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New monitoring technologies have now permitted the measurement of a variety of chemical species in airborne particulate matter with time resolution as high as 10 min to 1 h. There are still species that are measured with longer integration periods such as several hours to a day. These data from different measurement methods produce a data set of mixed time resolution. Traditional eigenvalue-based methods used in solving multivariate receptor models are unable to analyze this kind of data set since these data cannot form a simple matrix. Averaging the high time resolution data or interpolating the low time resolution data to produce data on the same time schedule is not acceptable. The former method loses valuable temporal information and the latter produces unreliable high resolution series because of the invalid assumption of temporal smoothness. In the present work, a solution to the problem of multiple sampling time intervals has been developed and tested. Each data value is used in its original time schedule without averaging or interpolation and the source contributions are averaged to the corresponding sampling interval. For data with the highest time resolution, the contributions are not actually averaged. The contribution series are smoothed by regularization auxiliary equations especially for sources containing very little high resolution species. This new model will be explored using data from the Pittsburgh supersite. (C) 2004 Elsevier Ltd. All rights reserved.

215 Zhou, L. M., **P. K. Hopke**, et al. (2004). "Comparison of two trajectory based models for locating particle sources for two rural New York sites." Atmospheric Environment **38**(13): 1955-1963.

Two back trajectory-based statistical models, simplified quantitative transport bias analysis and residence-time weighted concentrations (RTWC) have been compared for their capabilities of identifying likely locations of source emissions contributing to observed particle concentrations at Potsdam and Stockton, New York. Quantitative transport bias analysis (QTBA) attempts to take into account the distribution of concentrations around the directions of the back trajectories. In full QTBA approach, deposition processes (wet and dry) are also considered. Simplified QTBA omits the consideration of deposition. It is best used with multiple site data. Similarly the RTWC approach uses concentrations measured at different sites along with the back trajectories to distribute the concentration contributions across the spatial domain of the trajectories. In this study, these models are used in combination with the source contribution values obtained by the previous positive matrix factorization analysis of particle composition data from Potsdam and Stockton. The six common sources for the two sites, sulfate, soil, zinc smelter, nitrate, wood smoke and copper smelter were analyzed. The results of the two methods are consistent and locate large and clearly defined sources well. RTWC approach can find more minor sources but may also give unrealistic estimations of the source locations. (C) 2004 Elsevier Ltd. All rights reserved.

214 Zhou, L., E. Kim, et al. (2004). "Mining Airborne Particulate Size Distribution Data by Positive Matrix Factorization." Journal of Geophysical Research-Atmospheres **110**: Art. No. D07S19.

213 Zhou, L., E. Kim, et al. (2004). "Advanced Factor Analysis on Pittsburg Particle Size Distribution Data." Aerosol Science and Technology **38**(Supplement 1): 118-132.

212 Zhou, L., **P. K. Hopke**, et al. (2004). "Advanced Factor Analysis for Multiple Time Resolution Aerosol Composition Data." Atmospheric Environment **38**: 4909-4920.

210 Zhou, H., B. P. Farrell, et al. (2004). "Nanopatterns of Poly(styrene-block-butyl acrylate) Black Copolymer Brushes of the Surface of Exfoliated and Intercalated Clay Layers." Polymer **45**: 4473-4481.

209 Zhou, H., S. D. Argoti, et al. (2004). "Polymer- Silicate Nanocomposites Produced by in situ Atom Transfer Radical Polymerization." J. Polym. Sci Part A: Polym. Chem. **42**: 916-924.

208 Zhao, W. X. and **P. K. Hopke** (2004). "Source apportionment for ambient particles in the San Gorgonio wilderness." Atmospheric Environment **38**(35): 5901-5910.

Recent factor analysis studies of data from the Interagency Monitoring of Protected Visual Environments (IMPROVE) network in which the separate carbon fractions have been used have found factors that have been assigned to emissions from diesel and spark-ignition vehicles. In this study, positive matrix factorization (PMF) was applied to the chemical composition of PM_{2.5} collected at the San Gorgonio IMPROVE site, downwind of the Los Angeles area. Therefore, in addition to the general identification of the possible emission sources of the ambient aerosols at this site, this study explicitly examines the feasibility of separating diesel emission from gasoline emission using the organic and elemental carbon (OC/EC) thermal fractions. The results suggest the feasibility of separating diesel/gasoline emission profiles based on the species concentration data including the OC/EC fractions. Also in the analysis of these data, two crustal factors were identified with one being associated with local suspended soil and the other being associated with transported Asian desert dust. The other sources include secondary sulfate/OC, secondary nitrate, and reacted sea salt. (C) 2004 Elsevier Ltd. All rights reserved.

207 Tasdemir, Y., N. Vardar, et al. (2004). "Concentrations and Gas/Particle Partitioning of PCBs in Chicago." Environ. Poll. **131**: 35-44.

206 Tasdemir, Y., M. Odabasi, et al. (2004). "Dry Deposition Fluxes and Velocities of Polychlorinated Biphenyls (PCBs) Associated with Particles." Atmospheric Environment **38**: 2447-2456.

205 Smorodin, V. Y. and **P. K. Hopke** (2004). "Condensation activation and nucleation on heterogeneous aerosol nanoparticles." Journal of Physical Chemistry B **108**(26): 9147-9157.

Measurements of heterogeneous nucleation of several different compounds on different composition nuclei have shown several distinct patterns of nucleation and growth. Some of the specific behaviors for condensation activation of heterophilic (energetically nonuniform) aerosol nanoparticles have been theoretically analyzed based on a model of double-barrier nucleation (DBN) with an emphasis on scale and supersaturation effects. A new "semiempirical" method for collecting nucleation data from the condensation size spectrum of CN was developed. These results have been used to provide a qualitative interpretation of experimental data on the transformation of the initial size distribution spectrum of nanoparticles in a turbulent mixing condensation nuclei counter.

204 Schmit, R. F., M. N. Glauser, et al. (2004). "Flow and turbulence conditions in the wake of a H-section in cross flow." Journal of Fluids and Structures **19**(2): 193-207.

Both steady and unsteady wakes of a torsional aeroelastic wind energy converter are examined. The converter consists of a H-section prism with attached pendulums for adjusting the natural frequency of the system. To provide an understanding of the wake characteristics of the device, a particle image velocimetry system was used to measure the mean and fluctuating velocity fields from which various single-point statistics were calculated. For the steady case, wake profiles were obtained at angles of attack from -30degrees to +30degrees (at 5degrees intervals) with the H-section fixed at each angle. In the unsteady case, the H-section was free to vibrate due to flow-structure interaction and a torsional vibration was produced with angles of attack from -30degrees to +30degrees. Turbulent wake profiles obtained for the H-section at fixed angles of attack are compared with the oscillating cases and the differences between the various single-point turbulence velocity statistics are discussed. The presented results indicate that the overall dynamic wake deficit for the oscillating case is less than the static wake deficit. Furthermore, the dynamic wake deficit, which is about 20% of U_{∞} is dispersed across the entire section; whereas, the static wake is concentrated around the trailing edge side of the converter. (C) 2003 Elsevier Ltd. All rights reserved.

203 **Rossner, A.**, S. D. Warner, et al. (2004). "Performance of small evacuated canisters equipped with a novel flow controller for the collection of personal air samples." Journal of Occupational and Environmental Hygiene **1**(3): 173-181.

Small evacuated canisters have become more common in industrial hygiene personal sampling in recent years. The smaller canisters necessitate a low flow rate to ensure a full-shift air sample can be collected. Evaluation of small evacuated canisters compared to sorbent sampling methods is essential to ensure that the canisters accurately monitor airborne contamination. This data, in a controlled environment, will provide practitioners with valuable reference information when considering air-sampling campaigns. Six 300-mL evacuated canisters were used to collect 6-hour breathing zone samples of styrene on volunteers in a large exposure chamber. The canisters were specially designed with a capillary flow controller developed at McGill University in the mid-1990s. Based on the geometry of the capillary the airflow into the canisters was controlled to a low flow rate, similar to 0.3 mL/min. This low sampling flow rate allowed for the use of small-volume canisters as personal samplers to collect styrene vapors. Charcoal tubes and diffusive badges were simultaneously used to collect side-by-side samples for comparison. In addition, an online gas chromatograph (GC) documented the concentration in the chamber throughout the duration of the exposure. The three methods did not disclose any significant statistical difference when compared to the online GC values and to each other. In addition, linear regression analysis between the charcoal tubes and the canisters resulted in a correlation ($R^2 > 0.95$). An evaluation of the bias and precision (overall uncertainty) of the capillary-canister method, charcoal tubes, and diffusive badges found them to be within criteria established by European Committee for Standardization 482. The results indicate that the capillary-canister sampling device can be an acceptable alternative to sorbent samplers as a personal sampler providing reliable results that are representative of exposures.

202 **Rossner, A.** and J. P. Farant (2004). "A novel personal air sampling device for collecting volatile organic compounds: A comparison to charcoal tubes and diffusive badges." Journal of Occupational and Environmental Hygiene **1**(2): 69-81.

Evacuated canisters have been used for many years to collect ambient air samples for gases and vapors. Recently, significant interest has arisen in using evacuated canisters for personal breathing zone sampling as an alternative to sorbent sampling. A novel flow control device was designed and built at McGill University. The flow control device was designed to provide a very low flow rate, <0.5 mL/min, to allow a sample to be collected over an extended period of time. Previous experiments run at McGill have shown agreement between the mathematical and empirical models to predict flow rate. The flow control device combined with an evacuated canister (capillary flow control-canister) was used in a series of experiments to evaluate its performance against charcoal tubes and diffusive badges. Air samples of six volatile organic compounds were simultaneously collected in a chamber using the capillary flow control-canister, charcoal tubes, and diffusive badges. Five different concentrations of the six volatile organic compounds were evaluated. The results from the three sampling devices were compared to each other and to concentration values obtained using an online gas chromatograph (GC). Eighty-four samples of each method were collected for each of the six chemicals. Results indicate that the capillary flow control-canister device compares quite favorably to the online GC and to the charcoal tubes, $p > 0.05$ for most of the tests. The capillary flow control-canister was found to be more accurate for the compounds evaluated, easier to use, and easier to analyze than charcoal tubes and passive dosimeter badges.

201 Raymond, H. A., S. M. Yi, et al. (2004). "Dry Deposition of Reactive Nitrogen and Sulfur Containing Species in Remote Areas Using a Surrogate Surface Analysis Approach." Atmospheric Environment **38**(17): 2687-2697.

200 Ramadan, Z., **P. K. Hopke**, et al. (2004). "Application of PLS and Back Propagation Neural Networks for the Estimation of Soil Properties." Environmental Science & Technology(B108): 9147-9157.

199 **Powers, S. E.** and J. Dewaters (2004). "Creating Project-Based Experiences for University-K12 Partnerships." Proceedings of the Frontiers in Education Conference.

198 Popp, P. J., R. S. Gao, et al. (2004). "Nitric acid uptake on subtropical cirrus cloud particles." Journal of Geophysical Research-Atmospheres **109**: Art. No. D06302.

197 Paatero, P., **P. K. Hopke**, et al. (2005). "A Graphical Diagnostic Method For Assessing the Rotation In Factor Analytical Models Of Atmospheric Pollution." Atmospheric Environment **39**: 193-201.

196 Oliver Chang, M. C., **P. Hopke**, et al. (2004). "Measurement of Ultrafine Particle Size Distribution from Stationary Combustion Sources of Coal, Oil, and Gas." Journal of Air Waste Management Association **54**: 1494-1505.

195 Moument, N., S. M. Yi, et al. (2004). "Quantifying the Dry Deposition of Ammonia in Ammonia-Rich and Ammonia-Poor Environments Using a Surrogate Surface Approach." Atmospheric Environment **38**(17): 2677-2686.

194 Monsoori, Z., M. Saffar-Avval, et al. (2004). "Experimental Study of Turbulent Gas-Solid Heat Transfer in at Different Particle Temperatures." Experimental Thermal and Fluid Science **28**: 655-665.

193 **McLaughlin, J.**, S. V. Sreenivasan, et al. (2004). "Rapid human-assisted creation of bounding models for obstacle avoidance in construction." Computer Aided Civil and Infrastructure Engineering **19**(1): 3-15.

192 McKinney, K. A., P. O. Wennberg, et al. (2004). "Trajectory studies of large HNO₃-containing PSC particles in the Arctic: Evidence for the role of NAT." Geophysical Research Letters **31**(5): Art. No. L05110.

Large (5 to > 20 μm diameter) nitric-acid-containing polar stratospheric cloud (PSC) particles were observed in the Arctic stratosphere during the winter of 1999 - 2000. We use a particle growth and sedimentation model to investigate the environment in which these particles grew and the likely phase of the largest particles. Particle trajectory calculations show that, while simulated nitric acid dihydrate (NAD) particle sizes are significantly smaller than the observed maximum particle sizes, nitric acid trihydrate (NAT) particle trajectories are consistent with the largest observed particle sizes.

191 McKay, R. M. L., G. S. Bullerjahn, et al. (2004). "Consideration of the bioavailability of iron in the North American Great Lakes: Development of novel approaches towards understanding iron biogeochemistry." Aquatic Ecosystem Health and Management(7): 1-16.

190 Mavliev, R., **P. K. Hopke**, et al. (2004). "Experimental studies of heterogeneous nucleation in the turbulent mixing condensation nuclei counter." Journal of Physical Chemistry B **108**(14): 4558-4564.

A method for varying the supersaturation in a turbulent mixing CNC has been used to examine heterogeneous nucleation of different compounds (working fluid) on various nuclei's compositions. Supersaturation was controlled by changing the vapor pressure of working fluid in nozzle flow, which was accomplished by saturating only a predetermined fraction of the flow while the keeping the total flow and temperature constant. This approach allows the partial pressure of the working fluid to be varied while maintaining a constant flow structure and temperature field. Experimental results characterizing the initial stages of heterogeneous nucleation are presented for NaCl, KCl, AgCl, and Ag particles. Heterogeneous nucleation was examined at various pressures of dibutylphthalate, octadecane, octadecanol, and octadecanoic acid. For octadecanoic acid as the working fluid, the size distribution of the grown particles is unimodal with the size increasing with increasing pressure of the working fluid. For the other working fluids, the initial size distribution splits into a bimodal distribution with one mode approximately the same as the initial distribution and a larger sized mode that grows with increasing pressure of the condensing vapor. For NaCl and octadecane and octadecanol, the initial unimodal size distribution splits into a trimodal size distribution.

189 Marzocca, P., L. Librescu, et al. (2004). "Nonlinear Open/Closed Loop Aeroelastic Analysis of Airfoils via Volterra Series." AIAA Journal **42**(2): 673-686.

188 Li, Z., **P. K. Hopke**, et al. (2004). "Sources of fine particle composition in New York City." Atmospheric Environment **38**(38): 6521-6529.

Fine particle composition data from samples collected at Queens College during July 2001 were studied using positive matrix factorization (PMF). The sampling systems are an integrated filter sampler with a 6-h sampling time interval, an aerosol mass spectrometer (AMS) with a 10-min sampling time interval and a particle-into-liquid sampler with ion chromatography (PILS-IC) with 15-min sampling time interval. The data from the AMS and the PILS-IC were aggregated to 6-h average values for the PMF calculation. Sulfate, ammonium, and nitrate data were compared among the different instruments. The PMF method uses the estimated errors in the data to provide optimal point-by-point weighting and permits efficient treatment of missing and below detection limit values. Six source categories were resolved SO₄²⁻; from the data. They are: secondary sulfate with high concentration 4 secondary nitrate with the presence of high concentration NO₃⁻; motor vehicle emissions with high concentration of OC and Zn; road dust represented by Al, Ca, Fe, and K; sea salt with high concentration of Cl and Na; and oil combustion marked by the presence of Ni and V. (C) 2004 Elsevier Ltd. All rights reserved.

187 Kvasnak, W., **G. Ahmadi**, et al. (2004). "An Engineering Model for the Fuel Spray Formation of Deforming Droplets." Atomization and Spray **14**: 289-339.

186 Kittelson, D. B., W. F. Watts, et al. (2004). "On-road exposure to highway aerosols. 1. Aerosol and gas measurements." Inhalation Toxicology **16**: 31-39.

On-road experiments were conducted to determine the sensitivities of rats to real-world aerosol. This article summarizes the on-road aerosol and gas measurements and provides background information for the companion paper on the rat exposures. Measurements were carried out over 10 days, 6 h/day, driving a route from Rochester to Buffalo. Aerosol instrumentation used in this study included two scanning mobility particle sizers; (SMPS) to determine the aerosol size distribution from 10 to 300 nm, 2 stand-alone condensation particle counters to determine the total aerosol number concentration, and an electrical aerosol detector to determine the aerosol length concentration. A thermal denuder (TD) was used with one of the SMPS instruments to determine the size distribution of the non-volatile fraction. Filter samples were collected and analyzed for elemental carbon, and gas analyzers measured ambient levels of CO, CO₂, and NO. Average daily total aerosol number concentration ranged from 200,000 to 560,000 particles/cm³. Past studies on urban highways have measured total number concentrations ranging between 10⁴ and 10⁶ particles/cm³. The average daily NO concentration ranged from 0.10 to 0.24 ppm and the corresponding CO₂ concentration ranged from 400 to 420 ppm. The average daily geometric number mean particle size determined by the SMPS ranged from 15 to 20 nm. The TD reduced the average SMPS number concentration between 87 and 95% and the SMPS volume between 54 and 83%, suggesting that most of the particles consisted of volatile material. The TD also increased the geometric number mean diameter from 15 to 20 nm to 30 to 40 nm.

185 Kim, E., **P. K. Hopke**, et al. (2004). "Analysis of Particle Size Distributions using UNMIX and Positive Matrix Factorization." Environmental Science & Technology(38): 202-209.

184 Kim, E., **P. K. Hopke**, et al. (2004). "Factor analysis of Seattle fine particles." Aerosol Science and Technology **38**(7): 724-738.

Ambient particulate matter less than or equal to 2.5 μm in aerodynamic diameter (PM_{2.5}) samples were collected at a centrally located urban monitoring site in Seattle, WA on Wednesdays and Saturdays using Interagency Monitoring of Protected Visual Environments (IMPROVE) samplers. Particulate carbon was analyzed using the thermal optical reflectance method that divides carbon into four organic carbon (OC), pyrolyzed organic carbon (OP), and three elemental carbon (EC) fractions. A total of 384 samples that were analyzed for 36 species were collected between March 1996 and February 2000. These data were analyzed with the standard factor analysis model using the Multilinear Engine (ME). Eleven sources were identified: sulfate-rich secondary aerosol (26%), diesel emissions (22%), wood smoke (16%), gasoline vehicle (10%), aged sea salt (8%), airborne soil (7%), nitrate-rich secondary aerosol (5%), sea salt (4%), oil combustion (3%), paper mill (2%), and ferrous metal processing (1%). The use of ME provided enhanced source separations, including the nitrate-rich aerosol source and two industrial sources that were not deduced in a previous PMF₂ solution. Conditional probability functions using surface wind data and resolved source contributions aid in the identifications of local sources. Potential source contribution function analysis tentatively shows southern Washington State, along the Canadian border, and southwestern British Columbia, Canada as the possible source areas and pathways that give rise to the high contribution of the sulfate-rich secondary aerosol.

183 Kim, E., **P. K. Hopke**, et al. (2004). "Analysis of ambient particle size distributions using unmix and positive matrix factorization." Environmental Science & Technology **38**(1): 202-209.

Hourly averaged particle size distributions measured at a centrally located urban site in Seattle were analyzed through the application of bilinear positive matrix factorization (PMF) and Unmix to study underlying size distributions and their daily patterns. A total of 1051 samples each with 16 size intervals from 20 to 400 nm were obtained from a differential mobility particle sizer operating between December 2000 and February 2001. Both PMF and Unmix identify four similar underlying factors in the size distributions. Factor 1 is an accumulation mode particle size spectrum that shows a regular nocturnal pattern, and factor 2 is a larger particle distribution. Factor 3 is assigned as a traffic-related particle distribution, based on its correlations with accompanying gas-phase measurements, and has a regular weekday-high rush-hour pattern. Factor 4 is a traffic-related particle size distribution that has a regular rush-hour pattern on weekdays as well as weekends. Conditional probability functions (CPF) were computed using wind profiles and factor contributions. The results of CPF analysis suggest that these factors are correlated with surrounding particle sources of wood burning, secondary aerosol, diesel emissions, and motor vehicle emissions.

182 Kim, E., **P. K. Hopke**, et al. (2004). "Improving source identification of Atlanta aerosol using temperature resolved carbon fractions in positive matrix factorization." Atmospheric Environment **38**(20): 3349-3362.

Daily integrated PM_{2.5} (particulate matter less than or equal to 2.5 μm in aerodynamic diameter) composition data including eight individual carbon fractions collected at the Jefferson Street monitoring site in Atlanta were analyzed with positive matrix factorization (PMF). Particulate carbon was analyzed using the thermal optical reflectance method that divides carbon into four organic carbon (OC), pyrolyzed organic carbon (OP), and three elemental carbon (EC) fractions. A total of 529 samples and 28 variables were measured between August 1998 and August 2000. PMF identified 11 sources in this study: sulfate-rich secondary aerosol I (50%), on-road diesel emissions (11%), nitrate-rich secondary aerosol (9%), wood smoke (7%), gasoline vehicle (6%), sulfate-rich secondary aerosol II (6%), metal processing (3%), airborne soil (3%), railroad traffic (3%), cement kiln/carbon-rich (2%), and bus maintenance facility/highway traffic (2%). Differences from previous studies using only the traditional OC and EC data (J. Air Waste Manag. Assoc. 53(2003a)731; Atmos Environ. (2003b)) include four traffic-related combustion sources (gasoline vehicle, on-road diesel, railroad, and bus maintenance facility) containing carbon fractions whose abundances were different between the various sources. This study indicates that the temperature resolved fractional carbon data can be utilized to enhance source apportionment study, especially with respect to the separation of diesel emissions from gasoline vehicle sources. Conditional probability functions using surface wind data and identified source contributions aid the identifications of local point sources. (C) 2004 Elsevier Ltd. All rights reserved.

181 Kim, E. and **P. K. Hopke** (2004). "Source apportionment of fine particles in Washington, DC, utilizing temperature-resolved carbon fractions." Journal of The Air & Waste Management Association **54**(7): 773-785.

Integrated ambient particulate matter less than or equal to 2.5 μm aerodynamic diameter (PM_{2.5}) samples were collected at a centrally located urban monitoring site in Washington, DC, on Wednesdays and Saturdays using Interagency Monitoring of Protected Visual Environments samplers. Particulate carbon was analyzed using the thermal optical reflectance method that divides carbon into four organic carbon fractions, pyrolyzed organic carbon, and three elemental carbon fractions. A total of 35 variables measured in 718 samples collected between August 1988 and December 1997 were analyzed. The data were analyzed using Positive Matrix Factorization and 10 sources were identified: sulfate (SO₄²⁻)-rich secondary aerosol I (43%), gasoline vehicle (21%), SO₄²⁻-rich secondary aerosol II (11%), nitrate-rich secondary aerosol (9%), SO₄²⁻-rich secondary aerosol III (6%), incinerator (4%), aged sea salt (2%), airborne soil (2%), diesel emissions (2%), and oil combustion (2%). In contrast to a previous study that included only total organic carbon and elemental carbon fractions, motor vehicles were separated into fractions identified as gasoline vehicle and diesel emissions containing carbon fractions whose abundances were different between the two sources. This study indicates that the temperature-resolved carbon fraction data can be utilized to enhance source apportionment, especially with respect to the separation of diesel emissions from gasoline vehicle sources. Conditional probability functions using surface wind data and deduced source contributions aid in the identifications of local sources.

180 Kim, E. and **P. K. Hopke** (2004). "Improving source identification of fine particles in a rural northeastern US area utilizing temperature-resolved carbon fractions." Journal of Geophysical Research-Atmospheres **109**(D9).

Integrated, 24-hour, ambient PM_{2.5} (particulate matter <2.5 μm in aerodynamic diameter) samples were collected at a rural monitoring site in Brigantine, New Jersey, on Wednesdays and Saturdays using Interagency Monitoring of Protected Visual Environments (IMPROVE) samplers. Particulate carbon was analyzed using the thermal optical reflectance method, which divides carbon into four organic carbon (OC), pyrolyzed organic carbon (OP), and three elemental carbon (EC) fractions. A total of 910 samples and 36 variables collected between March 1992 and May 2001 were analyzed using positive matrix factorization, and 11 sources were identified: sulfate-rich secondary aerosol I (48%), gasoline vehicle (13%), aged sea salt (8%), sulfate-rich secondary aerosol II (7%), nitrate-rich secondary aerosol (6%), sulfate-rich secondary aerosol III (5%), sea salt (4%), airborne soil (4%), diesel emission (3%), incinerator (2%), and oil combustion (1%). Temperature-resolved carbon fractions enhanced source separations including three sulfate-rich secondary aerosols and two traffic-related sources that had different abundances of carbon fractions different between sources. Conditional probability functions using surface wind data and deduced source contributions aid in the identification of local sources. Potential source contribution function (PSCF) analysis shows the regional influence of sulfate-rich secondary aerosols. Backward trajectories indicate that the highly elevated airborne soil impacts at the monitoring site were likely caused by either Asian or Sahara dust storms.

179 Kim, E. and **P. K. Hopke** (2004). "Comparison between conditional probability function and nonparametric regression for fine particle source directions." Atmospheric Environment **38**(28): 4667-4673.

The objective of this study is to examine the use of conditional probability function (CPF) and nonparametric regression (NPR) to identify directions of PM_{2.5} (particulate matter less than or equal to 2.5 μm in aerodynamic diameter) sources using data collected from multiple monitoring sites across the US. NPR has been used on cyclohexane data from Houston, TX and correctly showed the direction of the source. In recent source apportionment studies using positive matrix factorization (PMF), ambient PM_{2.5} compositional data sets from 24-h integrated samples including eight individual carbon fractions collected at four monitoring sites, Atlanta, GA, Washington, DC, Brigantine, NJ, and Seattle, WA, were analyzed identifying 10-11 sources. To analyze local point source impacts from various wind directions, CPF and NPR were calculated using the source contributions estimated from PMF coupled with wind direction measured on site. The comparison between CPF and NPR demonstrated that both methods agreed well with the locations of known local point sources. CPF was simpler and easier to calculate than NPR. In contrast, NPR provided PM_{2.5} concentrations and associated uncertainties. This study indicates that both methods can be utilized to enhance source apportionment study of ambient PM_{2.5}. (C) 2004 Elsevier Ltd. All rights reserved.

178 Jiang, W. Y., **B. Helenbrook**, et al. (2004). "Inertialess instability of a two-layer liquid film flow." Physics of Fluids **16**(3): 652-663.

The physical mechanism of instability in a superposed two-layer liquid film flow down an incline plane is analyzed. If the layer adjacent to the wall is sufficiently thin and less viscous in certain two-layer parallel Newtonian liquid flows of the same density with an interface but without a free surface, the flows are stable with respect to long waves. This is the so-called "thin lubrication layer effect." However, when a free surface exists in the two-layered flow, the flow becomes unstable even when the Reynolds number approaches zero. Thus the thin-layer

lubrication effect is lost due to the presence of the free surface, and inertialess instability occurs. The reason for the loss of the lubrication effect and the mechanism of inertialess instability are explained by use of the energy budget in the mechanical energy equation. Contrary to the case of two-layer flows without a free surface, the flow with a free surface is stable if the layer adjacent to the solid wall is more viscous. The stabilization is achieved even without help from surface or interfacial tension. The mechanism of stabilization is also elucidated from an energy consideration. Navier-Stokes simulations are then performed to determine the effect of the layer viscosity ratio when nonlinear effects are included. (C) 2004 American Institute of Physics.

177 Jeong, C. H., D. W. Lee, et al. (2004). "Measurement of real-time PM_{2.5} mass, sulfate, and carbonaceous aerosols at the multiple monitoring sites." Atmospheric Environment **38**(31): 5247-5256.

Continuous or semi-continuous concentrations Of PM_{2.5}, organic carbon (OC), elemental carbon (EQ, black carbon (BC), and sulfate were measured during the summer of 2002 in two northeastern US cities, Rochester, New York and Philadelphia, Pennsylvania, for 2 and 4 weeks, respectively. Daily, 24-h samples were collected on quartz filter media for filter-based OC/EC and sulfate concentrations. The semi-continuous and daily integrated OC and EC were measured using a thermal-optical transmittance (TOT) method while BC was measured using an Aethalometer. Continuous sulfate concentrations were determined using a continuous sulfate analyzer and evaluated with daily filter-based sulfate data obtained using an ion chromatography (IC). In Rochester, semi-continuous OC and continuous sulfate accounted for more than 57% and 23%, respectively, of the PM_{2.5} mass with a mean of 16.2 $\mu\text{g m}^{-3}$ while OC and sulfate in Philadelphia accounted for 21% and 38% of the PM_{2.5} mass with a mean of 22.6 $\mu\text{g m}^{-3}$. The semi-continuous OC values in Philadelphia were somewhat correlated with real-time PM_{2.5} mass concentrations, whereas EC values were relatively lower and tended to be independent of the PM_{2.5} mass at the sites. Good agreement was found between the reconstructed mass based on chemical composition of the filter samples and the real-time PM_{2.5} mass at the sites. The continuous analysis and the filter-based IC analysis of sulfate was highly correlated. Comparing with result including the Canadian forest fire episode obtained with the filter-based analysis, the filter-based OC quite increased by the factor of four, whereas the average EC concentration increased by a factor of two. The non-denuded filter measurements of total carbon (TC) were always higher than the denuded semi-continuous TC values in Philadelphia. Significant differences were observed during a forest fire and haze events suggesting a positive artifact due to the adsorption of semi-volatile organic compounds. (C) 2004 Elsevier Ltd. All rights reserved.

176 Jeong, C. H., **P. K. Hopke**, et al. (2004). "The comparison between thermal-optical transmittance elemental carbon and Aethalometer black carbon measured at multiple monitoring sites." Atmospheric Environment **38**(31): 5193-5204.

Continuous and semi-continuous measurements of organic carbon (OC), elemental carbon (EC) and PM_{2.5} were performed during the summer of 2002 in Rochester, NY and Philadelphia, PA. During the study period in Philadelphia, high concentrations of wood smoke from a Canadian forest fire were transported to the monitoring site. Two-hour integrated thermal EC (EC)/optical EC (BCS) using a Sunset Lab OC/EC analyzer and continuous Aethalometer optical EC (BCA) using a two-wavelength Aethalometer were compared in various environments. The weekdays diurnal average for EC peaked during the morning rush-hour and was much higher than the value during weekends, whereas the OC results showed no diurnal

variation of OC during either weekdays or weekends at both sites. The diurnal variations of BCA were also strongly correlated with the rush-hour traffic. The correlation coefficient between EC and BCA in Rochester ($r(2) = 0.84$) was higher than in Philadelphia ($r(2) = 0.60$) while the BCA/EC slopes were 3.3 and 2.7 in Rochester and Philadelphia, respectively. The difference in the slopes indicates that the specific attenuation cross-section used for the optical carbon analysis depends on the physical and chemical characteristics of elemental carbon. During the Canadian forest fire, the BCA/EC slope dramatically dropped to 0.4 with a correlation coefficient of 0.60. The decrease of the proportionality between EC and BCA demonstrates the variability of the absorption coefficient. The level of UV absorbing organic compounds significantly increased during the fire aerosol episode suggesting the presence of abundant organic compounds in the forest fire smoke particles. (C) 2004 Elsevier Ltd. All rights reserved.

175 Jeong, C. H., **P. K. Hopke**, et al. (2004). "Characteristics of nucleation and growth events of ultrafine particles measured in Rochester, NY." Environmental Science & Technology **38**(7): 1933-1940.

Number concentrations and size distributions of particles in the size range of 0.010-0.500 μm were measured in Rochester, NY, from December 2001 to December 2002. The relationships between the number concentrations, gaseous pollutants, and meteorological parameters were examined during particle nucleation events. More than 70% of measured total number concentration was associated with ultrafine particles (UFP, 0.011-0.050 μm). Morning nucleation events typically peaking UFP number concentrations at around 08:00 were apparent in winter months with CO increases. These particles appear to be formed following direct emissions from motor vehicles during morning rush hour. There were also often observed increases in this smaller-sized range particles in the late afternoon during the afternoon rush hour, particularly in winter when the mixing heights remain lower than in summer. Strong afternoon nucleation events ($>30,000 \text{ cm}^{-3}$) peaking at around 13:00 were more likely to occur in spring and summer months. During the prominent nucleation events, peaks of SO₂ were strongly associated with the number concentrations of UFP, whereas there were no significant correlations between these events and PM_{2.5} and CO. Increased SO₂ concentrations were observed when the wind direction was northwesterly where three SO₂ sources were located. It is hypothesized that UFP formed during the events are sulfuric acid and water from the oxidation of SO₂. There were also a more limited number of nucleation events followed by particle growth up to approximately 0.1 μm over periods of up to 18 h. The nucleation and growth events tended to be common in spring months especially in April.

174 Huang, K. L., **T. M. Holsen**, et al. (2004). "The use of air fuel cell cathodes to remove contaminants from spent chromium plating solutions." Environmental Technology **25**(1): 39-49.

Results from experiments using an impregnation-reduction (I-R) Pt \ Nafion membrane electrode assembly (MEA) in an air fuel cell cathode to remove contaminants (Cu(II), Ni(II), and Fe(III)) from spent chromium electroplating baths are presented in this study. A platinum-carbon (Pt-C) \ Nafion MEA and a Pb planar cathode were also used for comparison. The average removal rates of Cu(II) and Ni(H) were almost the same (0.39 and 0.40 mM hr⁻¹) (or 0.117 and 0.12 mmol hr⁻¹), respectively) but higher than that of Fe(III) (0.16 mM hr⁻¹, or 0.048 mmol hr⁻¹) in accordance with the Nernst-Planck flux equation. The removal rates for the same cation were independent of the cathode used. The average removal rate of each impurity was approximately proportional to the product of its initial concentration and separator area/anolyte

volume ratio using Pb cathodes. Under constant current conditions the system using the Pt-C \ Nafion cathode needed the highest cell voltage, about 3 V more than needed for the system with the Pt \ Nafion cathode. The cell voltage required using the Pt \ Nafion cathode was similar to that using the conventional planar Pb cathode. Analyses of cathode deposits by SEM/EDS and XpS techniques indicated they were minimal on the Pb and Pt \ Nafion cathode and more apparent on the Pt-C \ Nafion cathode. The primary deposits on the Pb cathode were chromium oxides (e.g., Cr₂O₃) with minor amount of lead chromate (lead dichromate or lead trichromate) and other chromium solids (Cr black). As expected, the dominant deposit on the lead anode surface was PbO₂.

173 Han, Y. J., **T. M. Holsen**, et al. (2004). "Atmospheric gaseous mercury concentrations in New York State: relationships with meteorological data and other pollutants." Atmospheric Environment **38**(37): 6431-6446.

Ambient vapor-phase mercury concentrations including total gaseous mercury (TGM) and reactive gaseous mercury (RGM) were measured at three locations in rural New York State: Potsdam, Stockton, and Sterling. The RGM concentrations (4.2 +/- 6.4, 5.7 +/- 9.2, 6.0 +/- 10.8 pg m⁻³) at the Potsdam, Stockton, and Sterling sites, respectively) were about 0.2-3% of the total gaseous phase mercury concentration (TGM: 1.84 +/- 1.24, 1.83 +/- 1.32, 3.02 +/- 2.14 ng m⁻³), respectively) at the three monitoring sites. Standard deviations of RGM concentrations indicate that their daily variation was larger than that of TGM at all sites. This larger variation is probably because RGM is influenced by local sources to a greater extent than elemental mercury, which makes up to majority of TGM. There was no significant correlation between ozone and mercury concentrations. However, there was a significant positive correlation between water vapor mixing ratio and elemental mercury concentrations, suggesting that reduction of Hg²⁺ to Hg⁰ occurred in liquid water contained in clouds and fogs near the three monitoring sites. TGM concentrations had a generally negative correlation with ambient temperature, whereas RGM concentrations had a positive relationship. The negative relationship between TGM and temperature may be due to seasonal differences in emission rates of coal-fired power plants (winter maximum) in the northern hemisphere. This assumption was supported by a positive correlation between TGM and sulfur concentration, one of the major pollutants emitted from coal-fired power plants. (C) 2004 Elsevier Ltd All rights reserved.

172 Han, Y. J., **T. M. Holsen**, et al. (2004). "Identification of source locations for atmospheric dry deposition of heavy metals during yellow-sand events in Seoul, Korea in 1998 using hybrid receptor models." Atmospheric Environment **38**(31): 5353-5361.

Elemental dry deposition fluxes were measured using dry deposition plates from March to June 1998 in Seoul, Korea. During this spring sampling period several yellow-sand events characterized by long-range transport from China and Mongolia impacted the area. Understanding the impact of yellow-sand events on atmospheric dry deposition is critical to managing the heavy metal levels in the environment in Korea. In this study, the measured flux of a primarily crustal metal, Al and an anthropogenic metal, Pb was used with two hybrid. receptor models, potential source contribution function (PSCF) and residence time weighted concentration (RTWC) for locating sources of heavy metals associated with atmospheric dry deposition fluxes during the yellow-sand events in Seoul, Korea. The PSCF using a criterion

value of the 75th percentile of the measured dry deposition fluxes and RTWC results using the measured elemental dry deposition fluxes agreed well and consistently showed that there were large potential source areas in the Gobi Desert in China and Mongolia and industrial areas near Tianjin, Tangshan, and Shenyang in China. Major industrial areas of Shenyang, Fushun, and Anshan, the Central China loess plateau, the Gobi Desert, and the Alashan semi-desert in China were identified to be major source areas for the measured Pb flux in Seoul, Korea. For Al, the main industrial areas of Tangshan, Tianjin and Beijing, the Gobi Desert, the Alashan semi-desert, and the Central China loess plateau were found to be the major source areas. These results indicate that both anthropogenic sources such as industrial areas and natural sources such as deserts contribute to the high dry deposition fluxes of both Pb and Al in Seoul, Korea during yellow-sand events. RTWC resolved several high potential source areas. Modeling results indicated that the long-range transport of Al and Pb from China during yellow-sand events as well as non-yellow-sand spring daytimes increased atmospheric dry deposition of heavy metals in Korea. (C) 2004 Elsevier Ltd. All rights reserved.

171 Ferer, M., C. Ji, et al. (2004). "Cross-Over from Capillary Fingering to Viscous Fingering for Immiscible Unstable Flows: Experiment and Modeling." Physical Review E **70**(016330): 1-7.

170 Elder, A., R. Gelein, et al. (2004). "On-Road Exposure to Highway Aerosols 2. Exposure of Aged, Comprised Rats." Inhalation Toxicology **16**(Suppl. 1): 41-53.

169 **Dhaniyala, S.**, P. O. Wennberg, et al. (2004). "Stratospheric aerosol sampling: Effect of a blunt-body housing on inlet sampling characteristics." Aerosol Science and Technology **38**(11): 1080-1090.

During a campaign to study ozone loss mechanisms in the Arctic stratosphere (SOLVE), several instruments on NASA's ER-2 aircraft observed a very low number density (0.1 1(-1)) of large, nitric-acid-containing particles that form the polar stratospheric clouds (PSCs). For effective physical and chemical characterization of these particles, the measurements from these instruments have to be intercompared and integrated. In particular, proper interpretation requires knowledge of the sampling characteristics of the particles into the instruments. Here, we present the calculation of the sampling characteristics of the one of the instruments on the ER-2, the NOAA NOy instrument. This instrument sampled ambient particles and gas from two forward-facing inlets located fore and aft on a particle-separation housing (the football) and measured total NOy in the sample. In recent studies, ambient aerosol mass has been estimated by the difference of the measurements of the two inlets with the assumption that the rear inlet observations represent the gas-phase NOy and small particles and the front inlet samples represent gas-phase NOy and all particle sizes with varied efficiency (anisokinetic sampling). This knowledge was derived largely from semiempirical relations and potential flow studies of the housing. In our study, we used CFD simulations to model the compressible flow conditions and considered noncontinuum effects in calculating particle trajectories. Our simulations show that the blunt body housing the inlets has a strong and complex interaction with the flow and particles sampled by the two inlets. The simulations show that the front inlet characteristics are influenced by the effect of the blunt body on the upstream pressure field. The rear inlet sampling characteristics are influenced both by the shape and size of the inlet and its location on the blunt body. These interactions result in calculated inlet characteristics that are significantly different from previously assumed values. Analysis of the SOLVE data, considering the ambient

conditions and the calculated inlet sampling characteristics, in conjunction with thermodynamic growth modeling of super-cooled ternary solution (STS) particles, provides validation of the CFD results.

168 Chueinta, W., **P. K. Hopke**, et al. (2004). "Multilinear model for spatial pattern analysis of the measurement of haze and visual effects project." Environmental Science & Technology **38**(2): 544-554.

A multilinear model was developed for the analysis of the spatial patterns and possible sources affecting haze and its visual effects in the southwestern United States. The data from the project Measurement of Haze and Visual Effects (MOHAVE) collected during the late winter and midsummer of 1992 at the monitoring sites in four states (i.e., California, Arizona, Nevada and Utah) were used in the study. The three-way data array was analyzed by a four-product-term model. This study makes a direct effort to include wind patterns as a component in the model in order to obtain the information of the spatial patterns of source contributions. The solution is computed using the conjugate gradient algorithm with applied non-negativity constraints. For the winter data set, reasonable solutions contained six sources and six wind patterns. The analysis of summer data required seven sources and seven wind patterns. The ME results are compared to the prior single-species empirical orthogonal function analysis results and prior work describing the transport pathways.

167 Chrigui, M., A. Sadiki, et al. (2004). "Study of the Interaction in Sprat between evaporating Droplets and Turbulence Using Second Order Turbulence RANS modeling and a Lagrangian Approach." Progress in Computational Fluid Dynamics **4**: 162-174.

166 Biegalski, S. R. and **P. K. Hopke** (2004). "Total potential source contribution function analysis of trace elements determined in aerosol samples collected near Lake Huron." Environmental Science & Technology **38**(16): 4276-4284.

Aerosol samples were collected at the rural Burnt Island Ontario Integrated Air Deposition Network air sampling station on the northern shore of Lake Huron from 1992 through 1994. The samples were analyzed for trace elements by neutron activation analysis, and the air concentrations of over 30 elements were determined. Total potential source contribution function analysis (TPSCF) was used to determine the most probable geographical location of these aerosols' origin. The TPSCF results for As, In, Sb, Se, Sn, and Zn are highlighted in this paper. Source regions for these elements ranged from Alma, Quebec, Canada to Carrollton, GA. Because of large seasonal variations in the concentrations of the atmospheric concentrations of these elements, TPSCF values were calculated for the summer and winter halves of the year as well as the entire year.

165 Begum, B. A., E. Kim, et al. (2004). "Investigation of sources of atmospheric aerosol at urban and semi-urban areas in Bangladesh." Atmospheric Environment **38**(19): 3025-3038.

Samples of fine and coarse fractions of airborne particulate matter (PM) were collected in a semi-residential (AECD) area from June 2001 to June 2002 of Dhaka and in an urban area of Rajshahi, a city in northwestern region of Bangladesh from August 2001 to May 2002. The samples were collected using a 'Gent' stacked filter sampler in two fractions of < 2.5 μm fine and 2.5-10 μm coarse sizes. The samples were analyzed for elemental concentrations by PIXE. The data sets were then analyzed by positive matrix factorization technique to identify the

possible sources of atmospheric aerosols in these areas. The best solutions were found to be six and seven factors for elemental compositions for coarse and fine PM fractions in semi-residential Dhaka and five factors for elemental compositions of each of the coarse and fine PM respectively in the urban area of Rajshahi. The sources are soil dust, road dust, cement, sea salt, motor vehicles and biomass burning. The PMF results show that a large fraction of about more than 50% of the PM_{2.5-10} mass at both sites comes from soil dust and road dust. The motor vehicle including two strokes contributes about 48% of the PM_{2.5} mass in case of semi-residential area Dhaka. On the other hand, the biomass-burning factor contributes about 50% of the PM_{2.5} mass in Rajshahi. (C) 2004 Elsevier Ltd. All rights reserved.

164 Ally, M. R., J. Braunstein, et al. (2004). "Solubility and Vapor Pressures of Dissolved CO₂ in [bmim] [PF₆] and in [C8mim] [BF₄] Predicted by the Irregular Ionic Lattice Model IILM." Ind. Eng. Chem Research **43**: 1296-1301.

163 Ally, M. R., J. Braunstein, et al. (2004). "Irregular ionic lattice model for gas solubilities in ionic liquids." Industrial & Engineering Chemistry Research **43**(5): 1296-1301.

The irregular ionic lattice model (IILM) is applied to predict the vapor pressures and solubilities of carbon dioxide dissolved in 1-n-butyl-3-methylimidazolium hexafluorophosphate ([bmim] [PF₆]) and in 1-n-octyl-3-methylimidazolium tetrafluoroborate ([C8mim] [BF₄]) ionic liquids at temperatures ranging from 298.15 to 333.15 K. The model contains only two parameters; they are shown to be independent of an arbitrarily chosen reference state. The parameters show a slight dependence on temperature, but this dependence is ignored in computations to demonstrate the rigor of the IILM in predicting CO₂ solubility at high and low pressures at various temperatures. Model predictions are compared against the experimental data of Anthony et al. (J. Phys. Chem. B 2002, 106, 7315) and of Blanchard et al. (J. Phys. Chem. B 2001, 105, 2437). The usefulness of the model is in predicting CO₂ solubilities at temperatures and pressures where experimental data are unavailable.

162 **Ahmadi, G.**, C. Ji, et al. (2004). "Numerical solution for natural gas production from methane hydrate dissociation." Journal of Petroleum Science and Engineering **41**(4): 269-285.

This paper describes a one-dimensional model for natural gas production from the dissociation of methane hydrate in a confined reservoir by a depressurizing well. The approach accounts for the heat released by hydrate dissociation and convection - conduction heat transfer in the gas and hydrate zone. The system of governing equations is solved using a finite-difference scheme. For different well pressures and reservoir temperatures, the gas flow, the pressure and temperatures conditions in the reservoir are simulated. Distributions of temperature and pressure in the hydrate and gas regions and time evolutions of natural gas output also are evaluated. It is shown that the gas production rate is a sensitive function of well pressure. In addition, both heat conduction and convection in the hydrate zone is important. The simulation results are compared with the linearization approach and the shortcomings of the earlier approach are discussed. (C) 2003 Elsevier B.V. All rights reserved.

161 **Ahmadi, G.**, C. Ji, et al. (2004). "Numerical Simulation of Natural Gas Production from Methane Hydrate Dissociation." Journal of Petroleum Science and Engineering **41**: 269-285.

160 Zhao, H. and **D. A. Shipp** (2003). "Preparation of Poly(styrene-block-butyl acrylate) Block Copolymer-Silicate Nanocomposites." Chem. Mater. **15**: 2693-2695.

159 Zheng, J. and **S. E. Powers** (2003). "Identifying the Effects of Polar Constituents in Coal-Derived DNAPLs on Interfacial Tension." Environmental Science & Technology **37**(14): 3090-3094.

158 Yli-Tuomia, T., L. Venditte, et al. (2003). "Composition of the Finnish Arctic aerosol: collection and analysis of historic filter samples." Atmospheric Environment **37**(17): 2355-2364.

Week-long samples of total suspended particles have been collected between October 1964 and February 1978 from the Finnish Arctic. Neutron activation analysis, ion chromatography, and light-absorption techniques have been used to analyze the concentration of several heavy metals and other elements, major ions, methane sulfonate (MSA), and black carbon. Kevo is located near the Kola Peninsula and the effect of the industrial area can be seen. Compared to previous studies of Arctic aerosols carried out in North American Arctic, the Kevo results show higher concentration of anthropogenic pollutants and the seasonal variability for most constituents is weaker than the typical Arctic haze pattern. MSA, a marker of biogenic activity, has a clear seasonal cycle with a peak from April to August. (C) 2003 Elsevier Science Ltd. All rights reserved.

157 Yli-Tuomia, T., **P. K. Hopke**, et al. (2003). "Atmospheric aerosol over Finnish Arctic: source analysis by the multilinear engine and the potential source contribution function." Atmospheric Environment **37**(31): 4381-4392.

Week-long samples of total suspended particles were collected between 1964 and 1978 from Kevo at the Finnish Arctic and analyzed for a number of chemical species. The chemical composition data was analyzed using a mixed 2-way/3-way model. The results of receptor modeling were connected with the back trajectory data in a Potential Source Contribution Function analysis to determine the likely source areas. Nine sources, namely silver emissions, coal/ oil shale combustion, biomass burning, non-ferrous smelters (two sources), crustal elements from remote sources, excess silicon from local sources, sea salt particles and biogenic sulfur emissions from marine algae were found. Although the emissions from industrial areas in the Kola Peninsula had an effect on the concentration of anthropogenic pollutants at Kevo, the highest concentrations during winter were transported from the sources in the mid-latitudes. The yearly strength of the biogenic sulfur emissions showed no dependence on the Northern Hemisphere temperature anomaly and thus, a climatic feedback loop could not be confirmed. (C) 2003 Elsevier Ltd. All rights reserved.

156 Winkler, B. H. and **R. E. Baltus** (2003). "Modification of the Surface Characteristics of Anodic Alumina Membranes Using Sol-Gel Chemistry." Journal of Membrane Science **226**: 573-582.

155 Wilhelm, S. W., J. M. DeBruyn, et al. (2003). "Effect of phosphorous amendments on present day plankton communities in pelagic Lake Erie." Aquatic Microbial Ecology **32**: 275-285.

154 **Welsh, R.**, B. Hubbell, et al. (2003). "Agro-food System and Restructuring and the Geographic Concentrations of U.S. Swine Production." Environment and Planning(35): 215-229.

153 Wang, J., **P. Hopke**, et al. (2003). "Application of Modified Alternating Least Squares Regression to Spectroscopic Image Analysis." Analytica Chimica Acta **476**: 93-109.

152 **Shipp, D. A.**, D. H. Solomon, et al. (2003). "The Chain Length Dependence of Radical-Radical Termination in Free Radical Polymerization: A Pulsed Laser Photolysis Investigation." Macromolecules **36**: 2032-2040.

151 **Shen, H. T.**, Q. Xu, et al. (2003). "Modeling Lampricide Transport in the St. Mary's River." Journal of Great Lakes Research **29**(Supplement 1): 134-142.

150 **Shen, H. T.** and L. Liu (2003). "Shokotsu River Ice Jam Formation." Cold Regions Science and Technology **37**(1): 35-49.

149 **Shen, H. T.** (2003). "Research on River Ice Processes: Progress and Missing Links." Journal of Col Regions Engineering, ASCE **17**(4): 134-142.

148 Ramadan, Z., B. Eickhout, et al. (2003). "Comparison of Positive Matrix Factorization and Multilinear Engine for the source apportionment of particulate pollutants." Chemometrics and Intelligent Laboratory Systems **66**(1): 15-28.

New approaches to solving the factor analysis (FA) problem have recently been developed by recognizing that factor analysis is fundamentally a least-squares (LS) problem. This approach is called Positive Matrix Factorization (PMF). Two programs have been written to implement different algorithms for solving the problem. These programs are PMF2 and Multilinear Engine (ME-2). The two programs use different algorithms to obtain the least-squares solution and the constraints are imposed in different ways. Elemental composition data for particle samples collected in Phoenix, AZ from June 1996 through June 1998, were used to compare the source apportionment of these two programs. The ME-2 results presented in this paper are compared with the previously published PMF2 results. The identification of the eight PMF sources returned one questionable source: wood burning and some peculiar mass contributions. The extra features of ME-2 made it possible to also investigate the sources responsible for the fine particles. The mixed-way approach indicated the existence of incinerators in the Phoenix area. Like PMF, ME-2 identified high source contributions for biomass burning, motor vehicles (with higher contribution in winter), coal-fired power plants (secondary particles with higher contributions in summer), soil, and nonferrous smelting process. Sea salt and heavy-duty diesel were identified by the ME two-way analysis, but they disappeared in the three-way analysis of the dual fine particle sequential sampler (DFPSS) and DICHOT data. Instead, an obvious incinerator source was identified again. Thus, PMF and ME-2 identified the same major sources responsible for the PM_{2.5} in Phoenix, but some of the sources identified by PMF2 appear to be uncertain. The three-way analysis provided additional information about possible sources, but also returned unexplainable sources. (C) 2002 Elsevier Science B.V. All rights reserved.

147 **Powers, S. E.**, T. Graham, et al. (2003). "Diversity in K-12 Initiatives to Attract a Diverse Pool of Engineering Students." Proceedings of the Frontiers in Education Conference.

146 Paatero, P., **P. K. Hopke**, et al. (2003). "Advanced factor analysis of spatial distributions of PM_{2.5} in the eastern United States." Environmental Science & Technology **37**(11): 2460-2476.

This work analyzes PM_{2.5} 24-h average concentrations measured every third day at over 300 locations in the eastern United States during 2000. The non-negative factor analytic model, Positive Matrix Factorization, has been enhanced by modeling the dependence of PM_{2.5} concentrations on temperature, humidity, pressure, ozone concentrations, and wind velocity vectors. The model comprises 12 general factors, augmented by 5 urban-only factors intended to represent excess concentration present in urban locations only. The computed factor components or concentration fields are displayed as concentration maps, one for each factor, showing how much each factor contributes to the average concentration at each location. The factors are also displayed as flux maps that illustrate the spatial movement of PM_{2.5} aerosol, thus enabling one to pinpoint potential source areas of PM_{2.5}. The quality of the results was investigated by examining how well the model reproduces especially high concentrations of PM_{2.5} on specific days at specific locations. Delimiting the spatial extent of all such factors that exhibit a clear regional maximum surrounded by an almost-zero outer domain lowered the uncertainty in the computed results.

145 Paatero, P. and **P. K. Hopke** (2003). "Discarding or downweighting high-noise variables in factor analytic models." Analytica Chimica Acta **490**(1-2): 277-289.

This work examines the factor analysis of matrices where the proportion of signal and noise is very different in different columns (variables). Such matrices often occur when measuring elemental concentrations in environmental samples. In the strongest variables, the error level may be a few percent. For the weakest variables, the data may consist almost entirely of noise. This paper demonstrates that the proper scaling of weak variables is critical. It is found that if a few weak variables are scaled to too high a weight in the analysis, the errors in computed factors would grow, possibly obscuring the weakest factor(s) by the increased noise level. The mathematical explanation of this phenomenon is explored by means of Givens rotations. It is shown that the customary form of principal component analysis (PCA), based on autoscaling the original data, is generally very ineffective because the scaling of weak variables becomes much too high. Practical advice is given for dealing with noisy data in both PCA and positive matrix factorization (PMF). (C) 2003 Elsevier Science B.V. All rights reserved.

144 Nambi, I. M. and **S. E. Powers** (2003). "Mass Transfer Correlations for NAPL Dissolution from Regions with High Initial Saturations." Water Resources Research **39**(2): (SBH 4-1)-(4-11).

143 McDowell, C. J. and **S. E. Powers** (2003). "Mechanisms Affecting the Infiltration and Redistribution of Ethanol-Blended Gasoline in the Vadose Zone." Environmental Science & Technology **39**(9): 1803-1810.

142 McDowell, C. J., T. Buscheck, et al. (2003). "Behavior of Gasoline Pools Following a Denaturated Ethanol Spill." Ground Water **41**(6): 746-757.

141 Mazaheri, A. R., **G. Ahmadi**, et al. (2003). "Hot-gas flow and particle transport and deposition in a candle filter vessel." Advanced Powder Technology **14**(1): 111-125.

Hot-gas flow and particle transport and deposition in an industrial filtration system are studied. The special example of the Siemens-Westinghouse filter vessel at the Power System Development Facility at Wilsonville, Alabama is treated in detail. This tangential flow filter vessel contains clusters of 91 candle filters, which are arranged in two tiers. The upper tier containing 36 candle filters is modeled by six equivalent filters. Seven equivalent filters are used in the computational model to represent the 55 candle filters in the lower tiers. The Reynolds stress turbulent model of FLUENT(TM) code is used, and the gas mean velocity and root mean square fluctuation velocities in the filter vessel are evaluated. The particle equation of motion used includes drag and gravitational forces. The mean particle deposition patterns are evaluated and the effect of particle size is studied. The computational results indicate that large particles of the order of 10 μm or larger are removed from the gas due to the centrifugal forces exerted by rotating flow between the shroud and the refractory.

140 Liu, W., **P. K. Hopke**, et al. (2003). "Origins of fine aerosol mass in the western United States using positive matrix factorization." Journal of Geophysical Research-Atmospheres **108**(D23): 4716.

In order to evaluate the impact of Asian dust to the air quality of North America, a relatively new type of factor analysis, positive matrix factorization (PMF), was applied to the PM_{2.5} particle composition data obtained at two high elevated sampling sites in the western United States from Interagency Monitoring of Protected Visual Environments (IMPROVE) program. These two sites are Crater Lake National Park (1981m) and Lassen Volcanic National Park (1798m). PMF can provide optimal point-by-point weighting by using the estimates uncertainty in the data and can permit efficient treatment of missing and below detection limit values. It also imposes the nonnegativity constraint on the factors. Seven and six sources were resolved from the Crater Lake National Park and Lassen Volcanic National Park data, respectively. The factors were normalized by using aerosol fine mass concentration data through multiple linear regression so that the quantitative source contributions for each resolved factor were obtained. Among the sources resolved at the two sites, six are common. These six sources exhibit not only similar chemical compositions but also similar seasonal variations at both sites. The Asian dust was represented by Al, Ca, Fe, NO₃, S, K, and Ti with strong seasonal variation. Secondary sulfate with a high concentration of S and strong seasonal variation correlated with the Asian dust. Wood smoke was represented by organic carbon (OC), elemental carbon (EC), and K; sea salt with the high concentrations of Na, S and NO₃. Nitrate was dominated by NO₃ and motor vehicle with high concentrations of OC, EC, and dust elements. A incinerator source with the presence of Cu and Zn also was resolved from the Crater Lake site. Generally, most of the sources at these two sites showed similar chemical composition profiles and seasonal variation patterns. The source profile of Asian dust resolved from this study agreed reasonably well with the source characteristics found in other Asian dust studies. This study indicated that PMF was a powerful factor analysis method to extract sources from the ambient aerosol concentration data.

139 Liu, W., **P. K. Hopke**, et al. (2003). "Application of receptor modeling to atmospheric constituents at Potsdam and Stockton, NY." Atmospheric Environment **37**(36): 4997-5007.

A measurement program in this study has been undertaken to measure the concentrations of particles and Hg-0 in rural areas of New York State during the summer of 2000 and 2001. Sampling was performed at sites in southwestern (Stockton, NY) and northern New York (Potsdam, NY) where these materials may be transported into the New York from the central United States and from Canada. The data from these measurements were used in paired receptor models to assess the origins of the measured concentrations. Factor analysis in the form of positive matrix factorization (PMF) was used to obtain information about possible sources of the aerosol. Six and seven sources were resolved from Stockton and Potsdam sites, respectively. Six of the sources are common to the two sites in these two summers. They are secondary sulfate, secondary nitrate, soil, wood smoke, zinc smelter and copper smelter. A nickel smelter source is also resolved at Potsdam. Potential source contribution function (PSCF) analysis which combines the aerosol data with the air parcel backward trajectories was applied to identify possible source areas and pathways from these sources at the two sites. The combination of the two receptor modeling methods, PMF and PSCF, provides an effective way in identifying atmospheric aerosol sources and their likely locations. Emissions from different anthropogenic activities as well as secondary aerosol production are the main source measured in Potsdam and Stockton. (C) 2003 Elsevier Ltd. All rights reserved.

138 Librescu, L., G. Chiocchia, et al. (2003). "Implications of Cubic Physical/ Aerodynamic Nonlinearities on the Character of the Flutter Instability Boundry." International Journal of Nonlinear Mechanics **38**: 173-199.

137 Lee, D. W., **P. K. Hopke**, et al. (2003). "Comparison of experimental and theoretical heterogeneous nucleation on ultrafine carbon particles." Journal of Physical Chemistry B **107**(50): 13813-13822.

Using a modified turbulent mixing CNC, the heterogeneous nucleation of different compounds (working fluids) on nanometer sized carbon particles was examined. The working fluids were dibutyl phthalate, octadecane, octadecanol, and octadecanoic acid. Based on the particle size distributions measured with a scanning mobility particle sizer system, nucleation and consequent growth were examined with respect to different temperature and vapor pressure for each working fluid. Nucleation rates for all conditions were calculated from the fitted size distribution data by subtracting the residual nonactivated particle concentration for each condition. Experimental nucleation rates were compared to the calculated ones based on Fletcher's heterogeneous nucleation theory. This theory matches well with the experiments with octadecanol and octadecanoic acid, and at high supersaturation ratios for dibutyl phthalate. However, the theory shows discrepancies with the observed phenomena at low supersaturation for dibutyl phthalate, and especially for octadecane. Several possible hypotheses for the discrepancies and observed particle growth are discussed.

136 Kim, E., T. V. Larson, et al. (2003). "Source identification of PM_{2.5} in an arid Northwest US City by positive matrix factorization." Atmospheric Research **66**(4): 291-305.

Spokane, WA is prone to frequent particulate pollution episodes due to dust storms, biomass burning, and periods of stagnant meteorological conditions. Spokane is the location of a long-term study examining the association between health effects and

chemical or physical constituents of particulate pollution. Positive matrix factorization (PMF) was used to deduce the sources of PM_{2.5} (particulate matter less than or equal to 2.5 μm in aerodynamic diameter) at a residential site in Spokane from 1995 through 1997. A total of 16 elements in 945 daily PM_{2.5} samples were measured. The PMF results indicated that seven sources independently contribute to the observed PM_{2.5} mass: vegetative burning (44%), sulfate aerosol (19%), motor vehicle (11%), nitrate aerosol (9%), airborne soil (9%), chlorine-rich source (6%) and metal processing (3%). Conditional probability functions were computed using surface wind data and the PMF deduced mass contributions from each source and were used to identify local point sources. Concurrently measured carbon monoxide and nitrogen oxides were correlated with the PM_{2.5} from both motor vehicles and vegetative burning. (C) 2003 Elsevier Science B.V. All rights reserved.

135 Kim, E., **P. K. Hopke**, et al. (2003). "Incorporation of parametric factors into multilinear receptor model studies of Atlanta aerosol." *Atmospheric Environment* **37**(36): 5009-5021.

In prior work with simulated data, ancillary variables including time resolved wind data were utilized in a multilinear model to successfully reduce rotational ambiguity and increase the number of resolved sources. In this study, time resolved wind and other data were incorporated into a model for the analysis of real measurement data. Twenty-four hour integrated PM_{2.5} (particulate matter less than or equal to 2.5 μm in aerodynamic diameter) compositional data were measured in Atlanta, GA between August 1998 and August 2000 (662 samples). A two-stage model that utilized 22 elemental species, two wind variables, and three time variables was used for this analysis. The model identified nine sources: sulfate-rich secondary aerosol 1 (54%), gasoline exhaust (15%), diesel exhaust (11%), nitrate-rich secondary aerosol (9%), metal processing (3%), wood smoke (3%), airborne soil (2%), sulfate-rich secondary aerosol 11 (2%), and the mixture of a cement kiln with a carbon-rich source (0.9%). The results of this study indicate that utilizing time resolved wind measurements aids to separate diesel exhaust from gasoline vehicle exhaust. For most of the sources, well-defined directional profiles, seasonal trends, and weekend effects were obtained. (C) 2003 Elsevier Ltd. All rights reserved.

134 Kim, E., **P. K. Hopke**, et al. (2003). "Source identification of Atlanta aerosol by positive matrix factorization." *Journal of The Air & Waste Management Association* **53**(6): 731-739.

Data characterizing daily integrated particulate matter (PM) samples collected at the Jefferson Street monitoring site in Atlanta, GA, were analyzed through the application of a bilinear positive matrix factorization (PMF) model. A total of 662 samples and 26 variables were used for fine particle (particles less than or equal to 2.5 μm in aerodynamic diameter) samples (PM_{2.5}), and 685 samples and 15 variables were used for coarse particle (particles between 2.5 and 10 μm in aerodynamic diameter) samples (PM_{10-2.5}). Measured PM mass concentrations and compositional data were used as independent variables. To obtain the quantitative contributions for each source, the factors were normalized using PMF-apportioned mass concentrations. For fine particle data, eight sources were identified: SO₄²⁻-rich secondary aerosol (56%), motor vehicle (22%), wood smoke (11%), NO₃⁻-rich secondary aerosol (7%), mixed source of cement kiln and organic carbon (OC) (2%), airborne soil (1%), metal recycling facility (0.5%), and mixed source of bus station and metal processing (0.3%). The SO₄²⁻-rich and NO₃⁻-rich secondary aerosols were associated with NH₄⁺. The SO₄²⁻-rich secondary

aerosols also included OC. For the coarse particle data, five sources contributed to the observed mass: airborne soil (60%), NO₃-rich secondary aerosol (16%), SO₄²⁻-rich secondary aerosol (12%), cement kiln (11%), and metal recycling facility (1%). Conditional probability functions were computed using surface wind data and identified mass contributions from each source. The results of this analysis agreed well with the locations of known local point sources.

132 Ji, C., **G. Ahmadi**, et al. (2003). "Constant rate natural gas production from a well in a hydrate reservoir." Energy Conversion and Management **44**(15): 2403-2423.

Using a computational model, production of natural gas at a constant rate from a well that is drilled into a confined methane hydrate reservoir is studied. It is assumed that the pores in the reservoir are partially saturated with hydrate. A linearized model for an axisymmetric condition with a fixed well output is used in the analysis. For different reservoir temperatures and various well outputs, time evolutions of temperature and pressure profiles, as well as the gas flow rate in the hydrate zone and the gas region, are evaluated. The distance of the decomposition front from the well as a function of time is also computed. It is shown that to maintain a constant natural gas production rate, the well pressure must be decreased with time. A constant low production rate can be sustained for a long duration of time, but a high production rate demands unrealistically low pressure at the well after a relatively short production time. The simulation results show that the process of natural gas production in a hydrate reservoir is a sensitive function of reservoir temperature and hydrate zone permeability. Published by Elsevier Science Ltd.

131 Hwang, S. and **S. E. Powers** (2003). "Using Particle-Size Distribution Models to Estimate Soil Hydraulic Properties." Soil Sci. Soc. Am. J. **67**(7): 1103-1112.

130 Hwang, S. and **S. E. Powers** (2003). "Lognormal Distribution Model for Estimating Soil Water Retention Curves for Sandy Soil." Soil Science **168**(3): 156-166.

129 Hwang, S. and **S. E. Powers** (2003). "Estimating Unique Soil Hydraulic Parameters from Multi-Step Outflow Experiments with Sandy Media." Adv. Water Res. **26**(4): 445-456.

128 Huang, K. L., **T. M. Holsen**, et al. (2003). "Impurity Diffusion Through Nafion and Ceramic Separators used for the Electrolytic Purification of Spent Chromium Plating Solutions." Journal of Membrane Science(221): 135-146.

127 Huang, K. L., **T. M. Holsen**, et al. (2003). "Anion Partitioning In and Diffusion Through a Nafion Membrane." Ind. Eng. Chem Research(42): 3620-3625.

126 Huang, K. L., **T. M. Holsen**, et al. (2003). "Comparing Nafion and Ceramic Separators Used in Electrochemical Purification of Spent Plating Solutions: Cationic Impurity Removal and Transport." Environmental Science & Technology(37): 1992-1998.

125 Hsu, Y. K., **T. M. Holsen**, et al. (2003). "Response to comment on "Locating PCB sources in Chicago: Receptor modeling and field sampling"." Environmental Science & Technology **37**(24): 5838-5838.

124 Hsu, Y. K., **T. M. Holsen**, et al. (2003). "Locating and quantifying PCB sources in Chicago: Receptor modeling and field sampling." Environmental Science & Technology **37**(4): 681-690.

Potential source contribution function (PSCF) modeling using polychlorinated biphenyl (PCB) concentrations measured in the Chicago area resolved three PCB source sectors. They were (i) the direction northwest of Chicago, (ii) the direction southwest of Chicago, and (iii) the south side of Chicago in the neighborhood of Lake Calumet. The area south of Chicago was further examined by taking upwind/ downwind samples near a landfill and sludge drying beds. Results identified the sludge drying beds and a large landfill as PCB sources to the atmosphere. Another PCB source identified in Chicago was a transformer storage yard. This site had the highest upwind/downwind concentration increments in this study (downwind PCB concentrations were more than 5 times those in the upwind air). These PCB sources were characterized in terms of inventories, emission rates, contributions, and PCB congener profiles (fingerprints). Preliminary results indicate that the sludge may emit up to 90 kg/yr of PCBs to the air. This amount is probably not a significant contribution of PCBs to the Chicago atmosphere on the basis of dispersion modeling results and a simple box model.

123 Hsu, Y. K., **T. M. Holsen**, et al. (2003). "Comparison of hybrid receptor models to locate PCB sources in Chicago." Atmospheric Environment **37**(4): 545-562.

Results of three hybrid receptor models, potential source contribution function (PSCF), concentration weighted trajectory (CWT), and residence time weighted concentration (RTWC), were compared for locating polychlorinated biphenyl (PCB) sources contributing to the atmospheric concentrations in Chicago. Variations of these models, including PSCF using mean and 75% criterion concentrations, joint probability PSCF (JP-PSCF), changes of point filters and grid cell sizes for RTWC, and, PSCF using wind trajectories started at different altitudes, are also discussed. Modeling results were relatively consistent between models. However, no single model provided as complete information as was obtained by using all of them. CWT and 75% PSCF appears to be able to distinguish between larger sources and moderate ones. RTWC resolved high potential source areas. RTWC and JP-PSCF pooling data from all sampling sites removed the trailing effect often seen in PSCF modeling. PSCF results using average concentration criteria, appears to identify both moderate and major sources. Each model has advantages and disadvantages. However, used in combination, they provide information that is not available if only one of them is used. For short-range atmospheric transport, PSCF results were consistent when using wind trajectories starting at different heights. Based on the archived PCB data, the modeling results indicate there is a large potential source area between Joliet and Kankakee, IL, and two moderate sources to the northwest and south of Chicago. On the south side of Chicago in the neighborhood of Lake Calumet, several PCB sources were identified. Other unidentified potential source location(s) will require additional upwind/downwind field sampling to verify modeling results. (C) 2002 Elsevier Science Ltd. All rights reserved.

122 **Hopke, P. K.**, Z. Ramadan, et al. (2003). "Receptor modeling of ambient and personal exposure samples: 1998 Baltimore Particulate Matter Epidemiology-Exposure Study." Atmospheric Environment **37**(23): 3289-3302.

Sources of particulate matter exposure for an elderly population in a city north of Baltimore, MD were evaluated using advanced factor analysis models. Data collected with versatile air pollutant samplers positioned at a community site, outside and inside of

an elderly residential facility were analyzed with a three-way analysis to identify the source(s) that contributed to all sample types. These sources were secondary sulfate, secondary nitrate, motor vehicles, and a organic carbon (OC). The OC source contained 96% OC and most likely represents positive volatile organic carbon artifact and other unidentified sources. No soil source was found that contributed significantly to these samples. A second set of data was collected with personal samplers (PEM) from 10 elderly subjects, their apartments, a central indoor location, and outdoors. The PEM data were analyzed using a complex model with a target for soil that included factors that are common to all of the types of samples (external factors) and factors that only apply to the data from the individual and apartment samples (internal factors). From these results, the impact of outdoor sources and indoor sources on indoor concentrations were assessed. The identified external factors were sulfate, soil, and an unknown factor. Internal factors were identified as gypsum or wall board, personal care products, and a factor representing variability not explained by the other indoor sources. The latter factor had a composition similar to outdoor particulate matter and explained 36% of the personal exposure. External factors contributed 63% to personal exposure with the largest contribution from sulfate (48%). (C) 2003 Elsevier Science Ltd. All rights reserved.

121 **Hopke, P. K.,** W. Liu, et al. (2003). "Measured summertime concentrations of particulate components, Hg-0, and speciated polycyclic aromatic hydrocarbons at rural sites in New York State." Environmental Pollution **123**(3): 413-425.

Daily PM_{2.5} samples, Hg-0 and speciated polycyclic aromatic hydrocarbon (PAH) were simultaneously collected at Potsdam and Stockton site in NY during the summers of 2000 and 2001. Samples for determination of the mass concentration and chemical composition of the PM_{2.5} were obtained with a speciation network PM_{2.5} sampler. Chemical composition including trace elemental composition, water-soluble ions, and elemental carbon were analyzed. Elemental mercury and PAHs were sampled separately. Daily PM_{2.5} concentrations ranged from 0.47 to 53.7 $\mu\text{g m}^{-3}$ at the Potsdam site, and from 0.82 to 47.23 $\mu\text{g m}^{-3}$ at the Stockton site with large daily differences between the two sites. Potsdam consistently had lower mass values than Stockton. The greatest contributors to the PM_{2.5} mass (generally $> 0.1 \mu\text{g}/\text{m}^3$) were sulfate, nitrate, ammonium, and BC at both sites. Seventeen PAHs were identified at each site in 2000 and the average total concentrations were 3.2 ng/m^3 and 2.9 ng/m^3 at the Potsdam and Stockton sites, respectively. The mean vapor phase mercury concentration at the Potsdam site (2.4 \pm 1.2 ng m^{-3} , n = 93) was higher than that at the Stockton site (1.2 \pm 1.0 ng m^{-3} , n = 60) in 2000, whereas in 2001, the average concentrations were 1.1 ng m^{-3} and 1.6 ng m^{-3} at the Potsdam and Stockton sites, respectively. In general, vapor phase mercury concentrations increased with increasing ambient temperature at the Stockton site in 2000. These differences in values between 2000 and 2001 can be largely explained by distinct differences in the meteorological regimes that dominated in the different years. (C) 2003 Elsevier Science Ltd. All rights reserved.

120 **Hopke, P. K.** (2003). "Recent developments in receptor modeling." Journal of Chemometrics **17**(5): 255-265.

Receptor modeling is the application of data analysis methods to elicit information on the sources of air pollutants. Typically, it employs methods of solving the mixture resolution problem using chemical composition data for airborne particulate matter samples. In such

cases, the outcome is the identification of the pollution source types and estimates of the contribution of each source type to the observed concentrations. It can also involve efforts to identify the locations of the sources through the use of ensembles of air parcel back trajectories. In recent years, there have been improvements in the factor analysis methods that are applied in receptor modeling as well as easier application of trajectory methods. These developments are reviewed. Copyright (C) 2003 John Wiley Sons, Ltd.

119 **Hopke, P.** (2003). "The Evolution of Chemometrics." *Analytica Chimica Acta* **500**: 365-377.

118 Holland, D. M., W. M. Cox, et al. (2003). "Spatial Prediction of Air Quality Data: A Primer." *EM*(August): 31-35.

117 Hinrichs, C. and **R. Welsh** (2003). "The Effects of Industrialization of U.S. Livestock Agriculture on Promoting Sustainable Agriculture Practices." *Agriculture and Human Values* **20**: 125-229.

116 Gan, F. and **P. K. Hopke** (2003). "New convergence criterion for multi-variable curve resolution." *Analytica Chimica Acta* **495**(1-2): 195-203.

The traditional convergence criterion of the minimized sum of squared residuals does not always provide sufficient information to properly terminate the iterative process used in the multi-variable curve resolution problem. Thus, a new convergence criterion is proposed. The resolution results for both simulated and the real chromatographic system data show that the new convergence criterion can provide a better indication of the completion of the resolution process. (C) 2003 Elsevier B.V. All rights reserved.

115 Gan, F. and **P. K. Hopke** (2003). "Data mining of the relationship between volatile organic components and transient high ozone formation." *Analytica Chimica Acta* **490**(1-2): 153-158.

The aim of this study is to identify relationships between volatile organic components (VOCs) and transient high ozone formation in the Houston area. The ozone is not emitted to the atmosphere directly but is formed by chemical reactions in the atmosphere. In Houston, short-term (1h) sharp increases are observed followed by a rapid decrease back to typical concentrations. Automatic gas chromatographs (GCs) are operated at several sites which cryogenically collect VOCs during an hour and then the compounds are flash evaporated into the GC for analysis. Chromatographic data for more than 65 VOCs are stored in analysis report text files. A program has been developed to read the amount of each component in the measurements such that a data set is generated that includes the concentrations of each VOC for each hourly sample. A subset of the data is selected that corresponds to the period of the positive ozone transient and these data are used in the data mining (DM) process. Based on a chemical mass balance (CMB) analysis, a linear model was established between the subset of the VOCs data and the positive ozone transition. Non-negative least squares (NNLS) was used to calculate the regression coefficient of the VOCs that have the most significant positive relationship to the positive ozone transition. The results show that more attention might be paid to several unknown VOCs, which have significant relationships to the transient high ozone formation. (C) 2003 Elsevier Science B.V. All rights reserved.

114 Faber, N. M., X. H. Song, et al. (2003). "Sample-specific standard error of prediction for partial least squares regression." Trac-Trends In Analytical Chemistry **22**(5): 330-334.

The development of an adequate expression for sample-specific standard error of prediction for partial least squares regression is a major trend in chemometrics literature. This article focuses on three generally applicable expressions, namely one recommended by the American Society for Testing and Materials (ASTM), one implemented in Unscrambler software and a simplification derived under the errors-in-variables (EIV) model. Results obtained for a near-infrared data set taken from the literature demonstrate that the EIV expression works best. (C) 2003 Published by Elsevier Science B.V.

113 Faber, N. M., R. Bro, et al. (2003). "Recent developments in CANDECOMP/PARAFAC algorithms: a critical review." Chemometrics and Intelligent Laboratory Systems **65**(1): 119-137. Several recently proposed algorithms for fitting the PARAFAC model are investigated and compared to more established alternatives. Alternating least squares (ALS), direct trilinear decomposition (DTLD), alternating trilinear decomposition (ATLD), self-weighted alternating trilinear decomposition (SWATLD), pseudo alternating least squares (PALS), alternating coupled vectors resolution (ACOVER), alternating slice-wise diagonalization (ASD) and alternating coupled matrices resolution (ACOMAR) are compared on both simulated and real data. For the recent algorithms, only unconstrained three-way models can be fitted. In contrast, for example, ALS allows modeling of higher-order data, as well as incorporating constraints on the parameters and handling of missing data. Nevertheless, for three-way data, the newer algorithms are interesting alternatives. It is found that the ALS estimated models are generally of a better quality than any of the alternatives even when overfactoring the model, but it is also found that ALS is significantly slower. Based on the results (in particular the poor performance of DTLD), it is advised that (a slightly modified) ASD may be a good alternative to ALS when a faster algorithm is desired. (C) 2002 Elsevier Science B.V. All rights reserved.

112 Ervin, D. R., S. B. Welsh, et al. (2003). "Towards an Ecological Systems Approach in Public Research for Environmental Regulations of Transgenic Crops." Agriculture, Ecosystems & Environment **99**: 1-14.\

111 Duquette, M. M. and **K. D. Visser** (2003). "Numerical Implications of Solidity and Blade Number on Rotor Performance of Horizontal-Axis Wind Turbines." Journal of Solar Energy Engineering **125**(4): 426-432.

110 Duquette, M. M., J. Swanson, et al. (2003). "Solidity and Blade Number Effects on Small Horizontal-Axis Wind Turbines." Wind Engineering **27**(4): 299-316.

109 **Dhaniyala, S.**, R. C. Flagan, et al. (2003). "Novel aerosol/gas inlet for aircraft-based measurements." Aerosol Science and Technology **37**(10): 828-840.

A novel inlet has been designed for selective sampling of gas and aerosol phases of volatile species from high-speed aircraft. A multistage flow system brings the flow nearly isokinetically towards the sampling port. Two small airfoil-shaped "blades" are placed close to the sample port to provide the flow conditions required for aerosol and gas sampling. Aerosols are sampled when these blades are positioned to operate the inlet as a counterflow virtual

impactor (CVI). The design enables sampling of particles as small as 0.1 μm from a high-speed aircraft under stratospheric conditions, a substantial improvement over that possible with previous CVI designs. For gas sampling, one of the blades is moved by a stepper motor to occlude the inlet opening and gas is sampled perpendicular to the bulk flow. Boundary layer suction is used to prevent the sampled gas from coming in contact with the impactor walls. This is one of the first designs of an inlet that enables gas sampling free of wall contact. The inlet was flown on the NASA ER-2 aircraft during the SOLVE 2000 campaign to study aerosol/gas partitioning of nitric acid in the lower stratosphere. Data from the flight tests show that the inlet flow characteristics are broadly in agreement with computational fluid dynamics (CFD) simulations.

108 Basunia, M. S., S. Landsberger, et al. (2003). "Ambient silver concentration anomaly in the Finnish arctic lower atmosphere." Environmental Science & Technology **37**(24): 5537-5544.

Mean silver concentrations in weekly particle samples collected at Kevo, northern Finland, were determined for the period of October 1964-March 1978 by neutron activation analysis. Two distinct periods were observed in the silver concentration levels over this time frame. During 1964-1970, mean weekly silver concentration levels were found in the range of 0.01-190 ng/m^3 with an arithmetic mean of 2.19 ng/m^3 . A few very high silver concentration levels ($>10 \text{ ng}/\text{m}^3$) were observed in this period, some of which simultaneously occurred with some of the highest bromine and iodine concentration levels. During 1971-1978, silver concentration levels were in the range of 0.02-0.89 ng/m^3 with a mean value of 0.09 ng/m^3 . The observed concentration levels in the later period matched well the data from the early 1990s reported at Severtijarvi, northern Finland, about 60 km east of Kevo. Data analysis, historical records for this region, and residence time analysis (RTA) using wind back-trajectories show that occasional smelting of silver-rich Norilsk ores at the Nickel smelter, Kola Peninsula, was probably a significant contributor to elevated mean silver concentration levels during 1964-1970. RTA alone was not able to unambiguously identify the most probable source region for highest silver impacts at Kevo due to the weekly integrated nature of the samples collected. Critical examination of wind back-trajectories (24 per day) for specific high silver, bromine, and iodine concentration weeks was carried out to supplement the ensemble RTA analysis (2 back-trajectories per day). The supplemental back-trajectory analysis revealed that deposition of the smelter component silver as well as the sea components (bromine and iodine) could occur together at Kevo during these weekly sampling periods. The study implies that data from weekly integrated samples are insufficiently time-resolved for RTA methods alone to unambiguously resolve the sources contributing to ambient atmospheric concentrations at Kevo, Finland.

107 Baeza, C., **A. Rossner**, et al. (2003). "Removal of EDTA by UV-C/hydrogen peroxide." Environmental Technology **24**(10): 1277-1281.

Mineralization of a 5 mM EDTA solution at pH 3 was evaluated via TOC removal under UV-C irradiation in the presence of H_2O_2 at various conditions. The highest TOC removal (78%) was obtained using a 40:1 H_2O_2 /EDTA molar ratio, after 540 min irradiation. However, a 20:1 ratio gave slightly lower results, being economically more attractive. Best results of TOC removal were obtained under pH controlled conditions. Addition of TiO_2 (1 g l^{-1}) was detrimental, even in the presence of H_2O_2 , indicating that at this concentration, TiO_2 inhibits the mineralization, probably by scattering or by screening of the light.

106 Anisimov, M. P., **P. K. Hopke**, et al. (2003). "General requirements and recommendations for vapor nucleation rate experiments." Aerosol Science and Technology **37**(2): 183-186.

Agreement between experimentally measured vapor nucleation rates and current theoretical predictions exists for only a limited number of systems. These inconsistencies can result from differences in measurement methods and assumptions used to interpret the experimental results. Usually the causes of these disagreements are unclear. The current state of the art is such that experimental results using different methods can lead to very different interpretations of the same phenomenon. In this note, well-defined standard systems are suggested as a means to verify experimental system performance. The combination n-pentanol-helium is suggested as a standard reference system. Using this system, measurements produced by multiple research groups have been compiled, and from these experimental results, a nucleation rate equation was developed that can serve as a standard basis for method comparison. This equation provides a scale to relate nucleation rates over a range of nucleation temperatures and is a useful basis of comparison even if the proposed equation is not fully accurate. It is further suggested that the nucleation rate measurements be performed using small steps in nucleation temperature of around 2degrees or less to identify the features in the system such as phase changes in the critical embryos. In this note, a method that uses monotonicity and continuity conditions for the nucleation rate surface to detect such singularities is outlined. These monotonicity and continuity criteria can be formulated as a dimensionless quantity. The semiempirical construction of nucleation rate surfaces can indicate conditions where multiple nucleation rate surfaces may be detected. Experimental systems that include size distribution measurements have the potential to discern particles produced through multiple nucleation channels such that nucleation rates can be measured for each channel. Detection of nucleation rate surface singularities is important because these singularities indicate the existence of two-channel nucleation where one-channel nucleation theory cannot be applied.

105 **Ahmadi, G.**, A. R. Mazaheri, et al. (2003). "A model for multiphase flows through poroelastic media." Journal of Porous Media **6**(4): 243-256.

A continuum model for multiphase fluid mixture flows through poroelastic media is presented. The basic conservation laws developed via a volume averaging technique are considered. Effects of phasic equilibrated forces are included in the model. Based on the thermodynamics of the multiphase mixture flows, appropriate constitutive equations are formulated. The entropy inequality is exploited, and the method of Lagrangian multiplier is used along with the phasic conservation laws to derive the constitutive equations for the phasic stress tensors, equilibrated stress vectors, and the interactions terms. The special cases of wave propagation in poroelastic media saturated with multiphase fluids, and multiphase flows through porous media, are studied. It is shown that the present theory leads to the extended Darcy's law and contains, as a special case, Biot's theory of saturated poroelastic media.

104 Ahmadi, A., B. Williamson, et al. (2003). "Life Cycle Inventory of Toner Produced for Xerographic Processes." Journal of Cleaner Production **11**(5): 573-582.

103 **Ababneh, A.**, F. Benboudjema, et al. (2003). "Chloride penetration in nonsaturated concrete." Journal of Materials In Civil Engineering **15**(2): 183-191.

The two governing equations that describe the diffusion of chloride ions into nonsaturated concrete are established. Material models for the four material parameters involved in the governing equations are developed, including chloride binding capacity, chloride diffusion coefficient, moisture capacity, and moisture diffusion coefficient. The planned attempt is to establish material models based on analytical results first, and if this is not possible, to develop empirical models based on dominant physical or chemical mechanism(s) at different scale levels and calibrate the individual model by related test data. The alternating-direction implicit (ADI) finite-difference method was employed for solving coupled two-dimensional moisture diffusion and chloride penetration equations. The numerical solutions are compared with the experimental results obtained by the 90-day ponding test (AASHTO T259-80). The numerical prediction agrees very well with the test data. Free chloride concentration profiles at different depths and different ages of concrete slab are presented. Two limiting cases for different initial relative humidity levels are analyzed in detail to study the dependence of the chloride diffusion on the moisture diffusion in nonsaturated concrete.

102 Zheng, L. and **P. D. Yapa** (2002). "Modeling Gas Dissolution in Deepwater Oil/Gas Spills." Journal of Marine Systems(March): 299-309.

101 **Zander, A. K.** (2002). "Protocol for Equipment Verification Testing for VOC Removal: Requirements for All Studies." EPA Document 02/9209/EPAWCTR.

100 Yip, W. K., M. Shen, et al. (2002). "Hydrodynamic modeling of short-channel devices using an upwind flux vector splitting scheme." Computer Methods In Applied Mechanics and Engineering **191**(47-48): 5427-5445.

Upwind flux vector splitting is presented for hydrodynamic modeling of 1D and 2D deep-submicron semiconductor devices. This approach splits the Jacobian matrices of the hydrodynamic system into two parts corresponding to forward and backward running fluxes, and an upwind difference is applied to each split flux. Influences of the boundary discontinuity of electric field and velocity on transport results in the 21) deep-submicron devices are discussed. The study demonstrates that the developed method is capable of handling large discontinuity of the boundary conditions, and highly non-linear source terms in short-channel semiconductor devices. (C) 2002 Elsevier Science B.V. All rights reserved.

99 Yi, Y., T. L. Theis, et al. (2002). "The effect of chlorination on organocyanide compounds." Water Environment Technology **74**(1): 51-56.

98 **Yapa, P. D.** and H. Xie (2002). "Modeling Underwater Oil/Gas Jets and Plumes: Comparison with Field Data." Journal of Hydraulic Engineering, ASCE(September): 855-860.

97 Xia, X. and **H. T. Shen** (2002). "Nonlinear Interaction of Ice Cover with Shallow Water Wave in Channels." Journal of Fluid Mechanics **467**: 259-267.

96 Vardar, N., M. Odabasi, et al. (2002). "Particulate Dry Deposition and Overall Deposition Velocities of Polycyclic Aromatic Hydrocarbons." Journal of Environmental Engineering **128**(3): 269-274.

95 Stone, B. and **H. T. Shen** (2002). "Hydraulic Resistance of Flow Channels with Cylindrical Roughness." Journal of Hydraulic Engineering **128**(5): 500-506.

94 Choi, H.-D. P. D. T. M. H., Ph.D. "Gaseous Mercury Emissions from Unsterilized and Sterilized Soils: The Effect of Temperature and UV Radiation." Elsevier Editorial System(tm) for Environmental Pollution Manuscript Draft.

Mercury (Hg) emissions from the soils taken from two different sites (deciduous and coniferous forests) in the Adirondacks were measured in outdoor and laboratory experiments. Some of the soil samples were irradiated to eliminate biological activity. The result from the outdoor measurements with different soil suggests the Hg emission from the soils is partly limited by fallen leaves covering the soils which helps maintain relatively high soil moisture and limits the amount of heat and solar radiation reaching the soil surface. IN laboratory experiments exposure to UV-A (365 nm) has no significant effect on the Hg emissions while the Hg emissions increases dramatically during exposure to UV-B (302 nm) light suggesting UV-B directly reduced soil-associated Hg. Overall these results indicate that for these soil biotic processes have a relatively constant and smaller influence on the Hg emission from the soil than the more variable abiotic processes.

93 Shams, M., **G. Ahmadi**, et al. (2002). "Computational modeling of flow and sediment transport and deposition in meandering rivers." Advances In Water Resources **25**(6): 689-699.

A computational modeling analysis of the flow and sediment transport, and deposition in meandering-river models was performed. The Reynolds stress transport model of the FLUENT(TM) code was used for evaluating the river flow characteristics, including the mean velocity field and the Reynolds stress components. The simulation results were compared with the available experimental data of the river model and discussed. The Lagrangian tracking of individual particles was performed, and the transport and deposition of particles of various sizes in the meandering river were analyzed. Particular attention was given to the sedimentation patterns of different size particles in the river-bend model. The flow patterns in a physical river were also studied. A Froude number based scale ratio of 1: 100 was used, and the flow patterns in the physical and river models are compared. The result shows that the mean-flow quantities exhibit dynamic similarity, but the turbulence parameters of the physical river are different from the model. More strikingly, the particle sedimentation features in the physical and river models do not obey the expected similarity scaling. Published by Elsevier Science Ltd.

92 Shahin, U. M., **T. M. Holsen**, et al. (2002). "Dry Deposition Measured with a Water Surface Sampler: A Comparison to Modeled Results." Atmospheric Environment **36**: 3267-3276.

91 **Rossner, A.**, S. P., et al. (2002). "Development of a flow controller for long-term sampling of gases and vapors using evacuated canisters." Environmental Science & Technology **36**(23).

90 **Rossner, A.**, J. P. Farant, et al. (2002). "Development of a flow controller for long-term sampling of gases and vapors using evacuated canisters." Environmental Science & Technology **36**(22): 4912-4920.

Anthropogenic activities contribute to the release of a wide variety of volatile organic compounds (VOC) into microenvironments. Developing and implementing new air sampling technologies that allow for the characterization of exposures to VOC can be useful for evaluating environmental and health concerns arising from such occurrences. A novel air sampler based on the use of a capillary flow controller connected to evacuated canisters (300 mL, 1 and 6 L) was designed and tested. The capillary tube, used to control the flow of air, is a variation on a sharp-edge orifice flow controller. It essentially controls the velocity of the fluid (air) as a function of the properties of the fluid, tube diameter and length. A model to predict flow rate in this dynamic system was developed. The mathematical model presented here was developed using the Hagen-Poiseuille equation and the ideal gas law to predict flow into the canisters used to sample for long periods of time. The Hagen-Poiseuille equation shows the relationship between flow rate, pressure gradient, capillary resistance, fluid viscosity, capillary length and diameter. The flow rates evaluated were extremely low, ranging from 0.05 to 1 mL min⁻¹. The model was compared with experimental results and was shown to overestimate the flow rate. Empirical equations were developed to more accurately predict flow for the 300 mL, 1 and 6 L canisters used for sampling periods ranging from several hours to one month. The theoretical and observed flow rates for different capillary geometries were evaluated. Each capillary flow controller geometry that was tested was found to generate very reproducible results, RSD < 2%. Also, the empirical formulas developed to predict flow rate given a specified diameter and capillary length were found to predict flow rate within 6% of the experimental data. The samplers were exposed to a variety of airborne vapors that allowed for comparison of the effectiveness of capillary flow controllers to sorbent samplers and to an online gas chromatograph. The capillary flow controller was found to exceed the performance of the sorbent samplers in this comparison.

89 Paatero, P., **P. K. Hopke**, et al. (2002). "Understanding and controlling rotations in factor analytic models." Chemometrics and Intelligent Laboratory Systems **60**(1-2): 253-264.

Positive Matrix Factorization (PMF) is a least-squares approach for solving the factor analysis problem. It has been implemented in several forms. Initially, a program called PMF2 was used. Subsequently, a new, more flexible modeling tool, the Multilinear Engine, was developed. These programs can utilize different approaches to handle the problem of rotational indeterminacy. Although both utilize non-negativity constraints to reduce rotational freedom, such constraints are generally insufficient to wholly eliminate the rotational problem. Additional approaches to control rotations are discussed in this paper: (1) global imposition of additions among "scores" and subtractions among the corresponding "loadings" (or vice versa), (2) constraining individual factor elements, either scores and/or loadings, toward zero values, (3) prescribing values for ratios of certain key factor elements, or (4) specifying certain columns of the loadings matrix as known fixed values. It is emphasized that application of these techniques must be based on some external information about acceptable or desirable shapes of factors. If no such a priori information exists, then the full range of possible rotations can be explored, but, there is no basis for choosing one of these rotations as the "best" result. Methods for estimating the rotational ambiguity in any specific result are discussed. (C) 2002 Elsevier Science B.V. All rights reserved.

88 Paatero, P. and **P. K. Hopke** (2002). "Utilizing wind direction and wind speed as independent variables in multilinear receptor modeling studies." Chemometrics and Intelligent Laboratory Systems **60**(1-2): 25-41.

The problem of identifying sources of airborne pollutants and providing quantitative estimates of the contributions of each of those sources is important for airborne particulate matter. Various forms of factor analysis have been applied to this problem. However, in factor analysis, there is the fundamental problem of rotational ambiguity that makes the problem ill-posed. Thus, the incorporation of additional information can be useful in improving the solutions. Especially for identifying local sources, wind data (direction and speed) could be valuable additional information in such receptor modeling. However, wind data cannot be used directly as dependent variables in factor analytic modeling because the dependence of observed concentrations on wind variables is far from linear. An expanded multilinear model has been developed in which the wind direction, speed and other variables are included as independent variables. For each source, the analysis computes a directional profile that indicates how much of the concentrations are explained by the factors depending on wind direction, speed, and other values. This model has been tested using simulated data developed by the U.S. Environmental Protection Agency as part of a workshop to test advanced factor analysis methods. For most of the local sources, well-defined directional profiles were obtained. (C) 2002 Elsevier Science B.V. All rights reserved.

87 Northway, M. J., R. S. Gao, et al. (2002). "An analysis of large HNO₃-containing particles sampled in the Arctic stratosphere during the winter of 1999/2000." Journal of Geophysical Research-Atmospheres **107**(D20).

Large (>2 μm diameter) HNO₃-containing polar stratospheric cloud (PSC) particles were measured in situ by the NOAA NOy instrument on board the NASA ER-2 aircraft during seven flights in the 1999/2000 Arctic winter vortex. Here we discuss the detection of these large PSC particles, their spatial distribution, the ambient conditions under which they were detected, and our methods for interpreting NOy time series with respect to particle sizes and number concentrations. The particles were observed through the use of two NOy inlets on a particle separator extending below the ER-2 aircraft. The particle phase is assumed to be nitric acid trihydrate (NAT) or nitric acid dihydrate (NAD). Over a 48-day period, particles were sampled in the Arctic vortex over a broad range of latitudes (60-85degreesN) and altitudes (15-21 km). Typically, regions of the atmosphere up to 4 km above the observed large particle clouds were saturated with respect to NAT. Occasionally, large particles were measured in air subsaturated with respect to NAT, suggesting ongoing particle evaporation. Vortex minimum temperatures in the observation period suggest that synoptic-scale ice saturation conditions are not required for the formation of this type of particle. Three analytical methods are used to estimate size and number concentrations from the NOy time series. Results indicate particle sizes between 5 and 20 μm diameter and concentrations from 10⁽⁻⁵⁾ to 10⁽⁻³⁾ cm⁽⁻³⁾. These low number concentrations imply a selective nucleation mechanism. Particle sizes and number concentrations were greater during the midwinter flights than the late winter flights. Knowledge of the geographical extent of large particles, actual sampling conditions, and particle size distributions offers multiple constraints for atmospheric models of PSC formation, which will lead to a better understanding of the process of denitrification and improvements in modeling future ozone loss.

86 **Menz, F. C.** (2002). "The U.S. Experience with Motor Vehicle Pollution Control: Implications for China: Part II." World Environment **77**(5): 33-36.

85 **Menz, F. C.** (2002). "The U.S. Experience with Motor Vehicle Pollution Control: Implications for China: Part I." World Environment **77**(4): 26-28.

84 **Menz, F. C.** (2002). "The U.S. Experience with Controlling Motor Vehicle Pollution: Lessons for China." International Journal of Environment and Pollution **18**(1): 1-22.

83 Marzocca, P., L. Librescu, et al. (2002). "Aeroelasticity of a Two Dimensional Lifting Surfaces Via Indicial Function Approach." The Aeronautical Journal(March): 147-153.

82 Marzocca, P., L. Librescu, et al. (2002). "Aeroelastic response of a 2-D Airfoil in Compressible Flight Speed Regimes Exposed to Blast Loadings." Aerospace Science and Technology **6**(4): 259-272.

81 Lee, J. H., Y. Yoshida, et al. (2002). "Identification of sources contributing to Mid-Atlantic regional aerosol." Journal of The Air & Waste Management Association **52**(10): 1186-1205.

Source types or source regions contributing to the concentration of atmospheric fine particles measured at Brigantine National Wildlife Refuge, NJ, were identified using a factor analysis model called Positive Matrix Factorization (PMF). Cluster analysis of backward air trajectories on days of high- and low-factor concentrations was used to link factors to potential source regions. Brigantine is a Class I visibility area with few local sources in the center of the eastern urban corridor and is therefore a good location to study Mid-Atlantic regional aerosol. Sulfate (expressed as ammonium sulfate) was the most abundant species, accounting for 49% of annual average fine mass. Organic compounds (22%; expressed as 1.4 x organic carbon) and ammonium nitrate (10%) were the next abundant species. Some evidence herein suggests that secondary organic aerosol formation is an important contributor to summertime regional aerosol.

80 Krewski, D., J. H. Lubin, et al. (2002). "Projection of residential radon lung cancer risks: The BEIR VI risk models." Radiation Protection Dosimetry **102**(4): 371-373.

79 Kerr, D. J., **H. T. Shen**, et al. (2002). "Evolution and Hydraulic Resistance of Anchor Ice on Gravel Bed." Cold Regions Science and Technology **32**(2): 101-114.

78 Hwang, S., K. Lee, et al. (2002). "Models for Estimating Soil Particle Size Distributions." Soil Sci. Soc. Am. J. **66**(4): 1143-1150.

77 Hugaboom, D. A. and **S. E. Powers** (2002). "Recovery of Coal Tar and Creosote from Porous Media: The Influence of Wettability." Ground Water Monitoring and Remediation **22**(4): 83-90.

76 Huang, K. L., **T. M. Holsen**, et al. (2002). "Impurity partitioning of Nafion and Ceramic Separators Used for Electrolytic Purification of Spent Chromium Plating Solutions." Journal of Membrane Science **210**(1): 133-141.

75 **Hopke, P. K.** and P. Paatero (2002). "Remarks on the article 'Bilinear estimation of pollution source profiles and amounts by using multivariate receptor models'." Environmetrics **13**(7): 803-805.

74 Hirayama, K., M. Yamazaki, et al. (2002). "Aspects of River Hydrology in Japan." Hydrological Processes **16**(4): 891-904.

73 Hanisco, T. F., J. B. Smith, et al. (2002). "Quantifying the rate of heterogeneous processing in the Arctic polar vortex with in situ observations of OH." Journal of Geophysical Research-Atmospheres **107**(D20).

We present simultaneous in situ observations of OH, HO₂, ClONO₂, HCl, and particle surface area inside a polar stratospheric cloud undergoing rapid heterogeneous processing. A steady-state analysis constrained by in situ observations is used to show that concentrations of OH calculated during a processing event are extremely sensitive to the assumptions regarding aerosol composition and reactivity. This analysis shows that large perturbations in the abundance of OH are consistent with the heterogeneous production of HOCl via ClONO₂ + H₂O → HOCl + HNO₃ and removal via HOCl + HCl → Cl₂ + H₂O in a polar stratospheric cloud. If the cloud is composed of supercooled ternary solution (STS) aerosols and solid nitric acid trihydrate (NAT) particles, comparison with observations of OH show that modifications to surface reactivity to account for high HNO₃ content in STS aerosols and low HCl coverage on NAT particles are appropriate. These results indicate that with the low HCl levels in this encounter and in a processed polar vortex in general, reactions on STS aerosols dominate the total heterogeneous processing rate. As a consequence, the formation of NAT does not lead to significantly faster reprocessing rates when HCl concentrations are low and STS aerosols are present. Model calculations that include these modifications to uptake coefficients for STS and NAT will lead to significantly slower reprocessing and faster recovery rates of chlorine in the springtime Arctic polar vortex.

72 Giese, S. W. and **S. E. Powers** (2002). "Using Polymer Solutions to Enhance the Recovery of Coal Tar and Creosote DNAPLs." Journal of Contamination Hydrology **58**(1-2): 147-167.

71 **Dhaniyala, S.**, K. A. McKinney, et al. (2002). "Lee-wave clouds and denitrification of the polar stratosphere." Geophysical Research Letters **29**(9): Art. No. - 1322.

[1] We present a hypothesis that the known formation of nitric acid hydrates in lee-wave ice clouds produces a "standing crop" of nitric acid trihydrate (NAT) particles, and that growth and sedimentation of these particles efficiently denitrifies the polar stratosphere. Simulations using a simple two-dimensional model illustrate that the large NAT number concentrations produced in lee waves (>0.1 cm⁻³) lead to low gas-phase HNO₃ concentration in the cloud layer, limiting subsequent particle growth. Provided the NAT existence temperature is not exceeded, these particles slowly sediment out of the cloud layer, at which point further growth is initiated. As a result of the long residence time and vertical wind shear, NAT particles produced

in geographically selective regions over a short duration can cause extensive denitrification throughout the lower stratosphere. Our model illustrates that a single hypothetical lee-wave nucleation event [10 hours, 1000 km width (along a longitude) x 100 m altitude] is sufficient to produce significant denitrification (similar to 25%) vortex-wide.

70 Cleveland, C. T., T. F. Seacord, et al. (2002). "Standardized Membrane Pore Characterization by Polyethylene Rejection." Journal of Environmental Engineering **128**(5): 399-407.

69 **Baltus, R. E.** and B. K. Lavine (2002). "Kinetic Modeling of Micellar Liquid Chromatography, Sep." Science & Technology **37**: 3443.

68 Ahmed, M. I., J. R. Selman, et al. (2002). "Electrochemical Choric Acid Regeneration Process: Fitting of Membrane Transport Properties." Journal of Membrane Science **197**: 63-74.

67 **Ahmadi, G.** and D. H. Smith (2002). "Analysis of steady-state filtration and backpulse process in a hot-gas filter vessel." Aerosol Science and Technology **36**(6): 665-677.

The need to develop a technology for clean and efficient electric power generation has led to the development of advanced pressurized fluidized bed combustors (PFBC) and integrated gasification combined cycles (IGCC). The effective filtration of hot gases for removal of ash and sulfur sorbent, however, is the key to the success of these advanced coal energy systems. Recently, attention has been given to the use of ceramic candle filters for hot-gas cleaning. The ash cake formation on these filters needs to be removed by the backpulse for their successful operation. In this paper, steady-state filtration as well as the transient gas flow during the backpulse process in the integrated gasification and cleanup facility (IGCF) (located at the National Energy Technology Laboratory, NETL) is studied. The steady-state filtration condition is first evaluated, using a compressible heat-conducting flow analysis. Particle transport patterns are studied, and the deposition patterns of 1-30 μm particles on the ceramic filters and the vessel surfaces are analyzed. To simulate the backpulse process, the pressure at the filter exit is increased sharply in a period of about 0.01 s pressure. The stress transport model of the FLUENT code is used to evaluate the time evolution of the transient gas flow velocity, pressure and thermal fields, as well as turbulence intensities and stresses inside the candle filter and in the IGCF filter vessel. Contour plots of the hot-gas flow conditions from the start of the pressure buildup to its saturation level are presented. The results show the rapidly changing flow conditions during the initial stages of the backpulse. The pressure wave propagates along the length of the filter until a monotonic increase of pressure with time is achieved; that is, the pressure field inside the filter at the initial stages of the backpulse is strongly nonuniform. Therefore the potential for incomplete filter cake removal exists. Motions of particles that enter the vessel and/or are ejected from the candle filter during the backpulse process are also studied, and illustrative particle trajectories are presented.

66 **Ababneh, A.** and Y. Xi (2002). "An experimental study on the effect of chloride penetration on moisture diffusion in concrete." Materials and Structures **35**(254): 659-663.

Chloride penetration and moisture diffusion are two important transport processes for studying the long-term durability of concrete. The chloride penetration and moisture transfer in concrete are considered as two coupled transport processes. An experimental study was

conducted for determining, the related material parameters in the coupled transport processes. For the coupled moisture diffusion, we consider that the total moisture flux $J(H)(t)$ is resulted from two driving forces: the gradient of moisture H , and the gradient of free chloride $C-f$, that is, $J(H)(t) = -D(H-H)\text{grad}(H) - D(H-Cl)\text{grad}(C-f)$. In this formulation, two transport parameters are involved: the moisture diffusion coefficient $DH-H$, and the coupled moisture diffusion coefficient due to chloride diffusion $DH-Cl$. A seepage test was designed specifically for determining the two transport parameters. The test data showed that the chloride penetration accelerates the moisture diffusion significantly. The two transport parameters were determined using the present test data. The result showed that $DH-Cl$ is not a constant, but depends linearly on the free chloride concentration.

65 Zheng, J. and **S. E. Powers** (2001). "Asphaltenes from coal tar and creosote: Their role in reversing the wettability of aquifer systems." Journal of Colloid and Interface Science **224**(2): 365-371.

64 Zheng, J., S. Behrens, et al. (2001). "Predicting the Wettability of Quartz Surfaces Exposed to Dense Non-aqueous Phase Liquids." Environmental Science & Technology **35**(11): 2207-2213.

63 **Zander, A. K.** and N. K. Curry (2001). "Membrane and Solution Effects on Solute Rejection and Productivity." Water Research **35**(18): 4426-4434.

62 Yi, S. S., E. Y. Lee, et al. (2001). "Dry Deposition Fluxes and Size Distribution of Heavy Metals in Seoul, Korea During Yellow-Sand Events." Aerosol Science and Technology **35**: 569-576.

61 Yi, S. M., U. M. Shahin, et al. (2001). "Overall Elemental Deposition Velocities Measured Around Lake Michigan." Atmospheric Environment **35**: 1133-1140.

60 **Yapa, P. D.**, L. Zheng, et al. (2001). "A Model for Deepwater Oil/Gas Blowouts." Marine Pollution Bulletin (The International Journal for Marine Environmental Scientists/Engineers) **43**(7): 234-241.

59 Wang, J. H. and **P. K. Hopke** (2001). "Equation-oriented system: an efficient programming approach to solve multilinear and polynomial equations by the conjugate gradient algorithm." Chemometrics and Intelligent Laboratory Systems **55**(1-2): 13-22.

The factor analysis problem can be conceptualized as an expansion of polynomial equations that are solvable using least-squares methods. The equation-oriented system (EOS) is introduced as a method for solving polynomial equations using a preconditioned conjugate gradient (CG) algorithm for the normal equations, EOS is a fast, easy to program, low computer memory requirement method for accomplishing this task. EOS can be used to solve multilinear and PARAFAC problems. The practical aspects of implementing EOS in MATLAB are discussed. (C) 2001 Elsevier Science B.V. All rights reserved.

58 Tolve, N. S. and **T. C. Young** (2001). "Interactions of natural colloidal material and phenanthrene in the aquatic environment." **11**(3): 35-47.

57 Song, X. H., A. V. Polissar, et al. (2001). "Sources of fine particle composition in the northeastern US." Atmospheric Environment **35**(31): 5277-5286.

Fine particle composition data obtained at three sampling sites in the northeastern US were studied using a relatively new type of factor analysis, positive matrix factorization (PMF). The three sites are Washington, DC, Brigantine, NJ and Underhill, VT. The PMF method uses the estimates of the error in the data to provide optimal point-by-point weighting and permits efficient treatment of missing and below detection limit values. It also imposes the non-negativity constraint on the factors. Eight, nine and 11 sources were resolved from the Washington, Brigantine and Underhill data, respectively. The factors were normalized by using aerosol fine mass concentration data through multiple linear regression so that the quantitative source contributions for each resolved factor were obtained. Among the sources resolved at the three sites, six are common. These six sources exhibit not only similar chemical compositions, but also similar seasonal variations at all three sites. They are secondary sulfate with a high concentration of S and strong seasonal variation trend peaking in summer time; coal combustion with the presence of S and Se and its seasonal variation peaking in winter time; oil combustion characterized by Ni and V; soil represented by Al, Ca, Fe, K, Si and Ti; incinerator with the presence of Pb and Zn; sea salt with the high concentrations of Na and S. Among the other sources, nitrate (dominated by NO₃⁻) and motor vehicle (with high concentrations of organic carbon (OC) and elemental carbon (EC), and with the presence of some soil dust components) were obtained for the Washington data, while the three additional sources for the Brigantine data were nitrate, motor vehicle and wood smoke (OC, EC, K). At the Underhill site, five other sources were resolved. They are wood smoke, Canadian Mn, Canadian Cu smelter, Canadian Ni smelter, and another salt source with high concentrations of Cl and Na. A nitrate source similar to that found at the other sites could not be obtained at Underhill since NO₃⁻ was not measured at this site. Generally, most of the sources at the three sites showed similar chemical composition profiles and seasonal variation patterns. The study indicated that PMF was a powerful factor analysis method to extract sources from the ambient aerosol concentration data. (C) 2001 Elsevier Science Ltd. All rights reserved.

56 Song, X. H., N. M. Faber, et al. (2001). "Source apportionment of gasoline and diesel by multivariate calibration based on single particle mass spectral data." Analytica Chimica Acta **446**(1-2): 329-343.

The mass apportionment of gasoline and diesel particles in ambient aerosol samples is a difficult problem because both sources exhibit very similar chemical composition. However, individual particle analysis could provide additional information and help achieve source apportionment with good accuracy. Aerosol time-of-flight mass spectrometry (ATOFMS) has proven to be a powerful technique capable of simultaneously determining both the size and chemical composition of single particles in real time. Thus, samples of gasoline and diesel particles were analyzed by ATOFMS for their single particle information. In addition to the aerodynamic diameter from which the individual particle mass can be estimated, positive and negative mass spectra were obtained for each particle. A novel data analysis approach based on the combination of an adaptive resonance theory-based neural network (ART-2a), and a multivariate calibration method, partial least squares (PLS), has been developed to apportion the

mass contributions of gasoline and diesel sources to mixture samples. The ART-2a neural network was used first to classify the particle-by-particle mass spectral data. The source profile for each source (gasoline/diesel) was obtained in terms of the mass fractions of the classified particle types. Next, PLS was applied to build a model relating the mass fractions of different particle classes and the mass contributions of the two sources to mixture samples. Artificial mixture samples obtained by randomly mixing some particles from the two source samples have been used to examine the feasibility of the proposed method. Satisfactory predictions for the mass contributions of gasoline and diesel exhaust to the mixture samples have been obtained. A recently proposed formula for prediction error variance is successfully modified to quantify the uncertainty in the PLS predictions. This study exemplifies the potential promise of multivariate calibration as applied to the aerosol source apportionment problem. (C) 2001 Elsevier Science B.V. All rights reserved.

55 **Sokolov, I.**, D. S. Smith, et al. (2001). "Cell surface electrochemical heterogeneity of the Fe(III)-reducing bacteria *Shewanella putrefaciens*." Environmental Science & Technology **35**(2): 341-347.

Acid-base titration experiments and electrostatic force microscopy (EFM) were used to investigate the cell surface electrochemical heterogeneity of the Fe(III)-reducing bacteria, *Shewanella putrefaciens*. The acid-base titrations extended from pH 4 to 10; and the titration data were fit using a linear programming pK(a) spectrum approach. Overall, a five-site model accounted for the observed titration behavior with the most acidic sites corresponding to carboxylic groups and phosphodiester groups, intermediate: sites phosphoryl groups, and two basic sites equivalent to amine or hydroxyl groups. The pH for the point of zero charge on the bacteria was 5.4. In EFM images of cells rinsed in solutions at pH 4.0, 7.0, and 8.0, a pronounced increase in small (less than or equal to 100 nm diameter) high contrast patches was observed on the cells with increasing pH. The pH dependence of EFM image contrast paralleled the pattern of cell surface charge development inferred from the titration experiments; however, quantitative analysis of high Contrast regions in the EFM images yielded lower surface charge values than those anticipated from the titration data. For example at pH 7, the calculated surface charge of high contrast regions in EFM images of the bacterial cells was $-0.23 \mu\text{C}/\text{cm}^2$ versus $-20.0 \mu\text{C}/\text{cm}^2$ based on the titration curve. The differences in surface charge estimates, between the EFM images and titration data are consistent not only with charge development throughout the entire-volume of the bacterial cell wall (i.e., in association with functional groups that are not directly exposed at the cell surface) but also with the presence of a thin structural layer of water containing charge-compensating counterions. In combination, the pK(a) spectra and EFM data demonstrate that a particularly high degree of electrochemical heterogeneity exists within the cell wall and at the cell surface of *S. putrefaciens*.

54 Sofuoglu, A., M. Odabasi, et al. (2001). "Temperature Dependence of Gas-Phase Polycyclic Aromatic Hydrocarbon and Organochlorine Pesticide Concentrations in Chicago Air." Atmospheric Environment **35**: 6503-6510.

53 **Shen, H. H.** and Y. Zhong (2001). "Theoretical Study of drift of small rigid floating objects in wave fields." ASCE/ J. Waterway, Port, Coastal, and Ocean Engineering **126**(6): 343-351.

52 **Shen, H. H.**, S. F. Ackley, et al. (2001). "A conceptual model for pancake-ice formation in a wave field." Ann. Glaciol. **33**: 361-367.

51 Shams, M., **G. Ahmadi**, et al. (2001). "Transport and deposition of flexible fibers in turbulent duct flows." Journal of Aerosol Science **32**(4): 525-547.

Transport, dispersion, and deposition of flexible fibrous particles in the near-wall coherent vortices in a turbulent duct flow are studied. The vortical flow field is modeled as a sequence of plane stagnation point flows. Fibers are assumed to be inextensible but completely flexible. That is, fibers have no stiffness and offer no resistance to bending. In the simulation, a flexible fiber is divided into many segments. Interactions of each element with the adjacent elements are through interfacial forces that are evaluated as part of the solution. For different fiber diameters, aspect ratios, and initial configurations, deposition velocities are evaluated, and the fiber dispersion is analyzed. An empirical equation for the deposition velocity of flexible fibers is also developed. The results for flexible fiber deposition rate are compared with those for rigid straight fibers and the empirical equation predictions. (C) 2001 Elsevier Science Ltd. All rights reserved.

50 Ramadan, Z., X. H. Song, et al. (2001). "Variable selection in classification of environmental soil samples for partial least square and neural network models." Analytica Chimica Acta **446**(1-2): 233-244.

Two variable selection methods were evaluated by comparing their predictions with respect to differentiating among environmental soil samples. The focus of this work is to determine which input variables are most relevant for prediction of soil sources using discriminant partial least square (D-PLS) and back-propagation artificial neural network (BP-ANN) models. The methods investigated were stepwise variable selection method and genetic algorithms (GAs). Microbial community DNA was extracted from 48 environmental soil samples derived from different field crops and soil sources. After amplification of bacterial ribosomal RNA genes by polymerase chain reaction (PCR), the products were separated by gel electrophoresis. Characteristic complex band patterns were obtained, indicating high bacterial diversity. Two hundred and twenty-three DNA band patterns produced in the gels of the soil samples were used in the analysis, after removal of included DNA standard markers. Based on the brightness of the bands, densitometric curves of the selected DNA band pattern were extracted from the gel images. The curves were smoothed using Savitsky-Golay method and scaled to the DNA standard markers. The prediction results based on the two variable selection methods for PLS and ANN models are presented and compared. Both methods gave good results before any variable selection methods, with the ANN being better than D-PLS. The prediction performance of both methods especially the D-PLS were improved by applying the stepwise variable selection and the GA variable selection method. The study also shows that GA variable selection had a significant improvement of the predictive ability than the stepwise variable selection method. (C) 2001 Elsevier Science B.V. All rights reserved.

49 **Powers, S. E.**, D. Rice, et al. (2001). "Replacing MTBE with Ethanol as a Gasoline Oxygenate-How Many Ground Water Resources Be Impacted?" Environmental Science & Technology **35**(1): 79-123.

48 Powers, S. E., C. S. Hunt, et al. (2001). "The transport and fate of ethanol and BTEX in groundwater contaminated by gasohol." Critical Reviews in Environmental Science and Technology **31**(1): 79-123.

47 Polissar, A. V., P. K. Hopke, et al. (2001). "Atmospheric aerosol over Vermont: Chemical composition and sources." Environmental Science & Technology **35**(23): 4604-4621. Aerosol chemical composition data for PM_{2.5} samples collected during the period from 1988 to 1995 at Underhill, VT, were analyzed. Sulfur and black carbon mass concentrations ranged from 0.01 to 6.5 $\mu\text{g m}^{-3}$ and from 0.05 to 2.2 $\mu\text{g m}^{-3}$, respectively, while the total fine aerosol mass concentration ranged from 0.2 to 51.1 $\mu\text{g m}^{-3}$. Seasonal variations with maxima during the summer and minima in winter/spring were observed for sulfur and the fine mass concentrations. No annual pattern was observed for black carbon. Seasonal variations for most of the other anthropogenic species had maxima in winter and spring and minima in the summer. A factor analysis method, positive matrix factorization (PMF), utilizing error estimates of the data to provide optimum data point scaling was used to obtain information about possible sources of the aerosol. An 11-factor solution was obtained. The six sources representing wood burning, coal and oil combustion, coal combustion emissions plus photochemical sulfate production, metal production plus municipal waste incineration, and emissions from motor vehicles were identified. Emissions from smelting of nonferrous metal ores, arsenic smelting, and soil particles and particles with high concentrations of Na were also identified by PMF. Potential source contribution function (PSCF) analysis combines the aerosol data with the air parcel backward trajectories. PSCF was applied to identify possible source areas and pathways that give rise to the observed high particulate mass concentrations from these 11 sources. The CAPITA Monte Carlo trajectory model was used to obtain 10 sets of 5-day air parcel back trajectories arriving every 2 h for the 7-yr period from 1988 to 1995. The PSCF plot for the black carbon factor shows high probabilities in the area surrounding the sampling site, indicating a strong local influence from residential wood combustion in northern New England and southwestern Quebec. Similar large potential source areas in the midwestern United States were identified for the two coal combustion factors. The midwestern United States was also identified as the source region for the Zn-Pb factor. The oil combustion factor was associated with the east coast of the United States. The results for the Pb-Mn factor suggests high probability over the nearby Montreal urban area and the areas in the midwestern United States. The windblown dust emissions from the areas to the north are significant contributors for the soil factor. Canadian Ni smelters are the main sources for the As factor, although there is some contribution from coal-fired power plants to the south and west of Underhill, VT. It is concluded that the combination of the two receptor modeling methods, PMF and PSCF, provides an effective way. In identifying atmospheric aerosol sources and their likely locations. Emissions from different anthropogenic activities as well as secondary aerosol production are the main sources of aerosol measured in Vermont. Fuel combustion, local wood smoke, municipal waste incineration, and the secondary sulfate production collectively accounted for about 87% of the fine mass concentrations measured in Vermont.

46 Polissar, A. V., **P. K. Hopke**, et al. (2001). "Source regions for atmospheric aerosol measured at Barrow, Alaska." Environmental Science & Technology **35**(21): 4214-4226.

Aerosol data consisting of condensation nuclei (CN) counts, black carbon (BC) mass concentration, and aerosol light scattering coefficient at the wavelength of 450 nm (SC) measured at Barrow, AK, from 1986 to 1997 have been analyzed. BC and SIC show an annual cycle with the Arctic haze maxima in the winter and spring and the minima in the summer. The CN time series shows two maxima in March and August, Potential source contribution function (PSCF) that combines the aerosol data with air parcel backward trajectories was applied to identify potential source areas and the preferred pathways that give rise to the observed high aerosol concentrations at Barrow. Ten-day isentropic back trajectories arriving twice daily at 500 and 1500 m above sea level were calculated for the period from 1986 to 1997. The PSCF analyses were performed based on the 80th percentile criterion values for the 2- and 24-h averages of the measured aerosol parameters. There was a good correspondence between PSCF maps for the 2- and 24-h averages, indicating that 1-day aerosol sampling in the Arctic adequately represents the aerosol source areas. In winter, the high PSCF values for BC and SIC are related to industrial source areas in Eurasia. The trajectory domain in winter and spring is larger than in summer, reflecting weaker transport in summer. No high PSCF areas for BC and SIC can be observed in summer. The result is related to the poor transport into the Arctic plus the strong removal of aerosol by precipitation in summer. In contrast to the BC and SC maps, the CN plot for summer shows high PSCF areas in the North Pacific Ocean. High CN values appear to be mostly connected with the long-range transport from Eurasia in winter and spring and with the reduced sulfur compound emission from biogenic activities in the ocean in the summer. PSCF analysis was found to be effective in identifying potential aerosol source areas.

45 Poirot, R. L., P. R. Wishinski, et al. (2001). "Comparative application of multiple receptor methods to identify aerosol sources in northern Vermont." Environmental Science & Technology **35**(23): 4622-4636.

This study applies and compares results of four receptor modeling techniques to a common set of speciated fine particle measurement data collected at a remote site in northwestern Vermont between 1988 and 1995. Two multivariate mathematical models, positive matrix factorization and UNMIX, were applied to the measurement data and identified seven "common" sources that had similar compositions and similar fine mass contributions in both models. Two ensemble backward trajectory techniques, potential source contribution function and residence-time analysis, were also applied to evaluate and interpret the mathematical model results. The trajectory techniques indicate a strong regional character to the upwind locations associated with aerosol contributions from most of the sources identified independently by the mathematical models and help in the interpretation of those results. The process of model comparison provides insights on the strengths and limitations of the individual and combined source attribution techniques. Convergent results among the multiple methods provide a degree of confidence that each of the receptor methods may represent useful tools for future air quality management. Divergent or inconsistent results among the models can help identify limitations of the individual models and of the underlying aerosol and meteorological data sets.

44 Ortmeyer, T. H. and P. Pillay (2001). "Trends in Transportation Sector Technology Energy Use and GHG Emissions." Proceedings of the IEEE **89**(12): 1837-1847.

43 Odabasi, M., A. Sofuoglu, et al. (2001). "Mass Transfer Coefficients for Polycyclic Aromatic Hydrocarbons (PAHs) to the Water Surface Sampler: Comparison to Modeled Results." Atmospheric Environment **35**(9): 1655-1662.

42 **Menz, F. C.** and H. M. Siep (2001). "Acid Rain in Europe and the United States: An Update." Environmental Science & Policy **7**(4): 253-265.

41 **Menz, F. C.** (2001). "Green Electricity Policies in the United States: Policy Analysis and Case Study." Energy Journal: IN PRESS.

40 Mavliev, R., **P. K. Hopke**, et al. (2001). "A transition from heterogeneous to homogeneous nucleation in the turbulent mixing CNC." Aerosol Science and Technology **35**(1): 586-595.

A new method for changing the supersaturation in the Turbulent Mixing CNC has been developed and used to examine the transition from heterogeneous nucleation of test particles to homogenous nucleation of working fluid: dibutylphthalate (DBP). Supersaturation was controlled by changing the DBP vapor pressure in the nozzle flow by saturating only a predetermined part of the flow, while the total flow and temperature remain constant. This approach allows for the changing of the initial DBP vapor pressure, while keeping the flow structure and temperature field unchanged. The DBP concentration in the outlet of the vapor generator was measured experimentally for different ratios of saturated and bypass flows and found to be close to estimated values. Experimental results for transitions from heterogeneous nucleation to homogeneous nucleation are presented for NaCl and WO_x particles at various DBP vapor pressures. With an increasing of the DBP vapor pressure, the concentration of enlarged particles increases until it reaches a plateau. At higher initial values of DBP pressure, homogeneous nucleation prevails, and the number concentration of particles follows a curve typical for homogeneous nucleation recorded in the absence of nuclei. Nuclei with different mobility diameters were activated at different values of vapor pressure. There are significant differences in the slopes of particle activation curves for NaCl and WO_x particles. The reasons for such differences are a subject for continuing research.

39 Matyjaszewski, K., H. J. Paik, et al. (2001). "Free Radical Intermediates in Atom Transfer Radical Addition and Polymerization: Study of Racemization, Halogen Exchange, and Trapping Reactions." Macromolecules **34**: 3127-3129.

38 Lucey, D., L. Hadjiiski, et al. (2001). "Identification of sources of pollutants in precipitation measured at the mid-Atlantic US coast using potential source contribution function (PSCF)." Atmospheric Environment **35**(23): 3979-3986.

Potential source contribution function (PSCF) was employed to study the source receptor relationships for 14 chemical species (Mn, SO₄²⁻, Zn, Al, Fe, Cu, Cr, Ni, Cd, NO₃, NH₄⁺, K⁺, Mg²⁺, and Pb) found in precipitation collected at Lewes, Delaware. This study identified areas of the Eastern United States as possible emission source areas that could have contributed to the 14 element concentrations observed at Lewes. The identified regions in the Eastern United States generally coincide well with known emission source areas. The likely emission sources for these chemical species include oil- and coal-fired power plants, incinerators, motor vehicles, and iron and steel mills. (C) 2001 Elsevier Science Ltd. All rights reserved.

37 Hopkins, M. A. and **H. H. Shen** (2001). "Simulation of pancake-ice dynamics in a wave field." Ann. Glaciol. **33**: 355-360.

36 **Hopke, P. K.**, C. H. Liu, et al. (2001). "Multiple imputation for multivariate data with missing and below-threshold measurements: Time-series concentrations of pollutants in the Arctic." Biometrics **57**(1): 22-33.

Many chemical and environmental data sets are complicated by the existence of fully missing values or censored values known to lie below detection thresholds. For example, week-long samples of airborne particulate matter were obtained at Alert, NWT, Canada, between 1980 and 1991, where some of the concentrations of 24 particulate constituents were coarsened in the sense of being either fully missing or below detection limits. To facilitate scientific analysis, it is appealing to create complete data, by filling in missing values so that standard complete-data methods can be applied. We briefly review commonly used strategies for handling missing values and focus on the multiple-imputation approach, which generally leads to valid inferences when faced with missing data. Three statistical models are developed for multiply imputing the missing values of airborne particulate matter. We expect that these models are useful for creating multiple imputations in a variety of incomplete multivariate time series data sets.

35 **Hopke, P. K.**, S. Landsberger, et al. (2001). "Stepping back in time: Neutron activation analysis of Finnish filters collected between 1964 and 1978." Abstracts of Papers of The American Chemical Society **221**: U88-U88.

34 Frankenstein, S., S. Loset, et al. (2001). "Wave-Ice Interactions in Barents Sea Marginal Ice Zone." ASCE/ J. Cold Regions Engineering **15**(2): 91-102.

33 Fergenson, D. P., X. H. Song, et al. (2001). "Quantification of ATOFMS data by multivariate methods." Analytical Chemistry **73**(15): 3535-3541.

Aerosol time-of-flight mass spectrometry (ATOFMS) is capable of measuring the sizes and chemical compositions of individual polydisperse aerosol particles in real time. A qualitative estimate of the particle composition is acquired in the form of a mass spectrum that must be subsequently interpreted in order to draw conclusions regarding atmospheric relevance. The actual problem involves developing a calibration that allows the mass spectral data to be transformed into estimates of the composition of the atmospheric aerosol. A properly calibrated ATOFMS system should be able to quantitatively determine atmospheric concentrations of various species. Ideally, it would be able to accomplish this more rapidly, accurately, with higher size and time resolution, and at a far lower marginal cost than the manual sampling methods that are currently employed. Attempts have already been made at using ATOFMS and similar techniques to extract the bulk chemical species concentration present in an ensemble of particles. This study represents the use of a multivariate calibration method, two-dimensional partial least-squares analysis, for calibrating single-particle mass spectral data. The method presented here is far less labor-intensive than the univariate methods attempted to date and allows for less observer bias. Because of the labor savings, this is also the most comprehensive calibration performed to date, resulting in the quantification of 44 different chemical species.

32 Farhan, S., **T. M. Holsen**, et al. (2001). "The Interaction of Soil Air Permeability and Soil Vapor Extraction." Journal of Environmental Engineering **127**(1): 32-36.

31 Farhan, S., **T. M. Holsen**, et al. (2001). "Experimental Investigation of the Interaction Soil Air Permeability and Soil Extraction." Journal of Environmental Engineering **1**(32-37): 1133-1140.

30 Fahey, D. W., R. S. Gao, et al. (2001). "The detection of large HNO₃-containing particles in the winter arctic stratosphere." Science **291**(5506): 1026-1031.

Large particles containing nitric acid (HNO₃) were observed in the 1999/2000 Arctic winter stratosphere. These in situ observations were made over a Large altitude range (16 to 21 kilometers) and horizontal extent (1800 kilometers) on several airborne sampling flights during a period of several weeks. With diameters of 10 to 20 micrometers, these sedimenting particles have significant potential to denitrify the Lower stratosphere. A microphysical model of nitric acid trihydrate particles is able to simulate the growth and sedimentation of these Large sites in the Lower stratosphere, but the nucleation process is not yet known. Accurate modeling of the formation of these Large particles is essential for understanding Arctic denitrification and predicting future Arctic ozone abundances.

29 **Dhaniyala, S.** and B. Y. H. Liu (2001). "Theoretical modeling of filtration by nonuniform fibrous filters." Aerosol Science and Technology **34**(2): 170-178.

Modeling commercial filter media using classical theories results in incorrect filter pressure drop and efficiencies and this is attributed to media inhomogeneity. The use of an arbitrary inhomogeneity factor is seen to be inadequate in accounting for the effect of operating conditions on the performance of inhomogeneous filter media. A simplistic theoretical modeling approach is described here to account for the variations in filter packing densities and to estimate their effect on the media particle capture characteristics, The theoretical modeling results are used in obtaining an equivalent filter packing density distribution from media local efficiency measurements, Considering this variation in the theoretical models is seen to result in better prediction of media performance over a wide range of operating conditions. The observed deviation of experimental efficiencies from the theory at smaller Peclet numbers can be explained from the results of the theoretical analysis.

28 **Dhaniyala, S.** and B. Y. H. Liu (2001). "Experimental investigation of local efficiency variation in fibrous filters." Aerosol Science and Technology **34**(2): 161-169.

Classical filtration models consider filter media as homogeneous and use an arbitrary inhomogeneity factor to account for the differences between theory and experiments, The variations in media-packing density have been experimentally observed and seen to be significant. There is minimal experimental information on the effect of these variations on filter performance, In this paper, local efficiency variations in commercial fibrous filters have been obtained for varying operating conditions. A filter scanner was developed to measure local filter efficiencies, and the features of the scanner are described in detail. The variations in local efficiencies are seen to have a Gaussian distribution, and the operating conditions and media behavior Influence the variability in the local efficiency data. Theoretical modeling can he used to obtain two-dimensional packing density distribution data from the local efficiency measurements.

27 Chueinta, W. and **P. K. Hopke** (2001). "Beta gauge for aerosol mass measurement." Aerosol Science and Technology **35**(4): 840-843.

Within the International Atomic Energy Agency's coordinated research programs involving air quality monitoring, the participants have been provided with equipment for aerosol sampling and measurement. For aerosol mass measurements, a beta gauge was designed and constructed to provide the necessary performance in collected aerosol mass measurement at the minimum cost. A calibration for the beta gauge was performed to determine the precision of this unit. Two experiments with different size particles were conducted to calibrate the system. This calibration shows that the system provides satisfactory precision with a maximum deviation of approximately 8%. The bias between beta gauge and gravimetric method was found to be 6% on average when examining particles of different composition.

26 Chiarenzelli, J., J. Pagano, et al. (2001). "Enhanced airborne polychlorinated biphenyl (PCB) concentrations and chlorination downwind of Lake Ontario." Environmental Science & Technology **35**(16): 3280-3286.

Air samples were collected simultaneously at three sites downwind of Lake Ontario and at a control site near Lake Erie from March to July of 1999. The Lake Erie site (Stockton, NY) had PCB concentrations similar to rural Integrated Atmospheric Deposition Network(IADN) sampling sites across the Great Lakes, exhibited limited seasonal variation, and approximates regional background. Samples taken along Lake Ontario's southeastern shore (Rice Creek and Sterling, NY) had elevated PCB concentrations averaging similar to 1 ng/m³ and were more chlorinated than air collected at IADN sites and at Stockton. Air samples from Potsdam (similar to 75 km inland) had similar concentrations but were less chlorinated. Clausius-Clapeyron plots revealed a strong correlation between PCB fugacity and temperature near Lake Ontario; however, the extent of chlorination of the air samples rules out volatilization from the lake as a major source. It is hypothesized that volatilization from local surfaces, enriched in higher chlorinated congeners by meteorological or geographic factors, drives both the concentration and composition of airborne PCBs along Lake Ontario's southeastern shore.

25 Chen, F. H. and **P. D. Yapa** (2001). "Estimating Hydrate Formation and Decomposition of Gases released in a Deepwater Ocean Plume." Journal of Marine Systems **30**(1-2): 21-32.

24 Anisimova, L., **P. K. Hopke**, et al. (2001). "Two channel vapor nucleation in the vicinity of the triple point." Journal of Chemical Physics **114**(22): 9852-9855.

Considering the topology of semiempirical nucleation rate surfaces originate from lines describing the appropriate phase equilibria, there will be two nucleation rate surfaces that exist for the different physical states of the critical embryo phases that are formed near the triple point. Each rate surface is independently related to a nucleation channel and is described by individual equations for nucleation rates. Because of the differences in the sticking probability of vapor molecules when they collide with a physical surface (in this case, with the surface of the nucleation embryos) in the different phases, the growth rates of the different phase clusters will be different. As a result of this difference, one expects to find different sized particles for two cluster phases in the vicinity of the triple point for first order phase transitions. In the present study, particle size distributions were measured near glycerin triple point. A clearly bimodal size distribution was observed. This result suggests that there are two independent nucleation channels that exist near the triple point. This experimental system has the ability to discern

particles produced through the two separate nucleation channels so that the nucleation rates can be measured for each channel. (C) 2001 American Institute of Physics.

23 Anisimov, M. P., **P. K. Hopke**, et al. (2001). "Binary N-octanol-sulfur hexafluoride nucleation." Journal of Chemical Physics **115**(2): 810-816.

Recently, the accuracy of vapor nucleation rate measurements has increased substantially. However, when experimental conditions become close to the values to the critical parameters of investigated systems, significant discrepancies were found between the experimental results and theoretical predictions. Some studies have found agreement between results and theory only within a narrow range of nucleation conditions. Therefore, it is appropriate to investigate the nucleation of additional systems to obtain new information to guide nucleation theory development. Alcohols are the most studied class of chemical compounds, but currently there are no experimental data on n-octanol vapor nucleation. The present study is devoted to the investigations of the homogeneous nucleation of the n-octanol in sulfur hexafluoride. Comparison of the critical pressures for binary mixture with the Laplace pressure calculated in the droplet approximation using the bulk liquid surface tension shows that the carrier gas has a more active role in the nucleation than assumed by classical theory. A very high Laplace pressure in the critical embryo is calculated in the droplet approximation. When compared with the highest possible critical pressure for the binary system under investigation, the problems associated with calculating the critical embryo excess energy using the bulk liquid surface tension are revealed. Disagreement of the experimental results with predictions of classical nucleation theory, Dillmann-Meier theory, or any other theory reveals the same basic problems. These results suggest that it is appropriate to consider the general problem of vapor-liquid nucleation in a carrier gas including the estimation of the size and temperature dependence of the critical embryo excess energy as a binary nucleation problem instead of that of a single component. Theories for single-component vapor nucleation should be compared with the truly single-component vapor nucleation experimental results. (C) 2001 American Institute of Physics.

22 Anisimov, M. P. and **P. K. Hopke** (2001). "Nucleation rate surface topologies for binary systems." Journal of Physical Chemistry B **105**(47): 11817-11822.

Recent experiments have found that two nucleation rate surfaces can be observed for two different critical embryo phases (solid and liquid) near the triple point of the condensing species. Direct experimental evidence was presented of the existence of two independent nucleation rate surfaces with one of them existed over metastable vapor-liquid-phase equilibrium lines. These results force more careful consideration of the role of metastable phase equilibria in the topology of nucleation rate surfaces. In the present study, the topology of the nucleation rate surface for a binary vapor in which partial solubility of the condensed components is considered. Schematic multiple surfaces over the phase diagram with a eutectic point, presenting two-channel nucleation, are constructed. Vapor-liquid nucleation in a carrier gas in most cases is a binary system with partial solubility of condensate. It is reasonable to propose that multiple nucleation rate surfaces are common phenomena for many systems. Sulfur hexafluoride-n-pentanol nucleation was experimentally studied using a flow diffusion chamber. The experimental results for n-pentanol-sulfur hexafluoride at total pressures of 0.10, 0.20, and 0.30 MPa are presented. All experimental conditions were recalculated to correspond to a nucleation temperature of 255.0 K. The observed convoluted lines of $\ln J$ plotted against $\ln S$ provide experimental evidence of the existence of multiple nucleation rate surfaces. It can be anticipated that a variety of multiple

nucleation rate surfaces, such as presented here, will be detected soon. Obviously, the application of one-component nucleation theory for such systems with multiple nucleation rate surfaces will not be consistent with the data. Separation of the multiple nucleation surfaces reduces the problem to a simpler one-channel treatment of nucleation. It will then be possible to construct a consistent nucleation theory for a given series of compounds.

21 Ahmed, M. I., J. R. Selman, et al. (2001). "Chromic Acid Regeneration Process with Fuel-Cell Electrode Assistance, Part II: Electrochemical Characterization, Material Compatibility and Energy Consumption." Journal of Applied Electrochemistry **31**: 1389-1394.

20 Zheng, L. and **P. D. Yapa** (2000). "Buoyant Velocity of Spherical and Non-spherical Bubbles/ Droplets." Journal of Hydraulic Engineering(November): 852-855.

19 Zhang, H. F. and **G. Ahmadi** (2000). "Aerosol particle removal and re-entrainment in turbulent channel flows - A direct numerical simulation approach." Journal of Adhesion **74**(1-4): 441-+.

Aerosol particle removal and re-entrainment in turbulent channel flows are studied. The instantaneous fluid velocity field is generated by the direct numerical simulation (DNS) of the Navier-Stokes equation via a pseudospectral method. Particle removal mechanisms in turbulent channel flows are examined and the effects of hydrodynamic forces, torques and the near-wall coherent vorticity are discussed. The particle resuspension rates are evaluated, and the results are compared with the model of Reeks. The particle equation of motion used includes the hydrodynamic, the Brownian, the shear-induced lift and the gravitational forces. An ensemble of 8192 particles is used for particle resuspension and the subsequent trajectory analyses. It is found that large-size particles move away roughly perpendicular to the wall due to the action of the lift force. Small particles, however, follow the upward flows formed by the near-wall eddies in the low-speed streak regions. Thus, turbulent near-wall vortical structures play an important role in small particle resuspension, while the lift is an important factor for reentrainment of large particles. The simulation results suggest that small particles (with $\tau^+(p)$ less than or equal to 0.023) primarily move away from the wall in the low-speed streaks, while larger $\tau^+(p)$ greater than or equal to 780) are mostly removed in the high-speed streaks. particles (with $\tau^+(p)$ greater than or equal to 780) are mostly removed in the high-speed streaks.

18 Wang, J. H. and **P. K. Hopke** (2000). "Estimation of the heteroscedastic noise in large data arrays." Analytica Chimica Acta **412**(1-2): 177-184.

An approach has been developed to estimate the uncertainties in experimental data that follows a heteroscedastic model. The method presented is based on a hypothesis that the size of data is sufficiently large such that the data values over a limited domain have approximately homoscedastic variance. The implementation of the procedure has two steps. The first step is to estimate an approximate error for each data element. The second step is to estimate the standard deviation for the data points using the errors estimated for the neighboring data. The related mathematical theory is presented, and several simulated data examples are used to illustrate this approach. (C) 2000 Elsevier Science B.V. All rights reserved.

17 Shao, J. H. and **R. E. Baltus** (2000). "Effect of solute concentration on hindered diffusion in porous membranes." Aiche Journal **46**(7): 1307-1316.

The effect of solute concentration on hindered diffusion was investigated by measuring diffusion rates of dextran and polyethylene glycol (PEG) in track-etched polycarbonate membranes at concentrations up to 60 mg/mL. Results were interpreted using a model that incorporates a first-order virial coefficient to describe the concentration dependence of the equilibrium partition coefficient, as well as the intrapore diffusivity. For dextran, both virial coefficients were positive, indicating that the effective diffusivity increases with solute concentration. Measured values of the virial coefficient for equilibrium partitioning agreed with a model that includes attractive van der Waals interactions between dextran and the pore wall. For PEG, both virial coefficients were negative, indicating that the diffusivity decreases as solute concentration increases. These observations may be due to chain entanglement or aggregation that occurs with increasing PEG concentration.

16 Shahin, U. M., S. M. Yi, et al. (2000). "Long Term Elemental Dry Deposition Fluxes Measured Around Lake Michigan with an Automated Dry Deposition." Environmental Science & Technology **34**(10): 1887-1892.

15 Ramadan, Z., X. H. Song, et al. (2000). "Identification of sources of Phoenix aerosol by positive matrix factorization." Journal of The Air & Waste Management Association **50**(8): 1308-1320.

Chemical composition data for fine and coarse particles collected in Phoenix, AZ, were analyzed using positive matrix factorization (PMF). The objective was to identify the possible aerosol sources at the sampling site. PMF uses estimates of the error in the data to provide optimum data point scaling and permits a better treatment of missing and below-detection-limit values. It also applies nonnegativity constraints to the factors. Two sets of fine particle samples were collected by different samplers. Each of the resulting fine particle data sets was analyzed separately. For each fine particle data set, eight factors were obtained, identified as (1) biomass burning characterized by high concentrations of organic carbon (OC), elemental carbon (EC), and K; (2) wood burning with high concentrations of Na, K, OC, and EC; (3) motor vehicles with high concentrations of OC and EC; (4) nonferrous smelting process characterized by Cu, Zn, As, and Pb; (5) heavy-duty diesel characterized by high EC, OC, and Mn; (6) sea-salt factor dominated by Na and Cl; (7) soil with high values for Al, Si, Ca, Ti, and Fe; and (8) secondary aerosol with SO₄²⁻ and OC that may represent coal-fired power plant emissions; For the coarse particle samples, a five-factor model gave source profiles that are attributed to be (1) sea salt, (2) soil, (3) Fe source/motor vehicle, (4) construction (high Ca), and (5) coal-fired power plant. Regression of the PM mass against the factor scores was performed to estimate the mass contributions of the resolved sources. The major sources for the fine particles were motor vehicles, vegetation burning factors (biomass and wood burning), and coal-fired power plants. These sources contributed most of the fine aerosol mass by emitting carbonaceous particles, and they have higher contributions in winter. For the coarse particles, the major source contributions were soil and construction (high Ca). These sources also peaked in winter.

14 Nambi, I. M. and S. E. Powers (2000). "NAPL Dissolution in Heterogeneous Systems: Experimental Results in a Simplified System." Journal of Contamination Hydrology **44**(2): 161-184.

13 Morshed, J. and **S. E. Powers** (2000). "Regression and Dimensional Analysis for Two-Phase Flow Modeling." Transport in Porous Media **38**(1-2): 205-221.

12 Matyjaszewski, K., **D. A. Shipp**, et al. (2000). "Water-Bourne Block and Statistical Copolymers Synthesized Using Atom Transfer Radical Polymerization." Macromolecules **33**: 2296-2298.

11 Matyjaszewski, K., **D. A. Shipp**, et al. (2000). "Simple and Effective One-Pot Synthesis of (Meth)Acrylic Block Copolymers Through Atom Transfer Radical Polymerization." J. Polym. Sci Part A: Polym. Chem. **38**: 2023-2031.

10 Matyjaszewski, K., J. Qiu, et al. (2000). "Controlled/ "Living" Radical Polymerization Applied to Water-Bourne Systems." Macromol. Symp. **155**: 15-29.

9 **Hopke, P. K.**, T. B. Borak, et al. (2000). "Health risks due to radon in drinking water." Environmental Science & Technology **34**(6): 921-926.

Following more than a decade of scientific debate about the setting of a standard for Rn-222 in drinking water, Congress established a timetable for the promulgation of a standard in the 1996 Amendments to the Safe Drinking Water Act. As a result of those Amendments, the EPA contracted with the National Academy of Sciences to undertake a risk assessment for exposure to radon in drinking water. In addition, the resulting committee was asked to address several other scientific issues including the national average ambient Rn-222 concentration and the increment of Rn-222 to the indoor-air concentration arising from the use of drinking water in a home. A new dosimetric analysis of the cancer risk to the stomach from ingestion was performed. The recently reported risk estimates developed by the BEIR VI Committee for inhalation of radon decay products were adopted. Because the 1996 Amendments permit states to develop programs in which mitigation of air-producing health-risk reductions equivalent to that which would be achieved by treating the drinking water, the scientific issues involved in such "multimedia mitigation programs" were explored.

8 Hadjiski, L. and **P. Hopke** (2000). "Application of Artificial Neural Networks to Modeling and Prediction of Ambient Ozone Concentrations." Journal of Air Waste Management Association **50**: 894-901.

7 Grimberg, J. J., M. J. Rury, et al. (2000). "Trinitophenol Treatment in Hollow Fiber Membrane Bioreactor." Water Science and Technology **41**(4-5): 235-238.

6 Frenich, A. G., M. M. Galera, et al. (2000). "Resolution of multicomponent peaks by orthogonal projection approach, positive matrix factorization and alternating least squares." Analytica Chimica Acta **411**(1-2): 145-155.

The application of orthogonal projection approach (OPA), alternating least squares (ALS), and positive matrix factorization (PMF) to resolve HPLC-DAD data into individual concentration profiles and spectra is discussed. OPA was initially described as a purity method but the inclusion of an ALS procedure allows its application as a curve resolution method. PMF is a least square approach to factor analysis that in this study has been used as a tool to tackle the problem of curve resolution. OPA, ALS and PMF have been applied using a single matrix (two-

way data) or an augmented matrix containing several data matrices simultaneously. The results obtained with the different resolution methods are compared and evaluated using measures of dissimilarity between the real and the estimated spectra. The study is performed in three data subsets, obtained by segmentation of the original data matrix. Within each data subset, there is a reduced number of species present which makes the resolution easier. (C) 2000 Elsevier Science B.V. All rights reserved.

5 Fitzgerald, B. and **P. K. Hopke** (2000). "A prospective assessment of the Po-210 surface collection for estimating Rn-222 exposure." Journal of Environmental Radioactivity **51**(1): 79-98.

Previous studies have examined the utility of measuring the embedded Po-210 in solid materials as an indicator of long-term Rn-222 exposure. However, in those studies, existing surfaces were employed. In this prospective study, pairs of glass surfaces were placed in homes around the United States along with an LR-115-II-etched track radon detector for each piece of glass. A subset of these glass samples has been analyzed for Po-210 activity, The results of measurements on a subset of samples are presented. The independent Rn-222 measurements are compared with the Po-210 measurements and a relationship is obtained between the two results using a model for the accumulation of activity within an enclosed space. The data are interpreted in terms of (a) the usefulness of the Po-210 measurements as a long-term Rn-222 detector and (b) the value of a new interpretation scheme to make retrospective assessments of the Rn-222 exposure within rooms. (C) 2000 Elsevier Science Ltd. All rights reserved.

4 Davis, S. W. and **S. E. Powers** (2000). "Evaluation of Alternative Sorbents for Removal of MTBE from Groundwater." Journal of Environmental Engineering **126**(4): 354-360.

3 Chueinta, W., **P. K. Hopke**, et al. (2000). "Investigation of sources of atmospheric aerosol at urban and suburban residential areas in Thailand by positive matrix factorization." Atmospheric Environment **34**(20): 3319-3329.

Samples of fine and coarse fractions of airborne particulate matter were collected in an urban residential area of metropolitan Bangkok from June 1995 to May 1996 and in a suburban residential area in Pathumthani, Bangkok's boundary province, from September 1993 to August 1994. The samples were analyzed for elemental concentrations by instrumental neutron activation analysis. The data sets were then analyzed by positive matrix factorization followed by rotation to identify the possible sources of atmospheric aerosols in both areas. The best solutions were found to be six factors for elemental compositions of each of the fine and coarse particulate matter fractions at the urban site and five factors each for both fine and coarse fractions at the suburban location. Soil was the major source of airborne particulate matter identified for all data sets. The motor vehicle factor showed much higher concentration for Br in urban than in suburban area. A motorcycle factor with high concentrations of Zn and Mn were found at the urban site. The factor containing highest concentrations of Na and Cl was attributed to sea-salt and was clearly seen in the urban atmosphere. The site was located 35 km to the north from the Gulf of Thailand and was influenced by wind from the south and southwest for most of the year. Charcoal/wood burning and incineration factors were likely to be the local sources. A factor with high concentration of Ca was attributed to a construction near the urban residential site and from two plaster manufacturing factories close to the suburban residential site. (C) 2000 Elsevier Science Ltd. All rights reserved.

2 Anisimov, M. P., **P. K. Hopke**, et al. (2000). "n-Pentanol-helium homogeneous nucleation rates." Journal of Chemical Physics **113**(5): 1971-1975.

An international collaboration to examine the effects of different experimental systems on nucleation measurements has resulted in a series of nucleation experiments on the n-pentanol-helium system. In particular, using a laminar flow diffusion chamber, nucleation rate data were obtained for temperatures between 258 and 266 K and total pressures of 0.10, 0.20, and 0.30 MPa. These results are compared with other data on nucleation measured experimentally using an expansion wave tube, a two-piston expansion chamber, a flow diffusion chamber, and a static diffusion chamber. The influence of the carrier gas pressure on nucleation rates was explored. It was concluded that the critical embryo phase transitions should be detectable in an analogous manner to the recently reported phase transitions in the glycerin-carbon dioxide system. The experimental detection of the melting point is suggested as a critical test for the ability of an experimental system to provide adequate measurements of nucleation rates. For example, the glycerin melting point can be used for these tests. A reference equation for nucleation rates of n-pentanol-helium is proposed as a practical test of any experimental measurement system for total pressures of 0.10, 0.20, and 0.30 MPa. The use of this equation is recommended even if the reference equation is not completely accurate, because it provides a scale for comparison of the results for different research groups and methods. (C) 2000 American Institute of Physics. [S0021-9606(00)50322-5].

1 **Ahmadi, G.**, C. H. He, et al. (2000). "Air flow and particle transport in a triboelectric coal/ash cleaning system-counter flowing straight duct design." Particulate Science and Technology **18**(3): 213-256.

The process of triboelectric coal/ash cleaning is outlined and a new design for scale-up to industrial systems is described. A straight rectangular duct forms the mixing chamber and the main body of this triboelectric separator. To improve mixing and to generate a uniform concentration in the main electrostatic separator duct, the mixture enters the mixing box in the form of two opposing jets. The stress transport model of the FLUENT code is used for simulating the mean gas flow and to guide the overall design of the electrostatic coal/ash separator. The three-dimensional computational grid covers the mixing chamber with the opposing inlets and the upper part of the main separator duct. The gas flow field conditions including the directional intensities of turbulence are evaluated. The instantaneous fluctuating velocity field was simulated by a Gaussian filtered white noise model. A recently developed computational model for Lagrangian particle tracking is used to study the transport of particles from the inlets to the main body of the separator duct. The model accounts for the drag and lift forces acting on the particle, in addition to the Brownian motion and gravitational sedimentation effects. The particles are also dispersed by the action of the high level of turbulence that is generated in the mixing chamber. The computational results show that the new design generates roughly uniform flow conditions in the triboelectric separator duct. Furthermore, the larger 100 μm particles will have a more uniform distribution when compared with the smaller (40 μm) particles. The effect of the presence of an electric field perpendicular to the flow direction is also studied. It is shown that the charged particles are significantly deflected by the action of the electrostatic forces. As a result, the system could separate coal and ash particles that carry different charges. The simplicity and effectiveness of the straight duct separator makes it a prime candidate for scale-up for use in industrial applications for online coal beneficiation and separation of minerals from ash in combustion product.

