MODELLING EMISSION CONTRIBUTIONS TO AIR QUALITY CONCENTRATIONS DURING A COVID-19 LOCKDOWN

Roberto San José
Juan L. Pérez-Camanyo
Environmental Software and Modelling Group
Computer Science School, Technical University of Madrid (UPM),
Madrid, Spain
E-mail: roberto@fi.upm.es

KEYWORDS
Source Apportionment, COVID-19, lockdown, CAMx, WRF/Chem

ABSTRACT

In this work two air quality simulations are run to analyze the impacts of the reduction of anthropogenic emissions during COVID-19 lockdown over Madrid (Spain) area: one simulation considers the emission reductions during the lockdown (COVID simulation) and a second simulation," business as usual" (BAU simulation) with an emissions scenario without restrictions. Source apportionment techniques are used to identify and quantify the contributions from main pollution sources with the purpose to provide understanding on what measures should be taken to address them and this work shows the potential of these technique. This study helps to elucidate the complex and nonlinear response of O3 and PM concentrations after a reduction of emissions mainly from the transport sector, during the COVID-19 lockdown period.

INTRODUCTION

The atmospheric dispersion of pollutants released to the atmosphere depends on many factors that must be modelled, therefore the modelling of pollutant dispersion is a complex engineering problem involving several disciplines such as mathematics, computation, physics and chemistry (Lateb et al., 2016). Many physical and chemical processes are involved in the movement of air pollutants, such as turbulence, wind drag, buoyancy forces, diffusive effects, etc. Air quality models (AQM) use mathematical and numerical techniques to simulate these physical and chemical processes (Gery et al., 1989).

Air quality models are important tools for air quality management systems because they can be used to identify source contributions to pollutant concentrations and to help design effective strategies to predict and reduce adverse air pollutants (Atkinson et al., 2013). As a modelling tool it allows us to simulate theoretical scenarios to understand their impacts before implementing them in reality, e.g. air quality models can be used during the licensing process to verify that a new emission source will not exceed ambient air quality norms or, if necessary, to determine additional appropriate control measures, it also allows us to evaluate the effectiveness of emission reduction strategies before implementing them and to determine which is the most robust for the population (Bell et al., 2025).

In most cities, the decrease in economic activities during the COVID-19 lockdown triggered a reduction in anthropogenic emissions. This situation provides a unique opportunity to check the performance of our numerical modelling tools. This exceptional situation, which has never been observed before, has made it possible to quantify in a real environment the decreases in concentrations of some pollutants and increases in other pollutants following a significant reduction in emissions, demonstrating the absence of a direct, and linear, relationship between emissions and concentrations (Oostendorp et al., 2019). Understanding how air quality responds to emission reductions will provide important information for the future development of emission control strategies. In this situation, to understand the air pollution concentrations attributed to both source regions and emission categories, the source apportionment of PM and O3 is applied. The brute force method was also applied to quantify the impacts of emission reductions on concentrations.

In a first analysis of the impacts of anthropogenic emission reductions during the COVID-19 lockdown on the Madrid area (Spain), a significant reduction of NOx levels was found, but O3 and PM concentrations increased. In this work the causes of the increases are examined using the Source Apportionment Technology (SAT) included in the Comprehensive Air Quality Model with Extensions (CAMx).

Source apportionment techniques are used to identify and quantify the contributions of major pollution sources in order to understand what measures should be taken to address them, and this work shows the potential of these techniques. SAT was used to estimate the contributions of multiple sources and pollutant types (NOx and VOCs) to ozone and particulate matter formation in a single model run.

Communications of the ECMS, Volume 37, Issue 1,
Proceedings, ©ECMS Enrico Vicario, Romeo Bandinelli,
Virginia Fani, Michele Mastroianni (Editors) 2023
ISBN: 978-3-937436-80-7/978-3-937436-79-1 (CD) ISSN 2522-2414

MODELLING TOOLS

The air quality simulations were performed using the regional Weather Research and Forecasting model (WRF) with Chemistry (WRF/Chem) model (Grell et al., 2005) and the CAMx (Comprehensive Air quality Model with eXtensions) with its extension SAT (Source Apportionment) to study the impact of the COVID-19 lockdown measures on air quality in Madrid city. CAMx is also driven by the WRF model (meteorological part of the WRF/Chem model). Both models use a Carbon Bond scheme as a gas-phase chemical mechanism. Two-sectional method for the particle size was selected to calculate the aerosol concentrations.

WRF/Chem and CAMx are numerical Eulerian (gridded) regional photochemical dispersion model, which could simulate the emission (from emission inventories), dispersion, chemical reaction, and removal of pollutants by marching the Eulerian continuity equation forward in time for each chemical species on a system of nested three-dimensional grids under different complex terrain and meteorological conditions.

The chemical initial and boundary conditions were extracted from the output (WACCM 0.9º x 0.-125º) of the Whole Atmosphere Community Climate Model (Marsh et al., 2013). WRF is driven by initial and boundary conditions provided every 6 h by the Global Forecast System (GFS) produced by the European National Centers for Environmental Prediction (NCEP), NCEP GDAS Final Analysis 0.25º (ds083.3).

We obtain anthropogenic emissions in Europe without the influence of COVID-19 lockdown measures from the CAMS-REG-AP (Granier et al., 2019) European emission inventory (v4.2_ry 2019) with a 0.05º by 0.1º spatial resolution, processed by the EMIMO (UPM) tool to produce WRF/Chem (Zavery e tl., 2008) and CAMx ready emissions (CMBZ-MOSAIC and CB06-CF), (San José et al., 2015).

The models were applied over three computational domains, one covering all Iberian Peninsula with a spatial resolution of 25 km, a second nested domain covering Madrid Community with 5 km of spatial resolution and finally the last nested domain with 1 km of spatial resolution over Madrid city. All domain with 35 vertical levels.

EXPERIMENT

The air quality models have been run for February, 1, 2020 to April, 12, 2020 with two days spin up period. On March, 8, 2020, the first emission reductions were observed. On March, 15, 2020, the national lockdown was effective. On March, 28, 2020, the Spanish government banned all non-essential activity. On April, 13, 2020, workers in some non-essential sectors, such as construction and industry, who could not work remotely were allowed to return to work. Based on this date we have split the simulation time period in two symmetric periods with 36 days each one, the first one 01/February – 07/March called as pre-lockdown period and 08/March-12/April called lockdown period.

Two emission scenarios were prepared to retrieve the impacts of lockdown measures on pollutant levels and composition.: one is the business as usual scenario (BAU) and a rescaled emission scenario after March 8, referred to as COVID simulation, where anthropogenic emissions were reduced according to the lockdown meauseres. BAU ignores the changes due to the lockdown measures and is thus representative of what would have happened under BAU conditions.

Emissions reductions estimations during the lockdown period (COVID simulation) were published in a recent article (Guevara et al., 2021). Here, we have specific daily reduction rates for the following emission activities: public power, industry, road transport and aviation for each European country.

RESULTS

We have compared the hourly simulated concentrations with observational hourly data from the Madrid municipality and regional air quality observation networks with 48 monitoring station to analyze the WRF/Chem simulations performance. To have a representative and unique value, statistical performance indicators are calculated using the average values of the 48 monitoring stations and the corresponding model values for the COVID simulation.

Figure 1 and Figure 2 show the hourly time series of the concentrations estimated by the WRF/Chem and WRF-CAMx models for the pollutants NO2 and O3 compared with the measured data to analyze the performance of both modeling tools. The simulation period includes a period prior to the lockdown (pre-lockdown) and another corresponding to the lockdown itself to see how the models behave before two totally different situations from the point of view of emissions.

The two figures also provide an indication of the effects of lockdown on the concentrations of the two pollutants. In the lockdown period, a significant reduction in NO2 concentrations is observed, but O3 concentrations increase.

A summary of the performance of the WRF/Chem and WRF-CAMx models for the main four pollutans: NO2,O3, PM10 and PM2.5 is showed in Table 1. The performance is measured with the following statistical parameters: Normalized Mean Nias (NMB), root mean square error (RMSE) and square correlation coefficient (R2). Both RMSE and R2 quantify how well a regression model fits a dataset. The RMSE tells us how well a regression model can predict the value of the response variable in absolute terms while NMB tells us how well a model can predict the value of the response variable in percentage terms. In general, the performance results of both models show that the simulations capture the magnitude and temporal evolution of the two key air pollutants reasonably well, with the statistical indicators within the expected ranges.

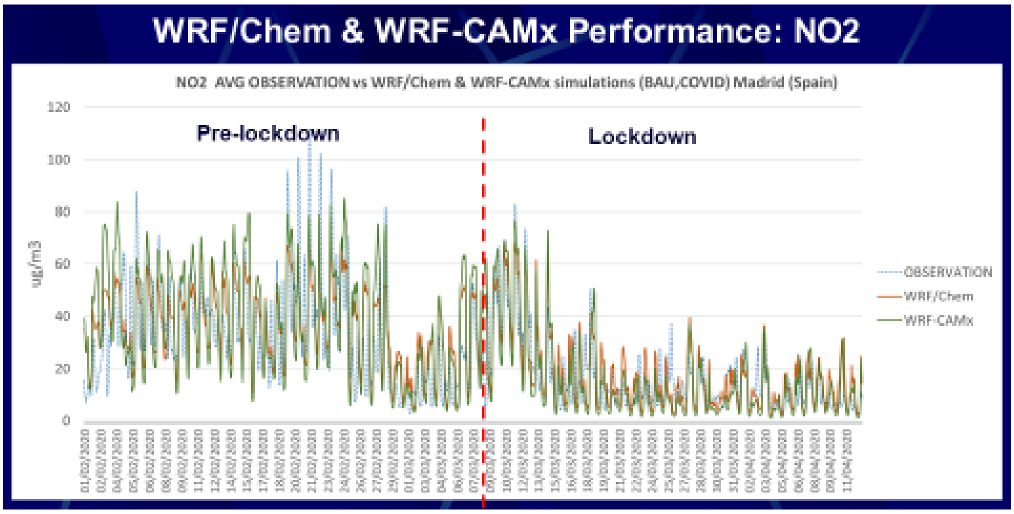

Figure 1: NO_2 (ug/m^3) time series of the WRF/Chem, WRF-CAMx models and mean of the 48 observations from de Madrid monitoring networks. Period: 01/02/2020 – 11/04/2020

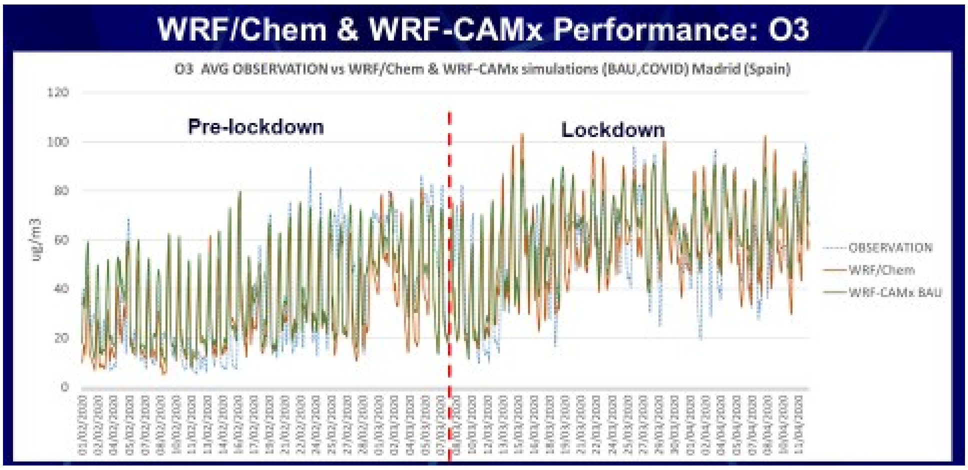

Figure 2: O_3 (ug/m^3) time series of the WRF/Chem, WRF-CAMx models and mean of the 48 observations from de Madrid monitoring networks. Period: 01/02/2020 – 11/04/2020

Table 1: Performance of the model simulations

		NMB (%)		**RMSE (µg/m3)**		**R^2 [0,1]**	
	Model	Pre-lockdown	Lock-down	Pre-lockdown	Lock-down	Pre-lockdown	Lock-down
NO_2	WRF/Chem	18	9	14	9	0.67	0.72
	WRF-CAMx	15	-5	19	10	0.57	0.76
O_3	WRF/Chem	-14	-2	15	13	0.75	0.78
	WRF-CAMx	3	7	15	13	0.74	0.76
PM10	WRF/Chem	18	-18	14	20	0.67	0.46
	WRF-CAMx	-18	-11	20	9	0.46	0.67
PM2.5	WRF/Chem	27	24	11	6	0.53	0.57
	WRF-CAMx	-16	-14	9	5	0.48	0.55

Good results have been obtained for NO_2 and O_3 with a small overestimation of NO_2 and underestimation of O_3 in the WRF/Chem simulation. For particulate matter the WRF-CAMx simulation obtains poorer R^2 results and a small underestimation below 20%. Model performance for is influenced by uncertainties in emission inventories. The best performance corresponds to the lockdown period. Simulated results for the lockdown period, using the adjusted emission inventory agree better with surface observations than the pre-lockdown period, where the BAU emission inventory is applied. NMB numbers and correlation coefficient is found to be better than in the pre-lockdown period. The improvement in model performance in the lockdown period demonstrate the good accuracy of the emission restriction estimated in Guevara et al., 2020. This air quality simulation is somehow a validation approach of the emission reductions proposed by Guevara et al., 2021.

The proposed approach compares two simulations: COVID simulation which tries to reproduce the observed data in the monitoring stations with emission reductions respect to the BAU simulation (no lockdown restriction) with the the simulation tools WRF-CAMx. Figure 3 and Figure 4 present the impacts (absolute difference between COVID and BAU simulations) of lockdown measures on the O_3 and NO_2 time average concentrations for the period March 08 to April 12.

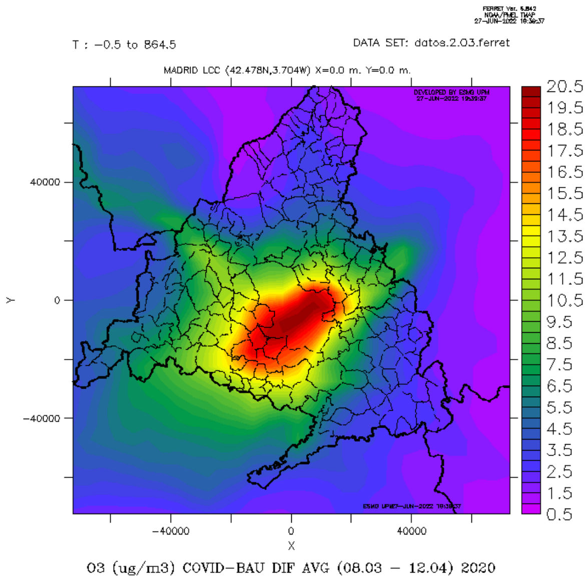

Figure 3: Map of differences (COVID-BAU) of average surface concentrations (μg m−3) for the period March, 08 to April, 12 for ozone with WRF-CAMx (right).

Figure 3 shows that there is an increase in O3 concentrations of up to 20 ug/m3 in the central area of the Community of Madrid, just where there has been a larger reduction in emissions, especially from traffic. We can also see that there is almost no impact on the outside of Madrid and therefore the reduction in emissions has not affected it.

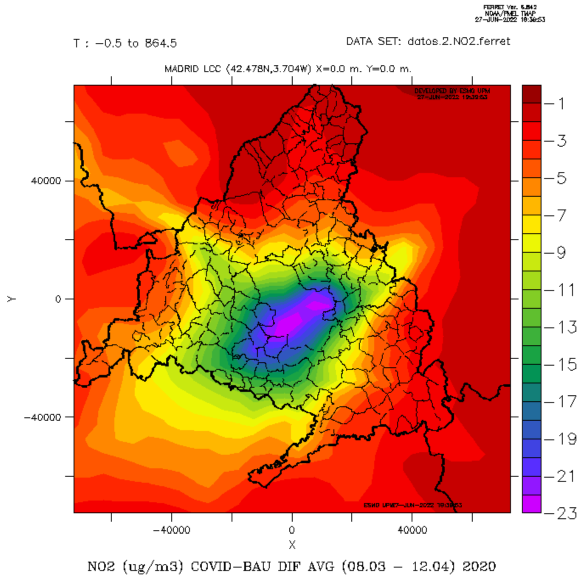

Figure 4: Map of differences (COVID-BAU) of average NO2 surface concentrations (μg m−3) for the period March, 08 to April, 12 for ozone with the WRF-CAMx .

Figure 4 shows how the impacts on NO_2 concentrations from emission reductions due to lock-down The largest reduction is seen in the city of Madrid due to the decrease in traffic emissions, in the area of the city of Madrid. Reductions were larger in urban areas and mainly localized along major traffic highways and highly populated areas. As NO decreases, the depletion of O3 during nighttime proceeds less efficiently, resulting in more O3 available at night particularly around urban areas and major highways.

We have applied the technique the Source apportionment (SAT) to estimates the contributions from 4 source areas: North-West (Z1), North-East (Z2), South-West (Z3) and South-East (Z4) quadrants of the computational domain, and 12 emissions categories: Public power (S1), Industry(S2), Other Stationary combustions (S3), Fugitives (S4), Solvents (S5), Road transport (S6), Shipping (S7), Aviation (S8), Off road (S9), Waste (S10), Agricultural livestock (S11) and Other agricultural (S12). The SAT also allows to know the contribution of the boundary conditions. In case of O3 the SAT methodology also estimates the fractions of ozone formed under VOC- or NOX-limited conditions. In Madrid O3 formation is dominated by VOC limited conditions it is when the rate of OH production is less than the rate of production of NOx, ozone production is VOC-limited. Here, ozone is most effectively reduced by lowering VOCs in case of NOx reductions, there will be O3 increments. Figure 5 shows the contribution (%) of the analysed elements with the SAT technology.

In Figure 5 we can see that 50% of the O3 comes from the boundary conditions. Solvent use is the main emission source and the contribution is larger in the south of the Madrid region (zone 3 and 4). During the lockdown period (COVID simulation) there is a reduction of the contribution of road transport (S6), but increase the contribution of solvents (S5) under VOC limited conditions. When the rate of OH production is less than the rate of production of NOx, ozone production is VOC-limited. Here, ozone is most effectively reduced by lowering VOCs. Between the NOx- and VOC-limited extremes there is a transitional region where ozone is nearly equally sensitive to each species. When the rate of OH production is greater than the rate of production of NOx, indicating that NOx is in short supply, the rate of ozone production is NOx-limited. In this situation, ozone concentrations are most effectively reduced by lowering current and future NOx emissions, rather than lowering emissions of VOCs. Solvents in products such as coatings, inks, and consumer products can emit substances into the air known as Volatile Organic Compounds (VOCs). VOC emissions from solvent-based products are regulated to protect air quality.

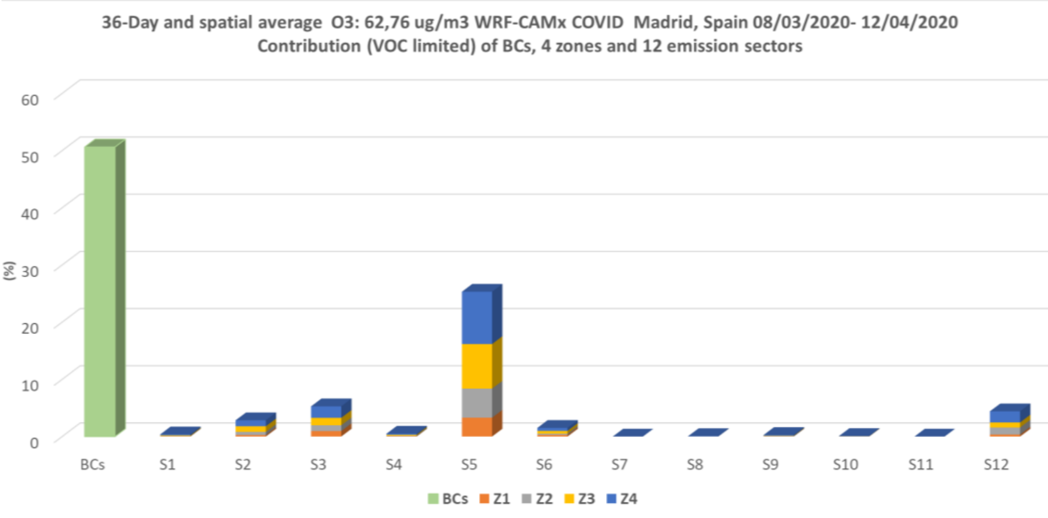

Figure 5: Contribution of the boundary conditions, four zones and twelve emission sources to O3 average concentration under VOC limited conditions in the simulation COVID.

CONCLUSIONS

Using the COVID-19 as an unprecedented experiment with substantial emission reductions from multiple sectors (in particular the transport sector), This study helps to elucidate the complex and nonlinear response of chemical composition of the air pollution through a sensitivity analysis. The impact of COVID lockdown on Madrid Community (Spain) air quality is estimated by running two simulations, one simulation considers the emission reductions during the lockdown (COVID simulation) and a second simulation, ”business as usual” (BAU simulation) with an emissions scenario without restrictions with two air quality models: WRF/Chem and WRF-CAMx Simulated results for the lockdown period, using the adjusted emission inventory agree better with surface observations than the pre-lockdown period, where the BAU emission inventory is applied.

In general, the performance results show that the simulations capture the magnitude and temporal evolution of the four key air pollutants reasonably well, with the statistical indicators within the expected ranges. WRF/Chem underestimates O3 concentrations (-14%) and WRF-CAMx gets better results (+3%) with a small overestimation. WRF/Chem overestimates PM concentrations and WRF-CAMx underestimates them. WRF/Chem gets better correlation coefficients than WRF-CAMx.

The reduction of emissions mainly from the transport sector, during the COVID-19 lockdown period in all Spain, has produced significant changes in the air quality in the Madrid city in term of reduction of NO2 concentrations (high reduction), PM10 and PM2.5 concentrations (moderate reduction) and increase in O3 concentrations (secondary pollutant). BAU-COVID results reflect an important reduction in NOx concentrations and important ozone increases. Such non-linear behavior was attributed to the less efficient O3 titration. Boundary conditions are the main source of the air pollution concentration (50%). The O3 formation is dominated by VOC limited situation. This produces increases of O3 during the lockdown period (NOx reduction).

The lesson from the COVID-19 lockdown showed that improvement in air quality requires the reduction in NOx emissions accompanied by a well-balanced reduction in VOC emissions to avoid the side effect on urban O3 pollution. The results evidence that emission mitigation strategies have to be a coordinated and balanced strategy for controlling multiple pollutants and the possible strategies can be simulated before its implementations with air quality modelling tools as used in this experiment.

In this experiment it was also found that 50% of the O3 concentration that citizens breathe in comes from outside the city, which means that large cities have little chance of reducing O3 pollution as their area of action is the city, hence the need for coordinated mitigation actions between the different authorities, local, regional and national. In this specific case, if the city of Madrid wanted to reduce its O3 concentrations, it would have to act on emissions from solvents produced to the south of the city, but it would only be able to reduce concentrations by 50%. In the case of NO2, as there is a more local effect, cities have a greater range of action and, as has been demonstrated in this study, reducing emissions from road traffic will reduce NO2 concentrations and local authorities have the capacity to reduce these emissions by facilitating the change of the vehicle fleet to electric and ECO vehicles.

REFERENCES

Atkinson, R., Carey, I., Kent, A., van Staa, T., Anderson, H. and Cook, D., 2013. Long-Term Exposure to Outdoor Air Pollution and Incidence of Cardiovascular Diseases. Epidemiology, 24(1), pp.44-53. https://doi.org/10.1097/ede.0b013e318276ccb8

Bell, M., Dominici, F. and Samet, J., 2005. A Meta-Analysis of Time-Series Studies of Ozone and Mortality With Comparison to the National Morbidity, Mortality, and Air Pollution Study. Epidemiology, 16(4), pp.436-445. https://doi.org/10.1097/01.ede.0000165817.40152.85.

Gery, M., Whitten, G., Killus, J., & Dodge, M. 1989. A photochemical kinetics mechanism for urban and regional scale computer modeling. Journal Of Geophysical Research, 94(D10), 12925. https://doi.org/10.1029/jd094id10p12925

Granier, C.; Darras, S.; Denier van der Gon, H.; Doubalova, J.; Elguindi, N.; Galle, B. et al. (2019): The Copernicus Atmosphere Monitoring Service global and regional emissions (April 2019 version). Available online at https://atmosphere.copernicus.eu/sites/default/files/2019-06/cams_emissions_general_document_apr2019_v7.pdf, checked on 2/6/2020.

Grell, G., Peckham, S., Schmitz, R., McKeen, S., Frost, G., Skamarock, W. and Eder, B., 2005. Fully coupled “online” chemistry within the WRF model. Atmospheric Environment, 39(37), pp.6957-6975.

Guevara, M., Jorba, O., Soret, A., Petetin, H., Bowdalo, D., Serradell, K., Tena, C., Denier van der Gon, H., Kuenen, J., Peuch, V. and Pérez García-Pando, C., 2021. Time-resolved emission reductions for atmospheric chemistry modelling in Europe during the COVID-19 lockdowns. Atmospheric Chemistry and Physics, 21(2), pp.773-797.

Lateb, M.; Meroney, R.N.; Yataghene, M.; Fellouah, H.; Saleh, F.; Boufadel, M.C.2016. “On the use of numerical modelling for near-field pollutant dispersion in urban environments—A review”. Environ. Pollut. 2016, 208, 271–283

Marsh, D., Mills, M., Kinnison, D., Lamarque, J., Calvo, N. and Polvani, L., 2013. Climate Change from 1850 to 2005 Simulated in CESM1(WACCM). Journal of Climate, 26(19), pp.7372-7391.

Oostendorp, R., Krajzewicz, D., Gebhardt, L., & Heinrichs, D. (2019). Intermodal mobility in cities and its contribution to accessibility. Applied Mobilities, 4(2), 183-199. https://doi.org/10.1080/23800127.2018.1554293

San José, R., Pérez, J., Balzarini, A., Baró, R., Curci, G., & Forkel, R. et al. 2015. Sensitivity of feedback effects in CBMZ/MOSAIC chemical mechanism. Atmospheric Environment, 115, 646-656. https://doi.org/10.1016/j.atmosenv.2015.04.030

Zaveri, R., Easter, R., Fast, J., & Peters, L. 2008. Model for Simulating Aerosol Interactions and Chemistry (MOSAIC). Journal Of Geophysical Research, 113(D13). https://doi.org/10.1029/2007jd008782

ACKNOWLEDGEMENTS

The UPM authors thankfully acknowledge the computer resources, technical expertise and assistance provided by the Centro de Supercomputación y Visualización de Madrid (CESVIMA).

AUTHOR BIOGRAPHIES

ROBERTO SAN JOSE completed his PhD in 1982 related to the unstable surface turbulent boundary layer parameterisation. He has been involved in air pollution modelling mainly using three-dimensional mesoscale models, such as MM5 and CMAQ. He created the Environmental Software and Modelling Group at Computer Science School of the Technical University of Madrid (UPM) in 1992. He spent one year at the Max-Planck Institute for Meteorology and two years at IBM-Bergen Environmental Sciences and Solution Centre. He has more than 150 publications in different national and international scientific journals. He has been a full professor since 2001

JUAN LUIS PÉREZ-CAMANYO graduated in Computer Sciences at Computer Science School of the Technical University of Madrid in 2000, and in 2005 he defended a PhD thesis related to operational modelling of the MM5-CMAQ system over the internet. He has been an associate professor since 2005 and permanent professor since 2011. He is involved in some international and national research projects about atmospheric simulations and has published many papers in journals and conference proceedings.