Disclaimer

The information in this presentation has been reviewed and approved for public dissemination in accordance with U.S. Environmental Protection Agency (EPA). The views expressed in this presentation are those of the author(s) and do not necessarily represent the views or policies of the Agency. Any mention of trade names or commercial products does not constitute EPA endorsement or recommendation for use.

Exposure Science STAR Grantee Abstracts

Abstract	First Author and Affiliation	Title	Key Words
1	**Deborah H. Bennett** *University of California – Davis*	Tracking Semivolatile Organic Compounds Indoors: Merging Models and Field Sampling to Access Concentrations, Emissions, and Exposures	▪ Indoor environment ▪ Measurement methods ▪ Modeling ▪ Organics
2	**Heather M. Stapleton** *Duke University*	Residential Exposure of Young Children to SVOCs	▪ SVOCs ▪ Children's exposure ▪ Dust ▪ Hand wipes
3	**Xudong Fan** *University of Michigan – Ann Arbor*	Three-dimensional Micro-gas Chromatography Device for Rapid and Sensitive Indoor Chemical Exposure Analysis	▪ Air sample ▪ Exposome ▪ Volatile organic compounds ▪ Environmental chemistry ▪ Engineering ▪ Analytical ▪ Measurement methods
4	**John C. Little** *Virginia Polytechnic Institute and State University*	Rapid Methods to Estimate Exposure to SVOCs in Indoor Environments	▪ Risk assessment ▪ Pollution prevention ▪ Toxics ▪ Environmental chemistry
5	**Tracey J. Woodruff** *University of California – San Francisco*	A Non-targeted Method for Measuring Multiple Chemical Exposures Amoung a Demographically Diverse Population of Pregnant Women in Northern California	▪ Endocrine disrupting chemicals ▪ Environmental organic acids ▪ Non-targeted testing ▪ LC-QTOF/MS ▪ LC-MS/MS ▪ Environmental justice ▪ Ethnic/racial disparities ▪ Pregnancy

1 – Tracking Semivolatile Organic Compounds Indoors: Merging Models and Field Sampling to Access Concentrations, Emissions, and Exposures

Investigators: Deborah H. Bennett, Hyeong-Moo Shin, and Thomas M. Young

University of California – Davis

- **EPA Grant Number:** R835641
- **Project Period:** 07/01/2014 – 06/30/2017

Objective:
The goals of this project are to (1) measure concentrations of a broad spectrum of target and non-target semivolatile organic compounds (SOVCs) in indoor dust to estimate emission rates and exposures, (2) refine and evaluate a multi-compartment indoor fate, transport, and exposure model, and (3) evaluate air-to-skin transdermal uptake models.

Approach:
First, we will develop and utilize liquid and gas chromatography and high resolution (time-of-flight) mass spectrometry to rapidly assess concentrations of a broad spectrum of SVOCs in indoor dust collected from participating homes in a field study. We will estimate emission rates of SVOCs for these homes using inverse modeling applied to SVOC levels in dust. With these emission rates, we will estimate exposures using our indoor exposure model. The robustness of such estimates will be greatly improved by the inclusion of a larger number and greater diversity of chemical constituents. We will also apply factor analysis to look for common source profiles. Second, we will provide a data set to evaluate indoor models by measuring half-lives of penta-brominated diphenyl ethers (BDEs) after removing sources in the study participant homes. We will also update critical model parameters, both by measuring dust loading and dust removal rates from a field study and by evaluating new model process equations and available data in the literature in order to refine our indoor model. Third, we will evaluate air-to-skin transdermal update models by measuring SVOC concentrations in human skin to determine if measured levels are similar to values anticipated by the models.

Expected Results:
The overall outcome of this research will be a significantly improved understanding of what chemicals and which pathways result in current exposures to the U.S. populations. The development of new analytical methods using high resolution (HR) mass spectrometric (MS) techniques and analysis of dust samples address the EPA's objective to develop and evaluate methods for rapid measurement of multiple compounds in the indoor environment. The improvements to the indoor exposure model through the development of the evaluation data set, collection of model input data, and evaluation of model processes, including the dermal pathway, address the EPA's objective to advance the scientific basis of exposure predictions.

Supplemental Keywords:
Indoor environment, measurement methods, modeling, organics

2 – Residential Exposure of Young Children to SVOCs

Heather M. Stapleton[1], P. Lee Ferguson[1], and Thomas F. Webster[2]

[1]*Duke University*
[2]*Boston University School of Public Health*

- **EPA Grant Number:** R835642
- **Project Period:** 07/01/2014 – 06/30/2017

Objective:

We hypothesize that residues measured in children's hand wipes will provide an improved measure of personal exposure to a wide range of semivolatile organic compounds (SVOCs) emitted from indoor sources. Furthermore we hypothesize that exposure levels will be related to chemical applications in specific consumer products commonly found in the home environment. To test these hypotheses we propose to: 1) Characterize SVOC sources in products by collecting surface wipes from consumer products (in the home) that may be potential sources of SVOCs (and other chemical additives) to the indoor environment (e.g. furniture, vinyl flooring, electronics, insulation, etc). 2) Characterize and quantify residential exposure of young children to SVOCs using hand wipes and determine how closely these measurements correlate with levels measured in paired samples of serum, urine, indoor air, and house dust from 50 children between the ages of 24-48 months of age. The hand wipes, air and dust samples will be analyzed for a suite of SVOC compounds using both targeted and nontargeted analytical methods. Additionally, we will: 3) Identify sources of variability in hand wipe measurements such as hand washing, lotions, etc.; 4) Examine the patterns of coexposure to multiple SVOCs (an important issue in the assessment of chemical mixtures); and 5) Compare our empirical results for SVOCs with predictions from indoor models.

Approach:

We will recruit 50 families into our study. Paired samples of serum, urine, hand wipes, consumer product surface wipes, and house dust will be collected for 50 children between the ages of 2-4 in central North Carolina and analyzed for organic contaminants using both targeted (i.e. measuring selected chemicals) and non-targeted (i.e. broadband screening) approaches. A detailed questionnaire will be administered to collect information on diet, home characteristics and behavioral aspects of the children that may contribute to exposure (e.g., mouthing behaviors). Associations among all matrices will be examined, and particular attention will be given to investigating correlations between SVOC measures in consumer product surface wipes with SVOC exposure levels. Statistical analyses will be conducted to determine how well i) SVOCs measured in consumer products, dust, and air predict measured hand wipe levels and ii) the degree to which hand wipes (a measure of personal exposure) predict SVOC levels in serum and urine (biomarkers of exposure) compared to measurements in home air and dust (measurements in microenvironment). Data collected from this study will be compared to exposure models to evaluate the predictive power of the models.

Expected Results:

As current knowledge regarding the occurrence, levels and even identity of SVOCs in consumer products is limited, our study will add substantially to that knowledge base. We anticipate observing significant associations among biomarkers of exposure, hand wipes and dust for a large number of SVOCs measured across a range of physicochemical properties. Results from this study will also provide the first data on novel SVOCs detectable in hand wipes and dust using high resolution mass spectrometry-based nontargeted analytical screening approaches. This aspect is particularly innovative and may provide insight into previously unknown or uncharacterized contaminant exposures in the home environment. Knowledge of patterns of joint exposures is a key research gap and this study will help improve our understanding of exposure to mixtures. We will also identify links between specific products in the home and children's exposure levels. Lastly, our study will be used to update screening models for indoor behavior and exposure to SVOCs and to compare the predictions with our empirical data.

Supplemental Keywords:

SVOCs, children's exposure, dust, hand wipes

3 – Three-dimensional Micro-gas Chromatography Device for Rapid and Sensitive Indoor Chemical Exposure Analysis

Xudong Fan, Katsuo Kurabayashi, and Rudy J. Richardson

University of Michigan – Ann Arbor

- **EPA Grant Number:** R835644
- **Project Period:** 06/01/2014 – 05/31/2017

Objective:
The objective of the proposed project is to develop a portable automated device for rapid (~20 min), sensitive (ppb to sub-ppb) and in-situ analysis of hundreds of (semi-)volatile organic compounds (VOCs) for indoor human exposure assessment.

Approach:
The device is based on the novel smart e-dimensional (3D) micro-gas chromatography (μGC) design and highly sensitive vapor sensor arrays. Unlike conventional portable GC on the market and comprehensive 2-D μGC being developed in research labs, both of which have limited peak capacity and handle only a small set or limited, well-defined classes of chemicals, the unique design of the smart μGC architecture significantly enhances the GC peak capacity while remaining compact in size, thus enabling real-time (20 min) and in-situ analysis of hundreds of VOCs associated with indoor chemical exposure at the ppb or sub-ppb level. In addition, the smart μGC architecture is highly scalable. If needed, high-dimensional separation (such as 4-D μGC) can be implemented easily, providing even larger peak capacity.

In the proposed work, a complete 3-D μGC device will be developed and built on chip, which will include pre-concentrator, micro-separation columns, flow control, and highly sensitive on-column vapor detector arrays. Operation and data analysis algorithms will also be developed for automation. Approximately 150 chemicals representing various categories of indoor exposures will be used as model systems to characterize and test the device's performance. A corresponding VOC reference library will be created for those chemicals. Finally, the device, in conjunction with the pre-built VOC reference library, will be used to quantitatively analyze 100-150 chemicals in actual indoor environments on the university campus. The device's performance will be benchmarked with a standard GC-Mass Spectrometer system.

Expected Results:
The proposed project addresses the urgent need for "technologies and methods to characterize the presence of hundreds of (semi-)volatile chemicals". Successful completion of the proposed project will provide quantitative information about temporal and spatial distribution of hundreds of indoor chemicals, which is vital in evaluating human exposure to those chemicals and in studying/mitigating health risks associated with such exposures.

Supplemental Keywords:
Air sample, exposome, volatile organic compounds, environmental chemistry, engineering, analytical, measurement methods

4 – Rapid Methods to Estimate Exposure to SVOCs in Indoor Environments

John C. Little and Linsey C. Marr

Virginia Polytechnic Institute and State University

- **EPA Grant Number:** R835606
- **Project Period:** 03/01/2014 – 02/28/2017

Objective:

(1) Develop novel methods to measure model parameters (C_0 and Y_0) for 20 representative sources that emit 27 SVOCs, and use the resulting data at five temperatures (from 25°C to 85°C) to establish the nature of the equilibrium relationship; (2) Develop novel methods to determine surface/air partition coefficients (K) for eight detected SVOCs and six interior surfaces including airborne particles (K_p) and dust (K_{dust}), and compare results to available correlations for K_s, K_p, and K_{dust}; (3) Conduct single-source chamber experiments to characterize emissions of target SVOCs from the 20 representative sources at five temperatures (from 25°C to 85°C); (4) Validate the single-source model using results from the chamber experiments for the 20 representative sources and the single-phase model using data collected from the literature; and (5) Evaluate assumptions on which the rapid single-source and single-phase methods are based and characterize the uncertainty inherent in model predictions, especially for the low volatility SVOCs.

Approach:

Modern indoor environments contain a vast array of products, many of which emit toxic semi-volatile organic compounds (SVOCs). There is an urgent need to estimate exposure to SVOCs, but the vast number of SVOC/product combinations poses a serious challenge. To solve this problem, we propose two distinct rapid methods to estimate exposure, both based on the same set of assumptions. The first is the "single-source" approach, in which we characterize a specific indoor product and then estimate exposure. The second is the "single-phase" approach, in which we characterize a particular indoor phase, for example, the indoor air, and then estimate exposure. Collectively, the single-source and single-phase approaches represent a very powerful way to solve the problem. The single-phase approach can be applied to get broad, population-wide, information about exposure to SVOCs in general. The single-source approach can rapidly characterize specific SVOC/product combinations, and estimate their contributions to exposure. This information can then be used to either remove specific products from the market, or make substitutions, introducing alternate low toxicity SVOCs that impart similarly desirable product performance at equivalent cost.

Expected Results:

Include: (a) A validated single-source model that can be used to make rapid estimates of exposure to SVOCs released from specific products used indoors; and (b) A validated single-phase model that can be used to make rapid estimated of exposure to a wide range of SVOCs, based only on the average concentration of SVOCs found in indoor air. Expected benefits are significant. When combined with the rapid estimates of toxicity being developed in ToxCast™, our rapid estimates of exposure will allow risk-based prioritization of a wide range of SVOCs, representing a powerful screening tool to rapidly estimate, prioritize and reduce, public health risks associated with SVOCs indoors.

Supplemental Keywords:

Risk assessment, pollution prevention, toxics, environmental chemistry

5 – A Non-targeted Method for Measuring Multiple Chemical Exposures Amoung a Demographically Diverse Population of Pregnant Women in Northern California

Tracey J. Woodruff, Roy Gerona, Rachel Morello-Frosch, and Saunak Sen

University of California – San Francisco

- **EPA Grant Number:** R835643
- **Project Period:** 02/01/2014 – 01/31/2017

Objective:

We propose to apply an innovative non-targeted biomonitoring method using liquid chromatography-quadrupole time-of-flight mass spectrometry (LC-QTOF/MS) to evaluate everyday exposure to over 700 chemicals classified as Environmental Organic Acids (EOAs) and the extent to which exposures vary amount different racial/ethnic and socio-economic groups of pregnant women. Our new LC-QTOF/MS non-targeted screening methodology has the capacity to directly (without enzymatic hydrolysis) and simultaneously screen for approximately 10-times more EOAs than what is currently being biomonitored in the National Health and Nutrition Examination Survey. We focus on EOAs, which are industrial compounds with at least one ionizable proton, because: 1) their chemical structure facilitates a higher rate of analytical detection; 2) many of their chemical structures are similar to hormones, increasing the potential for endocrine disruption, which can negatively affect fetal development; and 3) many are produced in high quantities and used in a wide range of consumer products, but have not been extensively biomonitored in pregnant women. We will use liquid chromatography tandem mass spectrometry (LC-MS/MS) to confirm the presence and levels of select EOAs identified through our non-targeted screening. Finally, we will assess differences in EOA exposures by race/ethnicity and socio-economic status. We hypothesize that pregnant women are exposed to more EOAs than previously documented, and that EOA exposure varies by race/ethnicity and SES, resulting in disproportionate EOA body-burdens among certain subpopulations.

Approach:

We will collect blood samples from 200 demographically diverse 2nd trimester pregnant women seeking prenatal care at two clinics at UCSF, San Francisco General Hospital (primarily low-income) and Moffitt-Long Hospital (primarily high-income). The population is about 30% Caucasian, 30% Latino, 10% African-American and 12% Asian. We will use our novel non-targeted biomonitoring method, LC-QTOF/MS, to screen for 729 environmental organic acids in 200 second-trimester maternal serum samples, We will conduct targeted analysis of four selected EOAs from our non-targeted screening using LC-MS/MS to confirm the presence and levels of chemicals identified through the QTOF analysis. Chemicals for the targeted analysis will be selected based on use in everyday consumer products and high production in the US, detected in high frequency in study participants, potential for developmental health risk, and novel exposures. Finally, we will evaluate potential differences in exposure levels by race/ethnicity and SES to six EOAs, four already identified and an additional two which are selected for targeted analysis based on screening data indicating high potential for racial/ethnic and/or SES disparities.

Expected Results:

We will have pioneered a screening method for over 700 environmental chemicals, and anticipate identifying chemicals previously unmeasured in biological samples. Further, we will provide novel data on the extent to which pregnant women are potentially exposed to these chemicals, and quantify exposures to six EOAs for which exposure has been poorly characterized in this vulnerable population. Finally, we will enhance understanding of racial/ethnic and economic differences in chemical exposures. Our innovative method of chemical screening will significantly advance biomonitoring science through its efficient approach that broadly characterizes multiple chemical exposures in ways that can help prioritize chemicals for identifying important sources of exposure, risk assessment and exposure education activities, and identify health risks to better protect public health.

Supplemental Keywords:

Endocrine disrupting chemicals, environmental organic acids, non-targeted testing, LC-QTOF/MS, LC-MS/MS. environmental justice, ethnic/racial disparities, pregnancy