## 20th Annual CMAS Conference

**November 2021**

## Oral Presentations

### Air Quality, Climate and Energy
**Tuesday, November 2 at 11:00 AM**

**Estimating heat related exposures: A case study of the 2012 Chicago Heatwave**

Kaiyu Chen
Author(s):

Kaiyu Chen, Mengjiao Huang, Colton Coon, Andrew J. Newman, Lyndsey A. Darrow, Matthew J. Strickland, Heather A. Holmes

Presenter(s): Kaiyu Chen

Format: Oral Presentation

Short Description: Heat-related impacts on human health have received increasing attention in recent years. Abnormal increases in temperature cause additional morbidity and mortality in highly urbanized regions and induce severe economic loss. Human activities, especially urban development, increase both the frequency and intensity of heatwaves (HW) and urban heat islands (UHIs). An extreme HW event occurred in 2012 summer that caused temperatures of more than 40? in Chicago, Illinois, USA, which is a highly urbanized city impacted by UHIs. Various numerical models, including the High Resolution Land Data Assimilation System (HRLDAS) and Weather Research and Forecasting (WRF) Model, were used to evaluate the model performance in simulating the HW and UHI. Sensitivity testing of three different WRF boundary layer physics options was done to determine the impact of increasing model complexity in simulating urban meteorology. The application of a multi-layer urban canopy model (MLUCM) in WRF performed best. MLUCM results showed that the HW caused rural temperatures to increase by ~4?, whereas urban Chicago had lower magnitude increases from the HW (~2-3? increases). Nighttime UHI intensity ranged from 1.44 to 2.83? during the study period. Spatiotemporal investigations of the temperature changes are used to quantify the excessive heat factor (EHF) that estimate heat-related exposure. The EHF during the HW episode provides a risk map indicating that while urban Chicago had higher heat-related stress during this event, the rural area also had high risk, especially during nighttime in central Illinois. This study provides a reliable method to estimate spatiotemporal exposures for future studies of heat-related health impacts.

## Future in- and out-of-state air pollutant emissions under decarbonization pathways for Massachusetts

Kaixin Huang
Author(s):

Kaixin Huang

Daniel H. Loughlin

Matthew J. Eckelman

Presenter(s): Kaixin Huang

Format: Oral Presentation

Short Description: Many U.S. states have adopted the goal of achieving carbon neutrality in the coming decades. Pathways for achieving these targets would likely yield a reduction of air pollutant emissions as well. We assess several state-level decarbonization pathways for Massachusetts, including electrification of buildings and transportation and decarbonization of the electric grid, estimating their impacts on in- and out-of-state emissions of carbon dioxide ($CO_2$) and several air pollutants. The analysis applies the GCAM-USA integrated assessment model with state-level resolution, and considers interactions between state and existing regional policies such as the Regional Greenhouse Gas Initiative and the Transportation and Climate Initiative. The most aggressive state decarbonization pathway that was examined would achieve only a 65% of reduction in $CO_2$ emissions by 2050, indicating the need for further decarbonization options within the industry and non-road transportation sectors. The air pollution co-benefits under these decarbonization pathways are significant, especially for PM2.5. While policies focusing only on MA are shown to produce in-state reductions of $CO_2$ and air pollutant emissions, a portion of these reductions was countered by emission increases in other states, indicating the need for coordinated planning to prevent leakage.

### Analyzing air emission co-benefits of transportation decarbonization scenarios for New York City using an energy systems model

Ozge Kaplan
Author(s):

Ozge Kaplan and Andrew Zalesak

Presenter(s): Ozge Kaplan

Format: Oral Presentation

Short Description: Many areas of the US require further emissions reductions to meet and maintain the National Ambient Air Quality Standards (NAAQS). Specifically, there has been a persistent NAAQS non-attainment issue surrounding the Northeast and Mid-Atlantic region. The majority of emissions that affect air quality originate from the energy system. New technologies for producing and using energy have the potential to dramatically alter future emissions. EPA recently developed an energy systems model for urban scale analysis for the State of New York focusing on New York City, City based Optimization Model for Energy Technologies (COMET), built on MARKAL/TIMES framework. In an earlier analysis, we highlighted the importance of increased energy efficiency and electrification of transportation at city scale to reach decarbonization targets where additional NOx reductions were observed due to reduced fuel consumption in heavy duty fleets and electrification of busses and LDVs. However, air pollutant emissions are estimated using regional average emission factors, emission factors from vehicles in NYC could be quite different from regional averages due to different driving conditions and vehicle type, age and condition. We will present a more refined analysis of light- and heavy-duty on-highway mobile emissions projections based on updated emission factors where we simulated county level data with the EPA's MOVES emissions model and other relevant sources. This includes the effects of EPA's Tier 3 standards set new vehicle emissions and fuel sulfur standards to reduce emissions beginning in 2017. The updated future year criteria air pollutant reductions due to decarbonization pathways would greatly aid in understanding future trends and help to refine policies so that greenhouse gas and air pollutant goals can be achieved in an equitable manner.

## Valuing the Impacts of Agricultural Soil Nitrogen Emissions on Air Quality and Climate

Lina Luo
Author(s):

Lina Luo, Rice University

Daniel S. Cohan, Rice University

Presenter(s): Lina Luo

Format: Oral Presentation

Short Description: Agriculture has long been neglected in air quality management and climate mitigation. However, fertilizer-intensive agriculture harms air quality and climate as the largest source of reactive nitrogen emissions in the United States (U.S.). Almost half of the nitrogen added to croplands is lost to the environment via runoff, sedimentation, or air emissions of nitric oxide (NO), ammonia (NH3), and nitrous oxide (N2O). Emission rates respond nonlinearly to meteorological conditions, soil properties, and farming practices. Once emitted to the air, NO and NH3 can contribute to the formation of ozone (O3) and fine particulate matter (PM2.5), with impacts that vary with atmospheric conditions. By contrast, N2O is a long-lived greenhouse gas whose radiative impact is independent of the timing and location of its origin. Thus, the relative emission rates and impacts of agricultural NO, NH3, and N2O may vary strongly by time and region. Understanding those variations can help inform the development of effective mitigation strategies. However, most prior studies have considered only individual pollutants or neglected the influences of farming practices and spatial and temporal variability. In this study, we develop an integrated assessment framework to compute emission rates and associated impacts of NO, NH3, and N2O from croplands, accounting for the influence of farming practices, atmospheric conditions, and interannual variability. This framework consists of a process-based biogeochemical model, Fertilizer Emission Scenario Tool for CMAQ (FEST-C), to simulate nitrogen emissions; a reduced-form air quality health effects model, Air Pollution Emission Experiments and Policy Analysis (APEEP), to estimate monetized impacts of NO and NH3 on air quality and health; and the social cost of N2O for comparing the relative importance of climate impacts with the air quality impacts. We have updated FEST-C by adjusting its crop demand-driven fertilizer database to consider fertilizer sales data and modifying its nitrogen schemes to include NO and N2O from nitrification NO from denitrification, adapting mechanisms from the DayCent model. Using this integrated framework, we compute adverse impacts of agricultural reactive nitrogen emissions across the contiguous U.S. for three years. We show that the social costs of greenhouse gases (N2O) are close to the monetized air pollution impacts associated with NO emissions but are lower than air pollution health impacts from NH3. Overall, climate impacts are relatively comparable to climate impacts for croplands in the Mountain and Northern Plains regions. However, in other regions, air quality impacts significantly exceed climate impacts. We also characterize how interannual variability of emissions rates and associated damages depend on both fertilizer input and meteorological conditions. Our results demonstrate that the selection of mitigation strategies should be regionally specific, due to the strong spatial variability in emission rates and the sensitivity of air quality and health to NO and NH3.

## Examining the Representation of Extreme Events in 4-km Dynamically Downscaled Simulations within the Southeast U.S.

Megan Mallard
Author(s):

Megan Mallard, Tanya Spero, Jared Bowden, Anna Jalowska, Geneva Gray, and Gregory Tierney

Presenter(s): Megan Mallard

Format: Oral Presentation

Short Description: As powerful computational resources become more available, finer resolution grid spacing can be used for long-term regional climate simulations. The use of increased spatial resolution to dynamically downscale global climate model output to finer regional domains has the potential to improve representation of extreme events. Presumably, the ability of the regional model to add value increases because mesoscale phenomena and finer-scale topographic and land use/land cover features can be better resolved. However, use of finer scale domains should be investigated to ensure that the chosen physics options are appropriate and that the computational expense is justified by improved results. Here, use of a 4-km domain for simulating extreme events with the Weather Research and Forecasting (WRF) model over the southeastern U.S. is explored and contrasted with results from a 12-km WRF simulation. A global reanalysis dataset, the 0.75° × 0.75° ERA-Interim, is used to drive 3-year simulations over a historical period (2015-2017). A 12-km domain covering the entire contiguous U.S. is run in a configuration similar to previous downscaling work, and then one-way nesting is used to implement a 4-km domain over the Southeast. This small ensemble of 4-km runs compares the use of the Multi-scale Kain–Fritsch scheme to an explicit approach to represent convective processes. These simulations will be compared with observation-based 2-m temperature and precipitation from PRISM (Parameter-elevation Relationships on Independent Slopes Model) data. The ability of these simulations to capture extremes in daily minimum and maximum temperatures, as well as heavy rainfall events, will be assessed.

## The impact of improving public transportation on decreasing air pollution and greenhouse gases emissions: the case of Sao Paulo, Brazil

Flavia Ribeiro
Author(s):

Flávia Noronha Dutra Ribeiro

Pedro Gerber Machado

Júlio Barboza Chiquetto

Dominique Mouette

Natasha Murgu Valdambrini

Jacyra Soares

Presenter(s): Flávia Noronha Dutra Ribeiro

Format: Oral Presentation

Short Description: The transportation sector is one of the major sources of greenhouse gases (GHG) emissions in the energy sector. In the Metropolitan Area of São Paulo (MASP), home to more than 20 million people, private cars contribute to 70% of vehicular air pollutants emissions and, even using biofuels such as ethanol, to more than 40% of GHG emissions. Therefore, the use of public transportation must be encouraged. However, to achieve this goal, investment in infrastructure is needed. An expansion of subway and metropolitan train lines was planned to take place until 2025, particularly towards the periphery of the MASP, but the actual implementation is delayed. The present work addressed the impact on air pollutants and GHG emissions of fully implementing the planned expansion of public transport. Emission scenarios were produced with SMOKE, using the expected emissions for the business as usual case and reduced emissions for the improved public transportation system case. Air quality simulations were performed using WRF-CHEM model and meteorology from 2018 was considered. While the general reduction of air pollutants concentration would be small, citizens near the planned stations would benefit from improved air quality. Considering GHG, the emission reduction is small but necessary to mitigate climate change. The results show that investment in public transportation has the potential to decrease GHG and air pollution emissions while increasing equality in transportation access.

## Modeling the Air Quality Impacts of Future Energy Scenarios

Uma Shankar
Author(s):

Uma Shankar[1,2], Kristen Brown[3], Ben Murphy[2], George Pouliot[2], Kristen Foley[2], Dan Loughlin[2], and Chris Nolte[2]

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[2]Office of Research and Development, U. S. Environmental Protection Agency, RTP, NC, USA

[3]Department of Civil Engineering, University of Texas at San Antonio, San Antonio, TX, USA

Presenter(s): Uma Shankar

Format: Oral Presentation

Short Description: Many areas of the United States remain out of compliance with the National Ambient Air Quality Standards. Additionally, some states have announced goals or adopted legislation to reduce emissions of carbon dioxide (CO2) and other greenhouse gases (GHGs). Human-Earth system models such as the Global Change Analysis Model (GCAM) can simulate the evolution of the energy system and estimate the associated emissions of both GHGs and traditional air pollutants. A tool has been developed to bridge GCAM and the Community Multiscale Air Quality Model using the Detailed Emission Scaling, Isolation, and Diagnostics (DESID) module, facilitating the simulation of the air quality impacts of alternative future energy scenarios, and better coordination of long-term air, climate and energy planning. In this work we demonstrate the application of this tool to examine the ozone and PM2.5 impacts at 2050 of a suite of GCAM scenarios, such as implementation of a Clean Energy Standard, high levels of electrification in the transportation and building sectors, and a moderate GHG reduction target.

## Air quality impacts of electric vehicle adoption in California

Nash Skipper
Author(s):

T. Nash Skipper, Armistead G. Russell

School of Civil & Environmental Engineering, Georgia Institute of Technology, Atlanta, GA

Presenter(s): Nash Skipper

Format: Oral Presentation

Short Description: Sales of electric vehicles (EVs) have increased in recent years and are expected to continue to rise. The governor of California has issued an executive order requiring, by 2035, all new cars and passenger trucks sold in California to be zero-emission vehicles. EVs are often touted for the climate benefits of reduced CO2 emissions, but EV adoption also has implications for air quality since emissions from onroad mobile sources contribute significantly to air pollution. We use the Community Multi-scale Air Quality Model (CMAQ) to estimate the impacts on PM2.5 and ozone of varying levels of EV adoption in the state of California. Simulations are conducted for one historic year (2016) and one future year (2028). The PM2.5 impacts of onroad emissions from tailpipe and non-tailpipe (i.e., brake and tire wear) emissions are also quantified. Results indicate that PM2.5 and ozone reductions from EV adoption scale approximately linearly with increasing EV adoption in much of California. Results also show that non-tailpipe emissions contribute up to 0.5 μg/m3 to annual mean PM2.5 concentrations.

## Life-Cycle Environmental Impacts of Liquid Hydrogen Production Pathways in La Guajira Colombia

Amanda Ullman
Author(s):

Amanda Ullman, Noah Kittner

Presenter(s): Amanda Ullman

Format: Oral Presentation

Short Description: As countries seek to transition their energy sectors towards zero-emissions energy systems, alternative energy carriers, like liquid hydrogen production, are becoming increasingly attractive for export and domestic use. Countries like Colombia, which export large levels of raw coal, must consider strategies to support a just transition for regions that depend economically on coal exports. Development of a hydrogen production industry is one such strategy discussed to support a just transition for coal dependent communities and to contribute to global environmental goals. This paper uses a life cycle assessment (LCA) methodology to examine the greenhouse gas emissions, water consumption, and trace metal emissions associated with six potential Colombian liquid hydrogen production strategies: (1) electrolysis powered by the country's national electricity grid, (2) onsite electrolysis powered by electricity produced by a wind farm, (3) offsite electrolysis powered by electricity produced by a wind farm, (4) electrolysis powered by electricity produced from a coal-fired power plant, (5) coal gasification without carbon capture and storage (CCS), and (6) coal gasification with CCS. The paper finds that wind-powered electrolysis outperforms the coal- and grid-powered scenarios in almost every environmental category, while coal-powered electrolysis consistently performs the poorest, with life-cycle mercury, nickel, and arsenic emissions of particular concern. While coal gasification with CCS reduced gasification $CO_2$ emissions by 35%, the scenario's VOC emissions were 62% greater than the gasification without CCS scenario, due to the increased inputs required to meet the same energy output. Wind-based power-to-hydrogen is also found to use at least 100 times less water than coal- or grid-based hydrogen production pathways. For Colombia to benefit from a hydrogen-based decarbonization transition, community-focused planning and wind-based hydrogen systems should be prioritized over grid- or fossil-fuel-based hydrogen production pathways.

## Impacts of Future Energy Transition on the U.S. Air Quality: Projections of Emissions and Air Quality in 2050

Kai Wang
Author(s):

Kai Wang[1], Yang Zhang[1], Shen Wang[2], Benjamin Hobbs[2], Hugh Ellis[2], Emily Fisher[2], Ken Gillingham[3], and Michelle Bell[3]

[1]Department of Civil and Environmental Engineering, Northeastern University, Boston, MA

[2]Department of Environmental Health and Engineering, Johns Hopkins University, Baltimore, MD

[3]School of Environment, Yale University, New Haven, CT

Presenter(s): Kai Wang

Format: Oral Presentation

Short Description: Understanding impacts of emission changes--especially those caused by the ongoing energy transition--on future air quality and human health is challenging due to the complex interactions among population and economic growth, energy demand, air pollution, and climate change. In this study, emission change factors (ECFs) of major air pollutants for energy-related sectors such as power plants, industrial, commercial, and residential, etc. are used in conjunction with the Sparse Matrix Operator Kernel Emissions model to project future emissions. The ECFs are generated through the downscaling approach based on the year 2050 projections from the National Energy Modeling System under a set of energy transition scenarios representing different drivers and shifts in the energy production/consumption in the future. The scenarios examined include a reference scenario without the clean power plan (refnocpp), a scenario with “abundant natural gas” (highNG), a scenario with “high electric vehicles penetration” (highEV), a scenario with “port electrification” (port), and a scenario with “high building energy efficiency” (highEE). Multiple 5-year (2008-2012) simulations using the Weather Research and Forecasting model with Chemistry (WRF/Chem) are carried out over the U.S. at a horizontal grid resolution of 36-km using current-year emissions based on the National Emission Inventory 2011 and projected future emissions in 2050. Our objectives are to 1) examine the emission changes for key air pollutants between future and past years under various energy transition scenarios, and 2) quantify the impacts of those emission changes on future air quality and human health. The preliminary results show large wide-spread reductions of CO, NOx, SO2, and primary PM2.5 emissions (~ 40-60% for gases and ~20% for aerosols) over the U.S. in 2050 for all scenarios, mainly due to coal power plants retirement and electric vehicles penetration, but much smaller reduction (~10%) for VOCs because the increases of their emissions from natural gas/oil production over source regions such as TX, PA, OH, and KY offset the decreases caused by power plant, industry, and transportation over the rest of domain. WRF/Chem predicts wide-spread domain-mean and maximum reductions of max 8hr O3 by < 2.0 ppb (~3.0%) and up to 8 ppb (~15%), respectively, and those for PM2.5 are by < 1.0 ug m-3 (~10%) and up to 6 ug m-3 (~50%), respectively, for all scenarios. The highEE scenario shows the largest reduction over the U.S. These reductions indicate the important impacts of energy transition on future air quality. The benefits of reduced air pollution on human health and economy under different scenarios will be further assessed in our future work.

**Air Quality, Climate and Energy (continued)**

## Decarbonization will lead to more equitable air quality in California

Shupeng Zhu
Author(s):

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Presenter(s): Shupeng Zhu

Format: Oral Presentation

Short Description: Climate policies enacted to mitigate emissions of greenhouse gases (GHG) further attain improvements in regional air quality that provide public health benefits to exposed populations. However, the current literature lacks an understanding of these co-benefits within the framework of socially vulnerable populations, including how portfolios of strategies within mitigation pathways can be designed to achieve maximum benefits within disadvantaged communities (DAC). Here, we introduce a Lorenz Curve based novel method (Suits Index) for quantifying and assessing the health co-benefits that accrue from regional air quality improvements associated with different long-term, low-carbon scenarios in California. The electrification of building appliances (HBE) yields 14.7% higher total co-benefits for DAC, as does the use of zero-emission renewable nature gas technologies (NBE). However, the considered distribution of co-benefits differs across DAC, e.g., the HBE is less progressive in promoting environmental justice compared to the NBE with a more flatted Lorenz Curve and a Suits Index 6.5% lower. Additionally, a cost/benefit analysis is performed to provide a comparison of the value of health benefits relative to the cost of implementing GHG mitigation strategies economy-wide. The results demonstrate the importance of including environmental justice analyses when evaluating climate mitigation policies.

## Cloud Computing

**Thursday, November 4 at 11:00 AM**

### Implementation and Testing of the Community Multiscale Air Quality (CMAQ) model on the Cloud

Elizabeth Adams
Author(s): Elizabeth Adams, Carlie Coats, Christos Efstathiou and Saravanan Arunachalam
UNC Institute for the Environment

Mark Reed and Robert Zelt
UNC Information Technology Services
Presenter(s): Liz Adams

Format: Oral Presentation

Short Description: Containers are lightweight, standalone, executable packages of software that offer a low-overhead method of building software such as the Community Multiscale Air Quality Modeling System (CMAQ) once, and then running across different cloud platforms and hardware. We developed methods to build, install, and run CMAQ as a Singularity container and Docker container. The container method scales well for the 12-km x 12-km Southeast U.S. domain on single node cloud computing environments including Amazon AWS and Microsoft Azure, using up to 96 processors with hyperthreading turned off. We also tested multi-node high performance computing on the cloud using the Amazon ParallelCluster command line interface and adapted CMAQ install scripts that mimic the container recipes to install and run CMAQ. The Azure Cycle Cloud benchmark (analogous to Amazon ParallelCluster) also showed good scalability using a containerized version of the 12-km x 12-km Continental U.S. (ConUS) domain benchmark case. The method to build the container required installing the software using the CMAS tutorial build instructions and then creating the container with the MPI libraries native to Azure's Cycle Cloud environment. This presentation will provide a summary of model performance for the benchmark simulations on the two different cloud computing environments for the two different modeling domains using single node as well as multinode configurations. Creating and sharing reproducible workflow methods for installing and building CMAQ for the 12-km x 12-km Southeast U.S. and ConUS benchmark cases using the Parallel Cluster and Azure Cycle Cloud will allow the CMAS community to learn how to provision resources, accurately forecast CMAQ modeling run time and storage requirements and further create reliable cost estimates for performing air quality modeling in the cloud for their individual use cases.

**Cloud Computing (continued)**

### Meteorology and Air Quality Modeling Using the AWS Parallel Cluster Cloud Service

Zac Adelman
Author(s): Zac Adelman and Tsengel Nergui
Lake Michigan Air Directors Consortium
Presenter(s): Zac Adelman

Format: Oral Presentation

Short Description: LADCO developed Weather Research Forecast (WRF) system and Comprehensive Air Quality Modeling System with Extensions (CAMx) modeling platforms on Amazon Web Services (AWS) for recent ozone and regional haze modeling projects. LADCO's motivation for using AWS was to take advantage of the scalable computing, memory, and data storage capabilities of the AWS cloud. LADCO modelers also envisioned that prototyping and deploying regional modeling capabilities on AWS would enable a new way to transfer modeling and high performance computing (HPC) capabilities to their member states. LADCO developed the AWS modeling platforms using the Parallel Cluster system for provisioning HPC resources. The system was developed to use AWS spot instances, which are as much as 75% less expensive than the on-demand AWS instances. This talk will describe the design of the AWS cluster used by LADCO, present performance statistics for relatively large-scale WRF and CAMx simulations, and show an analysis of the costs of the simulations. LADCO successfully used their AWS configuration for modeling to support and ozone attainment demonstration and regional haze state implementation plans (SIPs).

### CMAQ inverse modeling, WRF downscaling, and MPAS simulations on the cloud: Challenges and best practices

Matthew Alvarado
Author(s): Matthew Alvarado, Nicholas Heath, Chase Calkins, Rebecca Adams-Selin, John Henderson, Amy McVey, and Elizabeth Bettencourt
Atmospheric and Environmental Research (AER), Lexington, MA
Presenter(s): Matthew Alvarado

Format: Oral Presentation

Short Description: We will highlight three recent efforts to advance our air quality and meteorological modeling on the Amazon Web Services cloud. The first is our containerized CMAQ- and SMOKE-based inverse modeling system that optimizes NH3 emissions with Cross-track Infrared Sounder (CrIS) satellite observations. The second is our development of a cost-effective WRF-based downscaling system to produce high-resolution (4 km) climatologies from global climate model (GCM) output. The third is our on-going efforts to implementat the Model for Prediction Across Scales (MPAS) on AWS, which includes a discussion of the relative advantages and disadvantages of Amazon Batch and ParallelCluster for multi-node processing. Finally, we will discuss the policy and work flow changes we have made over the years to make cloud computing a regular part of our work, including staff training, investment in infrastructure development, resource tagging, and security policies.

**Cloud Computing (continued)**

## Migration and performance of CMAQ & WRF-CMAQ in the public cloud with commercial images

Arturo Fernandez
Author(s):

Arturo Fernandez (afernandez@odyhpc.com)

Presenter(s): Arturo Fernandez

Format: Oral Presentation

Short Description: Organizations interested in migrating their CMAQ & WRF-CMAQ workloads to the public cloud face several challenges including learning a new environment, cost prediction and performance optimization. The latter point is common when it comes to the migration of HPC (High Performance Computing) apps as public CSPs (cloud service providers) did not originally design their infrastructure with HPC in mind. Given these premises, system administrators and end-users have the choice to either prepare their own set-ups or use commercial images optimized for specific environments; these images integrate the app and its dependencies along with pre-processing and post-processing tools. The presentation will focus on the following aspects: Launching CMAQ & WRF-CMAQ with commercial images and scaling up to hundreds of cores Performance and scalability analysis Preliminary cost assessment AWS was the first commercial cloud platform and, since then, it has grown to offer multitude of services, which include several tailored to HPC needs. The first part of the presentation will cover how to run CMAQ with images in AWS infrastructure using either single instances or clusters composed by several instances; the latter option allows end-users to scale up CMAQ workloads up to hundreds or even thousands of cores. The presentation will also address the use of cluster monitoring tools. The second part of the presentation will cover performance and cost analysis. By using the U.S. Southeast test-case prepared by CMAS, it is possible to measure not only performance and cluster scalability, but also to perform comparisons vs. on-premises hardware. The evaluation of CMAQ performance in AWS infrastructure includes measurements with x86_64 and AArch64 (Graviton2) processors. These measurements provide side-by-side comparisons for both architectures as AArch64 processors are emerging as a cheaper alternative to x86_64 cores in the cloud market. The presentation will also make available data with Microsoft Azure infrastructure to provide measurements from a different CSP. Prediction of cloud costs is a non-trivial task that usually requires a TCO (total cost-of-ownership) analysis. A TCO analysis is beyond the scope of the presentation, but it is however possible to perform a cost assessment of computational power, which is the main contributor to overall cost. As CSPs offer a variety of payment options, the cost assessment will consider on-demand vs. reserved vs. spot prices. The cost assessment will also illustrate potential savings when using AArch64 vs. x86_64 infrastructure.

**COVID-19 and Impacts on Emissions and Air Quality**
**Wednesday, November 3 at 2:00 PM**

## Air Emission and Pollution Levels during the Pandemic in the Greater Athens Area, Greece

Athena Progiou
Author(s):

Athena G. Progiou a,b*, Ioannis Sempos b, Aikaterini-Maria Zarogianni c

Presenter(s): Athena G. Progiou

Format: Oral Presentation

Short Description: Lockdown restrictions due to the COVID-19 pandemic led to economic shudtdown and traffic limitations causing thus considerable reductions of air pollutant emissions and air quality levels. This work aims at studying the impact of traffic restrictions, due to pandemic, on air pollutant emissions and on atmospheric pollutant concentrations in the Greater Area of Athens, Greece. Data from the most representative air quality monitoring stations were collected and analysed for the period March to May 2017-2020 and were compared to the corresponding emission levels and emission reductions due to COVID-19 containment measures. Findings showed that road traffic emissions exhibit reductions, ranging for NOx, from 20 to 40% in March and April 2020, respectively. Likewise, PM10 emissions decreased by 25 and 40%. In the urban/traffic stations, significant reductions of NO2 (38-71%) and PM10 (30%) concentrations were determined in April 2020 compared to previous years. Reduction of C6H6 concentrations (50-80%) reflect emission decreases from petrol vehicles. In the analysis conducted, the relation between air pollutant levels and the corresponding emissions was identified. The conclusions drawn on air quality levels might provide policy makers with useful insights in order to plan and apply more efficient measures to reduce air pollution and comply with air quality standards and European Directives.This research was funded by the Natural Environment and Climate Change Agency (NECCA) of the Hellenic Ministry of Environment and Energy, under the framework of the project “Impact of restriction measures due to COVID-19 pandemic in terms of air pollution and climate change in the Greater Area of Athens (Greece)”.

## Emissions Inventories, Models, and Processes

**Wednesday, November 3 at 12:30 PM**

### Sensitivity of Particulate Matter Concentrations to Revised Estimates of Onroad Ammonia Emissions

Jesse Bash
Author(s):

Jesse Bash, Ben Murphy, Darrell Sonntag, Claudia Toro, Guy Burke, Karl Seltzer, Heather Simon, Kristen Foley, Alison Eyth, Chris Allen, Janice Godfrey

Presenter(s): Jesse Bash

Format: Oral Presentation

Short Description: In urban areas, mobile sources are important sources of ammonia (NH3) emissions that contribute to secondary formation of particulate matter. Recent studies have suggested that mobile ammonia emissions are underestimated in national and state emission inventories. In this study, we compared roadside, and tunnel ammonia measurements from light-duty gasoline and heavy-duty diesel vehicles to ammonia emission rates from EPA's latest version of the MOtor Vehicle Emission Simulator (MOVES3). The roadside and tunnel comparisons suggest that the ammonia emission rates for onroad vehicles are underestimated in MOVES3. From the evaluated roadside and tunnel data, we developed revised MOVES ammonia emission rates by vehicle class, model year, vehicle age, and operating mode for light-duty gasoline and heavy-duty vehicles for use in this study. We explored the effect of the revised onroad ammonia emission rates on US air quality using Community Multiscale Air Quality (CMAQ) simulations for the calendar year 2017 that were performed as part of the EPA's Air QUAlity TimE Series Project (EQUATES) to develop modeled meteorology, emissions, air quality and pollutant deposition for 2002 through 2017. Modeled datasets covering the Conterminous US (CONUS) were estimated using 12 km horizontal grid spacing, MOVES3 onroad emissions, Weather Research and Forecasting Model (WRFv4.1.1) meteorology, and CMAQv5.3.2 air quality modeling. A sensitivity simulation was performed with ammonia emissions from onroad non-diesel (primarily gasoline) vehicles scaled by a factor of 2.08 and onroad diesel vehicles scaled by a factor of 1.54; the factors were based on national-level MOVES output for calendar year 2017 using MOVES3 and the revised emission rates. All other model inputs and parameters were held constant. We explored the impact of these changes on PM2.5 concentrations. These updates increased three-month average PM2.5 by up to 0.5 ug/m3 in winter with regional impacts spread across the Eastern US and in some Western urban areas. Three-month average PM2.5 concentrations increased by up to 0.2 ug/m3 in summer with changes focused in major urban areas.

**Emissions Inventories, Models, and Processes (continued)**

## Using CrIS Ammonia Observations to Improve Decision Making on PM2.5 Control Policies

Nicholas Heath
Author(s):

Nicholas Heath, Matthew Alvarado, Amy McVey, Elizabeth Bettencourt, Chase Calkins, Karen Cady-Pereira, Jeana Mascio, Mark Shephard, Michael Sitwell, Jonathan Pleim, Limei Ran, Hansen Cao, Daven Henze

Presenter(s): Nicholas Heath

Format: Oral Presentation

Short Description: Ammonia (NH3) negatively affects air quality and human health, primarily through its role as a PM2.5 precursor. Therefore, accurate emissions estimates of NH3 are critical to air quality managers and forecasters. However, current emission inventories have significant uncertainties that inhibit reliable estimates of NH3. Observations from the satellite-based Cross-track Infrared Spectrometer (CrIS) provide an opportunity to improve NH3 emissions estimates using inversion-based modeling techniques. In the current study, CrIS NH3 observations are used in a finite-difference mass-balance inversion to constrain NH3 emissions in the Community Multiscale Air Quality (CMAQ) model. A unique aspect of our inversion is that it is applied using an NH3 bidirectional flux scheme. CMAQ is run over the continental United States using 12 km grid spacing for June 2015. A baseline simulation is made with unperturbed NH3 emissions. Then, a second simulation is performed with NH3 emissions perturbed by 20%. The resulting surface NH3 concentrations are compared to CrIS observations to derive a monthly-mean scaling factor for the a priori NH3 emissions. Lastly, an optimized simulation performed with the updated emissions improves agreement with CrIS observations. Encouragingly, the inversion also increases the correlation with independent NH3 observations from the Ammonia Monitoring Network (AMoN), increasing it from 0.66 to 0.7, while also reducing the overall error from 0.70 ug m-3 to 0.58 ug m-3. Similarly, we found that CMAQ simulations performed 36 km grid spacing spanning all of North America are also improved through this satellite-based inversion technique. Overall, this project illustrates the usefulness of applying satellite observations in a top-down inversion using NH3 bidirectional flux for improving NH3 emissions. The resulting emissions data will be made publicly available to air quality managers and other stakeholders for use in their air quality modeling applications.

**Emissions Inventories, Models, and Processes (continued)**

## Benefits from Low-NOx Omnibus and Advanced Clean Trucks (ACT) Adoption in 13 States and D.C. from 2020 to 2050

Jiaoyan(Joey) Huang
Author(s):

Jiaoyan (Joey) Huang[1], Jeff Houk[1], Shih-Ying Chang[1], Ray Minjares[2]
[1]Sonoma Technology, Petaluma, CA, USA

[2]International Council on Clean Transportation, San Francisco, CA, USA

Presenter(s): Jiaoyan (Joey) Huang

Format: Oral Presentation

Short Description: Fifteen states and the District of Colombia (D.C.) have signed a memorandum of understanding (MOU) that calls for 100% of new medium-duty (MD) and heavy-duty (HD) truck and bus sales to be zero emission vehicles by 2050, with an interim target of 30% by 2030. The California Air Resources Board (CARB) has adopted the Advanced Clean Trucks (ACT) and California HD Vehicle Phase II regulations and has proposed the low-NOx Omnibus regulation to accelerate MD and HD electric vehicle penetration and reduce on-road mobile source emissions in California. To understand the benefits of adopting these regulations and the resulting zero emission truck targets in other states, we designed a systematic method to estimate NOx, PM2.5, and CO2 equivalent (CO2e) benefits from these regulations. We developed five scenarios that used county-level on-road data for the year 2017 from the U.S. Environmental Protection Agency (EPA)'s MOVES3 model and EPA's Air QUAlity TimE Series Project (EQUATES), as well as data provided by state/local agencies, to model on-road emissions in 13 states (CO, CT, MA, MD, ME, NC, NJ, NY, OR, PA, RI, VT, WA) and D.C. for 2017, 2020, 2025, 2030, 2035, 2040, 2045, and 2050. The first scenario that was developed was a business-as-usual (BAU) scenario. We then post-processed total on-road NOx, PM2.5, and CO2e emissions for each state and D.C. based on four additional scenarios: • Scenario 2: Dual Harmonization (ACT Rule, Low-NOx Omnibus Rule with urban buses) from model year (MY) 2025 • Scenario 3: Only ACT Rule from MY2025 • Scenario 4: Only Low-NOx Omnibus Rule with urban buses from MY2025 • Scenario 5: Only California Phase II GHG Standard from MY2025 (benefits of Phase 2 trailer rule only) Emissions rates from the U.S. Department of Energy's Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies Model (GREET) model were used to calculate the impact on upstream emissions from electric utilities and petroleum fuel production. Compared to the BAU scenario, the typical NOx emission reduction (well-to-pump and vehicle emissions) is largest (25-30%) in scenario 2, and PM2.5 and CO2 emission reductions (well-to-pump and vehicle emissions) are 10-15% in scenarios 2 and 3. Some states had higher or lower reductions due to differences in fleet makeup and electrical grid emission rates. Detailed NOx, PM2.5, and CO2 emission reductions estimated for each state will be discussed, and the modeled future-year population of electric trucks will be presented. This information can help policymakers and scientists understand the benefits of zero-emission and low-NOx regulations.

**Emissions Inventories, Models, and Processes (continued)**

## Review of the PM2.5 source apportioning studies in the Megacity of Tehran

Hossein Khajehpour
Author(s):

Hossein Khajehpour, Farzaneh Taksibi, Mohammad Sadegh Hassanvand

Presenter(s): Hossein Khajehpour

Format: Oral Presentation

Short Description: The global trend of urbanization and limited environmental capacities have caused air pollution in Megacities, as one of the most prominent environmental concerns. In recent years, PM2.5 has been the major air pollutant in the Megacity of Tehran and the leading environmental risk factor causing health effects. Identification of the sources of this pollution is necessary for an effective environmental management program. Therefore, numerous studies have focused on source apportioning of PM2.5 in Tehran through emission inventory, source apportionment, and sensitivity analysis of the pollutants to the emission sources. A comparison of the methods and the derived results on relative shares of mobile and stationary sources in Tehran is studied in this short review. Our review shows that as the emission inventory approach is highly dependent on the geographic and sectoral coverage of the inventory, the results of this group of studies are not consistent. However, most of the source apportionment studies, although from different sampling locations and analytical methods, show similar shares of mobile and stationary sources in Tehran (in the range of 40% to 50%). This range is consistent with a published sensitivity analysis results which show that 47% of the PM2.5 concentrations in Tehran has resulted from mobile sources. The paper is concluded with a discussion on the methodological limitations of the methods, and finally, some suggestions for further developments of the study are proposed.

**Emissions Inventories, Models, and Processes (continued)**

## Assessment of Current and Future Airport-Related Emissions and their Impact on Air Quality in Atlanta, GA using CMAQ and TROPOMI

Abi Lawal
Author(s):

Abi Lawal, Armistead Russell (Ph.D.), Jennifer Kaiser (Ph.D.)

Presenter(s): Abi Lawal

Format: Oral Presentation

Short Description: Airports are high emitters of harmful pollutants species, leading to elevated concentrations and health implications as they tend to be located near city centers. Thus, better characterization of airport emissions is essential to understanding its effects on air quality. In this study, impacts of emissions from the Atlanta Hartsfield-Jackson airport (ATL) on ozone (O3), ultrafine particulates (UFPs) and particulate matter (PM2.5), are evaluated using the Community Multiscale Air Quality (CMAQ) model and high resolution satellite observations from TROPOMI. Two airport inventories are compared, an inventory using the default emissions where Landing and Take Off (LTO) processes are allocated at the same altitude and geolocation of the airport (default), and a modified (3D) inventory that has LTO and cruise emissions which are vertically and horizontally distributed, accounting for aircraft climb and descend rates. The 3D showed improved Normalized Mean Bias [NMB -46%/-43%] and Root Mean Square Error [RMSE 1.21/1.12 (1015 molecules/cm2)] between CMAQ and TROPOMI NO2 vertical column densities (VCDs), and improved agreement in ATL associated grids [RMSE 1.76/1.33 (1015 molecules/cm2)]. Close agreement of TROPOMI observations to modeled concentrations from measured sources (i.e. two power plants) was also observed. Our analysis indicated that ATL emissions yielded maximum increases in UFP particle number and PM2.5 mass by 6.5x108 #/m3 (~38%), and 0.7ug/m3 (~8%) respectively. Modelled Daily Maximum 8hr O3 with the modified inventory predicted an increase between 6ppb and 3ppb over the default inventory. Projected increases in future aviation emissions led to ozone increases up to 3 ppb around the airport as well. The results show 1) spatial allocation of airport emissions have notable effects on air quality and will be of further importance as airports become a larger part of the total urban emissions, 2) the applicability of high resolution satellite retrieval to better understand emissions from facilities such as airports.

## Emissions and Air Quality Implications of Upstream and Midstream Oil and Gas Operations in Mexicos Transforming Energy Sector

Elena Mcdonald-Buller
Author(s):

Elena C. McDonald-Buller, Gary McGaughey, John Grant, Tejas Shah, Yosuke Kimura, and Greg Yarwood

Presenter(s): Elena Mcdonald-Buller

Format: Oral Presentation

Short Description: Energy reform initiated under the Pacto por México in 2013 catalyzed transformational changes in Mexico's energy sector. Among the most significant outcomes was the allowance for private and foreign investment and participation for oil and gas exploration and extraction, reducing the influence of the state-owned monopoly of Petróleos Mexicanos (Pemex). Between 2015 and 2018, Mexico awarded more than 100 contracts for exploration and extraction of its onshore conventional, shallow water, and deepwater hydrocarbon resources. This study developed a bottom-up emissions inventory for criteria pollutants and precursors from upstream and midstream sector sources including onshore well sites, off-shore platforms, flaring, natural gas processing plants, and natural gas compressor stations for the 2016 base year and examined the status and spatial implications of blocks awarded to date through the bid rounds. The Comprehensive Air Quality Model with extensions (CAMx) was used with the base year inventory to examine contributions to ozone and fine particulate matter concentrations in Mexican and U.S. border states associated with onshore and offshore oil and gas producing regions in Mexico.

**Emissions Inventories, Models, and Processes (continued)**

## Application of the Reactive Organic Carbon Framework to Modeling VOC and PM Emissions

Ben Murphy
Author(s):

Ben Murphy[1], Karl Seltzer[2], Havala Pye[1], Emma D'Ambro[1], Colette Heald[3], and Jesse Kroll[3]

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[2]Office of Air and Radiation, Research Triangle Park, NC USA

[3]Massachusettes Institute of Technology, Cambridge, MA USA

Presenter(s): Ben Murphy

Format: Oral Presentation

Short Description: Organic emissions lead to ozone and particulate matter air pollution, which are known threats to both human and environmental health at global, regional, and local scales. Historically, the EPA has inventoried organic gas- and particle-phase emissions separately as VOC and PM-OC, respectively. However, the development of novel instrumentation and modeling capabilities has led to new terms and frameworks that often blur the line between gas- and particle-phase organics, which in turn have caused communication challenges between the regulatory and research-oriented air quality modeling communities. This is best highlighted by the inconsistent definition of "semivolatile." The emissions testing community definition is based on species that actively partition in concentrated stack, plume or tailpipe conditions (~50-10,000 µg m-3), while the atmospheric science community definition is based on ambient conditions (0.1-10 µg m-3). Overall, two core challenges for air quality modeling that result from these communication challenges are the inclusion of semivolatile primary organic aerosol and the emission of intermediate volatility organic compounds, which are known to efficiently produce additional aerosol after atmospheric oxidation. Given the influence and impact of regulatory and research data products, it is vitally important to resolve inconsistencies and decrease the barrier of incorporating new science to inform policy modeling, uncertainty analysis, and source attribution. We propose unifying VOC, semivolatile and organic PM emissions modeling tools under the reactive organic carbon (ROC) framework to consider the enormous breadth of sources, properties, and impacts relevant for these critical classes of air pollutants. This presentation will demonstrate the limitations in conventional methods for interpreting VOC and PM emissions, explain how these limitation are resolved with the ROC framework, share insights about potential emissions testing gaps that emerge using the ROC framework as a guide, and identify the specific modeling, data-reporting, and testing definition updates that should be made to fully realize the benefits of this comprehensive approach.

**Emissions Inventories, Models, and Processes (continued)**

## Whats New in SPECIATE 5.2?

George Pouliot
Author(s):

George Pouliot, Art Diem, Ying Hsu, Frank Divita, Venkatesh Rao, Casey Bray, Karl Seltzer, Havala Pye, Ben Murphy,Marc Menetrez

Presenter(s): G Pouliot

Format: Oral Presentation

Short Description: SPECIATE is a database of elements, compounds, particulate matter (PM) and other emissions from stationary and mobile sources. The SPECIATE project seeks to compile data from peer-reviewed literature or other sources on the identity of chemical species and composition of air pollutant emissions from all sources. Speciation profiles in the database contribute to emissions inventories and air quality modeling analyses that assess the impact of air emission sources on human health and the environment. For example, SPECIATE is used to support development of the National Emissions Inventory and associated modeling platforms, atmospheric modeling of regional haze, and prediction of human and ecological exposure. The SPECIATE database is a valuable tool used by air quality modelers, source-receptor modelers, emission inventory developers, and others who need a speciated breakdown of emissions. This presentation will summarize the newest updates to be included in SPECIATE 5.2 release including a major update to the species properties table.

**Emissions Inventories, Models, and Processes (continued)**

## Volatile chemical product enhancements to criteria pollutants in the United States

Karl Seltzer
Author(s):

Karl Seltzer, Ben Murphy, Elyse Pennington, Chris Allen, Kevin Talgo, Havala Pye

Presenter(s): Karl Seltzer

Format: Oral Presentation

Short Description: Volatile chemical products (VCPs) are a broad assortment of residential, commercial, institutional, and industrial sources of reactive organic carbon (ROC) emissions. Collectively, these sources currently contribute ~3.1 Tg of ROC emissions in the United States, with a substantial fraction of the sector (>20% by mass) serving as secondary organic aerosol (SOA) precursors. Here, we incorporate a new nationwide VCP inventory into the Community Multiscale Air Quality (CMAQ) model, with VCP-specific updates to better model air quality impacts. These CMAQ updates include representation of secondary air pollutant formation pathways for alkane-like intermediate volatility organic compounds (IVOCs), oxygenated IVOCs, and siloxanes. VCPs most enhance anthropogenic SOA formation in densely populated areas, with modeled, population-weighted annual average SOA increasing by 15 – 30% in Southern California and New York City due to VCP emissions (contribution of 0.2 - 0.5 μg m-3). Annually, VCP emissions enhance total population-weighted PM2.5 by up to 10% and generally ~5% in California, ~3% in New York, New Jersey, and Connecticut, and 1 – 2% in most other states. While the ozone enhancements from VCP emissions are more modest on average, their influence can cause a several ppb increase on select days in major cities and can account for up to 8.9% of annual-average maximum daily 8-hour ozone. Emissions from printing inks, cleaning products, paints and coatings contribute ~75% to the modeled VCP-derived SOA, and emissions from cleaning products, paints, coatings, and personal care products contribute ~81% to the modeled VCP-derived ozone. Overall, improved VCP emissions enhance modeled formation of multiple criteria pollutants throughout the United States, with the largest impacts in urban cores.

**Emissions Inventories, Models, and Processes (continued)**

## DIMENTIONING OF ATMOSPHERIC EMISSIONS CONTROL SYSTEM

Israel Soares
Author(s):

Israel Pestana Soares, Daniella Correa Gonçalves de Rezende and Karinnie Nascimento de Almeida*

Presenter(s): Israel Pestana Soares

Format: Oral Presentation

Short Description: One of the main challenges of the industry is to control fugitive emissions. Those can be defined as emissions that are not released by stacks, ducts or vents. Generation of fugitive emissions is intrinsic to the processes of steel plants and can be understood as a sequence of events, starting with feedstock preparation, transport and final product until its storage. Sinter plants and coal yard, for example, are areas that requires attention. There are a few alternatives that can be used to mitigate dust emissions in different areas of a steel plant. One of the most recent technology that is calling attention are the fog canyons. Those can spread a fine mist of water on the source of interest, increasing the density of the particles and consequently its sedimentation on the ground. This mechanism is called wet deposition and it acts similarly to rain, whereby particulate matter mix with water and wash out through atmosphere, minimizing pollutant dispersion. The main objectives of this study were determinate control systems (fog canyons) efficiency and criteria of its position in order to optimize the particulate matter control in critical areas of a steel plant. The OTM 32 (US EPA) - Exposure Profiling Method – is widely applied and is one of the best methods to monitor fugitive emissions. This method was developed to measure open source emissions of a pollutant, with exposure defined as the time-integrated mass flux of a pollutant at a sampling point. The mass flux is the product of pollutant concentration and wind speed, which gives the pollutant mass per unit of cross-section of the plume per unit of time. The total emissions from the source during the sampling period is found by spatial integration of the exposure over the cross-section of the plume. The efficiency of the control system performed relative to parameters such as wind speed, fog canyons high, angle and its position regarding the monitoring source of interest.

**Emissions Inventories, Models, and Processes (continued)**

## Adding the Model of Emissions of Gases and Aerosols from Nature (MEGAN) to the CMAQ Modeling System for inline biogenic emissions

Jeff Willison
Author(s):

Jeff Willison, Jonathan E. Pleim, David Wong, Francis S. Binkowski, and Christian Hogrefe

Presenter(s): Jeff Willison

Format: Oral Presentation

Short Description: Biogenic emissions of volatile organic compounds (BVOC) and nitric oxide can significantly contribute to surface concentrations of ozone and particulate matter. The current release of the Community Multiscale Air Quality (CMAQ) model offers the Biogenic Emission Inventory System (BEIS) as the only option for simulating inline biogenic emissions. This presentation will summarize the integration and performance of a second option, MEGAN v3.1, that will be included in CMAQ v6.0. We will present results from WRF-CMAQ simulations over the contiguous United States and from MPAS-CMAQ for a global domain. Comparisons with BEIS show that BVOC and nitric oxide production from MEGAN are strongly dependent on the configuration and runtime options. Enabling drought stress reduces BVOC production and PM2.5 concentration relative to BEIS, while improving the simulated organic carbon. Consistent with previous work, the Berkeley-Dalhousie Soil Nitric Oxide (NO) Parameterization simulates more NO and subsequently more ozone than the Yienger and Levy options that are available in both BEIS and MEGAN. The results from these sensitivity experiments will help CMAQ users improve the biogenic emissions configuration for their applications.

**Emissions Inventories, Models, and Processes (continued)**

## Impact of Recent Changes to Emissions Factors in BEIS on Estimation of Biogenic VOC Emissions for GEM-MACH

Junhua Zhang
Author(s):

Junhua Zhang, Verica Savic-Jovcic, Alexandru Lupu, and Michael D. Moran

Presenter(s): Junhua Zhang

Format: Oral Presentation

Short Description: Vegetation is an important source of VOC (volatile organic compound) emissions, accounting for about 80-90% of global total VOC emissions. Accurate estimation of biogenic VOC emissions is critical for air quality modeling, particularly for summertime when O3 production is high due to favorable meteorological conditions. The Canadian air quality model, GEM-MACH (Global Environmental Multiscale—Modelling Air-quality and Chemistry), employs the Biogenic Emission Inventory System (BEIS) for estimating biogenic emissions (https://www.epa.gov/air-emissions-modeling/biogenic-emission-inventory-system-beis). BEIS3.09 with updated VOC emissions factors for needleleaf trees is currently being used in GEM-MACH and VOC emissions estimated from BEIS3.61 are being tested. However, a new BEIS version, v3.70, developed within the Community Multiscale Air Quality (CMAQ) model has recently been released. Compared to BEIS3.61, emissions factors in BEIS3.70 have changed significantly for many types of vegetation. Leaf Area Index (LAI) value for crops have also been updated. In this presentation, changes to biogenic VOC emissions due to changes to emissions factors in various versions of BEIS will be investigated for the GEM-MACH regional 10-km North American grid. The impacts of these changes on GEM-MACH predictions will be discussed too.

## Machine Learning and Reduced Form Models Developments and Applications

**Tuesday, November 2 at 2:00 PM**

### A development of PM2.5 forecasting system using physicochemical models and ensemble machine learning

Younseo Koo
Author(s):

Youn-Seo Koo?Dae-Ryun Choi?Hui-Young Yun?Geon-Woo Yoon?Joung-Beom Lee?Hee Yong Kwon?Suk Hyun Yu?Ji-Seok Koo

Presenter(s): Younseo koo

Format: Oral Presentation

Short Description: Ambient exposure to PM2.5 is harmful effect on public health and the forecasting PM2.5 is essential to protect the public health in advance. Current PM2.5 forecasting systems in operation are mainly based on the physicochemical models such as CMAQ and WRF. The forecasting accuracy of them however, have substantial limits due to uncertainty of input data of anthropogenic emissions and meteorological fields as well as the physicochemical models themselves. In order to overcome the drawback of the prognostic model predictions and to take advantage of the recent advance in machine learning algorithm, the PM2.5 forecasting system using physicochemcal models of CMAQ and WRF as well as ensemble machine learning method is being developed and tested for national PM2.5 forecasting in Korea. The various levels of big data based on observation and model outputs and machine learning methods to reflect temporal variations and spatial characteristic PM2.5 between the source and receptor regions.

## Novel Higher-Order Sensitivities of Secondary Organic Aerosols with Respect to Their Precursor Concentrations using a Box Model Version of CMAQ-hyd

Jiachen Liu
Author(s):

Jiachen Liu, Eric Chen, Shannon L. Capps

Presenter(s): Jiachen Liu

Format: Oral Presentation

Short Description: Secondary organic aerosols (SOAs) are generated by complex transformations of organic molecule emissions and are often a significant portion of atmospheric particulate matter (PM) concentrations. High PM concentrations can lead to regional haze and pose health risks to the public. Understanding the sensitivities of SOA formation with respect to precursor concentrations is therefore essential for evaluating the highest priority of SOA precursor emissions to reduce. Existing methods of calculating the sensitivity coefficients include the finite difference method (FDM), the direct decoupled method (DDM), and the adjoint method. The FDM suffers from truncation and cancellation errors, while DDM and the adjoint method are relatively difficult to implement and maintain in chemical transport models. Here, we propose an alternative approach to calculating first- and second-order sensitivities. This method is an operator overloading approach which calculates the exact first- and second-order sensitivity coefficients of select precursors through one single run of the model (Fike & Alonso, 2011). We applied this method in the Community Multiscale Air Quality (CMAQ) model v.5.3.2 to formulate the CMAQ-hyd model. In this work, we apply a box model version of the CMAQ-hyd to compute the exact sensitivities of SOA concentrations with respect to their precursor concentrations. The sensitivity coefficient results could aid in evaluating the current Regional Haze Rule and potentially new NAAQS rules for the total atmospheric PM2.5 concentration in the future.

## Application of a Partial Convolutional Neural Network for Estimating Missing TROPOMI NO2 Remote Sensing Information

Yan Lops
Author(s):

Yannic Lops, Arman Pouyaei, Masoud Ghahremanloo, Yunsoo Choi, Arman Pouyaei, Jia Jung

Presenter(s): Yannic Lops

Format: Oral Presentation

Short Description: Nitrogen Oxides (NOX) are highly reactive and are one of the major criteria pollutants with significant negative impact on human health and the environment. The spatial coverage and quality of satellite remote sensing Nitrogen Dioxide (NO2) measurements are essential as an indicator for NOX concentrations. Unfortunately, satellite-derived measurements are negatively impacted by surface reflectivity and cloud cover, which lead to biases. Thus, these measurements would need to be discarded and significantly increase the amount of missing data within a satellite-derived image. This work employs the Partial Convolutional Neural Network to impute missing remote sensing data of the TROPOspheric Monitoring Instrument (TROPOMI) NO2 measurements efficiently and accurately for the entire Contiguous United States. The neural network model was trained by employing simulated NO2 from the Community Multiscale Air Quality Modeling System and missing masks from the TROPOMI dataset.

## From COVID-19 to future electrification: Assessing traffic impacts on air quality by a machine-learning model

Jiani Yang
Author(s):

Jiani Yang, Yifan Wen, Yuan Wang, Shaojun Zhang, Joseph P. Pinto, Elyse A. Pennington, Zhou Wang, Ye Wu, Stanley P. Sander, Jonathan H. Jiang, Jiming Hao, Yuk L. Yung, and John H. Seinfeld

Presenter(s): Jiani Yang

Format: Oral Presentation

Short Description: The large fluctuations in traffic during the COVID-19 pandemic provide an unparalleled opportunity to assess vehicle emission control efficacy. Here we develop a random-forest regression model, based on the large volume of real-time observational data during COVID-19, to predict surface-level NO2, O3, and fine particle concentration in the Los Angeles megacity. Our model exhibits high fidelity in reproducing pollutant concentrations in the Los Angeles Basin and identifies major factors controlling each species. During the strictest lockdown period, traffic reduction led to decreases in NO2 and particulate matter with aerodynamic diameters <2.5 μm by –30.1% and –17.5%, respectively, but a 5.7% increase in O3. Heavy-duty truck emissions contribute primarily to these variations. Future traffic-emission controls are estimated to impose similar effects as observed during the COVID-19 lockdown, but with a smaller magnitude. Vehicular electrification will achieve further alleviation of NO2 levels.

**Model Development**
**Wednesday, November 3 at 11:00 AM**

**Modeling Current and Future Windblown Utah Dust Events Using CMAQ v5.3.1**

Bradley Adams
Author(s):

Zachary Lawless, Bradley R. Adams

Presenter(s): Bradley Adams

Format: Oral Presentation

Short Description: Windblown dust events can be defined as windblown dust emitted from the Earth's surface to the atmosphere. These events have significant impact on local air quality. Predicting the location and magnitude of these events is important for air quality assessment and planning. Previous modeling studies have focused primarily on past dust events. This work utilizes a state-of-the-science software framework based on WRF v4.2.1, OBSGRID, and the Community Multiscale Air Quality (CMAQ) v5.3.1 modeling system to predict dust events in Utah. This approach is easily applied to other geographical regions as well. The framework was verified using previous studies for dust events in April 2017 and March 2010. Once verified, the framework was used to predict the impact of future land use properties on dust events. Two scenarios were studied – shrinking of the Great Salt Lake and the addition of large-scale solar farms west of the Wasatch Front. Both showed large increases in dust concentrations near dust sources and lesser but still significant increases over populated areas using the meteorological conditions from the April 2017 dust event. Such information from future impact studies can assess potential impacts from climate change and can guide government water and land use policies to mitigate dust event impacts.

**Model Development (continued)**

## CMAQ-MetEmis: Development of meteorology-sensitive emissions coupler with National Air Quality Forecasting Capability (NAQFC)

BH Baek
Author(s):

Baek, B.H., Wang, C.T., Ma, Siqi, Tong, Daniel and Coats, Carlie

Presenter(s): B.H. Baek

Format: Oral Presentation

Short Description: The National Oceanic and Atmospheric Administration (NOAA) and National Weather Services (NWS) have developed its operational National Air Quality Forecasting Capability (NAQFC). One of the NAQFC chemical transport models (CTMs) is the Community Multiscale Air Quality (CMAQ) model developed by the U.S. Environmental Protection Agency to forecast concentrations of ozone and particulate matter below 2.5 μm (termed PM2.5) over the contiguous continental U.S. (CONUS). One of the recent key developments in NAQFC is dynamically coupling the three major components: meteorology, emissions, and pollutant chemistry-transport. Simulating emissions inline is crucial especially for real-time air quality forecasting. It allows the model to include the influences of the most recently forecast meteorological fields on emissions from key emission sources. While biogenic emissions, bi-directional NH3 from fertilizer applications, and point-source plume rise are calculated inline in CMAQ, other important emissions sectors have little or no accounting of meteorological influences in current air quality forecasts. Sources such as onroad/off-network mobile, agricultural livestock, and fugitive dust use annual or monthly total emissions and standard weekly/daily temporal allocation profiles to disaggregate them on finer time scales for the hourly air quality forecasts. Especially, the onroad/off-network mobile emission sector is one of the most complicated and computationally expensive emission sectors in emission processing for CTMs. It requires the most computational resources and time to compute meteorologically sensitive mobile emissions from various processes (i.e., running exhaust, star-up, evaporative, idling, refueling, hot soak, etc.) This study aims to share the recent inline meteorology-sensitive emissions (MetEmis) module development within CMAQ (CMAQ-MetEmis) that can dynamically represent onroad mobile emissions without its computational requirements that are currently prohibitive in real-time air quality forecasting applications. We will illustrate its computational enhancements and air quality simulation performances, and confirm its feasibility for NAQFC applications.

**Model Development (continued)**

## The National Air Quality Forecast Capability Using the NOAA Global Forecast System: Model Developments and Community Applications

Patrick Campbell
Author(s):

Patrick C. Campbell, Youhua Tang, Pius Lee, Barry Baker, Daniel Tong, Rick Saylor, Ariel Stein, Jianping Huang, Ho-Chun Huang, Li Pan, Edward Strobach, Jeff McQueen, Ivanka Stajner, Jamese Sims, Jose Tirado-Delgado, Youngsun Jung, Fanglin Yang , Tanya L. Spero, Robert Gilliam, Michael Neish, and Paul Makar

Presenter(s): Patrick C. Campbell

Format: Oral Presentation

Short Description: The next-generation National Air Quality Forecast Capability (NAQFC) in the U.S. uses the advanced Finite Volume Cubed-Sphere (FV3) Global Forecast System (GFS) Version 16 to drive the 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 provides 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 a comprehensive analysis against the prior operational NAQFC for predictions of summer season ozone (O3) and winter season fine particulate matter (PM2.5). 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 O3 and PM2.5 predictions and diurnal patterns. New 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 O3 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.

**Model Development (continued)**

## CMAQ 5.3 PARALLEL PERFORMANCE FOR A 192-DAY SIMULATION

George Delic
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Presenter(s): George Delic

Format: Oral Presentation

Short Description: This presentation continues with a report of the thread parallel performance results for CMAQ 5.3 expanded here to include a 192-day simulation. This extends by far the results in [1] and will eventually reach the goal of the entire 2016 year-long scenario. Attention is focused on the Gear, Rosenbrock, and EBI solvers in the Chemistry Transport Model (CTM), by comparing both FSparse [1], and the legacy JSparse [2] algorithms. The former implements OpenMP thread parallelism for all three solvers in the CTM. Thread parallelism in the horizontal advection science procedures (HADV) is also included. The results discussed include execution performance and numerical precision for the first two quarters of the 2016 annual CONUS scenario provided by the U.S. EPA [3]. Both the legacy (EPA) JSparse and the FSparse thread parallel versions are compared in a hybrid MPI+OpenMP version on a heterogeneous cluster of 14 nodes with a total of 192 of the available 232 cores.[1] G. Delic, Modern Environmental Science and Engineering, Vol. 5, Nr.9, 2019, pp. 775-791. Full text available at: https://www.researchgate.net/publication/338581080_A_Thread_Parallel_Sparse_Matrix_Chemistry_Algorithm_for_the_Community_Multiscale_Air_Quality_Model[2] M. Jacobson and R.P. Turco (1994), Atmos. Environ. 28, 273-284.[3] The author gratefully acknowledges help from Kristen Foley (EPA), Ed Anderson (GDIT), and Elizabeth Adams (UNC) in providing model data and resolving implementation issues.

**Model Development (continued)**

## F0AM-CMAQ Model Framework for Secondary Organic Aerosol Development: F0AM Model integration of ISORROPIA and the CMAQ 5.3.2 Aerosol Modules

Jaime Green
Author(s):

Jaime R. Green, Yuzhi Chen, Jason D. Surratt, and William Vizuete

Presenter(s): Jaime R. Green

Format: Oral Presentation

Short Description: Field and laboratory measurement data have shown the importance of an aerosol's phase state in determining its interactions with gas-phase oxidation products derived from biogenic volatile organic compound (BVOC) emissions and on the formation and evolution of secondary organic aerosols (SOA), with implications on climate and air quality. Recent flow tube and smog chamber experiments systematically generated SOA and were subsequently collected by a particle-into-liquid sampler (PILS) for time-resolved chemical measurements. PILS samples were then analyzed for SOA constituents by either reverse-phase liquid chromatography (RPLC) or hydrophilic liquid interaction chromatography (HILIC) coupled to electrospray ionization-high resolution-quadrupole-time-of-flight mass spectrometry (ESI-HR-Q-TOFMS) and inorganic aerosol constituents by ion chromatography (IC). These experimental systems have produced new insights on how acidity, organic water, and phase state alters the formation of isoprene epoxydiols (IEPOX)- derived SOA. These SOA formation processes are not well represented in the current Community Multiscale Air Quality Model (CMAQ) model and could result in a significant under-prediction of the production of organic sulfur, affecting multiphase reactivity, phase state, aerosol growth, and reactive uptake of other chemical species. This work describes the development of the F0AM-CMAQ box model that will use these experimental data to evaluate and develop modifications to the existing CMAQ model. The F0AM-CMAQ model is based on the Framework for 0-D Atmospheric Modeling (F0AM) model and includes two critical updates. First is the integration of the inorganic aerosol thermodynamic equilibrium model (ISORROPIA 2.1) with the purpose of determining the acid-base activity of the inorganic components of the aerosols at varying percentages of relative humidity. The second is based on current implementation of SOA formation in CMAQ. Both of these modules will allow an evaluation of any explicit aerosol formation mechanism, developed based on field and laboratory data, alongside any mechanism developed for CMAQ. This model also has the capability of taking advantage of any explicit gas-phase chemical output from the F0AM model. Results presented here include the comparison of the predicted evolution of SOA mass loading between CMAQ and the observational data provided by our previous experiments using the F0AM-CMAQ model. These model runs will guide future updates to the CMAQ model related to isoprene derived SOA.

**Model Development (continued)**

## Implementation and evaluation of total vegetation data in the CMAQ windblown dust module

Xinyue Huang
Author(s):

Xinyue Huang, Hosein Foroutan

Presenter(s): Xinyue Huang

Format: Oral Presentation

Short Description: Simulation of windblown dust emissions in regional to global scale atmospheric models requires vegetation coverage as input to account for the alteration of dust flux by vegetation. Most of the current models merely consider the coverage of photosynthetically active (green) vegetation (PV) due to the availability of various remote sensing indices for estimating PV fractions and omit the non-photosynthetic (brown) vegetation (NPV), which is prevalent in dust source regions and potentially has significant impacts on simulated dust loads. In this study, we implemented a satellite-based dataset for total vegetation, which comprises NPV and PV, into the windblown dust module in CMAQ v5.3 model. The NPV and PV fractions were derived from the MODIS Nadir Bidirectional Reflectance Distribution Function-Adjusted Reflectance (NBAR) product MCD43A4 using spectral mixture analysis (SMA). The SMA method assumed that the seven bands of MODIS surface reflectance as well as their log-transformed and interactive terms were linear combinations of the synthetic reference reflectance of three pure components, namely NPV, PV, and bare soil, and resolved the fraction of each component. To examine the effects of NPV, we also conducted a control simulation using the PV-only data (i.e. the fraction of absorbed photosynthetically active radiation (fPAR) data based on MOD15A2GFS product). Simulations were conducted for the entire year 2016 over the conterminous United States at 12 km resolution. With the inclusion of NPV, the simulated dust concentrations decrease by above 10% over most of the southwestern U.S. during spring to autumn. Reductions in dust concentrations are the largest in spring, and when compared to observations from the IMPROVE sites, overpredictions of fine soil concentrations are attenuated at over 93% of the sites in the western U.S. Further analyses indicate that directly sheltering the surface and increasing the threshold velocity through drag partitioning are major mechanisms for NPV to suppress dust emissions. On the other hand, NPV causes the friction velocity to increase by more than 10% over most erodible lands during autumn and winter, which can amplify the dust flux. This study highlights the impact of total (PV+NPV) vegetation, which may be important to other parts of the model (e.g., dry deposition module).

**Model Development (continued)**

## Testing internally compressed netcdf-4 file format within SMOKE-IOAPI framework

Roger Kwok
Author(s):

Roger Kwok and Sarika Kulkarni

Presenter(s): Roger Kwok

Format: Oral Presentation

Short Description: The new Detailed Emissions Scaling, Isolation & Diagnostic (DESID) module that has been in place since the implementation of CMAQ5.3.1, offers great flexibility to CMAQ users on performing any number of model sensitivity studies by scaling multiple emission streams and exploring multiple regions/chemical species/PM size distribution combinations. Instead of allowing one single-layered, gridded emissions file with multiple inline emissions as in previous CMAQ versions, multiple emission streams together with the inline emissions can be ingested into the model. However, the arbitrary increase in the number of emission files poses disk space issues. Furthermore, windowing the emissions inventory into a subdomain has to be carried out offline, henceforth duplicating the emission files. The disk space constraint necessitates file size reduction. A conventional way to do this typically uses standalone compression tools (gzip, pbzip2, etc) on netCDF classic files before and after emission processing and/or AQ modeling, thus considerably increasing offline processing time. Therefore, research has been conducted at the California Air Resources Board (CARB) to offer a solution to the disk space problem with reduced overhead cost. This can be achieved via two one-time steps. First, recompile netCDF with additional libraries: Libz to enable compression, and Hierarchical Data Format (HDF5) to allow for more complex data structures with unlimited array size. Second, edit IOAPI source code to utilize the newly recompiled netCDF libraries, so that every Models3 program (CMAQ, MCIP, SMOKE, etc) can be recompiled with the updated libraries. Further code edits to IOAPI also provides end-users an additional option to choose the format of the netCDF outputs: either in compressed mode, or in 64-bit offset format to cater to large file sizes. The latter is particularly useful for CMAQ's regular or instrumental runs. Initial tests show that file size becomes 10% of its netCDF classic counterpart in compressed mode. More test results will be presented.

**Model Development (continued)**

## Modeling secondary organic aerosol formation from volatile chemical products in Los Angeles

Elyse Pennington
Author(s):

Elyse A. Pennington, Karl M. Seltzer, Benjamin N. Murphy, Momei Qin, John H. Seinfeld, Havala O.T. Pye

Presenter(s): Elyse A. Pennington

Format: Oral Presentation

Short Description: Volatile chemical products (VCPs) are commonly used consumer and industrial items that are an important source of anthropogenic emissions. Organic compounds from VCPs evaporate on atmospherically relevant time scales and include many species that are secondary organic aerosol (SOA) precursors. However, the chemistry leading to SOA, particularly that of intermediate volatility organic compounds (IVOCs), has not been fully represented in regional-scale models such as the Community Multiscale Air Quality (CMAQ) model, which tend to underpredict SOA concentrations in urban areas. Here we develop a model to represent SOA formation from VCP emissions. The model incorporates a new VCP emissions inventory and categorizes new SOA precursor emissions into three classes: siloxanes, oxygenated IVOCs, and nonoxygenated IVOCs. VCPs are estimated to produce 1.67 ug m-3 of noontime SOA, doubling the current model predictions and reducing the SOA mass concentration bias from -75% to -58% when compared to observations in Los Angeles in 2010. While oxygenated and nonoxygenated VCP species are emitted in similar quantities, SOA formation is dominated by the nonoxygenated IVOCs. This work suggests that VCPs contribute up to half of anthropogenic SOA and it is necessary to better represent SOA precursors from VCPs in CMAQ algorithms to predict the urban enhancement of SOA.

**Model Development (continued)**

## Implementation of Kain-Fritsch convective mixing scheme into CMAQ subgrid cloud modeling

Arman Pouyaei
Author(s):

Arman Pouyaei, Bavand Sadeghi, Yunsoo Choi, Jia Jung, Amir H. Souri, Chun Zhao, Chul Han Song

Presenter(s): Arman Pouyaei

Format: Oral Presentation

Short Description: To improve the representation of convective mixing of atmospheric pollutants in the presence of clouds, we developed a convection module based on Kain and Fritsch (KF) method and implemented it in the Community Multiscale Air Quality model. The KF-convection method is a mass flux-based model that accounts for updraft flux, downdraft flux, entrainment, detrainment, and the subsidence effect. The method is consistent with the convection parametrization of the meteorology model. We apply the KF-convection model to an idealized case and to a reference setup prepared for East Asia during the KORUS-AQ campaign period to investigate its impact on carbon monoxide (CO) concentration at various atmospheric altitudes. We investigate the impact of KF-convection on the horizontal distribution of CO concentrations by comparing it to aircraft measurements and the MOPITT CO column. We further discuss two types of impacts of KF-convection: the direct impact caused by vertical movement of CO concentrations by updraft or downdraft and the indirect impact caused by transport of lifted CO concentrations to another region. May 12 saw a high indirect impact originating from the Shanghai region at higher altitudes and a high direct impact of updraft fluxes at 1 km altitude. However, May 26 revealed an immense updraft increasing higher altitude concentrations (up to 40 ppbv) and diverse indirect impacts over the region of the study (±50 ppbv). The overall comparison shows a strong connection between differences in the amount of concentration caused by the direct impact at each altitude with the presence of an updraft at that altitude. The developed model can be employed in large domains (i.e., East Asia, Europe, North America, and Northern Hemisphere) with sub-grid scale cloud modeling to include the impacts of convection.

**Model Development (continued)**

## Integrating reactive organic carbon emissions into the Community Regional Atmospheric Chemistry Multiphase Mechanism (CRACMM)

Havala Pye
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George Pouliot, US EPA Office of Research and Development

William R. Stockwell, University of Texas at El Paso

Presenter(s): Havala Pye

Format: Oral Presentation

Short Description: The chemical mechanism of an atmospheric chemical transport model like the Community Multiscale Air Quality (CMAQ) system contains a condensed set of reactions that describe the interactions between emitted organic compounds and nitrogen oxides as well their reaction products. The Community Regional Atmospheric Chemistry Multiphase Mechanism (CRACMM) builds on the history of the Regional Atmospheric Chemistry Mechanism, Version 2 (RACM2) and aims to couple gas- and particle-phase chemistry by treating the entire pool of atmospheric reactive organic carbon (ROC) relevant to present-day emissions. Here, we develop CRACMM species to represent the total emissions of ROC, considering the OH reactivity, ability to form ozone and secondary organic aerosol (SOA), and other properties of individual emitted compounds. Compared to RACM2, we reduce the number of traditional volatile organic carbon species and increase the number of oxygenated and semivolatile to intermediate volatility precursors in the mechanism. In addition, we add explicit hazardous air pollutants to better characterize exposures relevant for human health. We contrast emissions of ROC in 2002 and 2017 from the EPA's Air QUAlity TimE Series project and their treatment in CRACMM to illustrate how precursors to ozone, SOA, and other endpoints are expected to propagate through the system. The CRACMM mechanism species will be operationalized in chemical transport models in future work.

**Model Development (continued)**

## Development and Initial Application of WRF-Chem-GHGs: Integrated Modeling of Air Quality, Carbon, and Climate

Yang Zhang
Author(s):

Yang Zhang1, Kai Wang1, Xiaoyang Chen1, Daniel Schuch1, Eeshan Basu1, Siqi Ma2, Daniel Tong2,3, and Ravan Ahmadov4,5

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Presenter(s): Yang Zhang

Format: Oral Presentation

Short Description: Mitigation of air pollution and carbon emissions in a changing climate requires an integrated modeling system that can dynamically simulate important feedbacks between climate/meteorology and atmospheric chemistry (i.e., so-called online-coupled models) and simultaneously track the evolution of criteria air pollutants (CAPs) (e.g., SO2, NO2, O3, CO, and PM) and greenhouse gases (GHGs) (e.g., CO2 and CH4). While online-coupled weather and chemistry models (e.g., the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem)) have been developed since early 2000's, regional/urban air quality modeling that can simultaneously track the atmospheric evolution of CAPs and GHGs has not been performed. In this work, to fill in the above model deficiency, we are developing an innovative integrated model system based on WRF/Chem to simultaneously simulate the atmospheric evolution of CAPs and GHGs and account for the chemistry-meteorology/climate feedback in one simulation (referred to as WRF-Chem-GHGs). WRF-Chem-GHGs integrates WRF-Chem with full chemistry and the WRF Greenhouse Gas Model (WRF-GHG) for the CO2/CH4 tracers. It can simulate the emissions, transport, removal, and chemical and physical processes for both CAPs and GHGs and their interactions via meteorology, radiation, cloud, and chemistry. In the initial application of WRF-Chem-GHGs, anthropogenic CAPs emissions are based on the US EPA's National Emission Inventory (NEI), and anthropogenic CO2 emissions are based on Vulcan version 3.0. Biogenic VOCs and CO2 emissions are generated online based on the Model of Emissions of Gases and Aerosols from Nature version 2 (MEGAN2) and the Vegetation Photosynthesis and Respiration model (VPRM), respectively. The simulation results will be evaluated using observations from the EPA's surface networks for CAPs such as (e.g., the Aerometric Information Retrieval Now (AirNow), the Aerometric Information Retrieval System– Air Quality System (AIRS-AQS), and the Chemical Speciation Network (CSN)) and the tall towers datasets for CO2 from the NOAA's Carbon Cycle Greenhouse Gases (CCGG) program. The enhanced model capability of WRF-Chem-GHGs allows simultaneous predictions of GHGs and CAPs in one simulation that is currently not possible and thus will provide a powerful tool to develop mitigation strategies for co-benefits of air quality, carbon, and climate change.

## Modeling to Support Exposure and Health Studies and Community-scale Applications

**Thursday, November 4 at 2:00 PM**

### Integrating Time-Activity and Air Quality Sensors and Models into Smartphone-based PM2.5 and Ozone Exposure Model (TracMyAir)

Michael Breen
Author(s):

Michael Breen, Vlad Isakov, Catherine Seppanen, Sarav Arunachalam, Miyuki Breen, Steven Prince, Thomas Long, David Heist, Parikshit Deshmukh, Wyat Appel, Christian Hogrefe, Benjamin Murphy, Chris Nolte, George Pouliot, Havala Pye, Jacky Rosati

Presenter(s): Michael Breen

Format: Oral Presentation

Short Description: Epidemiologic studies of ambient fine particulate matter (PM2.5) and ozone (O3) often use outdoor concentrations as exposure surrogates, which can induce measurement error. We developed an exposure model called TracMyAir, which is an iPhone application that determines eight tiers of individual-level exposure metrics in real-time for ambient PM2.5 and O3 using outdoor concentrations, home building characteristics, weather, time-locations, and time-activities. In this study, we extended TracMyAir by including (1) outdoor concentrations from an air quality model (CMAQ) and air monitoring network (OpenAQ), (2) indoor and outdoor PM2.5 concentrations from low-cost air sensors (PurpleAir), (3) microenvironment model (MicroTrac) based on time-resolved smartphone geolocations, and (4) inhaled ventilation models based on physical activity data from smartphone and smartwatch accelerometers and heart rate sensors. The exposure metrics for the extended TracMyAir include: residential air exchange rates (AER, Tier 1), infiltration factors (Finf_home, Tier 2), indoor concentrations (Cin_home, Tier 3); and personal outdoor concentrations (Cout, Tier 4), time spent in ME (TME, Tier 5), exposure factors (FPEX, Tier 6), exposures (E, Tier 7), and inhaled doses (D, Tier 8). We applied TracMyAir to determine hourly PM2.5 and O3 exposure metrics for two panel studies with nine participants living in central North Carolina: one study with 216 participant hours during November 2019, and another study with 648 participant-hours during September-October 2020. The TracMyAir predictions showed considerable temporal and house-to-house variability of AER, Finf_home, and Cin_home (Tiers 1-3), and person-to-person variability of Cout, TME, FPEX, E, and D (Tiers 4-8). Our study demonstrates the capability of extending TracMyAir with air quality and time-activity sensors and models to determine individual-level ambient PM2.5 and O3 exposure metrics, in support of epidemiologic studies and public health strategies to help individuals reduce their exposures to ambient air pollutants.

**Modeling to Support Exposure and Health Studies and Community-scale Applications (continued)**

## Air Quality Benefit from Accelerated EV Penetration in Southern California: A Case Study in the Interstate 710 Corridor

Shih Ying Chang
Author(s):

Shih Ying "Changsy" Chang[1], Jiaoyan Huang[1], Marcus Alexander[2], Doug Eisinger[1], Nathan Pavlovic[1], and Eladio Knipping[2]

[1] Sonoma Technology, Petaluma, CA

[2] Electric Power Research Institute, Palo Alto, CA

Presenter(s): Shih Ying Chang

Format: Oral Presentation

Short Description: As substantial progress is made on improving regional air quality, there is increased attention on addressing the ongoing challenge of reducing pollution exposure for individuals in disadvantaged communities living near heavily traveled roads such as major freeways and truck routes. Accelerated penetration of electric vehicles (EVs) into the vehicle fleet offers potential air quality benefits for near-road communities, but these benefits, to our knowledge, have not been previously quantified at a community scale. This case study aims to quantify the air quality benefit of EV penetration in environmental justice (EJ) communities in the Southern California Interstate 710 Corridor using a fine resolution modeling framework. Four future-year EV penetration scenarios in 2040 will be evaluated. These scenarios include Scenario A, business as usual (BAU); Scenario B, high EV penetration; Scenario C, medium EV penetration; and Scenario D, EV penetration for medium- and heavy-duty vehicle. The penetration of light-duty EV for each scenario is modeled with the Market Acceptance of Advanced Automotive Technologies (MA3T) model. The penetration of medium- and heavy-duty EV is based on policy analysis by the California Air Resource Board. The estimated EV penetration is used to adjust the emission factors modeled with the EMission FACtor mobile source emission model (EMFAC2017) to generate emission factors for each scenario. These emission factors will be combined with detailed travel activity data to estimate roadway emissions within a modeling domain covering Long Beach, California, and surrounding communities. These emissions will then be used by the Research LINE source dispersion model (RLINE) to estimate NOx and PM2.5 concentrations at a census block group level for both EJ and non-EJ communities in the modeling domain. The comparison between the four scenarios will provide information on how accelerated EV fleet penetration can close the gap in air quality between EJ and non-EJ communities.

**Modeling to Support Exposure and Health Studies and Community-scale Applications (continued)**

## Modeling Exposure of Diesel Particulate Matter in California

Shuming Du
Author(s):

Shuming Du, Sue Chen, Karry Liu, Zhen Liu, Abdullah Mahmud, Wenli Yang, Melissa Venecek, Roger Kwok, Pingkuan Di, and Jeremy Avise

Presenter(s): Shuming Du and/or Pingkuan Di

Format: Oral Presentation

Short Description: Diesel particulate matter (DPM) has been identified as a human carcinogen and toxic air contaminant (TAC) by many jurisdictions. In the past two decades, tremendous efforts have been made to reduce exposure of DPM to the public in California. However, since DPM cannot be directly measured, DPM concentrations and associated health risks need to be assessed using air quality models. Some existing studies unitized grid-based photochemical models such as CMAQ or CAMx to calculate DPM concentrations. Since most DPM emissions are emitted from on-road and off-road mobile diesel engines (such as trucks, locomotives, etc.), aggregated gridded emissions treated by CMAQ or CAMx may not fully reflect/represent actual emission source characterization. As such, accurate source-receptor relationships cannot be established, especially at a local/community scale. In this study, we utilize an air dispersion model - CALPUFF to simulate DPM concentrations for each emission source and category in 2017. Specifically, on-road mobile sources and some off-road mobile sources (such as OGV, locomotives, airport takeoff and landing, etc.) are characterized as individual line sources, major stationary sources are treated as individual point sources, and the remaining DPM emissions are simulated as area sources with fine resolution. DPM concentrations are calculated at every centroid of the census blocks and hundreds of explicit locations of interests, such as schools, daycare centers, elder centers, etc. As a comparison, CMAQ modeling is also conducted using the same emission inventory and meteorology but with different emission treatments (2km x 2km gridded). The similarities and differences of the modeling results between CALPUFF and CMAQ will be discussed. Both models' performance will be conducted by comparing to available observations. Elemental carbon (EC) is chosen as a surrogate of DPM because DPM cannot be measured directly, and it is understood that EC is likely to have a high correlation with DPM.

**Modeling to Support Exposure and Health Studies and Community-scale Applications (continued)**

## Reduction of air pollution concentrations due to a solid barrier downwind of a roadway: wind tunnel results and dispersion model development

Dianna Francisco
Author(s):

Dianna M. Francisco[1], David K. Heist[2], Akula Venkatram[3], Lydia H. Brouwer[4], and Steven G. Perry[2]

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Presenter(s): Dianna M. Francisco

Format: Oral Presentation

Short Description: Noise barriers have been proposed as a mitigation measure to reduce human exposure to traffic-related air pollutants. This paper presents new results from wind tunnel studies examining the effect of solid roadside barriers of varying heights (from 3 m to 9 m) on concentrations downwind of a roadway. These wind tunnel results are used to further develop a mixed-wake algorithm that accounts for barrier effects within a steady-state air dispersion model. The mixed-wake algorithm combines two flow regimes, one for flow above the barrier and one for the recirculation region that develops downwind of the barrier. The regime representing the recirculation region exhibits a uniform vertical concentration profile while the concentrations in the upper regime rise to a peak above the barrier before decreasing with height. Observations of the barrier-induced flow field and concentration patterns, and the mixed-wake algorithm implemented into the air dispersion model will be described. The algorithm was implemented in the U.S. EPA regulatory air dispersion model, AERMOD, using the non-regulatory line-source option, RLINEXT. Both the wind tunnel and mixed-wake algorithm show that relative to a roadway without a barrier, a solid barrier substantially reduces concentrations immediately downwind of the barrier with the greatest reductions occurring with the tallest barriers. Model performance will be evaluated using geometric mean (MG), geometric standard deviation (SG), and the fraction of model results that are within a factor of two of the observations (FAC2).

**Modeling to Support Exposure and Health Studies and Community-scale Applications (continued)**

## Estimating Risks due to Exposure to Toxic VOCs in Southern California Utilizing the Community Multi-scale Air Quality Model version 5.3.2 (CMAQv5.3.2)

Abdullah Mahmud
Author(s):

Abdullah Mahmud, Pingkuan Di, and Jeremy Avise

Presenter(s): Abdullah Mahmud

Format: Oral Presentation

Short Description: The Community Multi-scale Air Quality Model version 5.3.2 (CMAQv5.3.2) was utilized to simulate toxic Volatile Organic Compounds (VOCs) in the atmosphere for 2017 within major air basins in Southern California including the South Coast, San Diego, and Imperial. Formaldehyde, acetaldehyde, benzene, 1,3-butadiene, perchloroethylene, and p-dichloroethylebezene are some of the VOCs that have been identified as human carcinogens and toxic air contaminants (TACs) in California, which pose significant health risks through inhalation exposure. In this study, the annual average and population weighted concentrations of the toxic VOCs were calculated at a 2-km spatial resolution and at aggregated to population census tract levels within the model domain. The annual average concentrations were then applied to calculate cancer risks and burden with an objective to understand the distributions of toxic VOCs within southern California and to identify disadvantaged communities that are likely to experience higher pollution burden as required by the California community air protection Assembly Bill 617 (AB 617). In addition, the modeling results will be used to quantify the contribution of each toxic VOC to overall impact in Southern California. For formaldehyde and acetaldehyde, their relative contributions from primary (direct emissions) and secondary formed from atmospheric chemistry will be specified. The results of source attribution can be used to evaluate the benefits of emission reduction efforts the state has taken and to direct the efforts to further reducing toxic VOCs. The 2017 simulations were driven by the meteorological fields generated by the Weather Research Forecast version 3.9.1 (WRFv3.9.1) model. The gridded and speciated sector specific emissions were combined by the SMOKE emissions processing system. The air quality simulations were carried out separately using two emissions scenarios: 1) emissions that include sources within the US border only and 2) emissions within the US plus the sources adjacent to the southern border in Mexican side within the modeling domain. This was done to portray air quality as accurately as possible, particularly, within the communities that are near to the US-Mexican border. The boundary conditions for the 2-km model runs were generated from the state-wide 12-km model output. The model performance analysis was carried out using available data including satellite measurements and ground based monitored data for toxic VOCs, fine particulate matter (PM2.5), and ozone.

**Modeling to Support Exposure and Health Studies and Community-scale Applications (continued)**

## Influence of meteorological data on the health risk associated with PM10 Santa Catarina - Brazil

Clarissa May
Author(s):

Clarissa May, Robson Will, Vinicius Fin, Ana Paula Stein Santos, Otávio dos Santos, Leonardo Hoinaski

Presenter(s): Clarissa May

Format: Oral Presentation

Short Description: This study evaluated the influence of temperature and humidity data on the health risk associated with particulate matter (PM10) in two cities, Camboriú and Florianópolis, in the state of Santa Catarina, Brazil. We use data from hospital admissions for cardiorespiratory diseases and PM10 concentration data collected with a high volume sampler (AGV-MP10). We calculate the relative risk of cardiorespiratory diseases related to air PM10 in children under five years of age and adults over forty, due to their greater vulnerability. The health costs caused by these diseases associated with particulate matter are estimated by applying the Disability Adjusted Life Years (DALY) methodology. The highest calculated risks are found in the city of Florianópolis. In both cities, the annual risk variation is not significant, as well as the costs. The air pollution cost related to PM10 was larger in Florianópolis, whose population is about seven times larger than that of Camboriú. Analyzing the seasonally, there are some cases of significant variations in both cities, however, following different patterns. Children are the most affected as they have higher rates of variation. Comparing meteorological data from the respective cities, it was possible to observe that the humidity data had little relationship with the risk data. Temperature and humidity are inversely correlated to the risks.

## Effects of aircraft source characterization on AERMOD model performance for a major US airport

Chowdhury Moniruzzaman
Author(s):

Chowdhury Moniruzzaman, Gavendra Pandey, and Saravanan Arunachalam

Presenter(s): Chowdhury Moniruzzaman

Format: Oral Presentation

Short Description: Aircraft's landing and take-off (LTO) emissions contribute to surface air quality in and around an airport. Dispersion modeling helps to quantify the effects of aircraft emissions on surface air quality. We present results of two tasks: 1) effects of airborne aircraft emissions on surface air quality and 2) effects of varying number of sources in dispersion modeling. Although there are many studies on the effects of aircraft's surface emission on surface air quality, effects of airborne emissions on surface air quality in dispersion modeling remains poorly understood. In the first task, AERMOD modeling was performed for the Los Angeles International Airport (LAX) for SO2 for 1 month in February, 2012 for 2 cases: emissions with and without air-sources. The difference between the 2 cases gave the air emission's contribution to surface concentration which were found to be 3 to 6% at 3 monitors (AQ, CN and CS) and 13% at another monitor (CE) where all 4 monitors were within 2 km of the runway. The second task was motivated by a research need to reduce the number of sources in the Federal Aviation Administration's (FAA's) Aviation Environmental Design Tool (AEDT) produced AERMOD hourly emission file. Both the surface (idle, taxi and takeoff) and airborne sources were reduced by accumulating the emissions in an hour in a smaller number of sources based on their locations by developing a python-based emission processor which uses raw AEDT flight segment data as input. AEDT-segment surface emission data were extracted for 2 source characterizations: 1) 31-sources having 16 runway sources for landing and take-off in both direction with highly simplified 15 non-runway sources and 2) 138-sources having same 16 runway sources of 31-source case but having spatially detailed 122 non-runway sources having separate detailed taxiway, taxi-ramp, terminal and gate sources. AERMOD modeling was performed for the LAX airport for SO2 for Feb 1, 2012 for 3 surface source number sensitivity cases: 1) 1440, 2) 138 and 3) 31 surface sources. Based on 1 day's results for the 138-source run, the simulation found that 90% surface source reduction (from 1440 to 138) decreased computation time by 90% and changed the mean absolute error (MAE) by +8%, -10%, +1% at 3 sites (AQ, CN, CE) and +98% at 1 site (CS). For the 31-source run for 1 day's results, the simulation found that 98% surface source reduction (from 1440 to 31) decreased computation time by 95% and changed the MAE by -5%, -0.06%, -0.8% at 3 sites (AQ, CN, CE) and +85% at 1 site (CS). As airborne source's contribution is found to be 3-6% at 3 of the 4 sites, the number of airborne sources can be reduced significantly in AEDT for AERMOD modeling. The treatment of surface sources can also be reduced significantly to gain computational efficiency without affecting model performance in AERMOD predictions.

**Modeling to Support Exposure and Health Studies and Community-scale Applications (continued)**

## Modeling Aircraft Sources at sub-hourly time scales in AERMOD

Gavendra Pandey
Author(s):

Gavendra Pandey1, Chowdhury Moniruzzaman1, Saravanan Arunachalam1, and Akula Venkatram2

1Institute for the Environment, University of North Carolina at Chapel Hill 2University of California at Riverside

Presenter(s): Gavendra Pandey

Format: Oral Presentation

Short Description: Aircraft emissions from an airport are a significant source of total emissions that have an impact on air quality in the airport vicinity. These sources are unique due to the transient nature of the emissions from each source, as well as the buoyant exhaust. These sources emit the pollutants in short bursts especially during landing and takeoff operations (LTO). It is difficult to quantify these short bursts emissions and model the governing processes. An added complexity occurs when the wind speed is low and variable. In this condition, winds can go in several directions during an hour, resulting in multiple concentration “lobes”, and large plume spread. The classical steady-state model such as AERMOD does not account for the meandering effect and short bursts of aircraft emissions due to the hourly nature of inputs and outputs in typical applications. To account these features that characterize the dispersion of aircraft emissions, a sensitivity analysis based on the sub-hourly approach is being described in this paper. We used the SO2 concentration measurements from the LAX Air Quality Source Apportionment Study (AQSAS) conducted at the Los Angeles International Airport (LAX) on four core locations named AQ (Air Quality), CN (Community North), CS (Community South), and CE (Community East) for 42 days period during February and March 2012. This paper focuses on the effect of the sub-hourly approach on dispersion. We used AERMINUTEplus, the enhanced version of the AERMET preprocessor AERMINUTE that outputs sub-hourly wind averages. The output from AERMINUTEplus is used in AERMET, and then AERMOD is run multiple times for each portion of an hour, and output concentration files are simply averaged on that hour using a previously developed approach called SHARP (Sub-Hourly AERMOD Run Procedure). Hourly AERMOD simulations produced concentrations that were significantly greater than those at AQ and CS and significantly lower than those at CN and CE. The fractional bias based on top 26 robust highest concentrations improved from -1.50 and -1.37 to -0.91 and -0.79 respectively at sites AQ and CN sites, and showed little change at sites CS and CE. The ratio of medians of the observed to the modeled concentrations is improved from 3.6 to 2.2 at the CS site. In addition, the model performance improved substantially by replacing meteorological parameters such as friction velocity and Monin-Obukhov (M-O) length during stable and unstable conditions with those corresponding to neutral conditions. The use of the SHARP approach magnifies the mid to lower range concentrations and lower concentrations nearly match the observations. The fraction of model estimates within a factor of two of the observations improved from 32 to 55% at the CN site and at the CS site, by up to 46%. Overall, our sub-hourly modeling results using SHARP are relatively closer to observations and demonstrate that this alternate approach should be seriously explored in circumstances when low-wind meander conditions predominate and for treating aircraft sources.

**Modeling to Support Exposure and Health Studies and Community-scale Applications (continued)**

## Application of Photochemical Grid Models to Identify High Priority Locations for Health-Based Community Monitoring Needs

Marco Rodriguez
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Ralph Morris (Ramboll US Consulting Inc)

Presenter(s): Marco Rodriguez

Format: Oral Presentation

Short Description: Photochemical Grid Models (PGMs) are capable to assess the chemical formation and transport of secondarily formed pollutants, and this makes them suitable for use in a wide variety of regulatory and research purposes. PGM can produce vast amounts of data in the form of gridded air quality concentrations for multiple pollutants over a defined three-dimensional modeling domain. An advantage of data generated with PGMs is that enables scientists and regulators to have a more complete understanding of pollutant spatial variability than what is possible through monitoring data alone. However, the wealth of detailed information generated by PGMs is not commonly available to the broader public due to logistical constraints associated with transmitting, hosting, and visualizing large datasets. As the public and elected officials increasingly emphasize the importance of government transparency and equal access to clean air and water, so too our tools need to be upgraded and re-envisioned to serve these broader needs. PGMs data can aid regulatory agencies and communities make informed decisions for areas most in need of enhanced air monitoring funding to further Environmental Justice initiatives recently announced by the United States Environmental Protection Agency. In this presentation, we detail a method to develop an air quality screening tool based on local PGM results in combination with equity indicators to assist local and state government agencies identify areas most likely to have disproportionate air quality burdens that are a high priority for further monitoring efforts. This approach presents distinct advantages relative to federal screening tools, such as EJSCREEN, because is based on best available local data, rather than national defaults, and it exclusively uses air quality indicators, rather than have results confounded by other environmental variables. Further, the screening tool can be readily shared with the public to engage community members in meaningful and well-informed dialogue regarding potential air pollutant burdens as an important step to increase transparency, communication, and trust with historically underserved communities. Since many states and regions across the U.S. have access to PGM results from past analyses, leveraging local PGM data to assess environmental justice could provide a more robust method to prioritize future efforts and support informed community engagement.

**Modeling to Support Exposure and Health Studies and Community-scale Applications (continued)**

## Specifics of pollutant dispersion in street canyons

Margret Velizarova
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Presenter(s): Margret Velizarova

Format: Oral Presentation

Short Description: The urban area is a unique system, which includes all aspects of the natural environment, which was subsequently modified by the introduction of a build environment (so-called physical environment). Despite of all air quality studies conducted in Bulgaria during the last decades, the effect caused by the physical environment on the urban pollution hasn’t been studied till this day. The numerical experiments were conducted with the Air Quality Management & Assessment System: ADMS-Urban, which is a comprehensive system for air quality modeling in urbanized areas, and it is developed and supported by the private organization Cambridge Environmental Research Consultants (CERC). The main goal of this study is to present the spatial and temporal concentration distributions of atmospheric pollutants in street canyons, typical for Sofia city. In addition, the impact of the street canyon parameters on the pollutant concentrations from transport sources, was evaluated. The utilization of detailed spatial representation of the urban infrastructure (as 3D maps) can considerably affect the air quality modelling. It can describe the pollution field structure and help with locating the ‘hot spots’ of pollution, and by this way to secure valuable tools in favor of urban planning, design and management, in terms of creating regulations and guidance for future urban development projects, public works and activities in the urban environment.

## The U.S. Gulf region air toxicants (Styrene and BTEX) study: Emission estimate result by source types and concentration estimate

Chi-tsan Wang
Author(s):

Chi-Tsan Wang, William Vizuete, Marc Serre, Richard Strott, Jaime Green, Bok Haeng Baek*

Presenter(s): Chi-tsan Wang

Format: Oral Presentation

Short Description: These ambient toxicants, Styrene, Benzene, Toluene, Ethylbenzene, and Xylenes (SBTEX) , are emitted from the petrochemical industry, combustion process, transport emission, and solvent usage sources. There have been several SBTEX toxic assessment studies, but they mainly relied on the ambient measurements using GC-MS (Gas Chromatography-Mass Spectrometer)/FID (Flame Ionization Detector) combined with the statistical models or dispersion models to understand their behaviors in the atmosphere. However, the measurements are limited to specific locations only during the short monitoring period. To overcome the spatial and temporal coverage limitation, we have developed the long-term air quality modeling system over the U.S. gulf region using the state-of-science chemical transport model, Comprehensive Air Quality Model with Extensions (CAMx), the Sparse Matrix Operator Kerner Emissions (SMOKE), and the Weather Research and Forecasting (WRF) modeling systems. Our study will simulate the spatially and temporally enhanced SBTEX ambient concentrations over the U.S. gulf region over six years from 2011 to 2016. Because these individual SBTEX toxicants are not considered as the chemical model species with the complete chemical reactions in the atmosphere, we utilized the unique post-analysis feature called “Reactive Tracer” in the CAMx modeling system to simulate the ambient SBTEX concentrations. The Reactive Tracer applies the major oxidants concentration result (O3, OH, and NO3) to calculate the chemical reduction rate of SBTEX. Therefore, we can compare our SBTEX modeling outcomes against the Texas Commission on Environmental Quality (TCEQ) State Implementation Plan (SIP) air quality model results, and Ambient Monitoring Technology Information Center (AMTIC) data, to evaluate the model performance. The result of this study will be used in the human exposure assessment and epidemiological cohort study. In our preliminary result of the 2011 total annual SBTEX emission, the largest contribution section is the on-road transportation emission (32.5%), and the second largest is point fire emission (29.8%).

**Multiscale Model Applications and Evaluations**
**Tuesday, November 2 at 12:30 PM**

## Modeling of Nitrogen and Sulfur Deposition in the Chesapeake Watershed and Tidal Bay: Trends and Sources

Sarah Benish
Author(s):

Sarah E. Benish[1*], Jesse O. Bash[2], Kristen Foley[2], Sergey Napelenok[2], Christian Hogrefe[2], Wyat Appel[2], Lewis Linker[3]

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Presenter(s): Sarah Benish

Format: Oral Presentation

Short Description: Excess deposition of atmospheric nitrogen compounds can have harmful effects on vulnerable aquatic and terrestrial ecosystems. Chemical transport models, such as the Community Multiscale Air Quality (CMAQ) model, can simulate atmospheric deposition of compounds not routinely measured, such as organic nitrogen, as well as provide information about deposition in locations without measurements, like over complex terrain or over water bodies. Multiyear simulations from the EPA's Air QUAlity TimE Series (EQUATES) project provide a consistent modeling framework using CMAQv5.3.2 to provide stakeholders and partners with key information necessary for ecological evaluations and nutrient assessments. In this presentation, we assess trends of total inorganic nitrogen and sulfur from 2002-2017 in nine climatically consistent regions within the contiguous United States. We focus specifically on the Chesapeake watershed and tidal Bay, an area naturally sensitive to atmospheric nutrient deposition due to its geography and home to over 18 million residents. We present precipitation and bias adjustment of wet deposition fields to demonstrate improvements in modeling wet deposition compared to the National Atmospheric Deposition Program's (NADP) National Trends Network (NTN) wet deposition measurements and show how annual total nitrogen and sulfur budgets change over time and spatially. By applying the Integrated Source Apportionment Method (ISAM) in CMAQ to the Chesapeake Bay airshed, we identify key source regions and emission sectors to quantify their contribution to nutrient loading, one of the first ISAM applications for deposition. Preliminary results suggest mobile sources are responsible for ~24% of the total oxidized nitrogen deposition and non-poultry manure contributes ~17% to the total reduced nitrogen deposition in Winter 2016 throughout the Chesapeake Bay Watershed.

**Multiscale Model Applications and Evaluations (continued)**

## Enhanced representation of inter-continental pollutant transport by assimilating satellite NO2 and performing NOx emissions inversions

James East
Author(s):

James East, Barron H. Henderson, Sergey Napelenok, Shannon Koplitz, Brad Pierce, Allen Lenzen, Rob Gilliam, Golam Sarwar, Fernando Garcia Menendez

Presenter(s): James East

Format: Oral Presentation

Short Description: Long-range transport of ozone (O3) to the US has human health and regulatory impacts, and is produced, in part, from international nitrogen oxides (NOx) emissions. Accurately representing international O3 transport in hemispheric and global-scale air quality models requires accurate emissions inventories. However, developments of global bottom-up emissions inventories can be out-of-date and uncertain, particularly in developing countries, limiting the representation of international emissions and transport in air quality models. We introduce a satellite data assimilation system for inverse modeling of northern hemispheric NOx emissions which offers opportunities to improve representations of long-range O3 transport and model performance. The system can provide estimates of NOx emissions in China, India, Europe, and the US. We assimilate data from the Ozone Monitoring Instrument (OMI) and the TROPOspheric Monitoring Instrument (TROPOMI) separately in the Community Multiscale Air Quality (CMAQ) model for 2019 over the northern hemisphere and perform NOx emissions inversions for each assimilation. We analyze and compare model performance and long-range transported O3 in simulations: (1) without any satellite derived information, (2) with assimilated nitrogen dioxide (NO2), and (3) with satellite derived emissions updates. Results show large NOx emissions biases in India and China, and smaller biases in the US and Europe compared to satellite-inferred estimates. Assimilating NO2 and using satellite-inferred emissions both improve O3 and NOx model performance.
Disclaimer: The views expressed in this abstract are those of the authors and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency (EPA).

**Multiscale Model Applications and Evaluations (continued)**

## Exploring the Management Value of a Machine Learning-Based Model that Predicts Chlorophyll- Using Multi-Media Modeling Environmental Predictors

Christina Feng Chang
Author(s):

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Presenter(s): Christina Feng Chang

Format: Oral Presentation

Short Description: In the past, we presented a machine learning (ML) and multi-media modeling framework that was used to assess environmental variables (predictors) that affect water quality by using Lake Erie as a case study. We have since improved our water quality model by: (1) expanding our study period from an 11-year study period to a 16-year study period; (2) including additional in-lake observations with the addition of 6 monitoring stations (a total of 16 stations); and (3) utilizing outputs from updated versions of the numerical prediction models. These improvements have led to the development of a successful ML model that can predict chlorophyll-α (chl-α), a proxy for lake eutrophication and algal biomass, with a coefficient of determination of 0.81, bias of -0.12μg/l and RMSE of 4.97μg/l. In-situ chl-α measurements are provided by the Lake Erie Committee Forage Task Group and the University of Toledo for the 2002-2017 period. Meteorological weather variables from the Weather Research and Forecasting model, hydrological variables from the Variable Infiltration Capacity model, and agricultural management practice variables from the Environmental Policy Integrated Climate model for the 16-year period are used to fit a random forest ML model to predict chl-α concentrations. We discuss the importance of explanatory variables that originate from these individual modeling systems and analyze the contribution of each covariate in the model to better understand the occurrence of high chlor-α concentrations. Through various sensitivity tests, we focus on: (1) the influence of each set of predictors (meteorological, hydrological, and agricultural) by varying the usage of the ML-based model inputs; and (2) the ML model's ability to serve as a management tool through scenario evaluations (e.g., independent or concurrent changes in agriculture management, weather, and hydrology). Lessons learned from developing and testing this ML-based approach can be used to tackle water quality problems in other lakes or coastal areas and inform policy decisions.

**Multiscale Model Applications and Evaluations (continued)**

## EPAs Air QUAlity TimE Series Project (EQUATES): 2002-2017 meteorology, emissions, and air quality modeling for the Northern Hemisphere and the Conterminous United States

Kristen Foley
Author(s):

Kristen Foley, George Pouliot, Wyat Appel, Christian Hogrefe, Alison Eyth, Norm Possiel, Michael Aldridge, Chris Allen, Jesse Bash, Megan Beardsley, James Beidler, Sarah Benish, David Choi, Brian Eder, Caroline Farkas, Rob Gilliam, Janice Godfrey, Barron Henderson, Shannon Koplitz, Rich Mason, Rohit Mathur, Chris Misenis, Havala Pye, Lara Reynolds, Matthew Roark, Sarah Roberts, Donna Schwede, Karl Seltzer, Darrell Sonntag, Kevin Talgo, Claudia Toro, Jeff Vukovich

Presenter(s): Kristen Foley

Format: Oral Presentation

Short Description: The US EPA has developed a set of modeled meteorology, emissions, air quality and pollutant deposition spanning the years 2002 through 2017. Modeled datasets cover the Conterminous US (CONUS) at a 12km horizontal grid spacing and the Northern Hemisphere at a 108km using WRFv4.1.1 for meteorology and CMAQv5.3.2 for air quality modeling. New hemispheric and North American emissions inventories were developed using, to the extent possible, consistent input data and methods across all years, including emissions from mobile, fire, and oil and gas sources. This presentation will compare trends in the new emissions inventories to other emissions modeling platform data. Model estimates for ozone and PM2.5 over the CONUS will be compared to estimates from previous CMAQ version and to observational data. We will also highlight EQUATES datasets that are publicly available and can be used to support a wide variety of human health and ecological modeling applications as well as model evaluation and development.

**Multiscale Model Applications and Evaluations (continued)**

## CMAQv5.3.2 ozone simulations over the Northern Hemisphere: model performance and sensitivity to model configuration

Christian Hogrefe
Author(s):

Christian Hogrefe[1], Robert Gilliam[1], Rohit Mathur[1], Barron Henderson[1], Golam Sarwar[1], K. Wyat Appel[1], George Pouliot[1], Jeff Willison[1], Rebecca Miller[2], Jeff Vukovich[1], Alison Eyth[1], Kevin Talgo[3], Chris Allen[3], and Kristen Foley[1]

[1]U.S. Environmental Protection Agency

[2]Oak Ridge Associated Universities

[3]GDIT

Presenter(s): Christian Hogrefe

Format: Oral Presentation

Short Description: This presentation will provide an overview of the recently completed 2002 – 2017 Community Multiscale Air Quality (CMAQ) version 5.3.2 model simulations performed over the Northern Hemisphere for EPA's Air QUAlity TimE Series Project (EQUATES) project. After presenting a brief summary of the base model configuration which includes the Weather Research and Forecasting (WRF) version 4.1.1 model and an emissions dataset developed for EQUATES, model estimates of ozone will be compared against surface observations, satellite retrievals, and ozonesonde observations for different regions. Initial results indicate a persistent overestimation of summertime surface ozone and a tendency to underestimate springtime ozone both at the surface and aloft. Regional variations in modeled ozone trends are found to be in good agreement with observations. The presentation will also include an analysis of variability and trends in ozone and other longer-lived species simulated by hemispheric CMAQ at the boundaries of a 12km modeling domain covering the conterminous U.S. Finally, we will present results from sensitivity simulations performed for 2010 to investigate the impacts of several model configuration options (including biogenic volatile organic compound emissions, soil nitrogen oxide emissions, and WRF cumulus parameterization) on model estimates.

**Multiscale Model Applications and Evaluations (continued)**

## Uncertainty Analysis of CMAQ-derived Burden Estimation of PM2.5 Exposure with Bias Correction Technique

CHENG-PIN KUO
Author(s):

Cheng-pin Kuo, Joshua S. Fu

Presenter(s): Cheng-Pin Kuo

Format: Oral Presentation

Short Description: Ambient PM2.5 causing adverse effects on human health has been recognized as a major issue for regional air quality management in developing and developed countries. To quantify the impact of PM2.5 exposure to human health, the burden of disease (BD) is a commonly used assessment tool to provide references for air quality and health management. Technically, the BD estimation relies on reported PM2.5 exposure risks from existing literature and modeled or monitored PM2.5 concentration. Except for using monitoring data to access PM2.5 exposure, CMAQ modeling is also commonly employed to provide PM2.5 exposure estimations and has been intensively applied in previous studies. However, most CMAQ studies overlooked the bias between the CMAQ modeled results and monitoring data and failed to adjust the CMAQ results with monitoring data. Moreover, if CMAQ results were directly applied for BD calculation, the derived BD estimation could be also biased. In this study, we constructed a daily PM2.5 exposure matrix in 2013 with 3 km*3 km resolution in Taiwan and applied the inverse distance weighting (IDW) bias correction technique to adjust the CMAQ results with monitoring data. The BD was evaluated by the emergency visits of cardiovascular disease and estimated by CMAQ original and corrected results, respectively. Our objective is to quantify the difference between applying original and corrected CMAQ results for BD estimation and emphasize the importance of bias correction of CMAQ results and its potential bias for BD estimation. Our results showed that the average daily PM2.5 in the study regions has increased from 12.3 μg/m3 to 13.0 μg/m3, which implied underestimation (5%) of PM2.5 exposure if directly using CMAQ original results. For BD estimations, the emergency visits by using CMAQ results (2443 visits) would be 30% lower than those by using CMAQ-corrected results (3512 visits), especially for urbanized areas. The underestimation of CMAQ results and its derived BD estimation emphasizes the importance of bias correction of CMAQ modeling data. In addition, although most modeled estimations at monitoring sites had significant performance improvement, the CMAQ corrected estimations closer to the background sites had worse performance after bias correction, which suggests the IDW bias correction technique may be limited when applying in the region with complex terrain, and more data such as land-uses or satellite images should be involved for better modeling performance.

**Multiscale Model Applications and Evaluations (continued)**

## Assessment of the Impact of Lightning NOx on Air Quality over the Northern Hemisphere

Mike Madden
Author(s):

J. Mike Madden[1], Daiwen Kang[2], James East[1], Golam Sarwar[2], Christian Hogrefe[2], Rohit Mathur[2], and Barron H. Henderson[2]

[1]ORAU ORISE Research Participation Program hosted at the U.S. Environmental Protection Agency, Research Triangle Park, NC, USA.

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Presenter(s): J. Mike Madden

Format: Oral Presentation

Short Description: Lightning is a major natural source of nitrogen oxides (NOx), and as such, it is responsible for influencing the mixing ratios of tropospheric ozone (O3), a pollutant of interest to atmospheric scientists and regulators. Lightning-generated NOx (LNOx) is largely emitted in the mid- to upper-troposphere and is thus subject to long-distance transport that can affect O3 mixing ratios downwind. Uncertainties still exist regarding the production and distribution of LNOx, especially over hemispheric scales, and the importance of LNOx will increase as anthropogenic NOx emissions decrease over parts of the world. These concerns, therefore, merit further investigations of the release and fate of LNOx, as well as an assessment of its effects on air quality.This study uses the Community Multiscale Air Quality (CMAQ) model under varying LNOx emission configurations to analyze the effects of these emissions on tropospheric O3 mixing ratios across the Northern Hemisphere. Furthermore, this study focuses on the representation of LNOx and O3 in the mid- to upper-troposphere. Thus, performance evaluations using satellite (e.g., Ozone Monitoring Instrument (OMI)) and ozonesonde data will be conducted to examine the spread of results across the varying CMAQ configurations. Performance evaluations using surface O3 data (e.g., Air Quality System (AQS)) will also be conducted.Model simulations with and without lightning NOx are performed. In the simulations with LNOx, the original and adjusted data from the World Wide Lightning Location Network (WWLLN) are used to produce LNOx emissions. The adjustment factors for the WWLLN data are derived to reflect National Lightning Detection Network (NLDN) seasonal climatology over the contiguous United States, but the adjustment factors are interpolated onto the Northern Hemisphere. An additional LNOx case is conducted with Global Emissions InitiAtive (GEIA) climatological LNOx emissions. Preliminary results show differences in mid- and upper-tropospheric O3 mixing ratios that are especially pronounced during summer months across tropical and sub-tropical regions.Disclaimer: The views expressed in this abstract are those of the authors and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency (EPA).

## Modelling the impact of wood burning, road transport and agricultural emission reduction on total and secondary inorganic PM2.5 in the West Midlands, UK using WRF-CMAQ.

Andrea Mazzeo
Author(s):

Mazzeo A.[1], Zhong J.[1], Hood C.[2], Smith S.[2], Dai Y.[1], Stocker J.[2], Cai X.[1] and Bloss W.J.[1]

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2. 2. Cambridge Environmental Research Consultants, 3 King's Parade, Cambridge, CB2 1SJ, UK

Presenter(s): Andrea Mazzeo

Format: Oral Presentation

Short Description: Several progressive steps have been taken in the last decade to improve the air quality in the United Kingdom. Mitigation policies at the national level have led to significant reductions in PM2.5 concentrations, by 23 and 26% at urban and roadside locations respectively [1]. Despite this, air pollution levels exceeding the national legal threshold still represent a matter of concern for the rapid expansion evident in some places, such as the case of the West Midlands (WM). This area is the second-most populous region of the UK after Greater London, with more than 2,900,000 inhabitants. It includes the city of Birmingham as the UK's second-largest city, with 1.1 million inhabitants in the city alone. Moreover, according to UK government projections, the WM represents one of the highest population growth rates (+7.5%) in the period 2015-2025 [2]. Its rapid population growth, urbanisation, and consequent reduction in the air quality of urban areas led to an integrated approach to air pollution by West Midlands Combined Authority (WMCA) to reduce citizens' exposure to PM2.5 on the basis of the UK Clean Air Strategy 2019 [3]. According to the Air Quality Expert Group Report of 2012, 32% of the total PM2.5 level in the UK is generated by secondary inorganic aerosols; this percentage reaches 44% of the total concentration in the city of Birmingham [4]. Studies in the WM showed that NO3, SO2 and NH4 secondary inorganic fractions are the main constituents of PM2.5 in WM urban areas, followed by carbonaceous fractions of organic and elemental carbon (OC and EC) [5]. In order to maximise the effects of national and local environmental policies, it is important to analyse the influence that these reductions have not only on primary PM2.5 but also on the formation of secondary inorganic aerosols. In the context of the West Midlands Air Quality Project, the modelling system for meteorology and chemistry-transport processes, WRF-CMAQ [6-7], was implemented and validated to simulate annual concentrations of PM2.5 for a winter a summer period of the base case year 2016. The UK National Atmospheric Emission Inventory (NAEI) [8] was merged with the regional emission inventory CAMSv3.1 to account for the most up-to-date anthropogenic emissions for the UK and northwest Europe [9]. "What-if" scenarios with reduced primary emissions were designed and tested to assess the impact on annual concentrations of PM2.5 of both the UK Clean Air Strategy 2019 and WMCA mitigation policies related to road transport, agriculture and wood burning. The secondary inorganic fractions of PM2.5 were also quantified for the individual and combined reduced emissions scenarios. Results show that scenarios with combined mitigation policies lead to significant decreases in the air concentration of PM2.5, reducing both the primary PM2.5 and secondary inorganic aerosol fractions. In light of this, the combined transport and agriculture scenarios provide a high percentage of reduction for the whole region of the West Midlands, while the reduction of primary emissions of PM2.5 related to wood and coal burning only generates substantial concentration change in winter periods.

**Multiscale Model Applications and Evaluations (continued)**

## Upgrades to the Canadian Operational Regional Air Quality Deterministic Prediction Systems in 2021

Mike Moran
Author(s):

Michael Moran, Sylvain Ménard, Verica Savic-Jovcic, Jack Chen, Ayodeji Akingunola, Konstantinos Menelaou, Rodrigo Munoz-Alpizar, Dragana Kornic, Hugo Landry, Qiong Zheng, Junhua Zhang, and Paul Makar

Presenter(s): Michael Moran

Format: Oral Presentation

Short Description: Environment and Climate Change Canada (ECCC)'s operational Regional Air Quality Deterministic Prediction System (RAQDPS) has been operational since 2001 and has undergone frequent updates since then. A special parallel wildfire version called FireWork became operational in 2016. Both systems are built on a limited-area version of the GEM-MACH chemical weather model, an in-line chemistry model embedded in ECCC's GEM meteorological forecast model, and both use a 10-km North American grid. The 2021 upgrades to the RAQDPS and FireWork include a new set of anthropogenic emissions files based on a projected 2020 Canadian inventory and projected 2023 U.S. and Mexican inventories, improved representation of particle sedimentation, several GEM improvements, and new GEM meteorological and MACH chemical libraries. FireWork also benefits from an upgraded version of the Canadian Forest Fire Emission Prediction System (CFFEPS), which has an improved wildfire plume-rise parameterization and more detailed forest fuel parameters. This presentation will describe these changes in more detail and show their impact on air-quality forecast performance.

**Multiscale Model Applications and Evaluations (continued)**

## Evaluation of National Air Quality Forecast Capability for the Summertime: Case Studies of Year 2019-2020

Youhua Tang
Author(s):

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Presenter(s): Youhua Tang

Format: Oral Presentation

Short Description: The NOAA National Air Quality Forecasting Capability (NAQFC) has been upgraded with the CMAQ 5.3.1 with CB6r3-Aero7 mechanism driven by the operational Finite Volume Cubed-Sphere (FV3)-Global Forecast System (GFS), version 16, through the NOAA-EPA Atmosphere-Chemistry Coupler (NACC). We evaluated the new system, old NAQFC (CMAQ 5.0.2 driven by North America Mesoscale Model) and a downscaled GFSv16-driven WRF/CMAQ simulation with surface and airborne observations (Joint NOAA/NASA FIREX-AQ field campaign in summer 2019). Differing from the standard offline (i.e., WRF/MCIP/CMAQ) approach, the NAQFC systems use an interpolation-based meteorological coupler that can handle non-native grid meteorological inputs, as CMAQ is designed to handle various meteorological inputs with proper mass-conservation schemes. Compared with the CMAQ 5.0.2, CMAQ 5.3.1 drastically reduced the nighttime ozone overpredictions, and improved the overall ozone scores, also with help of a new emission inventory (NEI2016v1). The different meteorological drivers also showed strong impacts. The operational FV3-GFSv16 yielded better surface wind, compared to the overpredicted WRF 10-meter wind, but the GFS tended to underpredict 2-meter temperature. Correspondingly, GFS/CMAQ yielded the lowest ozone among the three models, and underpredicted the surface ozone over the western US. The GFS also tends to have stronger diurnal variations of planetary boundary layer (PBL), or higher daytime PBL and lower nighttime PBL. The comparison with FIREX-AQ aircraft data suggests that NEI2016v1 anthropogenic emissions are reasonable for most species except toluene and ethane. Overall, the WRF/CMAQ and GFS/CMAQ exhibited similar performance though their different meteorological inputs show influence on the predictions compared to the airborne observations.

**Multiscale Model Applications and Evaluations (continued)**

## Sensitivity Assessment of the Ozone and Fine Particulate Matter Pollution in the Greater Bay Area Using a Regional-to-Local Coupling Model

Xuguo ZHANG
Author(s):

Xuguo Zhang, Jenny Stocker, Kate Johnson, Yik Him Fung, Teng Yao, Christina Hood, David Carruthers, and Jimmy C. H. Fung

Presenter(s): Dr. Xuguo ZHANG

Format: Oral Presentation

Short Description: Ultrahigh-resolution air quality models resolving sharp concentration gradients benefit health calculations. Mitigating fine particular matter (PM2.5) in the past decade triggered the ozone (O3) deterioration in China. Effectively controlling the coupled two-pollutant from an ultrahigh-resolution perspective is still understudied. This study proposes a novel coupled regional-to-local scale air quality modeling system suitable for quantitative assessment of pollution mitigation pathways at various resolutions. Sensitivity scenarios relating to the control of nitrogen oxide (NOx) and volatile organic compounds (VOC) concentrating on traffic and industry sectors are explored. The results show the concurrent controls on both sectors lead to an overall 17%, 5%, and 47% emission reduction in NOx, PM2.5, and VOC pollutatant concentrations, respectively. The 50% less traffic scenario leads to reduced NO2 and PM2.5, but increased O3 concentrations in urban areas, revealing a VOC-limited chemical regime. The reduced industrial VOC scenario leads to reduced O3 concentrations throughout the mitigation domain. The maximum decrease in the median hourly NO2 metric is over 11 μg/m³, and the maximum increase in the median maximum 8-hour rolling O3 metric is over 10 μg/m³ for the reduced traffic scenario. When both the traffic and industrial control scenarios are applied, the impact on O3 reduces to an increase of less than 7 μg/m³. The daily-averaged PM2.5 decreases by less than 2 μg/m³ for the reduced traffic scenario and varies little for reduced VOC scenario. An O3 episode analysis for both controls scenario leads to O3 decreases by up to 15 μg/m³ (8-h metric) and up to 25 μg/m³ (1-h metric) in a rural area to the northeast of the mitigation domain.

**Regulatory Modeling and SIP Applications**
**Wednesday, November 3 at 2:00 PM**

## How much do various sources and states contribute to ambient ozone amounts over the northeastern U.S.? a source apportionment study with CAMx

Dale Allen
Author(s):

Dale J. Allen (University of Maryland)

Shan He (New Jersey State Department of Environmental Protection)

Eric Zalewsky, Winston Hao, and Jeongran Yun (New York State Department of Environmental Conservation)

Jin Sheng-Lin (Virginia Department of the Environment)

Mike Woodman (Maryland Department of the Environment)

Jeff Underhill (New Hampshire Department of Environmental Services)

Presenter(s): Dale J. Allen

Format: Oral Presentation

Short Description: Ozone concentrations from northern Virginia to Connecticut continue to exceed National Ambient Air Quality Standards (NAAQS). To provide guidance to air quality planners, the Ozone Transport Commission (OTC) states with the assistance of modeling centers at the University of Maryland and Rutgers University used the Comprehensive Air Quality Model with Extensions (CAMx) to examine the contribution of 322 tags (e.g., WV oil and gas, MD on-road non-diesel, PA Electrical Generating Units (EGUs)) to hourly ozone amounts over the eastern two-thirds of the U.S. under NOx-limited and NOx-saturated conditions. The simulations covered April to September and used 2016 meteorology and projected 2023 emissions based on the v1 2016 with ERTAC EGU emissions modeling platform developed by collaborative efforts between states, multi-jurisdictional organizations (MJOs), EPA and others. The relative importance of various sectors including mobile sources, Electrical Generating Units (EGUS), area non-point sources, oil-and-gas production, and commercial marine vessels (CMVs) to hourly and 8-hour maximum ozone will be examined using averages over several different measures of high ozone days. The role of meteorology will be highlighted by comparing day-to-day and hour-to-hour variations in the contributions of individual sectors and/or states to ozone amounts. Temporal and spatial variations in the contribution of NOx-limited versus NOx-saturated chemistry to 8-hour maximum ozone will be illustrated.

**Regulatory Modeling and SIP Applications (continued)**

## NO2 Impacts of Airport-Related Sources with AERMODs Five Chemistry Approaches

Melissa Buechlein
Author(s):

Melissa Buechlein, Michelle Snyder, R. Chris Owen

Presenter(s): Melissa Buechlein

Format: Oral Presentation

Short Description: A model sensitivity study was conducted by comparing monitoring data to modeling at an airport using source specific emission rates and NO2 chemistry algorithms in AERMOD to explore the sensitivity of each chemistry method. Temporal and spatial emissions were estimated for one year using AEDT, background NO2, NOx, and ozone concentrations were obtained from a nearby AQS monitor, and meteorology was from the on-site airport met tower. The Ozone Limiting Method (OLM), Ambient Ratio Method 2 (ARM2), Plume Volume Molar Ration Method (PVMRM), Travel Time Reaction Method (TTRM), and Generic Reaction Set Method (GRSM) were tested to understand: source parameter sensitivity, atmospheric stability sensitivity, and overall model performance.

**Regulatory Modeling and SIP Applications (continued)**

## Temporal source apportionment of PM2.5 over the Pearl River Delta region

Yiang Chen
Author(s):

Yiang Chen, Xingcheng Lu, Jimmy C.H. Fung

Presenter(s): Yiang Chen

Format: Oral Presentation

Short Description: The key problems in addressing air pollution include determining the source of the pollutants and developing a means to control them. In addition to the source area and source category of pollutants, the contribution of pollutants emitted during various periods is an important factor that must be better understood for effective and efficient policymaking. The source apportionment module in the Comprehensive Air Quality Model with Extensions (CAMx) was extended and applied to analyze the temporal contributions of emissions to the concentration of atmospheric particulate matter with a diameter ≤ 2.5 μm (PM2.5) in the Pearl River Delta (PRD) region. The results showed that in addition to cross-boundary transport, the PM2.5 concentration in the PRD region was generally influenced by emissions on the current day and previous day. Local emissions (within the local city) from 06:00 to 17:59 on the current day accounted for approximately 30% of the PM2.5 concentration, whereas regional sources (cross-city transport) had greater contributions during earlier emission periods. During the periods of episodic pollution, a weak wind situation hindered the transportation and diffusion of pollutants; thus, pollutants from 2 days earlier were trapped within the PRD region. Our results suggest that emission control measures should be implemented 2 days in advance when adverse meteorological conditions are predicted.

**Regulatory Modeling and SIP Applications (continued)**

## Emissions, reactions or bidirectional surface transfer? Gas phase formic acid dynamics in the atmosphere

Ziqi Gao
Author(s):

Ziqi Gao, Petros Vasilakos, Theodora Nah, Masayuki Takeuchi, Hongyu Chen, David J. Tanner, Nga Lee Ng, Jennifer Kaiser, L. Greg Huey, Rodney J. Weber, and Armistead Russell

Presenter(s): Ziqi Gao

Format: Oral Presentation

Short Description: Organic acids are among the many components produced from the secondary organic aerosol formation that can impact aerosol and cloud water acidity. The most abundant gas-phase organic acid in the atmosphere is formic acid, which has been observed in concentrations in excess of 2.5 ppbV in rural areas. However, atmospheric model simulations of formic acid are typically biased low, potentially due to biases in their direct emissions and/or chemistry. In this study, we used Community Multiscale Air Quality (CMAQ) to simulate gas-phase formic acid in Yorkville, Georgia during an intensive campaign that lasted from September to October 2016. Similar to previous studies, the diurnal trend of simulated formic acid did not match observations, being biased low with a dissimilar diel profile. Potential reasons for mismatch were investigated. Additional gas-phase reactions of isoprene and monoterpenes suggested by recent studies were added, leading to a small increase in acid concentrations, but having little impact on the diel profile. The surface reaction between OH and isoprene epoxydiols (IEPOX) was simulated, increasing the simulated concentration of formic acid by up to 150%; though the resulting simulated diurnal profile did not match the observed. Examination of the diel profile found that formic acid concentrations began to rise early in the morning before suspected precursors (e.g., isoprene, IEPOX, and methanediols) and the hydroxyl radical, and that concentrations decreased rapidly in the afternoon. The rapid, early morning rise could be reproduced with increased emissions. Given the long lifetime of formic acid, and that the condensed phase formate concentrations are small, the evening decrease is explained mainly by rapid dry deposition. This suggests that formic acid underwent bidirectional deposition/emission, e.g., depositing rapidly as dew formed at night, with subsequent re-emission during the following day as the dew evaporated. This also led to observed decreases in concentrations with height.

**Regulatory Modeling and SIP Applications (continued)**

## Sources Contribution to Ozone in Connecticut

Yukui Li
Author(s):

Yukui Li, Kristina Wagstrom

Presenter(s): yukui li

Format: Oral Presentation

Short Description: According to The American Lung Association “2021 State of the Air” report, most counties in Connecticut continue to receive failing grades for air quality, specifically due to high ozone levels. This has continued even after great effort has been made to control air pollution. As with all places, there are sensitive populations in Connecticut that are at high risk of health complications when ozone concentrations are high. This creates an urgent need to lower ozone concentrations in Connecticut. The first step to achieving this is to determine the major sources contributing to ozone in Connecticut. We use the Comprehensive Air Quality Model with Extensions with the Ozone Source Apportionment Tool (CAMx-OSAT), CAMx with the Decoupled Direct Method (CAMx-DDM), and the Community Multiscale Air Quality Modeling System with the Integrated Source Apportionment Method (CMAQ-ISAM) to estimate the impact of nine nearby point sources in New York and New Jersey and twelve nearby states on ozone concentrations in Connecticut. All three approaches estimate that boundary conditions and unapportioned sources (areas except for the selected sources inside the domain) contribute the most to ozone in Connecticut. The contribution of boundary condition remains fairly consistent, while unapportioned sources and the selected sources contribute more to ozone in Connecticut during periods with elevated levels. The nine point sources combined contribute little (<7%) to ozone in Connecticut, but emissions from the twelve states contribute substantially in Connecticut when ozone is high . Emissions from the twelve states contribute a substantial fraction (~50%) of the ozone in Connecticut, especially when levels exceed 70ppb. Among the twelve states, Ohio, Pennsylvania, and New York contribute the most to summertime average ozone. During periods of elevated ozone, New York contributes the most.

**Regulatory Modeling and SIP Applications (continued)**

## Health vulnerability due to atmospheric emissions: A study case in Santa Catarina State, Brazil

Julia Placido Moore
Author(s):

Julia Placido Moore

Leonardo Hoinaski

Presenter(s): Julia Placido Moore

Format: Oral Presentation

Short Description: The air pollution is a major threat to human health, and it is related to health diseases increase. The health hazard from air pollution is different to each human population. A recurring example is a higher probability of respiratory infections. That kind of hazard is highly influenced by population sensitivity, exposure, air pollution event and adaptive capacity. Santa Catarina state in Brazil presents a significant economic and industrial development scenario in the national context, which may influence human health consequently. However, little is known about the effects of air pollution on Santa Catarina population health, there are no recent research on the subject. Thus, the research aimed to evaluate the health vulnerability due to atmospheric emissions in the Santa Catarina state. A bivariate analysis was conducted, Pearson and Spearman correlation methods were utilized to verify the behavior between independent and dependent variables. The research utilized vehicular and burning emissions data and each municipality industry distribution to consider air pollution events. Also, for the vulnerability context were used socioeconomics index such as: Gross Domestic Product (GDP), Municipal Human Development Index (HDI-M) and Gini Coefficient. For the health data, were obtained respiratory hospitalization from Department of Computer Science of the Brazilian Unified Health System (DATASUS), segregate by ages. The analyses were performed considering all the municipalities in the Santa Catarina State and for each city's groups in the HDI-M state range.For the whole state, the vehicular emissions and the number of industries did not seemed to affect the number of hospitalizations. Moreover, the adults and elderly age group were liable to the burn emissions. The highest hospitalization rates were in municipalities with lower HDI-M. In addition, the segregated analysis by HDI-M showed that hospital admissions for adult and elderly populations, the vehicular emissions, and the number of industries in municipalities are linked with medium HDI-M (the lowest HDI-M in the state). The results display that municipalities that are in vulnerability (lowest HDI-M), may suffer the consequences from air pollution. However, municipalities with the highest HDI-M, despite not showing to have been affected by vehicle emissions, were affected by the wildfires. This shows that such municipalities may present a limit in relation to their adaptive capacity. Also, the elderly population demonstrated to be most affected in the analysis. The current research result on hypotheses that can guide future research at this subject and may help to understand about environmental risks to human health in Santa Catarina State.

**Regulatory Modeling and SIP Applications (continued)**

## Development of Ozone-NOx-VOC Emissions Isopleth using CMAQ-HDDM and Inverse Distance Weighted Method for Southern California and the Comparison with Empirically-based Method

Yu Qian
Author(s):

Yu Qian, Yongtao Hu, Petros Vasilakos, Zongrun Li, and Armistead G. Russell

Presenter(s): Yu Qian

Format: Oral Presentation

Short Description: We developed, applied, and evaluated different methods to estimate ozone-emission relationships, with a focus on the South Coast Air Basin in California (SoCAB). We conducted extensive air quality modeling of the SoCAB for a number of historical and future years to understand how well the current chemical transport models (CTMs) captured ozone dynamics and the response to controls of NOx and VOC. Those results, including the sensitivities, were analyzed independently and also used to construct ozone-emission isopleths using a modified inverse distance-weighted method. Both the 2011 and 2016 comparisons show high consistency between simulated and observed MDA8 ozone concentrations, suggesting that the CMAQ simulations capture peak ozone values in terms of their relationship to estimated emissions. We conducted a set of 15 CMAQ-HDDM simulations with different emissions levels, and 11 of the cases were used to develop ozone-NOx-VOC isopleth diagrams at locations across the basin. The CMAQ-derived isopleth for Crestline (the monitoring location with the highest modeled ozone for 2016) suggests that for much of the 1975–2018 period, peak ozone levels have been most sensitive to reducing VOCs, and, up until at least 2005, NOx controls would have led to ozone increases. Recent NOx emissions reductions, however, are pushing the SoCAB to a region where, on a percentage emissions basis, NOx emissions reductions will lead to greater ozone reductions than VOC emissions controls. We combined empirical and CTM modeling to comprehensively evaluate how well do chemical transport models capture observed ozone trends and sensitivities to emissions. The HDDM-based sensitivities capture much more spatial variation in the ozone-emissions responses. A similar trend is found for other far-inland monitoring sites (e.g., Azusa), and these are the locations that typically experience the highest observed levels in the SoCAB. This indicates that the HDDM-derived response over the emissions space is consistent with the empirically derived response, which describes the overall characteristics of the ozone-emissions relationship based on long-term estimated emissions and ODV observations.

**Regulatory Modeling and SIP Applications (continued)**

## Comparison of the performance of 2016 CMAQ platforms at 12km and 4km resolutions

Yuhong (Ruby) Tian
Author(s):

Yuhong (Ruby) Tian, Winston Hao, Jeongran Yun, Eric Zalewsky, Kevin Civerolo and Margaret LaFarr

Division of Air Resources, New York State Department of Environmental Conservation

Presenter(s): Yuhong (Ruby) Tian

Format: Oral Presentation

Short Description: Several states in the Ozone Transport Commission (OTC) region are in non-attainment status for the 2008 and/or 2015 ozone National Ambient Air Quality Standards (NAAQS) and as such are required to submit State Implementation Plans (SIPs). The Community Multiscale Air Quality (CMAQ) model was run for 2016 and the 2023 future year at both 4 and 12 kilometer resolutions. Ozone (O3) estimations were evaluated for 71 monitoring sites over the Northeastern Non-attainment areas. Using the EPA 2016 V1 (fi) inventory emissions at 12km and 4km resolutions, CMAQ underestimated O3 in May and June, and overestimated O3 in July and August. At 12km resolution, O3 concentrations were highly overestimated in some coastal grid cells, defined as water, due to difficulty in characterizing the land/water interface in both the air quality and meteorological models. Predicted O3 concentrations for July and August improved significantly at 4km resolution for three coastal monitors in Groton and Greenwich CT and Hart Miller Island MD. The differences in meteorological data and total emission of Nitrogen Dioxide (NO2) and Volatile Organic Compounds (VOC) between the two platforms were explored to examine the model performance at the six coastal CT sites. Either meteorological conditions or total emission changes explained the O3 concentration differences for most of the sites. In addition, we also compared the 2023 future design value (DVF) calculated from the 12km and 4km platforms. For most of the land monitoring sites, the 2023 DVFs from 4km platform are very similar to those from 12km platform. At 4km resolution, sites Greenwich, Stratford, Westport and Madison will have 2023 DVFs higher than 71 ppb; sites New Haven and Groton will have 2023 DVFs lower than 71 ppb. Our work suggests that for CMAQ model, grid resolution plays a crucial role in modeling O3 along the land/water interface area where more accurate allocating emissions at 4km resolution improved the O3 estimations when the meteorological conditions are not favorable for a good model performance.

**Regulatory Modeling and SIP Applications (continued)**

## Comparison of the CAMx performance of 2016 based modeling platforms at 12 km and 4 km resolution

Jeongran Yun
Author(s):

Jeongran Yun, Winston Hao, Eric Zalewsky, Yuhong (Ruby) Tian, and Kevin Civerolo

Division of Air Resources, New York State Department of Environmental Conservation

Presenter(s): Jeongran Yun

Format: Oral Presentation

Short Description: Grid cell sizes ranging from ~1 km to 12 km resolution have been used for various modeling applications for ozone. Previous works suggested that smaller grid cells with more detailed emissions and meteorological inputs do not always have better model performance than 12 km resolution. However, in our other work (see Tian et al, this conference), the Community Multiscale Air Quality (CMAQ) model at 4 km resolution performed better in simulating ozone than at 12 km resolution along the land/water interface area in the northern part of Long Island Sound with more accurate emissions allocation. This area is within the nonattainment area for the 2008 and 2015 8-hour ozone National Ambient Air Quality standards (NAAQS). Both the CMAQ and the Comprehensive Air quality Model with eXtensions (CAMx) photochemical models are commonly used for State Implementation Plan (SIP) attainment demonstration modeling. The 2016 emissions modeling platform for use in SIPs and other regulatory applications has been developed over the past several years through collaborative efforts between states, EPA, multi-jurisdictional organizations (MJOs), and others. In this study, CAMx performance will be compared between 2016 v1 based modeling platforms at 12 km and 4 km resolution focusing on the land/water interface along Long Island Sound. The model will be run for both 2016 and 2023, and future ozone design values will be compared between the two grid resolutions. Emissions allocations can be different at two grid resolutions; contributions to ozone from source apportionment modeling based on the emissions allocation differences will also be investigated.

**Remote Sensing/Sensor Technology and Measurements Studies**
**Tuesday, November 2 at 2:00 PM**

## Application of Remote Sensing Technology in Dust Detection and Air Quality Monitoring: A Case Study of the Middle East

Yusuf Alizade Govarchin Ghale
Author(s):

Yusuf Alizade Govarchin Ghale, Ismail Sezen, Goksel Demir, Ali Deniz and Alper Unal

Presenter(s): Yusuf Alizade Govarchin Ghale

Format: Oral Presentation

Short Description: The environmental problems around the world have been increasingly becoming larger-scale and planetary problems because the pollutants emitted are crossing borders and they affect different regions of the Earth that are actually not emitting these pollutants. The Middle East countries, such as Iraq and Syria suffer from air pollution, especially dust. Natural hazards such as drought and desertification have intensified this problem in recent years. The transported dust from these areas affects the air quality of neighboring countries such as Turkey. In this study, ground-level PM10 data and retrieval satellite products derived from MODIS, OMI and CALIPSO were used for aerosol type detection and understanding the source of aerosol pollution in the southern part of Turkey from 2010 to 2020. Based on the results of this study, transported dust from the Arabian Desert affects the air quality of Turkey and causes high aerosol concentration in the southern part of the country. The results indicated that dust storms mostly occur during spring and summer and local emission sources like fuel combustion account for air pollution, especially during winter.

**Remote Sensing/Sensor Technology and Measurements Studies (continued)**

## Performance Comparison of Electrochemical sensors across Six Cities in Continental United States

Md Hasibul Hasan
Author(s):

Md Hasibul Hasan, Yi Li, Haofei Yu

Presenter(s): Md Hasibul Hasan

Format: Oral Presentation

Short Description: Low-cost air quality sensors are being extensively used nowadays for community air quality monitoring. Most studies focused on installing low-cost sensors in a single geographical location for calibration and testing. How the performances of low-cost sensors vary across different geographical locations still remain largely under-investigated. In this study, performances of low-cost electrochemical air quality sensors installed in six different cities (Atlanta GA, New York City NY, Sacramento CA, Riverside CA, Portland OR, and Phoenix AZ) with different climatic and geographical conditions were compared. Several mathematical models were applied for calibration and testing in both local and other areas. The models selected include linear regression, polynomial regression and random forest. We also investigated the potential cross-interference of CO signal to NO2 and O3 in low-cost electrochemical gas sensors. We found that calibration parameters that are developed in one location are generally not suitable for other locations. We also found machine learning methods, when applied for calibration, performs generally better than conventional linear regressions. The incorporation of CO sensor data in calibration models increased model accuracy which suggested a possible cross-interference of CO-related gas to NO2 and O3.

## Changes in ozone chemical regime over the contiguous United States inferred by the inversion of NOx and VOC emissions using satellite observation

Jia Jung
Author(s):

Jia Jung[1], Yunsoo Choi[1*], Sayedali Mousavinezhad[1], Daiwen Kang[2], David C. Wong[2], Arman Pouyaei[1], Jincheol Park[1], Mahmoudreza Momeni[1], Masoud Ghahremanloo[1], and Hyuncheol Kim[3]

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Presenter(s): Jia Jung

Format: Oral Presentation

Short Description: To investigate the changes in ozone (O3) chemical production regime over the contiguous United States (CONUS) with accurate knowledge of ambient concentrations of its precursors, we applied an inverse modeling technique with the Ozone Monitoring Instrument (OMI) tropospheric nitrogen dioxide (NO2) and formaldehyde (HCHO) retrieval products in the summer of 2011, 2014 and 2017. The inclusion of dynamic chemical boundary conditions provided by hemispheric model simulation and the lightning-induced nitric oxide emissions significantly account for the contribution of the background sources in the free troposphere. Satellite-constrained nitrogen oxide (NOx) and non-methane volatile organic compounds (NMVOC) posterior emissions significantly mitigate the discrepancy between satellite-observed and modeled columns; nation-wide increases in tropospheric NO2 column by 34.95 – 48.18%, and the decrease in HCHO column over the southeastern US by -6.77 – -14.85%. Model-derived HCHO/NO2 column ratio with threshold values to identify O3 production regime classification (i.e., NOx-limited, NOx-saturated, and transition) showed gradual spatial changes in O3 production regime near urban cores during the study period, as well as apparent shifts from NOx-saturated regime to transition regime (or transition regime to NOx-limited regime) over most of the major cities in the western US between 2014 and 2017. In contrast, rural areas, especially in the southeastern US, exhibited an increased HCHO/NO2 column ratio by -1.30 ± 1.71 between 2011 and 2017, implying the change toward the NOx-saturated regime. The results of this study show that incorporating satellite observation into numerical modeling could be helpful to implement appropriate emission control policies for O3 air quality in time.Disclaimer: The views expressed in this abstract are those of the authors and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency (EPA).

**Remote Sensing/Sensor Technology and Measurements Studies (continued)**

### Estimation of the background PM2.5 concentrations in megacities in Iran

Hossein Khajehpour
Author(s):

Farzaneh Taksibi, Maryam Zare Shahne, Hossein Khajehpour

Presenter(s): Hossein Khajehpour

Format: Oral Presentation

Short Description: Particulate Matter with a diameter of 2.5 micrometers or smaller (PM2.5) pollution in megacities is a major environmental issue in developing countries. To manage this issue, pollutant dispersion modeling is an effective tool for simulating the distribution of the pollutant concentration and predicting the effectiveness of pollution control policies and measures. However, a prerequisite for a valid pollutant dispersion modeling is to consider the natural concentration of pollutants from non-anthropogenic emission sources. Though, due to lack of in-site measurements or source apportionment results, this information is merely available. In this research work, the remote sensing technique is used to estimate the background PM2.5 concentration from natural dust in eight megacities in Iran: Tehran, Isfahan, Ahvaz, Tabriz, Shiraz, Mashhad, Karaj, Kermanshah. The concentrations are estimated in points around the case studies which are located upstream of the anthropogenic emission sources via two methods: 1) calibration of the AOD values received from (MODIS) (combined Dark Target and Deep Blue) and (MISR), based on satellite Terra and 2) comparison of PM2.5 estimates from MODIS, MISR and SeaWiFS Aerosol Optical Depth (AOD) with GWR product. The monthly average concentrations are validated for Tehran through comparison with dust concentrations from source apportionment studies. The derived calibration factors are then applied to the remote sensing-based estimates of the other case studies. As a result, for the first time, the seasonal background PM2.5 concentrations are reported for the main megacities in Iran. This may serve as a valuable input for future pollution dispersion modelings in these case studies.

## Refining Ammonia Emissions Estimates with Satellite-based Observations Using a Novel Framework and an Air Quality Model

Congmeng Lyu
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Presenter(s): Congmeng Lyu

Format: Oral Presentation

Short Description: The Community Multiscale Air Quality (CMAQ) model calculates the impact of emissions on atmospheric composition, including inorganic aerosols, while considering the transport and reactions of chemical constituents. Adjusting emissions by comparing modeled concentrations with observations is justified when the science processes are well understood as is the case for inorganic species such as ammonia (NH3). The Finite Difference Mass Balance (FDMB) method and four-dimensional variational (4D-Var) data assimilation leverage differences in simulated and actual observations to revise estimates of emissions with spatial specificity. In this study, we evaluate the capability of a CMAQ-based data assimilation system to improve NH3 emissions, which are relatively uncertain given the diversity of emissions processes in the agricultural sector. To do so, the iterative FDMB and a Python-based four-dimensional variational framework (py4dvar) are integrated with CMAQ and its adjoint to constrain NH3 emissions with observations from the satellite-based Cross-track Infrared Sounder (CrIS). Observing System Simulation Experiments (OSSEs) are conducted with the CrIS observation operator to evaluate the extent to which emissions are expected to be recovered with the hybrid assimilation framework. The OSSE conducted with the 2007 modeling platform and 2016 CrIS data on a regional domain in Georgia results in promising recovery of the true emissions. The framework is then ported to a 2017 modeling platform for assimilation of 2017 CrIS NH3 observations to mitigate the mismatch between modeling platform and satellite observation years. Three suitable periods are selected from April through October 2017 for assimilation. Independent surface measurements are used to evaluate posterior modeled concentrations.

## Study on the effect of ventilation coefficient and anthropogenic emissions on PM2.5 concentration in the atmosphere above Tehran, Iran

Hossein Panahifar
Author(s):

Taheri Ahmad, Panahifar Hossein, Shahidzadeh Hossainreza

Presenter(s): Hossein Panahifar

Format: Oral Presentation

Short Description: Tehran (? 35.55◦–35.83◦ N, ? 51.09◦–51.59◦ E) is the capital and the most populated city in Iran. The current study intends to determine the share of ventilation coefficient and anthropogenic emission in the PM2.5 concentration rise in the atmosphere above Tehran. Many kinds of research have been done regarding urban air pollution in Tehran, but above question is rarely addressed in previous studies. The research includes in-situ PM concentration measurements supported by synoptic and reanalysis meteorological (ECMWF ERA5) as well as space-borne remote sensing data. The ventilation coefficient has been quantified based on measurements of mixing layer height and wind profiles for two successive years (2018-2019). The ground-based PM2.5 concentration measurements, as well as NO2 measurements by OMI and TROPOMI satellite, are used as an indicator to determine the air pollution episodes. The space-born CALIOP lidar measurements are used to derive the vertical profile of PM2.5 mass concentration from the backscattering coefficient profile. Meanwhile, the occurrence of heavy pollution in Tehran and the transport of pollutants from the densely industrial regions located on the west of Tehran is investigated. Finally, by the comparison of transport flux for heavily polluted episodes of each year, the impact of anthropogenic emission has been investigated. The results of this research are of broad interest to both the scientific community and policy-makers.

**Remote Sensing/Sensor Technology and Measurements Studies (continued)**

## Determination of the PM10 emission rate from an aerial grain conveyor belt by a set of SDS011 sensors by the upwind-downwind method

Débora Lia Perazzoli
Author(s):

**Andreas F. Grauer[1]; Débora L. Perazzoli[1]; Jacqueline A. Schraier[1]; André L. Malheiros[1]; Emílio G. F. Mercuri[2]; Lucas M. Malheiros[1]**

*[1] EnvEx Engineering and Consulting, Curitiba-PR, Brazil*

*[2] Federal University of Paraná - UFPR, Curitiba-PR, Brazil*

Presenter(s): Débora L. Perazzoli

Format: Oral Presentation

Short Description: Fugitive emissions of inhalable particles (PM10) from a grain conveyor belt were measured by a set of six low-cost sensors from the SDS011 model coupled to a Raspberry Pi microcomputer, which operate on an optical principle. These sensors were mounted downstream and upstream of the conveyor belt considering the predominance of the local wind direction. There were 4 sensors on a rod in two positions downstream of the belt, at distances of 5.35 and 7.35 m respectively, a sensor on the reference equipment side (TEOM) and an upstream sensor 3.25 m from the center of the source. At the same time, a meteorological station was installed to have information on the local wind speed and wind direction. In this configuration, the experiment recorded for 5 days the concentrations of PM10, meteorological data and operational data of the conveyor belt, that is, the operational periods and the quantities of grain transported. The SDS011 sensor readings were calibrated by the equation obtained by the sensor operating nearby the TEOM. Next, the dataset, usually available every minute, was summarized into 30-minute averages. The fugitive emissions quantification method was based on the Gaussian equation where the emission rate depends on the wind speed, the difference between the upstream and downstream concentration and the horizontal dispersion coefficients σy and σz. For the σy coefficient, a fixed value was adopted, corresponding to a source width of 1m. In this approach, the entire conveyor belt is considered a sequence of individual sources 1 m wide each. Thus, fugitive emissions were quantified per meter of belt in mg/(ms). The σz coefficient was calculated according to the ISC3 atmospheric dispersion model manual as a function of the atmospheric stability class. For the application of the fugitive emissions quantification algorithm, also known as the upwind-downwind method, it was necessary to filter the situations of the wind direction perpendicular to the conveyor belt, as this was the position of the rod with the sensors mounted. These situations where the wind lined up with the bar within a tolerance of ±45 degrees were filtered out. Filtering reduced the amount of data from 7056 measurements to 2682 measurements. Then, averages of thirty (30) minutes were calculated for standardization, which reduced the amount of data to 107 values corresponding to 53.5 hours. The average PM10 emission rate was 36.6 mg/(ms). In the same period, 5561.3 tons of grain were transported, which means an emission factor of 1266 mg/(tm). Statistical analysis of the data showed that the emission rate depended on the amount transported by the belt as well as on the intensity of the wind. Excluding the two highest and lowest emission rates significantly improved the correlation between the emission rate and transported mass and wind speed.

**Wildfire Emissions and Air Quality**
**Thursday, November 4 at 12:30 PM**

### Projections of Wildfire Impacts on Air Toxics in the Western US

Joshua Fu
Author(s):

Joshua Fu, Cheng-Pin Kuo, and Cheng-En Yang

Department of Civil and Environmental Engineering, The University of Tennessee, Knoxville, TN, USA

Presenter(s): Joshua Fu

Format: Oral Presentation

Short Description: Our CMAQ results have shown that the wildfire-induced air pollutant concentration changes could be as high as 102 ppb for O3 and 259 µg/m3 for PM2.5 at local scale in the western United States, under the Representative Concentration Pathway 8.5 (RCP8.5) climate scenario. Wildfires and climate change are increasingly causing a rise in air pollution and a human health impact. Future projections of wildfire emissions show a rise in pollutant concentrations between 2050 - 2059. Air pollutants have many important effects, such as influencing Earth' s radiative balance, diminishing human quality of life and exacerbating human health conditions, injuring ecosystems, damaging buildings and monuments, interfering with food safety, accelerating animal extinctions, altering Earth' s atmospheric composition, and impacting deposition rates. O3 and PM2.5 concentrations are damaging to human health and property, and there are long-term effects on climate change. In addition to O3 and PM2.5, air toxics such as formaldehyde (CH2O), methane (CH?), carbon monoxide (CO), and nitrogen dioxide (NO?) also impose threats to environmental and human health and are not paid too much attention. Since CH2O, CH?, CO, and NO? are projected to increase in the future over CONUS, it is essential to examine how wildfires would influence their concentrations. In this presentation, we will present the trends and correlations between wildfires and the concentrations of CH?, CO, CH2O, and NO?. Uncertainty of the projected pollutant concentrations will also be presented.

## Public Health Impacts of Prescribed Fires (PHIRE) Study - Baseline and Projected Prescribed Fire Smoke Exposures in California

ShihMing Huang
Author(s):

ShihMing Huang, Samantha Kramer, Melissa Chaveste, Crystal McClure, Fred Lurmann

Presenter(s): ShihMing Huang, Samantha Kramer

Format: Oral Presentation

Short Description: California has experienced increased catastrophic wildfires over the last decade, prompting the need for increased prescribed fires. We developed two prescribed fire emissions scenarios and assessed the public's exposure to fire smoke. In the baseline scenario, we established a 10-year (2008-2017) wildfire and prescribed fire inventory for California by merging satellite hotspots and agency records. The fire inventory and meteorological data were used to initialize daily PM2.5 smoke modeling in BlueSky Smoke Modeling Framework with HYSPLIT dispersion option. Dispersion modeling was completed independently for wildfires and prescribed fires. The modeled PM2.5 results were used to assign daily exposure for each California ZIP code. In the target prescribed fire scenario, we modeled PM2.5 exposures from multiple annual cycles of hypothetical prescribed fires. The representative distribution of prescribed fires by size and vegetation type was developed based on the baseline inventory and applied to the target acreage goals. Fire locations were randomly distributed within high-fire-risk areas. Fire dates were randomly assigned based on historical burn days for each air basin. The hypothetical fires were then used to initialize smoke modeling using the same representative climatology for each annual cycle. We will present the baseline fire history and modeled smoke exposures from each scenario.

## Toward Understanding Aerosol Vertical Distribution and Boundary Layer Dynamics During Wildfire Events

Jingting Huang
Author(s):

Jingting Huang, Kaiyu Chen, and Heather A. Holmes

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Presenter(s): Jingting Huang

Format: Oral Presentation

Short Description: Wildfire risks are accelerating at unprecedented rates in the western U.S. due to exceptional drought conditions. Short- and long-term human exposure to fine particles generated by wildfire smoke is projected to increase and will worsen population health outcomes. The issue of how plume emissions are vertically distributed through the atmosphere is a current knowledge gap for air quality modeling. The proper vertical emission profiles are necessary for accurate simulation of atmospheric transport and deposition. Whether aerosols are contained in or lofted above the planetary boundary layer height (PBLH) significantly affects the vertical placement and downwind transport of wildfire emissions. However, most existing plume rise parameterizations, based on Briggs' solutions (1969, 1975, 1984), are inappropriate for the physical characteristics of wildfire smoke plumes, especially for the large wildfires in the western U.S. In this study, we explore the plume injection height (PIH) for two large wildfire events [i.e., Rim Fire (2013) and Soberanes Fire (2016)] by evaluating notable and novel plume rise schemes with inputs from satellite remote sensing data, emission inventories, and numerical weather prediction. Simulated results from different plume rise algorithms are further compared to observations from field campaigns or aircraft measurements and satellite-derived PIH products. The final objective of this study is to develop a new plume rise model over the western U.S for use in 3-D chemical transport models.
Keywords: Air Quality; Wildfire Emissions; Smoke Plume Injection Height

## Status of New WMO North American Regional Vegetation Fire and Smoke Pollution Warning and Advisory Centre

Patrick M. Manseau
Author(s):

Patrick M. Manseau[1*], Radenko Pavlovic[2], Si Jun Peng[1], Jacinthe Racine[1], Michael Moran[3], and Jack Chen[3]

[1]Canadian Meteorological Centre Operations Division, Environment and Climate Change Canada (ECCC), Montreal, Quebec, Canada

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[3]Air Quality Research Division, ECCC, Toronto, Ontario, Canada

Presenter(s): Patrick M. Manseau

Format: Oral Presentation

Short Description: Concern about the health and socioeconomic impacts of wildfires and fire smoke is growing around the world, especially as wildfire frequency and severity are expected to increase under climate change. Vegetation fire danger warning and smoke forecast systems are a key component to increase societal resilience to wildfires and to raise awareness of the impact of fire smoke on air quality and population health. The World Meteorological Organization (WMO) is spearheading better international collaboration on this topic, including through the creation of several Regional Vegetation Fire and Smoke Pollution Warning and Advisory Centres (RVFSP-WACs). These centres will enhance the ability of countries to deliver timely and quality vegetation fire and smoke pollution forecasts, observations, information and knowledge to users through an international partnership of research and operational communities. The first RVFSP-WAC, which covers southeast Asia, was established in Singapore. Environment and Climate Change Canada (ECCC) is now working to create a North American RVFSP-WAC, the second to be established worldwide. For this project, ECCC is leveraging existing products from multiple agencies, including wildfire danger and fire weather index maps, operational North American air quality forecasts, which include near-real-time (NRT) vegetation fire emissions and smoke plume forecasts, and sub-seasonal temperature and precipitation forecasts. To date, to supplement its own products ECCC has accessed feeds of multiple global and regional NRT smoke-related forecasts from various agencies such as ECMWF, NASA, NOAA, FMI and JMA to generate a multi-model ensemble smoke forecast over North America. Development of this Centre is continuing, but some demonstration products are already accessible from a central web portal. This presentation will describe the status of the North American RVFSP-WAC, show examples of preliminary forecast and analysis products, and outline future work.

## An Evaluation of Biomass Burning Plumes on the Vertical Distribution of Tropospheric Ozone Over the Midwestern United States

Joseph Wilkins
Author(s):

Joseph L. Wilkins, Susan O'Neill, Ernesto Alvarado, Amber Soja, Hyundeok Choi, Emily Gargulinkski, Benjamin De Foy, George Pouliot, Thomas Pierce, Anne M. Thompson, David Peterson, Edward Hyer, Sim Larkin.

Presenter(s): Joseph L. Wilkins

Format: Oral Presentation

Short Description: Air quality models are used to assess the impact of smoke from wildland fires, both prescribed and natural, on ambient air quality and human health. However, the accuracy of these models is limited by uncertainties in the parametrization of smoke plume injection height (PIH), vertical distribution, and emission factors used for criteria pollutants. These errors can propagate, resulting in under or overestimations over large areas in public health analysis. We compared PIH estimates from the plume rise method (Briggs) in the Community Multiscale Air Quality (CMAQ) modelling system with observations from the 2013 California Rim Fire and 2017 prescribed burns in Kansas to study long range transport of smoke impacts to St. Louis, Missouri. We also examined PIHs estimated using alternative plume rise algorithms, model grid resolutions, and temporal burn profiles. For the Rim Fire, the Briggs method performed as well or better than the alternatives evaluated (mean bias of less than 5–20% and root mean square error lower than 1000 m compared with the alternative plume methods). PIH estimates for the Kansas prescribed burns improved when the burn window was reduced from the standard default of 12 h to 3 h. This analysis suggests that meteorological inputs, temporal allocation, and heat release are the primary drivers for accurately modelling PIH. Further our results indicate that long range transported smoke can add an additional smoke burden on a city, leading to 10 – 80 ppbv of ozone enhancement at the surface and ~15-30 % enhancement of the total column.

## Poster Presentations

### Poster Session: November 5 at 1:00 PM

### Air Quality, Climate and Energy

#### Modeling the Source Sectors Contribution to Nitrogen Deposition in U.S. Hydrological Regions

Sharmin Akter
Author(s):

Sharmin Akter and Kristina Wagstrom

Presenter(s): Sharmin Akter

Format: Poster

Short Description: The excessive deposition of atmospheric nitrogen containing species to aquatic systems and watersheds can lead to harmful algae growth and loss of biodiversity, particularly in coastal waterways. It increases the risk of acidification and hypoxia by reducing oxygen levels for living organisms in marine environments. It is important to determine the major species, source sectors, and source regions responsible for atmospheric nitrogen deposition to develop effective watershed management systems. We use the Comprehensive Air Quality Model with extensions (CAMx) version 6.0, along with the Particulate Matter Source Apportionment Technology (PSAT), to identify and separate source sector contributions to atmospheric nitrogen deposition. We model the amount of atmospheric nitrogen deposition from electricity generating units, biogenic emissions, area fugitive dust, on-road, residential wood combustion, agricultural emissions, non-point source oil and gas, point source oil and gas, fires, non-road mobile equipment sources, marine vessels and locomotives, and other non-point sources in the contiguous United States, southern Canada, and northern Mexico. We use emissions, meteorology, boundary conditions, and ozone column inputs from the United States Environmental Protection Agency's 2011 Modeling Platform. We evaluate the wet and dry deposited mass of atmospheric nitrogen containing species against measurements. This information will aid environmental regulators in developing watershed management plans to protect the health of aquatic and terrestrial ecosystems. The Upper Mississippi hydrologic region experienced the highest flux of gaseous ammonia deposition, and the dominant source sector was agricultural ammonia emissions. The Ohio region received the highest flux of reactive gaseous nitrogen, mostly from on-road emissions. Reactive gaseous nitrogen depositions from biogenic and electricity generating source sectors were significant throughout the United States.

## RESPONSE SURFACE METHODOLOGY TO EVALUATE THE EFFECTS OF GEOMETRIC PARAMETERS ON THE ELECTROSTATIC PRECIPITATION

Raíssa Andrade
Author(s):

Raíssa G. S. A. Andrade[1], Vádila G. Guerra[1]

[1]Department of Chemical Engineering, Federal University of São Carlos, São Carlos, SP, Brazil

Presenter(s): Raíssa G. S. A. Andrade

Format: Poster

Short Description: ABSTRACT – Electrostatic precipitator (ESP) is an equipment used on air pollution control systems to reduce the particulate material concentration. The main components of the ESP are the discharge and collecting electrodes, which are negatively charged and grounded, respectively. Due to the electrode different polarities, an electric field is generated inside the ESP duct and the particles are electrically charged and collected. The collection efficiency is influenced by operating conditions and geometric parameters, which have not been widely discussed for nanoparticles. In this study, the influence of the number and diameter of the discharge electrodes on the performance of the ESP, with different air velocities and electric field intensities, were evaluated through an ANOVA analysis and the response surface methodology. The inlet air that enters the experimental apparatus passes through purification filters, to remove impurities, while the NaCl aerosol is generated and mixed with the purified air. After that, the excess moisture is retained by a diffusion dryer and the particles are neutralized by a Krypton-85 source and enter the ESP, which is connected to a high voltage power supply. The phenomenon of electrostatic precipitation occurs inside the ESP duct and the particles are collected. The outlet airflow is neutralized, with a source of Americium-241, to prevent imprecise results. A Scanning Mobility Particle Sizer (SMPS) and an Ultrafine Condensation Particle Counter, operating for diameters between 5.83 and 228.8 nm, were used to determine the collection efficiency of ESP. The experiments were performed in a wire-plate single-stage ESP with two copper collecting plates spaced in 6.5 cm. The number of wires analyzed was 1 and 2, with the wire-spacing of 6.5 cm, for the wire diameters of 0.3 and 0.4 mm, the air velocities of 1.03 and 4.08 cm/s, and the electric fields of 3.08 and 3.38 kV/cm. The overall efficiencies results were applied on a 24 statistical analysis to determine the parameters with the most significant effects. It was evaluated the influence of each variable on the collection efficiency through the analysis of the effects, the standard error, and the statistical significance (p-value), with a confidence interval of 95%. The ANOVA analysis and the Pareto chart results showed that all factors were significant for the particle collection, especially the electric field and wire diameter. The wire diameter and the air velocity presented a negative effect, which means that the particle collection efficiency reduced (14-30%) with the increase of these parameters. On the other hand, the number of wires and electric field showed a positive effect, with an increase of over 36% on the particle collection. Through the analysis of the response surfaces, it was concluded that the highest collection efficiencies were achieved for the wire diameter of 0.3 mm and the electric field of 3.38 kV/cm. Therefore, it is possible to obtain collection efficiencies higher than 95% with a small number of wires and operating conditions that contribute to the electrostatic precipitation of particles.
Keywords: Electrostatic precipitator, geometric parameters, response surface.

## Atmospheric Dispersion Modeling of Emitted Pollutants from the Oil Refineries in the Gulf of Mexico Coastal Region using WRF-CALPUFF

Foroozan Arkian
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Presenter(s): Foroozan Arkian

Format: Poster

Short Description: The Gulf of Mexico coastal region (GCR) is home to numerous oil refineries, including the largest in North America, contributing significantly to environmental pollution in the region. The emitted pollutants from the oil refineries impact not only the local residents but can also be dispersed over a wide region depending on wind patterns. The primary objective of this research is to find the impact of sea breeze on concentrations and variability of sulfur dioxide (SO2), benzene, and nitrogen oxides (NOx) pollutants emitted from the oil refineries along the Gulf of Mexico Coastal Region (GCR). The Advanced Research WRF (ARW) model Regulatory Model has been used to simulate sea/land breeze condition and AMS/EPA Regulatory Model (AERMOD) model are being used to develop a better understanding of the transport and fate of the pollutants in the GCR. The penetration length of sea breeze and land breeze are estimated 25-30 miles and 20-25 miles in the coastal region, respectively. Thus, the influence/penetration length covers most of refineries along the GCR but most of the time the duration of sea breeze is 3-5 hours so it is seems not sufficient to transport and fate the majority of emitted pollutants from the oil refineries.
Key Words: Key Words: Benzene, NOX and SO2, Atmospheric dispersion, Sea/Land breeze circulation, Penetration length, WRF, AERMOD, Oil Refinery, the Gulf of Mexico.

### Simulating wildfire smoke transport in the western United States: Comparison of two fire emissions inventories

Kaiyu Chen
Author(s):

Kaiyu Chen, Jingting Huang, Samantha Faulstich, Heather Holmes

Presenter(s): Kaiyu Chen

Format: Poster

Short Description: The western U.S. has had increasing impacts from wildfire smoke in recent years due to global climate change. Emissions from wildfires contain large amounts of criteria air pollutants such as particulate matter (PM), sulfur dioxide ($SO_2$) and ozone ($O_3$). As one of the largest wildfires in 2016, the Soberanes Fire occurred in central California and caused profound impacts on air quality through its smoke plume transport. This research is an applied modeling study to estimate the impacts from Soberanes Fire using the Community Multiscale Air Quality (CMAQ) model with the meteorological inputs from the Weather Research and Forecasting (WRF) model. Wildfire emissions from the Fire INventory from NCAR (FINN) and the National Emissions Inventory (NEI) using the BlueSky framework are used in CMAQ and the outputs are evaluated using ground-based observations and satellite products. FINN uses thermal anomalies and land cover products from satellite remote sensing to estimate burned area and fuel loading, respectively. FINN uses emissions factors, for many chemical species, and vegetation estimates to provide fire emissions inputs to chemical transport models in near real-time. The NEI has point source day-specific fire emissions obtained from SMARTFIRE (Satellite Mapping Automated Reanalysis Toll for Fire Incident Reconciliation) with the estimated fire activities (fire locations, duration and size) serving as the initial data for the BlueSky framework. This framework is implemented in the Sparse Matrix Operator Kerner Emissions (SMOKE) modeling system to generate CMAQ ready fire emissions. In addition to the emissions inventory comparison, different speciation mechanisms (CB6 and SAPRC07) are also evaluated in this study to quantify the impacts of applying different speciation configurations on modeling wildfire smoke. Consequently, future work will use these results to develop a wildfire smoke forecasting framework and to simulate smoke transport to estimate the impacts on air quality and human health. Broadly, these findings are valuable to researchers interested in assessing fire and smoke impacts and provide evidence for further model studies of fire activities.

## PM2.5 variability with meteorology from reanalysis and ground-based monitors across locations

Shreya Guha
Author(s):

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Presenter(s): Shreya Guha

Format: Poster

Short Description: Air pollution is one of the most important eco-environmental?problems?throughout the world?and its?concentrations are sensitive to both source emission levels and meteorological fluctuations.?The purpose of this study is to identify?differences in covarying meteorological factors?between?reanalysis?and observed?meteorological data?sets across locations?such that?more effective and integrated air quality policies can be drafted in the future.We?utilize?two approaches to quantify the effects of?ground-based observed (from National Climatic Data Center [NCDC]) and?reanalysis model?values (taken from Climate Forecast System version 2?[CFSv2]) of meteorological variables on PM2.5?emission levels (downloaded from?AirNow?Beijing and the?US?Environmental Protection Agency?[EPA]website) for the years 2011?to?2020?for the cities Beijing, China and Washington DC, USA.?We?consider?temperature, precipitation, relative humidity, wind speed & direction at 2m above ground level and planetary boundary layer height.?The first approach applies?Kolmogorov-Zubrenko?filters and linear regression models to study long-term, seasonal, and short-term components of the pollutant signals?and its?meteorological components. The second approach?applies?general additive models to?quantify?relationships between meteorology and?PM2.5?fluctuations?at the given locations with the two different sets of meteorological?data.?We perform a?holdout analysis?to?evaluate?the predictive performances of?all?models.In?Beijing,? reanalysis?meteorological data show?very weak relationships with PM2.5?concentrations, whereas the observed data?are?very significant for the short-term scale, with the average daily?PM2.5?increasing by?1μg?m-3?per?~3.5??average temperature increase.?In?continuing analysis,?we are comparing the results?between?Beijing and Washington, DC.?

**Air Quality, Climate and Energy (continued)**

## Quantifying impacts of climate change and variability on future US PM2.5 by dynamically downscaling a global chemistry-climate model in WRF and CMAQ

Surendra Kunwar
Author(s):

Surendra Kunwar[1], Jared Bowden[2], George Milly[3], Michael Previdi[3], Arlene Fiore[3], Jason West[1]

[1]University of North Carolina at Chapel Hill, Chapel Hill, NC, USA

[2]North Carolina State University, Raleigh, NC, USA

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Presenter(s): Surendra Kunwar

Format: Poster

Short Description: Anthropogenic climate change and meteorology-sensitive natural feedback emissions like biogenic VOCs, lightning NOx and sea salt will likely affect future PM2.5 and O3 air quality. But the noise from variability in meteorological variables like temperature, precipitation and wind speed can confound the signal of climate change on air quality. Previous studies of the impacts of climate change on air quality in the US have often downscaled only a small number of years from global models, without understanding the broader distribution of possible effects, thereby not clearly separating the influence of variability from that of climate change.Here we use a combination of multidecadal global model ensemble simulations with downscaling by finer regional atmospheric models for selected years, to quantify the effects of climate change and variability on US PM2.5 in the 2050s under climate change from the RCP8.5 scenario. We use simulations of the global chemistry climate model GFDL-CM3 at 2o resolution for the period 2006-2100, where the three ensemble members vary only in initial conditions, providing an unprecedented dataset for defining PM2.5 probability distributions. These simulations held anthropogenic emissions of PM2.5 and O3 precursors constant at present day levels, to isolate the influence of RCP8.5 climate change. Empirical Orthogonal Function analysis of the global model dataset has helped identify the Eastern US regions where PM2.5 covaries spatiotemporally. We then select four present (2006-2020) and four mid-century (2050-2060) years representing median and high PM2.5 levels in different US regions for downscaling by regional models.We use the Weather Research and Forecasting (WRF) model version 3.9.1.1 to dynamically downscale the coarse GFDL-CM3 meteorology of the eight selected years to a finer 12 km resolution for the CONUS. The GFDL chemistry and the WRF meteorology are then provided as inputs to the regional air quality model CMAQ to obtain US PM2.5 levels at 12 km resolution for the selected years. CMAQv5.3.2 uses the BEIS model to generate biogenic emissions inline, and the Carbon Bond 6 (with Aerosol Module 7 and Aqueous Chemistry) chemical mechanism, which incorporates aqueous-phase and cloud aerosol chemistry. NEI emissions for year 2016 processed in SMOKE are used in all CMAQ simulations to represent present day emissions.We then combine the broad probability distribution of mean annual PM2.5 from the global model with the CMAQ-downscaled PM2.5 values in selected years, to construct PM2.5 distributions for the present and mid-century in individual 12 km grid cells. We do so by fitting distribution parameters that minimize percentile differences with the percentiles of the selected years from the global model. A Monte Carlo simulation of differences in fine resolution mean annual PM2.5 distributions between the present and the future will be used to quantify the impacts of climate change and variability on US PM2.5. Expressing the impact of climate change on PM2.5 as probability distributions will then allow us to calculate the impact of climate change and variability on human mortality and visibility.

## Analyzing the Transportation and Climate Initiative Program Using an Integrated Assessment Model

Zhuoran(Gray) Li
Author(s): Zhuoran "Gray" Li* (presenter) and Dan Loughlin+

* Conducted while a graduate student at Duke University
Currently with the Environmental Defense Fund, Beijing, China
+ U.S. EPA Office of Research and Development
Presenter(s): Zhuoran "Gray" Li

Format: Poster

Short Description: The Transportation & Climate Initiative (TCI) is a cap-and-invest program that is designed to reduce transportation-related CO2 emissions from the thirteen participating states. Electrification of the transportation sector has the potential to interact with the Regional Greenhouse Gas Initiative (RGGI) market, a cap-and-trade system for CO2 emissions from electricity generation. Potential impacts of this interaction could include leakage of CO2 emissions to other sectors and states. This study utilized a human-earth systems model to investigate TCI's regional emissions reduction potential and to quantify the impacts of the program under alternative assumptions. The results show that TCI would lower regional net CO2 emissions and increase market penetration of both heavy- and light-duty electric vehicles through 2050. Furthermore, emissions reduction and changes in transportation fuel mix would be accompanied by an increase in the RGGI CO2 allowance price, a moderate increase in the price of electricity, and an increase in the cost of on-road travel. In the freight sector, a portion of heavy-duty demand shifts from trucks to trains and marine vessels. Also, some of the CO2 reduction from on-road transportation is offset by the increases in emissions from non-road transportation and electricity generation. Pennsylvania, the only TCI state that does not currently belong to RGGI, experiences the highest increases in CO2 from the electric sector as well as the lowest percentage reduction of NOx emissions, reflecting both its own additional electricity demands from TCI and greater electricity exports to RGGI states. Extending the declining RGGI and TCI cap trends through 2050 leads to greater reductions in CO2 and air pollutant emissions. In addition, it further facilitates the energy transition from carbon-based fuels to electricity in the on-road transportation sector.

## Changes in Mortality in Response to Decreases in Ozone and PM2.5 Concentrations Across the United States from 1990 to 2019

Revathi Muralidharan
Author(s):

Revathi Muralidharan, Yuqiang Zhang, Omar Nawaz, Daniel Tong, Aaron van Donkelaar, Randall Martin, Marc L. Serre, and J. Jason West

Presenter(s): Revathi Muralidharan

Format: Poster

Short Description: O3 and PM2.5 concentrations in the United States have decreased significantly since 1990 due to the success of air quality regulations such as the 1990 Clean Air Act Amendments. It is estimated that between 1990 and 2019 maximum daily 8 hour average (MDA8) O3 decreased by 25%, and from 2000 to 2019 annual average PM2.5 concentrations decreased by 43%. A decrease in mortality is expected to correspond to this reduction in O3 and PM2.5 concentrations. In order to assess the health impacts of reduced air pollution across the United States, mortality attributable to O3 and PM2.5 in the continental United States is assessed each year from 1990 to 2019 using multiple concentration datasets for comparison. We create a 28-year dataset by performing Bayesian Maximum Entropy kriging on observations (1990-2017). We also use a long-term simulation (1990-2010) from a regional air quality model (CMAQ), as well as CMAQ simulations from the North American Chemical Reanalysis project (2009-2019), and a satellite-derived PM2.5 dataset (1999-2018). We also use annual county-level mortality statistics from the US Centers for Disease Control and Prevention, and separate the trends caused by the change in concentrations vs. the changes in population and baseline mortality rates. In using multiple concentration datasets, we aim to investigate whether trends in mortality are consistent across different concentration datasets and to account better for uncertainty. We hypothesize that the different datasets will show similar decreases in premature mortality.

## Influence of land use and occupationon aerosol chemical composition in the eastern part of Sao Paulo city

Maria Oliveira
Author(s):

Maria Carla Queiroz Diniz de Oliveira, Regina Maura de Miranda - University of São Paulo, São Paulo, SP, Brazil

Presenter(s): Maria Carla Queiroz Diniz de Oliveira

Format: Poster

Short Description: The city of São Paulo is one of the main financial and mercantile centers in South America, impacted mainly by heavy trafficand industrial emissions. Thus, to better understand the sources of pollution emissions, fine particulate matter (PM2.5) samples werecollected in the eastern region of the city of São Paulo during 2015. Particle concentrations, chemical composition, Wind speed and direction were related to land use and occupation in order identify the main sources that influence air quality at the site. Episodes with high concentrations of PM2.5 (concentrations above 25ug/m3) indicated higher concentrations of the species S, Si, K and SO4-2. During 2015, World Health Organization (WHO) air quality standard for the pollutant (25ug/m3) has been exceeded for 17 days. The results indicated that vehicle traffic has the greatest influence on the site, but residential waste burning in the surrounding residences and the airport also have a strong contribution.

## Effectiveness of Decarbonization Pathways on Eleven Northeastern States Greenhouse Gas Reduction Goals

Sarah Simm
Author(s):

Sarah Simm[1], Carol Lenox[2], & Dan Loughlin[2]

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[2]U.S. EPA, ORD, CEMM, AESMD, ESAB

Presenter(s): Sarah Simm

Format: Poster

Short Description: Increased awareness of the impacts of global climate change has resulted in many US states committing to various greenhouse gas reduction (GHG) and decarbonization goals. In this study, GLIMPSE is used to analyze various decarbonization pathways in eleven Northeastern states. GLIMPSE is a decision support modeling tool being developed by the EPA to support state-level environmental and energy planning. GLIMPSE is a graphical interface for the Global Change Analysis Model (GCAM), an integrated assessment model (IAM) developed by the Pacific Northwest National Laboratory. GCAM links representations of the world's energy, economic, agriculture, and land use systems with a climate model, simulating their interactions and co-evolution. The aim of this study is to provide a greater understanding of the potential impacts these state GHG mitigation policies have on carbon dioxide (CO2) and air pollutant reductions and what additional efforts might be needed for states to reach their ultimate goals. The states studied in this analysis include Connecticut, Delaware, Massachusetts, Maine, Maryland, New Hampshire, New Jersey, New York, Pennsylvania, Rhode Island, and Vermont. The decarbonization pathways explored include: increased electrification and efficiency in the building sector, increased electrification in the passenger vehicle sector, renewable portfolio standards, clean energy standards including carbon capture and storage technologies and biomass use. These pathway choices are applied to each individual state, both alone and in combination, and the reduction in CO2 is analyzed at the state level, providing insight into what type of pathways could be most effective for each state.

## Envi Met Model Studies of Urbanization Impact on Climate Change

G S N V K S N SWAMY UNDI
Author(s):

G S N V K S N SWAMY UNDI

Presenter(s): G S N V K S N SWAMY

Format: Poster

Short Description: The present reflects the dynamics of urbanization on climate change. Sustainable urbanization includes environmental factors that need to be considered for urban development. The complexity of urban structure brings considerable changes to the urban atmosphere, micrometeorology, and dispersion conditions in a significantly considerable behavior known as urban hotspots. An increase in temperature and air pollution levels influence regional and global trends, so it is important to correlate urbanization's impact on climate change indicators. This present paper aims to present the concept of sustainable urban planning, the effects of climate change, and importance of urban heat islands (UHI) in territorial planning. This chapter draws attention to the impact of land use and land cover change on UHI characterization, measurements, and impact assessment have been discussed in the present chapter. The paper presents a system that can be used for the assessment of the land use pattern effect on the UHI. The system integrates analysis of land use modeling and an indicator-based assessment. The applicability of the model is illustrated through developing scenarios for the future land use allocation of the urban zone. The results show scenarios of the UHI effect and outdoor thermal comfort. Moreover, for each scenario of urban design patterns accounting for adaptation to climate change could be implemented. This study provides a guideline for local authorities to create more sustainable urban structures and adapt to climate change.

**Air Quality, Climate and Energy (continued)**

## US Clean Energy Futures - an analysis of different energy policies towards cleaner air

Petros Vasilakos
Author(s):

Petros Vasilakos, Huizhong Shen, Nash Skipper,  Armistead Russell

Presenter(s): Petros Vasilakos

Format: Poster

Short Description: In this presentation, we will be comparing different policies aimed at controlling EGU emissions between the present day and 2050. Most of these policies are aimed at reducing CO2 levels, but at the same time produce significant co-benefits for other criteria pollutants that we will be mostly focusing on. We find that even modest policies can provide both climate and air quality benefits at a small cost, indicating that an 80% clean energy sector by 2030 is both viable and financially beneficial (though the reduction in health associated mortality costs).

## Unexpected deterioration of ozone pollution in South Coast Air Basin of California: Role of meteorology and emission changes

Kai Wu
Author(s):

Kai Wu, Shupeng Zhu, Michael Mac Kinnon, Scott Samuelsen

Presenter(s): Kai Wu

Format: Poster

Short Description: Urban ozone (O3) pollution over the South Coast Air Basin (SoCAB) is a prominent environmental threat due to adverse impacts on vulnerable populations and ecosystems. In recent years, O3 concentrations have demonstrated surprisingly high trends which run counter to expected reductions from decreased precursor emissions. However, the driving factors behind these trends remain unclear. Therefore, providing insights into the potential roles of meteorological variability and precursor emissions on SoCAB O3 is urgently needed. In this work, we combined ambient measurements, satellite data, and air quality modeling to investigate O3 trends and the impacts of meteorological conditions and emission changes.

## COVID-19 and Impacts on Emissions and Air Quality

### The COVID-19 lockdown period in the Mexico Megalopolis: impact on surface SOA and Ozone

Victor Almanza
Author(s):

Victor Almanza[1] and Agustín García[1]

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Presenter(s): Victor Almanza

Format: Poster

Short Description: Despite the many challenges derived from the COVID19 pandemic, the current worldwide lockdown measures still represent a unique opportunity for the development and evaluation of mitigation measures aimed to abate air pollution. In Mexico, the lockdown coincided with periods of high temperature and intense solar radiation, which can result in ozone episodes and biomass burning emissions. In addition, given the highly nonlinear dynamics of ozone formation, the effects on air quality might be different among regions according to the magnitude and spatial distribution of emissions. In this work, the impact of emissions reductions will be presented for the Megalopolis area, which consists of the Mexico Megacity and the 5 surrounding states in Central Mexico. The variation in local emissions was estimated mainly on both official mobility data and on the adjustment factors developed as part of the CONFORM (COvid adjustmeNt Factor fOR eMissions) global emissions dataset [1]. The biomass burning emissions were included using the FINN inventory. The variations in surface ozone, fine particles and secondary organic aerosols obtained with the WRF-Chem model will be discussed for both the 3 main stages of the lockdown period and the first weeks of the so-called “new normal”, when some of the main economic activities began to re-open.References 1. Doumbia, T., Granier, C., Elguindi, N., Bouarar, I., Darras, S., Brasseur, G., Gaubert, B., Liu, Y., Shi, X., Stavrakou, T., Tilmes, S., Lacey, F., Deroubaix, A., and Wang, T.: Changes in global air pollutant emissions during the COVID-19 pandemic: a dataset for atmospheric chemistry modeling, Earth Syst. Sci. Data Discuss. [preprint], https://doi.org/10.5194/essd-2020-348, in review, 2021.

**COVID-19 and Impacts on Emissions and Air Quality (continued)**

## Assessing the impact of COVID-19 on power plants emissions in the United States using generalized synthetic control methods

Munshi Md Rasel
Author(s):

Munshi Md Rasel[1*], Kevin L. Chen[2], Rachel C. Nethery[2], and Lucas R.F. Henneman[1]

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[2]Department of Biostatistics, Harvard T.H. Chan School of Public Health, Boston, MA, USA
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Presenter(s): Munshi Md Rasel

Format: Poster

Short Description: Public health interventions implemented to reduce the spread of the Coronavirus Disease 2019 (COVID-19) impacted air quality globally due to change in emissions from transportations, industries, and energy sectors. Subsequent research has identified reduced on-road vehicle emissions as a reason for improved air quality in U.S. cities in early 2020, but the extent that emissions changes from large stationary sources influenced regional air quality has yet to be investigated in full. This study assesses emissions from 977 electric facilities across the United States using a generalized synthetic control (GSYNTH) causal inference model trained on daily facility emissions from January to April 2010-2019. Using historic emissions trends and meteorological covariates, the GSYNTH model estimates the counterfactual emissions at each facility, i.e., the emissions expected during the lockdown period in the absence of lockdown, and uses these to estimate changes in emissions due to lockdown. We apply GSYNTH to estimate lockdown effects on NOx and SO2 emissions at each facility. Overall, we find average increases of 254 (confidence interval will be presented at the poster presentation) tons of SO2 and 121 (confidence interval will be presented at the poster presentation) tons of NOx emissions per day during the COVID-19 lockdown period relative to expected emissions in the absence of lockdown. While some facilities emitted less than expected, other facilities emitted more—in Texas, Louisiana, and Pennsylvania, for instance, we find increases of 22, 15, and 18 tons of NOx per day. Conversely, Ohio, Tennessee, and Nebraska saw emissions reductions of 15, 4, and 3 tons of NOx per day. Louisiana, Arizona, and Indiana emitted 47, 38, and 29 more tons of SO2 per day than expected. We find that facilities in Ohio emitted, on average, reduced NOx and SO2 emissions more than facilities in other states relative to their expected emissions. Ongoing work will identify the location, fuel type, and other features related to facility-specific emissions changes across the lockdown period, and we will identify long-term effects. These findings provide a post-hoc assessment of the impacts of the lockdowns on electric utility emissions, and they serve as a blueprint for future studies of emission responses to large-scale interventions.

## Emissions Inventories, Models, and Processes

### DETERMINATION OF CONTROL SYSTEM EFFICIENCY USING LIQUID CO2 INJECTION

Israel Soares
Author(s):

Israel Pestana Soares, Daniella Correa Gonçalves de Rezende and Karinnie Nascimento de Almeida

Presenter(s): Israel Pestana Soares

Format: Poster

Short Description: Generation of fugitive emissions in a steel plant can be understood as a sequence of events, starting with feedstock preparation, transport and final product until its storage. One of the steelmaking processes that requires attention is the liquid pig iron production, which involves both its production as well as the converting process, when necessary. The converting of pig iron by torpedo cars only happens when the quality of the material are not within the established standards. When this occurs, they are directed to specific yards that are properly prepared to receive it. The fall of the pig iron causes great movement of liquid metal, promoting the detachment of particles and therefore the emission of particulate matter. In this study were monitored different fractions of particulate matter: Total Suspended Particles (TSP), Coarse Particles (PM10) e Fine Particles (PM2,5) on the pig iron dumping process in a Steel Plant in Belo Horizonte, Minas Gerais, to determinate the efficiency of the system control using liquid CO2 during the pig iron dumping. The OTM 32 - exposure profiling method (US EPA, 2013) is one of the best methods to monitor fugitive emissions. This method was developed to measure open source emissions of a pollutant, with exposure defined as the time-integrated mass flux of a pollutant at a sampling point. In order to evaluate the efficiency of the control system used on this study it were realized comparative tests on the pig iron converting Yard with and without liquid CO2 injection. The results of the tests without the application of liquid CO2 shown up that the high temperatures reached by pig iron elevates the vertical gradient plume dispersion, provoking a quick rise of the plume and less horizontal reach. As expected, it was noticed the increase of particulate matter concentration during the pig iron converting without the CO2 injection. Considering the overall average of particulate matter emission rate it was observed a percentage drop of 68% for TSP, 71,5% for PM10 and 66,5% for PM2,5.

## Machine Learning and Reduced Form Models Developments and Applications

### Applying CMAQ sensitivity analysis for the state of California: Reduced order modeling, source attribution, and process analysis

Zhen Liu
Author(s):

Zhen Liu, Pingkuan Di, Jeremy Avise

Presenter(s): Zhen Liu

Format: Poster

Short Description: We present results from our ongoing effort of investigating the potential of CMAQ sensitivity analysis in supporting air quality policy making and planning in the state of California. The model code for CMAQ-DDM-3D (v5.2) was adapted with the SAPRC07tic-AERO6i chemical mechanism, and then used for reduced order modeling (ROM), source attribution, and process analysis. A reduced order model (ROM) was constructed to establish first-order source-receptor relationships between emissions of NOx and VOCs from 58 counties in California and gridded surface concentrations for the full suite of CMAQ output species at a 12 km resolution. The ROM is shown to allow efficient projections of changes in air quality due to emission perturbations at 58 counties as resulting from a future regulation, while its accuracy is illustrated by comparing against results from full CMAQ modeling. Source contributions from 58 counties to PM and toxic VOC concentrations are estimated with the ROM, considering both transport and chemistry with a first-order approximation. Finally, we discuss the potential of using sensitivity analysis to help understand chemical and transport processes (e.g., nitrate formation and its dependency on emissions of precursors).

**Model Development**

# A NEW APPROACH ON FRACTIONARY DIFFERENTIAL EQUATIONS USING THE GILTT METHOD ON DISPERSION PROBLEMS AT THE ATMOSPHERIC BOUNDARY LAYER

André Luiz Santos Soledade
Author(s):

ANDRÉ LUIZ SANTOS DA SOLEDADE, JOSÉ ROBERTO DANTAS DA SILVA, PAULO HENRIQUE FARIAS XAVIER2, DAVIDSON MARTINS MOREIRA4, ANDRÉ LUIS COSTA PINTO

Presenter(s): André Luiz Santos da Soledade

Format: Poster

Short Description: This study aims to investigate the potential of fractional derivatives in modeling the dispersion of air pollutants. For this purpose, an analytical solution of the fractional two-dimensional advection-diffusion equation is proposed, using the GILTT and conformable derivatives methods. The novelty of this study is the insertion of fractional parameters in all derivatives of the equation considering conformable derivatives, taking into account the anomalous behavior in the diffusion process, resulting in a new methodology here called the α-GILTT method. The simulations were compared with the moderately unstable data from Copenhagen experiment and the best results are for the fractional parameters alfa = 0.99 (advective term) e beta = 0.964 (diffusive term).

## Modeling to Support Exposure and Health Studies and Community-scale Applications

### Improving Exposure Estimates in Urban Areas using a Multiscale Modeling Approach

Britney Russell
Author(s):

Britney Russell and Kristina Wagstrom

Presenter(s): Britney Russell

Format: Poster

Short Description: Urban populations are exposed to air pollutant concentrations that have been linked to adverse health outcomes. Exposure assessments have widely used air quality measurements from regulatory monitoring stations. However, the spatial distribution of the monitoring stations cannot capture the spatial variations of pollutants at these urban scales. Additionally, short-term and long-term exposure to air pollutants results in distinct health outcomes requiring concentrations at a high temporal resolution collected over extended periods. One approach to address these limitations is to use modeled concentrations as an alternative to monitoring data. In this work, we evaluate the use of a multiscale modeling system for generating pollutant and exposure estimates at the urban scale. The Comprehensive Air Quality Model with Extensions (CAMx) provided estimates of pollutant concentrations at a regional scale (12 x 12 km resolution) for the Contiguous United States. CAMx results were further resolved using the Model for Air Pollution (InMAP) to yield higher resolution pollutant concentrations. The performance of the modeling system was evaluated by comparing the results with monitoring data provided by the EPA. Exposure estimates generated using monitoring data and modeling results were compared. The multiscale modeling system provided concentration estimates with an improved spatial coverage when compared to monitoring data. The system also provides concentrations with a high degree of spatial and temporal resolution, which is crucial for exposure assessments.

## Multiscale Model Applications and Evaluations

### An evaluation of a two-decade CONUS and Northern Hemispheric timeseries of retrospective WRF simulations

Robert Gilliam
Author(s):

Robert Gilliam, Kristen Foley, Lara Reynolds, Jesse Bash, Christian Hogrefe, Rohit Mathur, Norm Possiel, Chris Misenis, Barron Henderson, Golam Sarwar, Wyat Appel and George Pouliot

Presenter(s): Robert Gilliam

Format: Poster

Short Description: The US EPA's Air QUAlity TimE Series (EQUATES) Project has developed a consistent set of modeled meteorology and emissions that are being used to produce multidecadal timeseries (2002-2017) of air quality model output using the Community Multiscale Air Quality (CMAQ) model. This CMAQ dataset will be leveraged for a diverse set of research and air quality management applications. To support this collective dataset that will be available for broad distribution, we present an evaluation of the nearly twenty years of meteorology that was produced using version 4.1.1 of the Weather, Research and Forecasting (WRFv4.1.1) model. WRFv4.1.1 was ran over the contiguous United States and the Northern Hemisphere for the 2002-2020 period using a horizontal grid-resolution of 12 km and 108 km, respectively, although the air quality was a few years shorter. We examine the simulated meteorology using a broad range of observations including upper-air and near-surface temperature, moisture and winds. We also use shortwave radiation observations to examine the model's ability to represent clouds. And finally, the US-based PRISM (Parameter-elevation Regressions on Independent Slopes Model) precipitation dataset is leveraged to understand how well the model characterizes seasonal and annual precipitation. Results of the evaluation show that the model output is suitable in terms of driving air quality models as error levels are within expected bounds of recent retrospective simulations that use data assimilation. As expected, the 12 km scale simulations reduce the level of error when compared to the coarser 108 km hemispheric domain. As such, the distribution and use of these meteorological modeling datasets can help air quality modelers by providing a robust and lengthly set of inputs for air quality applications.

**Multiscale Model Applications and Evaluations (continued)**

## Modeling potential odor sources in Brunswick, GA

Xiangyu Jiang
Author(s):

Xiangyu Jiang, Byeong-Uk Kim, Jim Boylan

Presenter(s): Xiangyu Jiang

Format: Poster

Short Description: Residents in Brunswick, GA reported foul smelling odors from December 2, 2020 to February 9, 2021. To locate potential emission sources associated with the odor complaints, we applied two modeling approaches along with a “hybrid” approach. The first modeling approach used a simple vector trajectory method with 1-minute wind speed and wind direction data from a single meteorological station to track air parcels back in time. The second approach used the HYSPLIT model to identify the hourly averaged movement of air parcels based on the 3-km HRRR meteorological data. Both approaches show that more than 80% of the back-trajectories passed through the 1-mile buffer zone surrounding a wood pulp mill and the adjacent wastewater treatment plant. When the meteorological monitoring station, potential odor sources, and odor complaints are relatively close together, the simple vector trajectory method captures more back-trajectories passing the 1-mile buffer zone compared to the HYSPLIT approach. The “hybrid approach” takes advantage of strengths from both modeling approaches. This approach showed that over 90% of the back-trajectories passed the 1-mile buffer zone. Based on this analysis, the odor source(s) are likely in and/or near the 1-mile buffer zone surrounding the wood pulp mill and the adjacent wastewater treatment plant.

**Multiscale Model Applications and Evaluations (continued)**

## Implementation of Lightning NOx production in CMAQ over the Northern Hemisphere with Lightning Flash Data from WWLLN

Daiwen Kang
Author(s):

Daiwen Kang, Mike Madden, James East, Golam Sarwar, Christian Hogrefe, Rohit Mathur, and Barron H. Henderson

Presenter(s): Daiwen Kang

Format: Poster

Short Description: Lightning NOx (nitrogen oxides) emissions based on lightning flash data from the National Lightning Detection Network (NLDN), a ground-based lightning detection network that covers the contiguous United States (CONUS) with high detection efficiency, have been included and analyzed in previous modeling studies using the Community Multiscale Air Quality (CMAQ) model over the CONUS domain. For modeling simulations beyond the CONUS domain, a potential alternative source of lightning flash dataset is the World Wide Lightning Location Network (WWLLN), albeit with low detection efficiency. In this study, a comparison between NLDN and WWLLN is performed over the CONUS domain, and an effort is made to adjust the WWLLN data based on the climatological ratios between WWLLN and NLDN. Lightning NOx emissions are then estimated using lightning flashes from NLDN, WWLLN, and the adjusted WWLLN flashes in CMAQ simulations over the CONUS domain. This presentation will focus on the development of a methodology for the adaptation of the WWLLN data and the assessment of model performance over the CONUS domain to demonstrate how the flash data from WWLLN can be used and how the simulations perform with different sources of data and quality. In addition, as an important component of the impact of lightning NOx on air pollution, the simulations of aerosol nitrate deposition are evaluated using data from the National Atmospheric Deposition Program (NADP)'s National Trends Network (NTN). Then, CMAQ simulations are performed over the Northern Hemisphere without any lightning NOx, and with lightning NOx produced by the original and adjusted WWLLN flashes and using the Global Emissions InitiAtive (GEIA) climatological lightning NOx emissions. The simulation results with lightning NOx emissions are compared to those obtained without lightning NOx and with climatological lightning NOx emissions. A follow-on presentation will focus on the assessment of hemispheric CMAQ simulations with varying lightning NOx emissions.

**Multiscale Model Applications and Evaluations (continued)**

## Evaluation of the Community Multiscale Air Quality (CMAQ) version 5.3.2 over California: Preliminary analysis

Sarika Kulkarni
Author(s):

Sarika Kulkarni and Chenxia Cai

Presenter(s): Sarika Kulkarni

Format: Poster

Short Description: The Community Multiscale Air Quality (CMAQ) version 5.3.2 (CMAQ532) that was released to the public in October 2020, has numerous scientific updates when compared to previous versions. This study will present preliminary findings from the ongoing evaluation of an air quality modeling system comprised of CMAQ532, Weather Research Forecasting v4.2.1 (WRF421) and Sparse Matrix Operator Kernel Emissions 4.8 (SMOKE48) applied over California. As a first step, the performance of CMAQ532, using State Air Pollution Research Center version 07tc with extended isoprene chemistry (SAPRC07tic) and aerosol module (AERO6) treatment of SOA, was evaluated by comparing simulated ozone and particulate matter (PM2.5) to observations as well as model results from a similarly configured modeling system which utilized the CMAQ version 5.2.1 (CMAQ521). Preliminary analysis has shown that ozone and PM2.5 predicted by CMAQ532 compare well with observed values and are able to capture the broad spatial patterns and temporal variability over the major air basins in California including San Joaquin Valley, Sacramento Metropolitan area and South Coast. However, the CMAQ532 simulated ozone and PM2.5 values are generally lower when compared to the corresponding values from the CMAQ521 simulation. Additional sensitivity analysis results will be presented to isolate the impact of specific science updates including but not limited to new aerosol module (AERO7) and the new Surface Tiled Aerosol and Gaseous Exchange (STAGE) deposition model on the simulated ozone and PM2.5 over California.

**Multiscale Model Applications and Evaluations (continued)**

## An evaluation of trends and variability in aerosol optical depth over the Northern Hemisphere simulated by CMAQv5.3.2 for the EQUATES project

Rebecca Miller
Author(s):

R. Miller[1], C. Hogrefe[2], R. Mathur[2], J. Pleim[2] and K. Foley[2]

[1] Oak Ridge Associated Universities

[2] AESMD, Environmental Protection Agency

Presenter(s): Rebecca Miller

Format: Poster

Short Description: Air quality models are important tools for studying atmospheric trace gases and aerosols. Their outputs are often used to quantify adverse impacts of air quality on human health and the environment. Model simulations were performed for 2002–2017 using CMAQv5.3.2 and WRFv4.1.1 over the Northern Hemisphere. Emissions were represented by a 2002–2017 emissions dataset developed for EPA's Air QUAlity TimE Series (EQUATES) project. In this presentation, we compare these simulations with monthly average aerosol optical depth (AOD) data from the Moderate Resolution Imaging Spectroradiometer (MODIS) on board the NASA Terra satellite to assess the model's ability to capture observed variability and trends in the tropospheric aerosol burden. Initial findings show regional and seasonal differences between model and satellite observations. Over CONUS, the annual AOD cycle is in general agreement with satellite observations for all seasons, except summer when CMAQ AOD values are lower than observed. Linear trends through the annual average AOD reveal a decrease in AOD over the southeastern United States, Europe, and China, and an increase over India. These linear trends are similar for both the model output and satellite observations. To provide further context for the AOD analysis, we also present an analysis of ground-based AOD from AERONET and PM2.5 concentrations measured at surface monitoring networks over North America and Europe.

## The Impact of Altering Emission Data Precision on Efficiency and Accuracy Regarding the Community Multiscale Air Quality Model

Michael Walters
Author(s): Michael Walters (US EPA)
Presenter(s): Michael Walters

Format: Poster

Short Description: The Community Multiscale Air Quality Model (CMAQ) has been a vital tool for regulatory work at the United States' Environmental Protection Agency (EPA), State government sectors, and at numerous, academic institutions. At the EPA specifically, CMAQ itself requires a copious amount of disk space in terms of input and output as a result of temporally long simulations initialized at a fine horizontal grid scale which encompasses the contiguous United States. As a result, disk space management is strict to ensure the uninterrupted progress of ongoing research projects at the EPA. Such disk space management includes optimal data compression techniques on input and output files for all CMAQ simulations when archiving is necessary. Currently, there are several such utilities' that compresses files using losslessness compression such as GNU zip (gzip) and Basic Leucine Zipper Domain (bzip2), however, a new approach has been created herein this study and ingested into CMAQ simulations to examine the impact on CMAQ model performance and data compression efficiency. In total, four simulations were conducted: Three using emission files which consist of 5, 4, or 3 significant digits, and the fourth case using original, unaltered emission files as the benchmark case. Results demonstrate that CMAQ runtime was consistently reduced by roughly 1-7% for simulations using altered emission files. Additionally, the altered emission files improved disk space by 5%, 25%, and 48% compared to the unaltered emission files when using the bzip2 compression utility for files containing 5, 4 and 3 significant figures respectively. As for simulation accuracy at in-situ locations via the United States Environmental Protection Agency's (USEPA) Air Quality System (AQS) and Ammonia Monitoring Network (AMON) stations, all 3 cases performed nearly identical to one another for ammonia (NH3), ozone (O3), and particulate matter (PM2.5). In fact, the normalized mean bias for all analyzed species differed by less than 0.01% for all bulk, regional, and temporally stratified calculations. In summary, we have shown that by reducing input CMAQ emission data to 5, 4, or 3 significant digits, simulation runtime slightly improved, disk space significantly improved, and model accuracy remained relatively unchanged with respect to the unaltered emission data CMAQ simulation.

## Wildfire Emissions and Air Quality

### Adding On-Line Photolysis Calculations to a 2D Lagrangian Model of Smoke Plume Chemistry to Investigate In-Plume Gradients

Matthew Alvarado
Author(s):

Matthew J. Alvarado[1], Marikate Mountain[1], and Archana Dayalu[1]

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Presenter(s): Matthew J. Alvarado

Format: Poster

Short Description: Plume-scale process models allow for explicit simulation and examination of the chemical and physical transformations of trace gases and aerosols within biomass burning smoke plumes, and they may be used to develop parameterizations of this aging process for coarser grid-scale models. One challenge for plume-scale models is to account for the horizontal and vertical gradients in smoke chemistry caused by differences in concentrations and photolysis rates within the plume. Here we present an update to the 2D Lagrangian plume-scale process model SAM-ASP to incorporate on-line photolysis calculations using the fast version of the Tropospheric Ultraviolet and Visible (TUV) aerosol model. The photolysis calculations are fully coupled to the aerosol concentrations within SAM-ASP to account for the impact of the changing aerosol properties on photolysis rates, and thus ozone and secondary organic aerosol chemistry, within the plume. We describe the coupled model and show some initial simulations of the impact of the more realistic photolysis on the plume chemistry.