Air Quality Research Abstracts

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1. Thermochemical properties of mono-ethanolamine salts to assess the impact of carbon capture on particulate matter pollution

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The use of mono-ethanolamine (MEA) for scrubbing of carbon dioxide from combustion flue gases may become the dominant technology for carbon capture by 2030. The widespread implementation of this technology will result in emissions of MEA to the environment that may increase the loading and modify the properties of atmospheric aerosols. The increase in aerosol concentration may hinder re-designation of the New Jersey portions of two multi-state fine particulate matter nonattainment areas to attainment. We have utilized combined experimental and computational aerosol microphysics approaches to derive thermodynamic properties of MEA sulfate and carboxylate salts, potentially the dominant forms of MEA in atmospheric particles. The derived saturation vapor pressures, vaporization enthalpies, surface free energies, and hygroscopicities are used to evaluate the role of MAE in the aerosol and haze formation. The stability and haze forming potential of MAE salts depend strongly on the chemical nature of the acid counterpart. The data can be incorporated in air quality models to assess potential environmental impacts of the MEA-based carbon capture technology.

2. Developing an Updated Statistical Ozone Model for Operational Air Quality Forecasting in the Philadelphia Metropolitan Area

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An updated statistical linear regression ozone model was developed to aid air quality forecasters in generating accurate operational ozone forecasts for the Philadelphia, Pennsylvania metropolitan area. The model calculates a maximum 8-hour average ozone mixing ratio in parts per billion (ppb) that can be used as forecast guidance for “tomorrow’s” operational ozone forecast. A statistical ozone model was previously utilized in Philadelphia, but it was discontinued in 2011 since a steady decline in emissions of ozone precursors associated with the NOx SIP rule made the model, trained on data prior to 2003, progressively less skillful. Recent stabilization of emissions across the Mid-Atlantic region has provided an opportunity to update the statistical ozone model. The foundation of the model is a historical dataset of over 60 key parameters for the period 2004–2014, which were selected based on local climatology and

atmospheric chemistry. A series of rejections and transformations were made to the historical dataset using the SYSTAT general purpose statistical software program to determine the 20 variables that were most highly correlated with observed maximum 8-hour average ozone. The regression model includes the 7 parameters from the subset of 20 that gave the most highly correlated and consistent predictions of maximum 8-hour average ozone mixing ratios. These 7 parameters include predicted and observed data, such as maximum air temperature, surface wind speed, and today's maximum observed ozone. The model will be tested during the 2015 summer ozone season to determine its forecast skill in an operational setting.

3. Modeling the Impact of Nanotechnology-based Diesel Fuel Additives on Air Quality and on Population Exposures to Diesel Exhaust Particles and Co-Occurring Pollutants

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Diesel engines are major contributors to ambient airborne fine and ultrafine particulate matter, that has significant inhalation potential for human populations, and is associated with a wide range of adverse health effects. A critical issue that requires study is the introduction of new nanotechnology-based diesel fuel additives, that are currently being increasingly used in various countries across the world as combustion promoters in diesel engines. The impact of these additives on both air quality and on associated exposures of populations to Diesel Exhaust particles (DEPs) and to co-occurring air pollutants, including airborne nanoparticles from constituents of the fuel additives, needs to be thoroughly characterized. This work presents a new set of modeling tools, developed as components of the Prioritization/Ranking of Toxic Exposures with GIS Extension (PRoTEGE) system, to support characterization of population exposures, intakes and uptakes DEPs. Case studies compare exposures to DEPs and co-occurring pollutants for situations without fuel additives and situations involving the use of different amounts of nano-ceria based fuel additives as combustion promoters. Local estimates of ambient DEP distributions across the contiguous United States (CONUS), developed through the most recent USEPA National Air Toxics Assessment (NATA), are combined here with new data on combustion rates, emission rates and particle size distributions of DEPs that are produced from combustion with nano-ceria additives. These new data on diesel combustion were collected by our team collaborators within the "Risk Assessment for Manufactured Nanoparticles Used in Consumer Products" (RAMNUC) project, and used to adjust simulation estimates of ambient

DEP concentrations across the CONUS. Human exposure characterization further employed intake fraction methods to characterize exposed populations and to to assess differences associated with gender, age, demographics, and CONUS climate regions. Resulting estimates of population intake incorporate and characterize uncertainties associated with the geographic distribution patterns of airborne DEPs as well as with inherent inter-individual variabilities in physiology, location and activity patterns. Distributions of inhalation intakes are then used to calculate biologically-relevant uptakes and target tissue doses through mechanistically-based gender and age-specific respiratory dosimetry modeling.

4. Assessing Peaking Unit Contributions to Air Quality and Related Societal Costs in the PJM Electricity Sector

Caroline M. Farkas, Michael D. Moeller, Frank A. Felder, Kirk R. Baker, Mark Rodgers, Annmarie G. Carlton

Electric generating units (EGUs) that operate under an average of 10% of their capacity over a three year period, and 20% under their capacity each of those three years is considered by the EPA to be a peaking unit[64]. Peaking units are used on high energy demand days (HEDDs), typically during the afternoon in the summer months, to supply extra electricity to high density areas. Generally speaking, these EGUs tend to be older, less efficient, and higher emitters of pollutants such as SO_2, NO_X, and PM than comparable base-load units. We explore the hypothesis that although peaking unit emissions are infrequent and sporadic, they contribute significantly to regional air quality when they are used, in particular on peak summer days when air quality is most likely to be poorest. In this work we investigate the population-weighted exposure and societal economic costs of peaking unit pollution during a heat wave stagnation event during July 2006 in the PJM region (regional electricity transmission organization) of the U.S

5. Temporalization of Peak Electric Generation PM Emissions during High Energy Demand Days

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Underprediction of peak ambient pollution by air quality models hinders development of effective strategies to protect health and welfare. EPA's Community Multiscale Air Quality (CMAQ) model routinely underpredicts peak ozone and fine particulate matter ($PM_{2.5}$) concentrations. Temporal mis-allocation of electricity sector emissions contributes to this modeling deficiency. Hourly emissions are created for CMAQ using temporal profiles applied to annual emission totals unless a source is matched to a continuous emissions monitor (CEM) in the National Emissions Inventory (NEI). More than 46% of CEMs in the Pennsylvania-New Jersey-Maryland (PJM) electricity market and 45% nationally are unmatched in the 2008 NEI. For July 2006, a U.S. heat wave with high electricity demand, peak electric sector emissions, and elevated ambient $PM_{2.5}$ mass, we match hourly emissions for 267 CEM/NEI pairs in PJM (approximately 65% and 15% of unmatched CEMs in PJM and nationwide) using state permits, electricity dispatch modeling and CEMs. Hourly emissions for individual facilities can differ up to 154% during the simulation when measurement data is used rather than default temporalization values. Maximum CMAQ $PM_{2.5}$ mass, sulfate, and elemental carbon predictions increase up to 83%, 103%, and 310%, at the surface and 51%, 75%, and 38% aloft (800 mb), respectively.

6. Modeling Pulmonary Effects of Inhaled Fine and Ultrafine Particles: A Multiscale Systems Biology Approach

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Inhalation of fine and ultrafine airborne particles represents a ubiquitous environmental health problem, in both indoor and outdoor settings, with situations correspondingly exacerbated by the presence of smokers or the use of gas cooking stoves indoors and by conditions of heave vehicular traffic outdoors. Once inhaled, fine and ultrafine particles are arrested at various stages of the respiratory system, via mechanisms protecting the human organism against such xenobiotics. However, most of the airborne ultrafine particles (UFPs), including (a) by-products of fossil fuel combustion and of atmospheric physicochemical transformation processes and (b) manufactured nanoparticles released during their manufacturing, use, or disposal, can reach the deeper regions of the lung and interact with alveolar cells and the bronchoalveolar fluid. These particles are thus known to induce oxidative stress, immune responses, and to eventually cause changes in lung function. Furthermore, chronic changes in lung function have been related to cardiovascular effects in humans. A multiscale computational model was developed for the physiologically and biochemically based mechanistic simulation of toxicodynamic processes associated with UFP inhalation. The model forms part of an integrative systems biology framework that is designed to be iteratively refined with new data from various *in vitro* and *in vivo* measurements. The model deals with the pulmonary tissue with explicit focus on the various cells and surfactant chemicals that regulate the process of breathing and respond to xenobiotics within the respiratory system. Toxicodynamic modules were developed to account for processes occurring at multiple scales, linking cellular and surfactant dynamics as a result of particle exposure and linking the cellular level effects to tissue level lung function changes. Particle properties such as size, surface chemistry, and zeta potential were explicitly included as parameters in the model. The model can provide significant insights into potential health impacts

of particulate matter inhalation, taking into account age and existing pulmonary conditions for specific individuals and for both general and sensitive populations.

7. Evaluation of regulatory and research models for estimating traffic-related ultrafine particles near an urban highway

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Numerous models are available for predicting air pollution levels near busy roads for epidemiological studies and policy-making. Our goal was to evaluate the ability of freely available regulatory (CALINE 4, AERMOD) and research (R-LINE, QUIC, regression) models to predict the hourly number concentration of ultrafine particles (PNC) – a major constituent of motor vehicle exhaust emissions – in a residential neighborhood (Somerville) and an urban center (Chinatown) near Interstate 93 in MA, USA. Traffic emission factors, meteorological data and highway traffic volumes were obtained from local and state sources. We measured PNC for model evaluation with a mobile laboratory during 2009-2010 in Somerville and 2011-2012 in Chinatown. Models were evaluated for hot and cold temperatures, and for parallel and perpendicular wind directions relative to the highway. Agreement between measurements and predictions was assessed with correlations (R^2), fraction within a factor of two (FAC2), normalized mean square error (NMSE), and fractional bias (FB). In Somerville, all statistics were typically within acceptable limits (FAC2 >45%, NMSE <0.2, FB <1, R^2 >0.6). An exception was for parallel winds on a cold day, where the R^2 was ≤0.5 for all models. All models predicted near-highway concentration gradients discernible above background extending 100-200 m from the roadway. Inter-model differences were generally within a factor of two and smaller than the noise in the measurements. Model performance in Chinatown was worse, mainly because of the contribution of local traffic to background PNC. Improving measurements and regional PNC estimates may be more important than model choice in urban areas.

8. Modeling Inhalation Exposures of US Populations to Air Pollutants of Emerging Concern: Case Studies - Nanoparticles in Consumer Products

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The number of chemicals manufactured or processed in the US is steadily increasing, with over 84,000 compounds currently being listed in the inventory of the Toxic Substances Control Act (TSCA) and between 700 to 900 new ones being added annually. At the same time, new uses and formulations are introduced for many “old” chemicals, an example being new Engineered Nanomaterials (ENMs) developed from carbon, metals, polymers, etc., and incorporated in many consumer and high technology products. These facts make it critical to understand and quantify the potential for exposures to both new and old “Chemicals of Emerging Concern” (COECs) during their Life Cycles, from their production to their use and then following their disposal. In particular, human exposures to Manufactured Nanoparticles (MNPs) are rapidly increasing as use of MNPs in consumer products becomes widespread. This work presents a new set of modeling tools, developed as components of the Prioritization/Ranking of Toxic Exposures with GIS Extension (PRoTEGE) system to support characterization of population exposures, intakes, uptakes, as well as associated potential risks from established or hypothesized Adverse Outcome Pathways (AOPs) involving a wide range of COECs. Example case studies focus on silver MNPs that are the engineered nanomaterials most widely used in consumer products, having the potential to become significant contributors to both indoor and outdoor air pollutant mixtures. Modules for simulating ambient and indoor settings have been developed, utilizing (a) available production, usage, and properties databases on MNPs and (b) new data on size distributions of MNPs in consumer products. Modeling of environmental and microenvironmental levels of MNPs employs material balances combined with product Life Cycle Analysis (LCA) to account for manufacturing, transport, usage, disposal, etc. processes. Human exposure characterization further employs intake fraction methods combined with Life Stage Analysis (LSA) for potentially exposed populations, to assess differences associated with gender, age, and demographics. Resulting population intake estimates incorporate and characterize uncertainties in the data associated with the production, market penetration, and usage of MNPs as well as inherent inter-individual variabilities in physiology and activity patterns. Distributions of inhalation intakes within the exposed populations are then used to calculate biologically-relevant uptakes and target tissue doses through a customized version of the human airway Multiple-Path Particle Dosimetry (MPPD) model.

9. Modeling Climate Change Effects on Spatiotemporal Dynamics of Emissions and Airborne Concentrations of Allergenic Pollens in a "One Atmosphere" Framework

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Allergenic pollen has been an increasing concern under the changing climate because its synergism with air pollutants to cause allergic airway disease. A modeling system incorporating pollen emission and transport has been developed to simulate the spatiotemporal distributions of allergenic pollen of representative trees, weeds and grasses, and common air pollutants such as ozone and particulate matter. The pollen emission module incorporated major physical processes such as direct emission and re-suspension of pollen particles and considering effects of meteorological parameters such as ground surface temperature, friction velocity and humidity, etc. Using the emission module, spatiotemporal distributions of pollen and air pollutants was simulated via the combined application of the Weather Research and Forecasting (WRF) model and an adapted version of the CMAQ model.

The estimated mean start dates and season length for birch, oak, ragweed, mugwort and grass pollen season in 1994-2010 are mostly within 0 to 6 days of the corresponding observations for the majority of the National Allergy Bureau (NAB) monitoring stations across the contiguous United States (CONUS). The simulated spatially resolved maps for onset and duration of allergenic pollen season in the CONUS are consistent with the long term observations. Changes of pollen season timing and airborne levels depend on latitude, and are associated with changes of growing degree days, frost free days, and precipitation. These changes are likely due to recent climate change and particularly the enhanced warming and precipitation at higher latitudes in the CONUS.