry and supporting informed environmental decision-making.

Conflicts of Interest: The author declares no conflicts of interest.

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