



# **10<sup>th</sup> International Workshop on Air Quality Forecasting Research**

Wednesday 20 October 2021 - Friday 22 October 2021

## **Book of Abstracts**



The purpose of the International Workshop on Air Quality Forecasting Research (IWAQFR) is to provide a forum to discuss science issues and advancements related to air quality forecasting and to promote collaborations among air quality forecasting researchers and practitioners. This workshop themes include progress and challenges of operational air quality forecasting with a focus on research and development to improve air quality forecast models, using observations for model evaluation/improvement and data assimilation, as well as urban air quality modeling.



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**Welcome and Opening Remarks / 1**

# Welcome and Opening Remarks

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## Keynote Presentation

### Advancing Atmospheric Composition Predictions and Related Services to Meet the Growing Societal Needs

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Changes in atmospheric composition impact air quality and human health and play key roles in the Earth's weather and climate systems. For example, aerosol amounts, and physical and chemical properties determine their toxicity, radiative and microphysical impacts. Recent advances in observations and models are significantly enhancing our ability to quantify the distribution and properties of aerosols, understand their impacts on atmospheric radiation and cloud distributions and properties, and their impacts on human health. Furthermore, tropospheric ozone levels remain high in many parts of the world, impacting human and ecosystem health. Smoke and wind-blown dust also impact transportation and renewable energy production. To meet societal needs atmospheric composition information is needed at higher resolution and with longer lead times (including seasonal to sub-seasonal). Improving air quality predictions requires further improvements in key processes, emission estimates, and the observing system. Advancements in Earth System models and coupled data assimilation are also needed. This talk draws on illustrative results from on-going activities to highlight areas where further advances in models and observations are needed to enhance seamless prediction of environmental, weather and climate services across relevant spatial and temporal scales. The talk emphasizes that the high-quality atmospheric composition infrastructure, consisting of observations, model predictions, data management, and people, and which delivers high quality open access, atmospheric composition information as described at this conference is of critical importance to society.

# Session 1. Operational Air Quality Forecasting: Progress and Challenges

## Introduction

**Moderator:** Mike Moran<sup>1</sup>

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## Overview of the ECCC Operational AQ Forecasting Program: Status, Recent Improvements, and Perspectives

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ECCC's operational air quality program is based on a multi-pollutant forecast and warning program and includes several Air Quality (AQ)-related products. Currently, AQ information is communicated through an Air Quality Health Index (AQHI) that is primarily based on forecasted and/or observed concentrations of O<sub>3</sub>, NO<sub>2</sub> and PM<sub>2.5</sub>. The ECCC national AQ program is supported by two operational forecast systems: the Regional Air Quality Deterministic Prediction System (RAQDPS) and FireWork, where the latter also includes near-real-time biomass combustion emissions. At the heart of these systems is a limited-area version of the GEM-MACH model, an online meteorology-chemistry model that is configured for a North American domain with a 10-km horizontal resolution. The other ECCC AQ-related products include the Regional Deterministic Air Quality Analysis (RDAQA) system for objective analyses of PM<sub>10</sub>, PM<sub>2.5</sub>, NO<sub>2</sub>, NO, O<sub>3</sub>, and SO<sub>2</sub> and several statistical post-processing packages.

The Canadian operational AQ program is continuously improving and some of the most recent upgrades will be covered by this presentation, including chemical process improvements, anthropogenic emission updates, wildfire emission module upgrades, extended forecast lead-times, etc. Some of the regional and/or WMO initiatives bringing together different entities to provide improved and timely AQ services tailored to user needs will also be discussed.

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## Development of NOAA's next Generation Air Quality and Aerosol Predictions

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NOAA provides operational predictions of air quality (AQ) for the United States and aerosols globally. We present recent progress in the development of NOAA's next generation AQ and aerosols predictions, within the new Unified Forecast System (UFS) framework.

Development of AQ predictions focuses on better representation of wildfire impacts. A new limited-area, high-resolution Rapid Refresh Forecast System weather model is online coupled with EPA's Community Multiscale AQ chemistry model to form the RRFS-CMAQ system. Anthropogenic emissions come from EPA's National Emissions Inventories and wildfire emissions from the NESDIS Blended Global Biomass Burning Emissions Product. Initial evaluations of RRFS-CMAQ use FIREX-AQ and routine AQ measurements. Planned model refinements include increased resolution, dynamic lateral boundary conditions, diurnal variations in wildfire emissions, and smoke plume rise. Data assimilation of AirNow PM<sub>2.5</sub> observations, VIIRS Aerosol Optical Depth (AOD) and TROPOMI NO<sub>2</sub> retrievals

constrain pollutant concentrations. A machine learning emulator is being developed for chemical transformations and explored for tracer transport to reduce computational requirements. A bias correction post-processing procedure is planned to improve prediction accuracy.

Aerosol prediction in the global coupled UFS under development uses the Goddard Chemistry Aerosol Radiation and Transport (GOCART) model from NASA's repository. The coupled UFS also includes the Finite Volume cubed sphere (FV3) dynamical core with the Global Forecast System (GFS) physics for atmosphere, Modular Ocean Model (MOM6), Los Alamos Sea Ice Model (CICE6), WAVEWATCH III for waves and NOAA-MP for land. Testing and evaluation of UFS aerosols during NASA's airborne Atmospheric Tomography campaign and FIREX-AQ field missions focuses on aerosol composition and vertical distribution. In combination with routine AOD and surface observations, this allows us to improve model representation of wildfires, plume rise or dust emissions as we develop coupled UFS aerosol prediction, include AOD data assimilation, explore aerosol-radiation interactions, and provide aerosol lateral boundary conditions for RRFS-CMAQ.

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## Progress and Challenges with Air Quality Forecasting in Europe

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A substantial fraction of R&D activities that underpin operational air quality forecasting in Europe takes place under the umbrella of the Copernicus Atmosphere Monitoring Service (CAMS). CAMS provides daily analyses and 3-day forecasts of the main air pollutants over Europe using a 9-member ensemble of state-of-the-art regional air quality systems. CAMS also provides twice daily global analyses and forecasts using a specific configuration of ECMWF's highly successful Numerical Weather Prediction model. Over 80 different satellite data streams (including about 15 for atmospheric composition variables) and surface air quality observations are assimilated to provide these products. This presentation will highlight some of the developments that have recently entered into operations and it will also showcase how the CAMS global and/or regional systems has performed over different cases of interest including wildfires, dust plumes and the impact of COVID-19 lockdown measures. The presentations will also highlight the current main lines of development on emissions, on modeling and on data assimilation aspects.

Session 1 / 9

## Development and Evaluation of the Aerosol Forecast Member in NCEP's Global Ensemble Forecast System (GEFS-Aerosols)

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NOAA's National Weather Service (NWS) is on its way to deploy various operational prediction applications using the Unified Forecast System, a community-based coupled, comprehensive Earth modeling system. An aerosol model component developed in collaboration among the Global Systems Laboratory, Chemical Science Laboratory, the Air Resources Laboratory, and Environmental Model center (GSL, CSL, ARL, EMC) was coupled online with the FV3 Global Forecast System (FV3GFS) using the National Unified Operational Prediction Capability (NUOPC)-based NOAA Environmental Modeling System (NEMS) software framework. This aerosol prediction system replaced the NEMS GFS Aerosol Component (NGAC) system in the National Center for Environment Prediction (NCEP) production suite in September 2020 as one of the ensemble members of the Global Ensemble Forecast System (GEFS) dubbed GEFS-Aerosols. The aerosol component of atmospheric composition in GEFS is based on the Weather Research and Forecasting model (WRF-Chem). GEFS-Aerosols include bulk modules from the Goddard Chemistry Aerosol Radiation and Transport model (GOCART). Additionally, the biomass burning plume rise module from WRF-Chem was implemented; the GOCART dust scheme was replaced by the FENGSHA dust scheme (developed by ARL); the Blended Global Biomass Burning Emissions Product (GBBEPx V3) provides biomass burning emission and Fire Radiative Power (FRP) data; and the global anthropogenic emission inventories are derived from the Community Emissions Data System (CEDS). All sub-grid scale transport and deposition is handled inside the atmospheric physics routines, which required consistent implementation of positive definite tracer transport and wet scavenging in the physics parameterizations used by NCEP's operational Global Forecast System based on FV3 (FV3GFS). This paper describes the details of GEFS-Aerosols model development and evaluation of real-time and retrospective runs using different observations from in situ measurement, satellite and aircraft data. GEFS-Aerosol predictions demonstrate substantial improvements for both composition and variability of aerosol distributions over those from the former operational NGAC system.

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## Real-time Air Quality Forecasting over the Eastern Mediterranean with WRF/Chem

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We employ the regional coupled meteorology-atmospheric chemistry WRF/Chem model to perform air quality forecasts over the Eastern Mediterranean, and inter-compare with the forecast from the EU Copernicus Atmosphere Monitoring Service – CAMS. The model forecast skill is evaluated using measurements the concentrations of atmospheric pollutants from a dense network of 9 ground stations in the island of Cyprus. The WRF/Chem model forecasts surface temperature, pressure, and wind speed

accurately, with minor differences in 10m wind speed between model and observations at coastal and mountainous stations attributed to limitations in the representation of the complex topography. Dust emissions from the major dust sources in the region, sea-salt and biogenic emissions are calculated online, while a high (1km, hourly) spatiotemporal resolution anthropogenic emission inventory is used for the island of Cyprus. Using higher resolution, and optimized chemistry mechanism and physical process parameterizations the WRF/Chem model achieves lower normalized mean bias between the predicted and observed NO<sub>2</sub> mixing ratios at the urban sites (-7% during winter and -44% during summer) compared to CAMS (-81% during winter and -84% during summer). Furthermore, the diurnal profiles of NO<sub>2</sub> and O<sub>3</sub> mixing ratios at the urban sites are captured more accurately by the WRF/Chem model. The presented advances in the predictive skill of real-time air quality forecasting models can reduce health risk and population exposure to air pollutants.

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## Effect of the Uncertainty in Meteorology on Air Quality Model Predictions

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An operational air quality forecasting model system has been developed and provides daily forecasts of ozone, nitrogen oxides and particulate matter for the area of Hungary and three big cities of the country (Budapest, Miskolc and Pécs). The core of the model system is the CHIMERE off-line chemical transport model. The AROME numerical weather prediction model provides the gridded meteorological inputs for the chemical model calculations. The horizontal resolution of the AROME meteorological fields is consistent with the CHIMERE horizontal resolution. The individual forecasted concentrations for the following 2 days are displayed on a public website of the Hungarian Meteorological Service. It is essential to have a quantitative understanding of the uncertainty in model output arising from uncertainties in the input meteorological fields. The main aim of this research is to probe the response of an air quality model to its uncertain meteorological inputs. Ensembles are one method to explore how uncertainty in meteorology affects air pollution concentrations. During the past decades, meteorological ensemble modeling has received extensive research and operational interest because of its ability to better characterize forecast uncertainty. One such ensemble forecast system is the one of the AROME model, which has a 11-member ensemble where each member is slightly perturbed by initial conditions. In this work we focus on wintertime particulate matter concentrations, since this pollutant is extremely sensitive to near-surface mixing processes. Selecting a number of extreme air pollution situations we will show what the impact of the meteorological uncertainty is on the simulated concentration fields using AROME ensemble members.

## Session 1 / 30

## Interpretation of Probabilistic Surface Ozone Forecasts: A Case Study for Philadelphia

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The use of probabilistic forecasting has been growing in a variety of disciplines because of its potential to emphasize the degree of uncertainty inherent in a prediction. Interpretation of probabilistic forecasts, however, is oftentimes a difficult endeavor and can deter users who may benefit from such forecasts. To encourage broader use of probabilistic forecasts and to show their practicality in the field of air quality, we explore possible ways of interpreting forecasts from a statistical probabilistic air quality surface ozone model known as Regression in Self-Organizing Map (or REGiS) in detail. Four procedures to convert probabilistic to deterministic forecasts are studied using the data from the Philadelphia metropolitan area in southeastern Pennsylvania. The procedures are based on calibrating threshold probability with 1) climatological relative frequency, 2) the more likely event, 3) the threat score, and 4) the bias ratio. REGiS is trained using 2000-2011 ozone season (May 1 to September 30) data, calibrated using 2012-2014 data, and evaluated using 2015-2018 data. Assessment of skill scores indicate that the way in which a probabilistic forecast is converted to a deterministic forecast matters. Using REGiS for the Philadelphia study area and time period, the greatest skill is derived from its probabilistic forecasts through a calibration process based on climatological relative frequency. For other probabilistic models and situations, different calibration procedures may be more beneficial.

## Session 1 / 31

## Environment and Climate Change Canada's FireWork Forecasts During the 2021 Fire Season and Recent System Upgrades

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2021 has been a very active year in North America for wildfires, especially in western and central Canada. More than 4 million hectares of forested land in Canada were burned as of September 2021, well above the average for the last 10 years. Over 40,000 people in several regions were evacuated from their homes, also above average, and dozens of residences were destroyed, notably in Lytton (British Columbia). Many densely populated urban centres downwind of fires, such as Edmonton (Alberta),

Winnipeg (Manitoba), and Toronto (Ontario), experienced high PM<sub>2.5</sub> concentrations and poor visibility conditions due to wildfire smoke.

Since 2016, Environment and Climate Change Canada's FireWork numerical air quality modeling system has been providing operational forecast guidance on the air quality impacts of wildland fire events across North America. FireWork is a collaborative system that obtains near-real-time fire information from the Canadian Forest Service's Canadian Wildland Fire Information System (CWFIS) and Canadian Forest Fire Emissions Prediction System (CFFEPS). The FireWork system captured several extreme air quality episodes in summer 2021 caused by wildfire smoke.

In this presentation we will show analysis and evaluation of results for the FireWork air quality forecasts for summer 2021 and discuss upcoming changes to the operational system expected later this year. We will also show results from some preliminary research work on wildfire aerosol feedbacks on meteorology, particularly surface temperatures, in summer 2021.

### Session 1 / 37

## Improving Collective Capability of Vegetation Fire and Smoke Pollution Forecasts over North America

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As the frequency and intensity of large forest fires continue to increase in the western North America, so do the costs of firefighting, health burdens, life and property losses. Smoke forecasting and early warning are effective tools to mitigate the harmful effects of wildfires and associated air pollution. This work presents a new international initiative, the North America Centre of the World Meteorological Organization (WMO) Vegetation Fire and Smoke Pollution Warning Advisory and Assessment System (VFSP-WAS), as an effort to improve our collective wildfire forecast capability and communication. VFSP-WAS was initiated by WMO, at the request of its members in several regional impacted by wildfires, to provide guidance and expert recommendations to address local needs and enhance data access to end users (web-site:<https://community.wmo.int/activity-areas/gaw/science/modelling-applications/vfsp-was>). As the second node of VFSP-WAS, the North American Centre aims at building a network of operational and research centers, such as Environment Canada and Climate Change (ECCC) and National Oceanic and Atmospheric Administration (NOAA), to provide wildfire related information to users in Canada, United States, and Mexico. VFSP-WAS leverages and facilitates collaborations among existing forecasting and observation programs to collect, enhance, share, and disseminate data of wildfire emissions, forecasts, and satellite observations. We will present the research and development work plan of the VFSP-WAS NA Centre, along with the high-priority research areas identified by the Steering Committee to improve wildfire forecast capabilities. A high-level summary of ongoing VFSP-WAS activities, including ensemble forecasting and multi-model intercomparison, will be discussed. Finally, we will provide information on how researchers and users can participate in this new exciting program, such as interacting with regional centers and joining VFSP-WAS NA Workgroups in the areas of wildfire emissions, ensemble forecast, verification, wildfire risk forecast, observations and detection, Arctic and other issues.



## Session 1 / 13

## Advancement of the National Air Quality Forecast Capability Using the NOAA Global Forecast System: Model Development and Community Applications

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The next-generation National Air Quality Forecast Capability (NAQFC) in the U.S. now uses the advanced Finite Volume Cubed-Sphere (FV3) Global Forecast System (GFS) Version 16 to drive the Community Multiscale Air Quality (CMAQ) model version 5.3.1. Development of the NOAA-EPA Atmosphere Chemistry Coupler (NACC) formed the bridge between the GFSv16 driving meteorology and CMAQ model chemical predictions (i.e., "NACC-CMAQ"). The NACC-CMAQ predictions are further extended from 48 to 72-hours for the first time, and provide numerous scientific advances in atmospheric chemistry modeling to state and local forecasters. NACC-CMAQ became operational at NWS/NOAA in July 2021, thus replacing the previous NAQFC configuration based on the North American Mesoscale Model (NAM)-CMAQv5.0.2. Here we present recent developments of NACC-CMAQ and analysis against the prior operational NAQFC for predictions of summer season ozone (O<sub>3</sub>) and winter season fine particulate matter (PM<sub>2.5</sub>). Results show that the NACC-CMAQ model has significant changes to the meteorological and chemical predictions compared to the prior NAQFC, and that NACC-CMAQ has generally more realistic ground-level O<sub>3</sub> and PM<sub>2.5</sub> predictions and diurnal patterns. Parameterization of in-canopy effects (e.g., canopy shading and modified turbulence) in NACC-CMAQ will also be assessed for their impacts on air quality predictions. Early results show that inclusion of in-canopy processes can substantially reduce model biases for North American surface O<sub>3</sub> forecasts, especially within contiguous forested regions of the eastern U.S. We also present the progress on migrating the GFSv16 data and NACC to the Amazon Web Services (AWS) Cloud and High Performance Computing (HPC) platform, which aims to facilitate community GFSv16-CMAQ applications for any regional domain across the globe.

## Session 2. Emissions and Inventories

### Introduction

**Moderator:** Nicolas Huneeus<sup>1</sup>

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**Session 2. / 29**

### Developing Near Real-time Emissions over the US during the COVID-19 Pandemic

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The COVID-19 pandemic has caused significant changes in emissions of ozone and aerosol precursors. This has been a challenge for air quality forecast models to adapt to evolving emissions associated with the lockdown and recovery periods. Traditionally, the development of bottom-up emission inventories is a time-intensive activity that often involves a multi-year lag. Here, we explore the use of monthly emission adjustments in near real-time using publicly available energy and economic datasets of the US. We update mobile source emissions, using the Fuel-based Inventory of Vehicle Emissions (FIVE), and point and area source emissions on a monthly basis. Our bottom-up inventory suggests that in April 2020, US nitrogen oxides (NO<sub>x</sub>) emissions fell by ~20% in 2020 versus 2019. The reduction was mainly contributed by mobile source engines, as well as industrial sources and electricity generation. In July 2020, emissions had rebounded, but were still lower by ~10% in 2020 versus 2019. We evaluate the emission inventory with satellite tropospheric nitrogen dioxide (NO<sub>2</sub>) columns from the Tropospheric Monitoring Instrument (TROPOMI). Over urban source regions, the inventory captures the COVID-19 perturbations in TROPOMI NO<sub>2</sub> observed from April through July. Over isolated point source regions, TROPOMI NO<sub>2</sub> fell by -42% in April and -29% in July, illustrating impacts on the economy from the pandemic. Overall, the monthly adjustment factors developed for mobile source and industrial point sources are promising for adjusting emission inventories in near real-time for air quality forecast models.

Session 2. / 48

## The Integrated Assessment of Air Pollution, Climate Change & Sustainable Development in Africa

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The impact of air pollution and climate change constitutes a serious and growing public health across Africa. Sustaining economic growth without a large increase in problems associated with air pollution and climate emissions will depend on whether policy makers in the region adopt and implement cost-effective solutions to air pollution and climate change. Furthermore, Africa is considered particularly vulnerable to climate change due to high levels of poverty, vulnerable water resources and dependency on rain-fed agricultural production. Not surprisingly, climate adaptation is a key issue in Africa's future development. Taking people out of poverty is a major goal, and this will need to be accompanied by increasing access to clean energy services, ramping up sustainable agricultural practices, tackling growing waste challenges and curbing transport and industrial emissions.

It is in this context, the Climate and Clean Air Coalition (CCAC) in partnership with the United Nations Environment Programme (UNEP), the African Union Commission (AUC) and the Stockholm Environment Institute (SEI) is developing an assessment on air pollution, climate change and sustainable development in Africa to identify priority measures that reduce emissions while maximizing the multiple-benefits for human well-beings, health, ecosystems, climate, and food security. The assessment is bringing together academics, experts, and practitioners working across Africa to address the growing air pollution and associated climate threats while promoting capacity mobilization and building, and action to reduce air pollution and climate change. The analysis being undertaken is framed around 'development pathways for Africa and their air quality and climate consequences' to determine how Africa can meet its development aspirations and priorities. The paper will outline how the Africa Assessment process has been actively linking to the atmospheric science community and highlight the capacity building and consultation processes to develop the modeling and scenarios and present the emerging results.

Session 2. / 22

## Transport Emissions in Chile, Current Situation and Looking ahead for a Carbon-Neutral Future?

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Emissions generated by the transportation sector continue to be one of the main causes of air pollution in Latin American cities. Despite major technological improvements in the automotive industry, motor vehicles continue to rely primarily on fossil fuels. Electromobility is emerging as a potential solution for the transport of the future, but there are still several decades of transition, during which conventional engines will coexist with zero-emission vehicles. Emission inventories from mobile sources must be able to incorporate these changes, with high-resolution spatial disaggregation, offering emissions of local and global pollutants, on urban and national scales. This paper presents results of three studies, where emission inventory estimation methodologies are combined with local information on activity and emission factors, as well as projections of new technologies and forms of mobility that seek to achieve carbon neutrality by the year 2050. A bottom-up, high-resolution national inventory of exhaust emissions for on-road transportation is presented for Chile, covering the period 1990-2020. Recent advances are also shown in the measurement of local emission factors, using portable emission measurement systems, as well as real-time vehicle counts with specialized algorithms and low-cost equipment. Finally, preliminary results of a forecast analysis for the years 2020-2050 are presented, which considers various official strategies for all modes of transport in Chile, with the aim of evaluating the feasibility of achieving carbon neutrality by 2050, while reducing emissions of criteria pollutants in urban areas.

Session 2. / 25

## Improving Black Carbon Modeling: Emissions and Model Evaluation

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Black carbon (BC) is a particulate matter component associated with adverse health impacts and contribution to global warming. Therefore, it is one of the priority air pollutants. Emissions of BC are however still subject to large uncertainties, in particular for residential wood combustion. In order to come to a reliable emission inventory, it is essential to verify the emissions through their use in models and consequent evaluation with observed BC concentrations. Here, we present results from a study aimed at the improvement of BC emissions for air quality modeling, focusing on Germany.

Several emission inventories exist for black carbon and a large range of PM emissions factors and BC fractions can be found in literature. Based on literature review, a new estimate for BC emissions of wood combustion and traffic country totals was derived for Germany. These were used in scenario simulations with LOTOS-EUROS using a labeling approach. Updated emission factors led to a better performance

of the model. In addition, several emission distribution scenarios were explored to improve the spatial and temporal distribution of residential combustion, agricultural machinery and road traffic.

Model evaluation for BC is non-trivial. It was done based on available aethalometer and EC observations, and dedicated observations with harmonized aethalometer data in Berlin, including separation of biomass burning and fossil fuel contributions. Using location-dependent factors is key to derive BC from optical measurements and to separate fossil fuel/biomass burning contributions, and the lack of harmonized data for the rest of Germany limited the evaluation of the spatial distribution of emissions.

Using the approach with dedicated observations, final model simulations with new emission distributions showed good consistency with the observations for Berlin.

# Session 3. Data Assimilation (Ground-based and Satellite Observations)

## Introduction

**Moderator:** Rajesh Kumar<sup>1</sup>

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**Session 3. / 44**

## Assimilation of Multiple Satellite Retrievals with Emissions Adjustment to Improve High Resolution Air Quality Forecast Skill and Predictability

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Poor air quality (AQ) is a most pressing international environmental problem. A soon-to-be-operational network of geostationary AQ satellites (GEMS, TEMPO, and Sentinel 5) that will effectively cover the Northern Hemisphere with hourly AQ observations at ~5 km resolution will revolutionize AQ forecasting/data assimilation. I will present preliminary results from two multi-constituent ensemble AQ forecast/assimilation experiments with WRF-Chem/DART: (i) FRAPPE – a 15 km grid space domain covering the western continental US (CONUS); and (ii) COLORADO – a 4 km grid space domain covering Colorado. These experiments will highlight some of the expected benefits from the geostationary array of AQ satellites.

WRF-Chem/DART incorporates the Weather Research and Forecast (WRF) model with on-line chemistry (WRF-Chem) into the ensemble Kalman filter assimilation system known as the Data Assimilation Research Testbed (DART). We assimilate the ground-based AQS CO, O<sub>3</sub>, NO<sub>2</sub>, SO<sub>2</sub>, PM<sub>10</sub>, and PM<sub>2.5</sub> observations together with MOPITT CO, IASI CO, MODIS AOD, OMI NO<sub>2</sub>, TROPOMI CO, NO<sub>2</sub>, and synthetic TEMPO NO<sub>2</sub> total/partial column and/or profiles retrievals. We use: (i) the state augmentation method for emissions adjustment, and (ii) state-space localization to enable cross-species adjustments by controlling which observations update which state variables.

I will discuss three basis experiments: (i) CONTROL – assimilates only meteorology; (ii) ALLCHEM – same as CONTROL but also assimilates AQS, MOPITT, IASI, MODIS, OMI, TROPOMI and/or synthetic TEMPO; and (iii) EMISADJ – same as ALLCHEM but also includes emissions adjustment. Our results show that: (i) assimilating chemical observations increases AQ forecast skill; (ii) including emissions adjustment increases forecast skill/predictability time; (iii) including emissions adjustment reduces the

magnitude and areal extent of the analysis increments; and (iv) assimilation of high-resolution retrievals from TROPOMI and TEMPO increases the magnitude of the increments. Based on the earlier work of my collaborators, we expect that assimilation of high-resolution retrievals will also increase predictability.

Session 3. / 23

## Assimilation of Atmospheric Composition Observations in the Global Copernicus Atmosphere Monitoring Service (CAMS) System

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The Copernicus Atmosphere Monitoring Service (CAMS) is implemented by ECMWF on behalf of the European Commission to provide operational analyses and 5-day forecasts of global atmospheric composition, including reactive gases, aerosols and greenhouse gases. For this, CAMS assimilates near-real-time satellite observations of key atmospheric constituents into the IFS and also operates an ensemble of regional air quality models over Europe to provide 4-day, daily forecasts of the main atmospheric pollutants at 10 km resolution. In addition to the operational products, CAMS has also produced a global reanalysis, currently available from 2003-2020, to provide spatially and temporally consistent 3-D fields of atmospheric composition. This talk gives some background about the satellite retrievals of atmospheric composition that are used in the CAMS system, with focus on the global system. The talk will present examples of the limitations of some of the used data sets, focussing on ozone, carbon monoxide and aerosol optical depth, as well as the benefits obtained when combining the information from different instruments in an assimilation system.

Session 3. / 20

## Development of a Regional multi-Air Pollutant Assimilation System (RAPASv1.0) and its Application to Emission Inversion

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Top-down atmospheric inversion uses spatially distributed observations of atmospheric compositions to provide estimates of surface-atmosphere fluxes. In this study, we constructed a Regional multi-Air Pollutant Assimilation System (RAPASv1.0) based on the Weather Research and Forecasting/Community Multiscale Air Quality Modeling System (WRF/CMAQ) model, the three-dimensional variational (3DVAR) algorithm and the ensemble square root filter (EnSRF) algorithm, which simultaneously assimilates spatially distributed hourly in-situ measurements of CO, SO<sub>2</sub>, NO<sub>2</sub>, PM<sub>2.5</sub> and PM<sub>10</sub> concentrations to quantitatively optimize gridded emissions of CO, SO<sub>2</sub>, NO<sub>x</sub>, primary PM<sub>2.5</sub> (PPM2.5) and coarse PM<sub>10</sub> (PMC) on regional scale. A “two-step” inversion scheme is adopted in each data assimilation (DA) window, in which the emission is inferred in the first step, and then, it is input into the CMAQ model to simulate the initial field of the next window, meanwhile, it is also transferred to the next window as the prior emission. In this way, the original emission inventory is only used in the first DA window, and

the 3D-Var algorithm used to optimizing the chemical IC is also run only in the first window. Besides, a “super-observation” approach is implemented based on optimal estimation theory to decrease the computational costs and observation error correlations and reduce the influence of representativeness errors. Based on this system, the emissions of CO, SO<sub>2</sub>, NO<sub>x</sub>, PPM2.5 and PMC in December 2016 are inferred using the corresponding nationwide observations over China. The 2016 Multi-resolution Emission Inventory for China (MEIC 2016) is used as the prior emission. The results showed that, compared to the prior emission (MEIC 2016), the posterior emissions increased by 129%, 20%, 5%, and 95% for CO, SO<sub>2</sub>, NO<sub>x</sub> and PPM2.5, respectively, in December, indicating that there was significant underestimation in the MEIC inventory.

Session 3. / 18

## Develop and Evaluate the AIRNow Assimilation in JEDI for RRFS-CMAQ: a Case Study for Summer 2019

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There are ongoing efforts to develop the operational regional inline air quality model, RRFS-CMAQ (Rapid Refresh Forecast System with CMAQ chemistry) based on the Finite Volume Cubed-Sphere Dynamic Core (FV3), under the NOAA Unified Forecast System. As part of these efforts, the chemical data assimilation (DA) capability is being developed to improve the model results. Here we present the preliminary results of using surface AIRNow in-situ measurements and a 3D-Var method in the Joint Effort for Data-Assimilation Integration (JEDI) to adjust the near-surface chemical initial conditions. Our test case for summer 2019 shows that assimilating in-situ measurements is a reliable method to reduce the bias in the aerosol and ozone initial conditions of RRFS-CMAQ. Unlike the satellite aerosol optical depth data assimilation, this DA with the in-situ measurements can be used at night or under the cloud, and is available at hourly intervals, matching well with the rapid refresh system. The duration of DA influence varied from region to region. Over polluted areas with strong emissions, the assimilation effect may fade quickly. The bias of the base model predicted PM<sub>2.5</sub> (particle matter with diameter < 2.5 μm) has strong diurnal variations, implying that some processes (e.g. dynamics, emission, and chemical processes) in RRFS-CMAQ could have systematic diurnal biases. Cycling the assimilation system every 6 hours reduced that bias, but did not completely eliminate it. This study shows that the DA adjustment on the chemical initial condition is useful with little side effects, and other efforts are needed to reduce the models' overall biases.



Session 3. / 33

## Near-Real-Time Global Aerosol Data Assimilation and Forecasting at NOAA/OAR/GSL

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A near-real-time (NRT) global aerosol data assimilation (DA) and forecast system has been developed to produce global aerosol analyses and forecasts at NOAA/OAR/GSL. The aerosol DA is performed using the Joint Effort for Data assimilation Integration (JEDI) led by the Joint Center for Satellite Data Assimilation (JCSDA). The GSL's Common Community Physics Package (CCPP) version of Global Ensemble Forecast System - Aerosols (GEFS-Aerosols) is used to produce global aerosol forecasts. This aerosol forecast model relies on the Finite-Volume Cubed-Sphere (FV3) dynamical core and the Global Forecast System (GFS) physics. The aerosol parameterization is based on the Goddard Chemistry Aerosol Radiance and Transport (GOCART) model. Daily Blended Global Biomass Burning Emissions Product (GBBEPx) and Fire Radiative Product (FRP) are used for wildfire emissions. In the DA that uses JEDI-based applications, the 3D ensemble-variational (3D<sub>En</sub>Var) approach is used to update our deterministic analysis and the local ensemble Kalman filter (LETKF) is used to update the ensemble members. It assimilates aerosol optical depth (AOD) retrievals at 550 nm derived from the Visible/Infrared Imager Radiometer Suite (VIIRS) instrument. AOD forward operator is calculated using NASA aerosol scattering lookup tables. To reduce modeled AOD bias and increase aerosol ensemble spread, a parameterization of scaling and stochastically perturbing emissions was developed and implemented in the GSL's CCPP version of GEFS-Aerosols model. Our recent cycled NRT experiments show that assimilation of VIIRS AOD retrievals at 550 nm efficiently reduces bias and error of simulated AOD compared to those from the Aerosol Robotic Network (AERONET) and the Moderate Resolution Imaging Spectroradiometer (MODIS) instrument. Furthermore, our aerosol analyses demonstrate comparable skills to NASA and ECMWF analyses, although our current system is run at a much lower resolution compared to the aerosol DA systems at these two meteorological centers. System development and our NRT experiment results will be presented.

Session 3. / 38

## Developing Aerosol Reanalysis at NOAA. Version 1.0: Methodology and Results.

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In collaboration with the Global Modeling and Assimilation Office at NASA and State University of New York at Albany, NOAA is developing capability to assimilate observations to create the first ever aerosol reanalysis at this institution. Initially, the reanalysis is being developed only for the year 2016. It will benefit scientists involved in aerosol forecasting, as well as the climate, health, and environmental communities. The observations include Aerosol Optical Depth (AOD) derived from Moderate Resolution Imaging Spectroradiometer (MODIS) and AErosol RObotic NETwork (AERONET) direct sun measurements. The model relies on Finite-Volume Cubed-Sphere (FV3) dynamical core, Global Forecast System (GFS) physics and the aerosol parameterization based on the Goddard Chemistry Aerosol Radiance and Transport (GOCART). The assimilation tools are from the Joint Effort for Data assimilation Integration (JEDI): the forward operator uses aerosol scattering tables from NASA/GMAO and the assimilation approach combines the variational solver and the Local Ensemble Transform Kalman Filter (LETKF). Reanalysis is compared to NASA's Modern-Era Retrospective analysis for Research and Applications Two (MERRA-2) and ECMWF's Copernicus Atmosphere Monitoring Service interim Reanalysis (CAM-SiRA) and evaluated against various observations from AERONET, and other independent satellite AOD retrievals.

# Session 4. Urban Air Quality Modeling

## Introduction

**Moderator:** Pablo Saide<sup>1</sup>

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**Session 4 / 45**

## Integrated Air Quality Forecasting and Decision Support System for Delhi

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This study reports a very high-resolution (400 m grid-spacing) operational air quality forecasting system developed to alert residents of Delhi and the National Capital Region (NCR) about forthcoming acute air pollution episodes. The system assimilates near real-time aerosol observations from in situ (260 stations) and space-borne platform in the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem) to produce a 72-h forecast daily in a dynamical downscaling framework. Such a high-resolution system has been developed for the first time and is evaluated during the winter seasons. The assimilation of aerosol optical depth and surface PM<sub>2.5</sub> observations improves the initial condition for surface PM<sub>2.5</sub>. Our forecast is found to be very skillful both for PM<sub>2.5</sub> concentration and unhealthy/very unhealthy air quality index categories and has been helping the decision-makers in Delhi make informed decisions. We have further extended the AQEWS with a Decision Support System (DSS) for air-quality management in Delhi. DSS provides quantitative information about a) The contribution of emissions from Delhi and the surrounding 19 districts to the air quality in Delhi, b) The contribution of emissions from 8 different emission sectors in Delhi to the air quality Delhi, c) The contribution from biomass-burning activities in the neighboring states to the degradation of air quality in Delhi, and d) The effects of possible emission source-level interventions on the forecasted severe air-quality event in Delhi. This information would explicitly highlight the most important emission sources responsible for the degraded air quality in Delhi and suggest possible solutions to the policymakers. With a plethora of quantitative data, the AQEWS integrated with DSS will be an essential tool for air-quality management in Delhi and the surrounding region.

**Session 4 / 28**

## Modeling COVID Perturbation on Urban Emissions over the US

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The COVID-19 outbreak has caused significant reductions in traffic and economic activities, impacting anthropogenic emissions and urban air quality. The covid perturbation on the emissions are estimated by comparing publicly available energy and economic datasets between 2019 and 2020. The perturbation impacts are then evaluated by comparing the Weather Research and Forecasting with Chemistry (WRF-Chem) model simulations with aircraft measurements from University of Maryland and Scientific Aviation, and with the satellite retrievals from the TROPOspheric Monitoring Instrument (TROPOMI) and Aura Ozone Monitoring Instrument (OMI). Compared to the aircraft measurements over New York City, Houston, and Denver, the emission perturbation has much larger impacts on concentrations of nitrogen dioxide (NO<sub>2</sub>) than CO, despite larger reductions in the CO anthropogenic emissions, suggesting the significant impacts through secondary formation from biogenic sources. Also, the impacts on NO<sub>2</sub> and CO concentrations are larger over New York City than Houston and Denver, suggesting the heterogenous responses from large cities across the US during the COVID-19 pandemic. Compared to satellite retrievals, our model is able to capture the observed changes in tropospheric NO<sub>2</sub> columns over urban source regions between 2019 and 2020, demonstrating the reasonable estimates of the COVID perturbation on the anthropogenic emissions. In addition, we find the emission perturbation dominates the observed reductions in tropospheric NO<sub>2</sub> over urban source regions, with meteorological impacts tending to increase tropospheric NO<sub>2</sub> by 2–8%.

**Session 4 / 14**

## Using multi-scale Modeling to Calculate Primary and Secondary Pollutant Concentrations in Urban Areas with a Street Resolution

**Authors:** Karine Sartelet<sup>1</sup>; Lya Lugon von Marttens<sup>2</sup>**Co-authors:** Olivier Chretien<sup>3</sup>; Youngseob Kim<sup>1</sup><sup>1</sup> (1) CEREAs, École des Ponts ParisTech, EDF RD<sup>2</sup> (1) CEREAs, École des Ponts ParisTech, EDF RD, (2) Paris Department of Green Spaces and Environment, (\*) Now at Max Planck Institute for Meteorology<sup>3</sup> (2) Paris Department of Green Spaces and Environment

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Atmospheric pollution is an important issue in urban areas, posing a major threat to health and climate. Streets, where populations are exposed, often present high concentrations of nitrogen oxides and fine particles composed by black carbon, organic and inorganic compounds. These pollutants may have important effects on human health, including asthma and cancer. Here, multi-scale simulations are performed over Paris city to calculate pollutant concentrations in the urban background (with the regional-scale model Polair3D) and in the streets (with the local-scale model MUNICH). Gas-phase chemistry and the formation of secondary aerosols are taken into account at both scales. Different aspects are investigated: (i) the difference between particle concentrations, size distribution and chemical compositions in the urban background and in the streets, (ii) the formation of secondary particles in the streets, and their influence in the total fine particle concentrations, (iii) the influence of non-exhaust emissions on black carbon concentrations. Simulations indicate that the ratio between concentrations in the streets and in the urban background can be, in average, 2 regarding nitrogen dioxide, 3 regarding black carbon and 1.8 regarding organic particles. Particle concentrations may also have more dangerous health impacts in the streets than in the urban background due to their size distribution, and to their chemical composition. Secondary particles represent an important average parcel of particle concentrations in the streets, and can reach until 18% of fine particles in Paris, depending on the street. A large contribution is observed regarding organic fine particles (reaching 38% according to the street). Traffic-related emissions of ammoniac may contribute by up to 26% of fine inorganic particle concentrations in the streets of Paris. Traffic exhaust emissions are not strong enough to explain the high black carbon concentrations observed in the streets, and non-exhaust emissions from tyre wear may need to be revisited.

**Session 4 / 21**

## **Analysis of Surface Ozone Exceedance Events in the Detroit/Windsor Area during the Michigan-Ontario Ozone Source Experiment (MOOSE)**

**Author:** Craig Stroud<sup>1</sup>

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The Michigan-Ontario Ozone Source Experiment (MOOSE) was designed to understand what contributes to ozone exceedance events in the southeastern Michigan and southwestern Ontario border region. Measurements were collected using advance remote sensing and mobile laboratories, which complement the existing hourly network measurements by both counties. High resolution, real-time meteorological and air quality forecasts were conducted by Environment and Climate Change Canada (ECCC) to guide the deployment of the mobile measurements during the field study. The air quality forecasts are based on ECCC's Global Environmental Multiscale model - Modeling Air quality and Chemistry (GEM-MACH) at 2.5-km grid spacing with the Town Energy Balance (TEB) urban surface parameterization.

In this study, we assess the impact of a new initialization method for the meteorology for each model forecast cycle. A new assimilation at a true 2.5-km grid spacing is now used instead of the prior simple downscaling from the 10-km regional analysis. The model meteorology is nudged to the analysis gradually over a 6-hr window at the start of cycle to avoid introducing instability. The impact of this new analysis method on high-resolution air quality predictions will be illustrated for the MOOSE study period.

We will also show model results for several of the ozone case study periods. We will first evaluate the model performance and then illustrate diagnostic ratios (e.g. radical-loss-via-NO<sub>x</sub>/total-radical-loss, HCHO/NO<sub>2</sub>) which can be used to assess ozone production sensitivity to its precursors (VOC and NO<sub>x</sub>). This will be used to assess whether VOC and/or NO<sub>x</sub> reductions will be most efficient at reducing ozone for the exceedance periods.

Session 4 / 35

## Recent Developments of a High Resolution Operational Air Quality System at ECCC

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Associated with increasing worldwide urbanization, and despite efforts made to reduce airborne concentrations of primary pollutants, air quality remains a concern in urban areas. Especially during short-term pollution episodes that can lead to exceedances of air quality standards. Furthermore, exposure to elevated levels of air pollution may result in various adverse health effects.

In Canada, a high percentage of the population (~81%, according to the 2011 Census) living in urban areas may be exposed to urban pollution. To improve services for Canadians, Environment and Climate Change Canada (ECCC) has developed a high-resolution air quality forecasting capability for urban areas. Because urban air quality (AQ) is influenced by a variety of factors including meteorology, urban infrastructure, local emissions and regional background, it is important to combine all the factors in an integrated model system.

As a part of the ECCC effort, the operational Regional Air Quality Deterministic Prediction System (RAQDPS) has been reconfigured to provide 48-hours air quality forecasts at model grid resolutions of 2.5km. The proposed urban AQ system, referred as High Resolution Air Quality Deterministic Prediction System (HRAQDPS), relies on the configurations of the operational High Resolution Deterministic Prediction System (HRDPS) for meteorology, and the Global Environmental Multiscale model - Modeling Air quality and Chemistry (GEM-MACH) system for chemistry. The HRDPS system also includes the Town Energy Balance (TEB) urban surface scheme.

The HRAQDPS uses initial surface and hydrometeor fields from a high-resolution land assimilation system and a forecast cycle at 2.5km respectively. The system has been tested on a small domain over east North America and compared to the operational RAQDPS system.

This presentation will describe the HRAQDPS system as well as sensitivity tests and model performance during the summer 2019 and winter 2020 periods. The planning for the short and long-term HRAQDPS development will also be discussed.

# Poster Session

## Introduction

**Moderator:** Megan Melamed<sup>1</sup>

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**Poster / 43**

## Estimation of Uncertainties in Model-Ready Emissions Inventories for Air Quality Modeling Applications

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Emissions inventories provide information on pollutants' mass contributions and emission characteristics during a given period for sources located in a geographic area. Researchers further transform them into model-ready files that are input to air quality models by aggregating emission rates for each pollutant and source in a computational domain. As such, emissions inventories used in air quality models are essential instruments for air quality management during the design and evaluation of emission control strategies, air quality forecasting, and evaluation of health and environmental impacts. Since all emissions inventories are estimates obtained by a combination of 1) limited source measurements, 2) emissions modeling, and 3) assumptions based on expert judgment, uncertainties from input parameters are introduced and irremediably propagated in the emission estimates. Therefore, there is a need to better characterize uncertainties estimates in model-ready emissions inventories used in air quality modeling applications. In this study, we 1) summarize the current state of statistical methods for quantifying uncertainties in emissions inventories, and 2) identify improved approaches that can be used to estimate uncertainties in model-ready emission inventories. The results of this analysis include recommendations of analytical techniques during the application of air quality models for assessing the impacts of emissions uncertainties in air quality predictions.

**Poster / 8**

## Carbonaceous Aerosol from Open Burning and its Impact on Regional Weather in South Asia

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Seasonal open biomass burning contributes to significant carbonaceous aerosol loading over South Asia. This study analyzes long-term trends in emissions in two hot spot regions, Myanmar and Punjab, based on data from the Global Fire Emissions Database (GFED4s) and Fire INventory (FINN) from the National Center for Atmospheric Research (NCAR). Our analysis reveals that emissions during active fire seasons increase by approximately 83–106% and 2338–3054% for Punjab and Myanmar, respectively, compared to the estimates of anthropogenic emissions obtained with FINN. We also examine the impact

of carbonaceous aerosol from open biomass burning on regional weather by using the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem) to conduct a year-long simulation of the post-monsoon and pre-monsoon periods when active fires were reported. The results indicate that the carbonaceous aerosol is vertically lofted by as much as 3–5 km into the atmosphere and, rising as high as the 850 hPa level from the surface, disperses horizontally throughout South Asia. Our calculations on the radiative forcing suggest that changes of up to  $-6.14 \text{ W m}^{-2}$  and  $-0.50 \text{ W m}^{-2}$ , and  $-42.76 \text{ W m}^{-2}$  and  $-1.91 \text{ W m}^{-2}$  occur at the surface and at the top of the atmosphere over Punjab and Myanmar, respectively. We also find that carbonaceous aerosol (black carbon + organic carbon), similar to black carbon (BC), reduces the surface temperature, despite the scattering effects of organic carbon (OC). Overall, open biomass burning causes the surface temperature to decrease by 2 K, the relative humidity to increase by 8% and the planetary boundary layer height to change by as much as 600 m. Changes in the precipitation patterns and volume due to the carbonaceous aerosol from open biomass burning, however, are negligible when considering only the direct radiative feedback.

Poster / 12

## A Data Assimilation Method Combined with Machine Learning and its Application to Anthropogenic Emission Adjustment in CUACE model

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A data assimilation method combined with machine learning has been developed and applied to adjust anthropogenic emissions and improve forecasting accuracy in Chinese unified atmospheric chemistry environment (CUACE) model. This is an attempt to combine data assimilation and machine learning. Nudging method was used to create the database of nudging gain matrixes, using simulations of CUACE and the ground-based observations. Then these data are employed to train a machine learning model using extremely random trees method (ExRT), and to store the relations between nudging gain matrixes and simulations in the trees. Observations was used again to find out the proper nudging gain matrixes using the trained machine learning model. The Nudging-ExRT emission inventories was calculated by the original emission inventories and the Nudging-ExRT gain matrixes. During its application for the operational CUACE five days forecasts in China in March 2021, the data assimilation of anthropogenic emissions had a good performance in most of the periods for PM<sub>2.5</sub> and O<sub>3</sub>, and the optimization did not weaken over time. As for PM<sub>2.5</sub>, the hourly average spatial correlation coefficient (R) increased from 0.39 to 0.45 and the root mean square error (RMSE) decreased from  $43.59 \mu\text{g}/\text{m}^3$  to  $40.71 \mu\text{g}/\text{m}^3$ . As for O<sub>3</sub>, R increased from 0.08 to 0.11, RMSE decreased from  $63.66 \mu\text{g}/\text{m}^3$  to  $56.70 \mu\text{g}/\text{m}^3$ . This simplicity, efficiently and extensibility framework of Nudging-ExRT method has been proved to be a good way to adjust anthropogenic emissions in CUACE and still remains much to be done in the future.



**Poster / 40**

## **Dispersion of Atmospheric Pollution from Surface Oil burns in the Gulf of Mexico**

**Author:** Cuauhtemoc Turrent<sup>1</sup>**Co-authors:** Alejandro Dominguez<sup>1</sup>; Agustín García<sup>2</sup>; Victor Almanza<sup>2</sup><sup>1</sup> *Centro de Investigación Científica y de Educación Superior de Ensenada (CICESE)*<sup>2</sup> *Instituto de Ciencias de la Atmósfera y Cambio Climático, UNAM***Corresponding Author:** turrentc@cicese.mx

The dispersion patterns and arrival times to the Mexican coast of the Gulf of Mexico (GoM) of atmospheric pollutants that would result from surface oil burns are studied using the WRF and FLEXPART models. Dispersion scenarios are analyzed under different meteorological conditions in the GoM basin: sea-breeze days (for winter, spring, summer, and autumn), cold fronts (Nortes), southerly wind, and tropical cyclones. The WRF model was used to dynamically downscale CFSR reanalysis fields to a horizontal resolution of 4 km. The positions for tens of thousands of particles released from different points over the GoM during multiple events for each meteorological condition were calculated with the FLEXPART Lagrangian model, using the high-resolution WRF wind fields. The initial positions of the particles were randomly distributed vertically over a 900 m high column at different locations over the GoM.

Of the meteorological conditions that were analyzed, sea-breeze days represent the most significant risk for the air quality of Mexican coastal communities in the event of a large-scale oil spill in the GoM. During those days, larger accumulations of atmospheric pollutants within the planetary boundary layer are expected compared to other synoptic conditions. Point sources located near the cities of Tuxpan and Poza Rica, Veracruz produced, during summer sea-breeze days, the distribution of atmospheric pollutants that has the highest probability of affecting air quality in coastal communities of the state of Veracruz, with arrival times of less than 12 hours. In contrast, emissions for summer sea-breeze days from point sources located near the border between the exclusive economic zones of Mexico and the United States produced a distribution of atmospheric pollutants mostly contained over marine regions, with a low probability of arrival of the polluting material to the Texan or Mexican coastlines.

# Session 5. Using Observations for Model Evaluation

## Introduction

**Moderator:** James Crawford<sup>1</sup>

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## The Building Blocks for Informative Model Evaluation Activities

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Verification and diagnostic activities are critical for the success of both numerical weather prediction and weather forecasting efforts at organizations around the world. There are several concerns that should be addressed before starting a model evaluation activity, including understanding the nature of observations that will be used for the evaluation. This information will determine what statistics and diagnostics may be computed to inform model development activities. Additionally, having reproducible results via a consistent framework is equally important for model developers and users alike. This presentation will identify those key questions that should be addressed and introduce several tools that can be used to in the evaluation of air quality forecast and the meteorological conditions driving them. The tools include the enhanced Model Evaluation Tools (METplus) as well as Model Evaluation using Observations, Diagnostics and Experiments Software (MELODIES) and Model and Observation Evaluation Toolkit (MONET).

Session 5. / 15

## Validation of the Copernicus Atmosphere Monitoring Service Forecasts and Reanalyses

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The Atmosphere Monitoring Service of the European Copernicus Programme (CAMS) is an operational service providing analyses, reanalyses and daily forecasts of aerosols, reactive gases and greenhouse gases on a global scale, and air quality forecasts and reanalyses on a regional scale. In CAMS, data assimilation techniques are applied to provide daily analyses using remote sensing and in-situ air quality observations. The global component is based on the Integrated Forecast System of the ECMWF, and the regional component on an ensemble of nine European air quality models. For more information: <http://atmosphere.copernicus.eu>

CAMS has a dedicated validation activity - implemented by a partnership of 13 institutes co-ordinated by KNMI - to document the quality of the atmospheric composition products. In our contribution we discuss this validation activity, including the measurement data sets, validation requirements, the

operational aspects, the upgrade procedure, the validation reports and scoring methods, and the model configurations and assimilation systems validated. Of special concern are the forecasts of high pollution concentration events (fires, dust storms, air pollution events, volcano eruptions).

Session 5. / 17

## Air Quality Evaluation System: Central México Case Study

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In order for an air quality model to better emulate and represent the atmospheric pollution in a region, its performance has to be evaluated to both identify uncertainties and reproduce ambient observations.

An air quality modeling system has been implemented at UNAM's Institute of Atmospheric Sciences and Climate Change with the main objective of generating air quality forecasts for the area of Central Mexico. This region encompasses a megalopolis that includes 5 states surrounding the Mexico Megacity. Central Mexico is chosen as a case study because of the interest in criteria pollutant emissions, evaluation of emissions inventories and greenhouse gases in the region.

The modeling system has been applied in studies related to improving emissions inventories and to evaluate mitigation scenarios. Part of the products have been used to support key decision-making processes both at a regional and national level. In order to better identify the uncertainties and improve the model performance, a verification system based on the NCEP Unified Post Processing System (UPP), Model Evaluation Tools (MET), Fortran codes, grads, R and bash scripts, has been implemented. The system aims to address the following questions: 1) at which monitoring stations does the model perform best? 2) Are the chemical/meteorological regimes impacting the model performance? 3) Is the forecast capturing the meteorology natural variability correctly? 4) What is the best way to present the results to the public?

A description of the observational dataset used for validation will be presented. It includes data from several platforms: surface air quality network, satellite products for CO and CO<sub>2</sub> and additional surface meteorological observations. In addition, a comparison between model results and satellite products will be presented.

## Session 5. / 11

## Development and Evaluation of North America Wildfire Ensemble Forecast: Initial Application to the 2020 Western United States “Gigafire”

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Wildfires are important emission sources that generate large amounts of aerosols into the atmosphere. These hazardous events have been increasing rapidly due to the climate change effects, leading to poor air quality, which causes impacts on the society, including adverse health effects, life and property losses, and the economic burden. To mitigate these effects, many regional and global numerical models have been developed and used by state and local agencies to study and predict the dispersion of aerosols to protect the public from poor air quality. However, the accuracy of these forecast models is dominantly affected by uncertainties in errors in emission and meteorological input data as well as model simulation. Therefore, in addition to individual models, ensemble forecast is increasingly being used to reduce model uncertainties and improve model forecasting performance. This study aims to develop a multi-model ensemble forecast of wildfires using models from different institutes, including the three National Air Quality Forecast Capability (NAQFC) regional models: GMU-CMAQ, NACC-CMAQ, and HYSPLIT, and the three International Cooperative for Aerosol Prediction (ICAP) global models: GEOS-5, GEFS-Aerosol, and NAAPS. Aerosol optical depth (AOD) and particulate matter less than 2.5  $\mu\text{m}$  in diameter ( $\text{PM}_{2.5}$ ) forecasting performances of individual models, and ensemble mean were evaluated by analyzing statistical metrics using the ground observations (AirNOW) and satellite data sets (MAIAC and VIIRS) for the 2020 Giga fire period (August-September 2020) over the Continental United States (CONUS). The ensemble then will be used to improve the real-time wildfire forecasting system over North America to support the key-decision making processes for the air quality at local and national levels.

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## Routine Multi-model Performance Analysis over North America for Six Operational Air Quality Forecast Systems

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Three agencies that produce daily operational air quality forecasts for North America began to exchange their forecasts on a routine basis in 2017, allowing a side-by-side comparison and ongoing evaluation of four different forecasts. The three agencies were Environment and Climate Change Canada (ECCC), which produces two slightly different forecasts, the U.S. National Oceanic and Atmospheric Administration (NOAA), and the European Centre for Medium-range Weather Forecasts (ECMWF). ECCC developed the multi-model verification system that receives and ingests the North American AQ forecasts from each centre and then evaluates the forecasts using near-real-time North American hourly surface measurements of O<sub>3</sub>, NO<sub>2</sub>, and PM<sub>2.5</sub> levels. A set of monthly multi-model performance statistics for North American daily maximum forecasts of O<sub>3</sub>, NO<sub>2</sub>, and PM<sub>2.5</sub> are automatically generated at the end of each month and shared with the participating centres on a seasonal basis. More recently, two more global forecast systems run by the U.S. National Aeronautics and Space Administration (NASA) and the Finnish Meteorological Institute (FMI) have joined this international collaboration for a total of six forecast systems, three regional and three global. By exchanging forecast scores on a regular basis, this international collaboration provides useful information on multi-model performance, including peer performance, seasonal variations and trends, unusual periods, and the impacts of model upgrades implemented by each centre.

## Session 6. Impacts (Application of AQ Modeling and Forecasting)

### Introduction.

**Moderator:** Alexander Baklanov<sup>1</sup>

<sup>1</sup> WMO

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### Sand and Dust Storm Forecasts and the Extended R&D and Application of CUACE

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CUACE is the CMA Unified Atmospheric Chemistry Environment which is designed for the numerical chemical weather forecasting. Based on CUACE, two forecasting systems have been developed in CMA. One is the CUACE/Haze-fog which is for heavy pollution warning, the other is CUACE/Dust which has been operationally run since 2006 in CMA and began issuing products since late of 2008 for Asian Regional Center of WMO SDS WAS, transferred into RSMC-ASDF BEIJING later in 2017.

Great improvements of SDS forecast in RSMC-ASDF BEIJING have been made in terms of international collaboration, modeling system, forecast skills and service, for sand and dust storm and also for the extended applications of regional haze and global Chemical weather.

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### Assessment of Health Impacts in Bogota using an Air Quality Modeling Platform

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Air quality (AQ) is a major challenge in Bogota. Frequently, PM ambient standards are exceeded in the southwestern areas of the city. An AQ modeling platform was established in Bogota aiming to understand sources of pollution and evaluate control strategies. Modeling fields allow to estimate pollutant concentrations outside the AQ monitoring network range. Health impacts can be assessed at the city domain using results from the model, along with epidemiological and demographics data.

In this work, we estimate the health burden of air pollution in Bogota and assess the economic cost. A maximum value of  $67.5 \mu\text{g}/\text{m}^3$  of  $\text{PM}_{2.5}$  was estimated by the model in the southwestern areas of the city. The  $\text{PM}_{2.5}$  average concentration resulted in 1,746 city-wide deaths, with a cost of 1000 million of dollars.

The large impact of air pollution in Bogota has motivated the environmental authority to define Urban Zones for Better Air (ZUMA in Spanish), where intersectoral actions will be concentrated to improve air quality, mitigate emissions and reduce the risk to people's health from air pollution.

**Session 6. / 49**

## **Operational Forecasting of Smoke, Visibility and Smoke-Weather Interactions by the High-Resolution RAP/HRRR-Smoke Models**

**Authors:** Ravan Ahmadov<sup>1</sup>; Eric James<sup>1</sup>; HRRR and FIREX-AQ teams<sup>1</sup>; Jordan Schnell<sup>1</sup>

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The Rapid Refresh and High-Resolution Rapid Refresh coupled with Smoke (RAP/HRRR-Smoke) models are based on NOAA's RAP/HRRR numerical weather prediction modeling systems. The RAP model domain covers the entire North and Central Americas at 13.5km grid spacing. The HRRR domain covers the contiguous US at 3km grid spacing. The RAP-Smoke model provides boundary conditions for the meteorological and smoke variables to HRRR. The RAP/HRRR-Smoke models have been running operationally at NOAA/NCEP since December 2020. In RAP/HRRR-Smoke primary aerosols (smoke) emissions from wild-land fires are simulated by ingesting the fire radiative power data from the VIIRS (onboard S-NPP and NOAA-20) and MODIS (Terra and Aqua) satellite instruments.

In this presentation I will discuss the applications of these models to forecast smoke distributions on local, regional and continental scales, and how adding the smoke capability helped to improve weather and visibility forecasting over the regions, when they are impacted by dense smoke. The verification of the HRRR-Smoke model for July-August 2021 using various ground based and remote sensing aerosol measurements will be presented. For verification of the fire plume injection height simulations in HRRR-Smoke we use the aircraft LIDAR and in-situ measurements from the FIREX-AQ campaign during summer 2019. Finally, I will discuss the remaining challenges in smoke forecasting and future plans to develop next-generation smoke forecast models.

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## **Effect of Climate Change on Air Pollution**

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The impacts of climate change on air quality – and thus on human and ecosystem health – act through multiple pathways. The drivers of these impacts are primarily higher temperatures (influencing chemical reaction rates), but also changes in other meteorological factors such as clouds (influencing photochemistry), precipitation (influencing deposition), and winds (influencing pollutant dispersion). Other Earth system feedbacks caused by climate change that affect atmospheric pollutant loads directly have already been observed (e.g., increased forest fires, sand and dust storms, biogenic emissions from land and oceans, and the release of methane from thawing permafrost).

This contribution provides a brief review of these drivers, highlights their complexity, and discusses promising approaches that can help to unravel and attribute causes. Concrete examples are provided by the evaluation of past trends in stratosphere-troposphere exchange of ozone using chemistry-climate

models and the influence of meteorology on air pollutant concentrations during the Covid lockdown using a machine-learning approach. The implications of this complexity between climate change and air quality for future mitigation policies will conclude the discussion.

**Session 6. / 55**

## **The Challenges of the Application of Air Quality Modeling and Forecasting in Decision-Making in Mexico**

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As in many other countries, Mexico needs to develop the capacity to model air quality for various diagnostic and forecasting applications. These two applications categories have common challenges and needs specific to one or the other. Both require being able to evaluate the model performance in terms of the maximum pollutants values and their hourly profiles. This requires comparisons against observations.

Another challenge is that the high spatial and temporal resolution emissions model, which is derived from the emissions inventory, must also be evaluated against measurements and this is seldom done in Mexico and when done, the results do not always find their way to those who carry out inventories for their improvement.

A major challenge is to develop and sustain modeling capability in its two general applications, both in terms of personnel and modeling infrastructure.

Here, national capacities and opportunities are discussed to face these challenges in Mexico.



**Session 6. / 16****Use of the AERMOD Code to Estimate SO<sub>2</sub> Dispersion from Emissions of Turrialba Volcano, Costa Rica**

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A daily and monthly estimate of sulfur dioxide (SO<sub>2</sub>) dispersion emitted by the Turrialba volcano in Costa Rica was made between January and December 2019 with the help of the AERMOD code. The measured data at the emission source such as topography (digital elevation model of the area around the volcano) and other characteristics of the emission source were included in the computer program. Annual average flux of SO<sub>2</sub> emitted by the main vent of the volcano was taken as the emission parameter, which was 119 Mg/day. The modeling of the measured parameters is run to generate pollutant dispersion maps, obtaining as a result the receiving points and the towns with the greatest impact by volcanogenic pollution, according to the month of the year. A meteorological station provided data on wind direction and speed, global radiation, temperature, percentage of relative humidity, precipitation, and atmospheric pressure.

The SO<sub>2</sub> dispersion maps show an emission at 360° around the volcano throughout the year, with a predominance of emission towards the west and southwest, where the Central Valley is located, an area that concentrates around 60% of the inhabitants of Costa Rica. Accordingly, to AERMOD, SO<sub>2</sub> reached a maximum average concentration of 60 µg/m<sup>3</sup>day (at less than 2 km from the crater), in April 2019.

With the scatter diagrams, estimates were made of the places with the greatest influence from the pollutant expelled by the Turrialba volcano, even minutes before the possible impact on the communities, which has allowed to warn about possible risks associated with exposure to SO<sub>2</sub> emitted by the volcano and to take the necessary precautions to minimize effects on human health.

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## Operational Air Quality Model Version 6: New Updates and Performance Evaluation

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The National Weather Service (NWS) National Air Quality Forecast Capability (NAQFC) implemented a newer version of the operational air quality model, AQM version 6, at the National Center for Environmental Prediction (NCEP) in July 2021. NAQFC is a collaborative effort to improve operational air quality (AQ) forecast guidance among the Environmental Modeling Center (EMC), Air Resources Laboratory (ARL), and Physical Sciences Laboratory (PSL) within the National Oceanic and Atmospheric Administration (NOAA), and with the Environmental Protection Agency (EPA) through the Memorandum of Agreement (MOA). The major upgrade includes extending our predictions from 48 to 72 hours and upgrading to the EPA Community Multiscale Air Quality model (CMAQ) version 5.3.1. CMAQ is driven by NOAA's operational Global Forecast System (GFSv16). The Kalman Filter Analog (KFAN)-based bias-correction algorithm applied to both ozone and PM<sub>2.5</sub> is also upgraded. The operational Global Ensemble Forecast System (GEFS)-Aerosol member at 25 km provides aerosol lateral boundary conditions to account for dust and smoke aerosols influxes. Various products are publicly available through the operational AQ display system (<https://airquality.weather.gov/>) and an experimental display in the cloud (<https://digital.mdl.nws.noaa.gov/airquality/>).

The performance of the AQMv6 is monitored daily and assessed through monthly statistics over the Contiguous United States (CONUS) domain and ten sub-domains. Overall, day 3 forecast skills over the CONUS domain during August are similar to day 2 for ozone in terms of the critical success index, while a slight reduction in skills is observed with PM<sub>2.5</sub>. Skill scores show large variability among sub-domains. In general, the bias-correction algorithm significantly reduces forecast errors for both ozone and PM<sub>2.5</sub>, including day 3 forecasts. More detailed evaluation results since its implementation will be presented at the workshop.

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## **Comparative Evaluation of Gas-Phase Chemistry and Aerosol Representations for the U.S. Next-Generation National Air Quality Forecast Capability using GFSv15-CMAQv5.3.1**

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The National Oceanic and Atmospheric Administration (NOAA) National Air Quality Forecast Capability (NAQFC) utilizes the offline-coupled Global Forecast System (GFS) with the Community Multiscale Air Quality (CMAQ) modeling system (GFS-CMAQ). Although NAQFC has used carbon-bond (CB) series mechanisms, its capability of deploying different mechanisms for operational forecasting has not been demonstrated. In this work, we configured an experimental version of NAQFC, driven by meteorological forecast from GFS v15, to drive CMAQ v5.3.1 for four representative months (January, April, July, and October) in 2019. GFS-CMAQ simulations with the mechanisms of CB6r3\_AE6/7, RACM2\_AE6, SAPRC07tc\_AE6, and SAPRC07tic\_AE6i/7i are inter-compared to assess the underlying causes of their different performance and to identify further needs in reducing the biases in predictions of ozone, aerosol, and their key precursors. RACM2 and SAPRC07 give higher O<sub>3</sub> predictions comparing to CB6r3, due to the difference in reaction rate constants and photolysis rates. While RACM2 gives lower formaldehyde than CB6r3 due to a higher photolysis rate, SAPRC07 gives higher formaldehyde than RACM2 and CB6r3 due to greater chemical production. RACM2 coupled with AE6 aerosol mechanism yields overall higher secondary organic aerosol (SOA) and inorganic aerosols than CB6r3\_AE6 due to its higher OH radical concentrations, except in the Southeast due to a lack of the reactive uptake of dicarbonyls. The implementation of detailed isoprene chemistry in SAPRC07tic\_AE6i increases O<sub>3</sub> and aerosol concentrations compared to S07tc\_AE6. The updates of monoterpene-SOA in the AERO7 aerosol mechanism increase biogenic SOA significantly. Excluding potential SOA from combustion from the residential wood combustion emissions largely reduces the overprediction of organic carbon during cooler months. This work demonstrates the forecasting capability of various gas-phase and aerosol mechanisms in CMAQ v5.3.1, and identifies the key factors in causing biases for future development and improvement of NAQFC.

## **Concluding Remarks**

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