

DRAFT PROPOSAL

*Environmental Fate and Ozone Formation Potential of
Low Vapor Pressure – Volatile Organic Compounds from Consumer Products*

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ABSTRACT

Background: The South Coast Air Quality Management District (SCAQMD) and the California Air Resources Board (CARB) are considering changing current policy related to exemption from the low vapor pressure – volatile organic compounds (LVP-VOC) list for certain classes of compounds, because LVP-VOCs used in consumer products can contribute to formation of ozone and/or secondary organic aerosol. To evaluate ozone formation potential of LVP-VOCs used in consumer products, both what is emitted from the product and what remains in the air should be considered. Additionally, the fate of the portion of the compounds entering wastewater treatment facilities when they are disposed down the drain needs to be modeled to estimate the resulting percent of the product used that remains in the air.

Objectives: The goal of this project is to determine the fraction of LVP-VOC in consumer products that is available for ozone formation reaction.

Methods: First, we will conduct experiments to determine the emission rate of LVP-VOCs from consumer products during use. We will then determine if a model can be developed to predict the emissions from product use based on key physicochemical properties. Second, we will develop a wastewater fate and transport model to predict evaporation rates of LVP-VOCs that may occur at wastewater treatment facilities or in the discharge zone of the facilities as well as partitioning between gas and particle phases. Third, we will evaluate the need to integrate additional complexities into the model, specifically, the Bennett fugacity-based indoor model and a dynamic or multi-box spatial model. Fourth, we will integrate the wastewater model and necessary model components with the CalTOX model and develop a simple estimation tool of the fraction of LVP-VOC in consumer products that is available for ozone formation.

Implications: This project will provide CARB with emission data from specific consumer products and both a full model and a simple estimation tool to determine the impact of the emissions of LVP-VOCs on total ozone formation and to determine whether the exemption for LVP-VOCs in the Consumer Products Regulations should continue as is or be modified based on key physicochemical properties and release scenarios.

1. INTRODUCTION

1.1. Background

Volatile organic compounds (VOCs) have ozone (O_3) formation potential under the presence of sunlight and nitrogen oxides (NO_x). Exposure to ozone causes public health problems with serious consequences in the U.S. economy [1]. Thus, there has been increasing interest in evaluating the effect of volatile organic compounds from mobile sources, green waste composting, livestock and poultry waste emissions, consumer products, and municipal solid waste disposal sites on ozone formation [2-6]. Chen and Luo studied the effect of different sources of total organic gases (TOG) emissions on ozone formation in California's South Coast Air Basin (SoCAB) and identified that the top three reactivity-based TOG emission sources in SoCAB are light-duty passenger cars, off-road equipment, and consumer products, indicating that VOC emissions from consumer products could be a significant contributor to ozone formation [2]. This finding is important because currently exempt low vapor pressure – volatile organic compounds (LVP-VOCs) used in consumer products can be another contributor of ozone formation depending on the emission rate and reactivity of the compound.

The potential for ozone formation of VOCs can be evaluated from maximum incremental reactivity (MIR), which is the mass of ozone produced per unit mass of VOC precursor introduced [7-10]. A method used to derive MIR is well established in Kwok et al. [11] and updated MIR values are available for all VOCs in Carter [12]. Due to the extensive effort on estimating MIR values, there is only a need to determine the fraction of LVP-VOCs used in consumer products that is available for potential formation of ozone and/or secondary organic aerosol (SOA) during daylight hours.

The South Coast Air Quality Management District (SCAQMD) and the California Air Resources Board (CARB) are considering changing current policy related to exemption from the LVP-VOC list for certain classes of compounds, because some LVP-VOCs have higher MIR values than ethane, a baseline chemical between photochemically-reactive and non-reactive VOC compounds. The proposed changes are in response to uncertainty about whether LVP-VOCs used in consumer products can contribute to ozone and/or SOA formation. To evaluate ozone formation potential of LVP-VOCs used in consumer products, both what is emitted from the product and what remains in the air should be considered. Therefore, a detailed understanding of sources/sinks, transport, and distribution among gas and airborne particle phases is needed for LVP-VOCs.

However, for most chemicals, there is limited information available about how the use of the consumer products results in releases to indoor environments [13]. Specifically, we do not know the fraction of LVP-VOCs in consumer products that will be released over a relevant time period to participate in ozone forming atmospheric chemistry. The existing

methods for characterizing chemicals as volatile, semi-volatile or non-volatile often misclassify compounds leading to errors in the estimate of ozone forming potential of a product [14]. There is a need for careful measurement of evaporation rates for specific compounds in consumer product formulations at ambient conditions with the ultimate goal of developing a predictive model for volatility that can be used to select chemicals with low ozone forming potential.

In addition to emissions of LVP-VOCs from the use of consumer products, LVP-VOCs that are disposed down the drain might result in atmospheric releases from wastewater treatment facilities or from rivers to which effluent is released. This in turn may result in ambient ozone formation. DeLeo et al. recently estimated the “down-the-drain” load of consumer products to a wastewater treatment facility using the product formulation and market sales data and found that liquid laundry detergent contributes 69% of the total load alone [15]. However, emission rate estimates of LVP-VOCs from the treatment facilities are limited by the lack of understanding about the relationship among other competing processes including degradation, partitioning between gas and particle phases, and formation of SOA. Thus, there is a need to carry out research to explore the use of fugacity approach in combination with multimedia chemical mass-balance models to track emission rates from the use of consumer products and a wastewater treatment facility.

Multimedia mass-balance models have been used to simulate the fate and transport of environmental contaminants and determine the contribution of VOCs in ozone formation [16-19]. This is a critical step in evaluating the ozone forming potential because only the portion of emitted LVP-VOCs that remains in the air is available for forming ozone. The ozone formation potential must be modified by the fraction remaining in air. Therefore, there is a need to develop a comprehensive modeling approach to estimate emission rates of gas phase LVP-VOCs from a wastewater treatment facility by integrating wastewater as an essential model component in a multimedia mass-balance model such as the CalTOX [20].

The key element needed to understand the contribution of LVP-VOCs to ozone and particle formation is the emission rates from consumer product formulations, emission rates from down-the-drain disposal, and the multimedia environmental distribution of the target chemicals. We anticipate that careful measurement and modeling of these elements can provide a predictive model or bright line that differentiates chemicals that can participate in ozone formation atmospheric chemistry and those that are not likely to be available for ozone formation.

1.2. Related Previous Studies

Drs. Bennett, McKone, Shin, and Maddalena all have extensive modeling experiences and Dr. Maddalena has extensive laboratory experiences. All details are shown below.

Dr. Thomas McKone is an expert in the development, use, and evaluation of models and data for human-health and ecological risk assessments. To assist the California Environmental Protection Agency in its efforts to assess risks from human exposures to releases to multiple environmental media, i.e. air, soil, and water, McKone and his team developed the CalTOX model [20]. First issued in 1993 and updated in 1995 and 2002, with continued enhancements ongoing, CalTOX consists of two component models – a multimedia transport and transformation model and a multi-pathway human exposure model.

Drs. Bennett, McKone, and Maddalena worked together on spatially-dependent multimedia models [21, 22]. These three researchers also worked on a number of studies addressing model performance. These studies have provided tools and procedures for model performance evaluation [20, 23, 24], explicit characterization of uncertainty in exposure models [25, 26], optimum use of models by environmental decision-makers [27, 28], and Bayesian methods in model evaluation [29, 30]. In addition, these three researchers worked on experimental and theoretical efforts to address surface chemistry, surface processes, and partitioning. This has included efforts to model the uptake and penetration of particle-bound and semi-volatile organic chemicals on vegetation surfaces [31, 32], and the mass transfer of chemicals in surface soils [33]. Dr. McKone and Maddalena also worked to quantify emissions of VOCs and SVOCs from computer equipment [34].

Dr. Maddalena worked specifically on a project assessing the role of multimedia models in urban air quality with emphasis on ozone formation [16]. Dr. Maddalena has managed the Indoor Environment Group's volatile organic compound sampling and analysis lab at Lawrence Berkeley National Laboratory (LBNL) since 2006. Dr. Maddalena also has worked with investigators on high impact projects such as a recent study of air quality in day care settings [35]. Dr. Maddalena specializes in measuring emission factors from materials and processes using a variety of controlled environmental chambers and instrumentation. Using the LBNL emissions testing facilities, he has completed studies quantifying sources and exposure concentrations of VOCs and aldehydes in FEMA travel trailers [36, 37], measuring volatile sulfur compound emissions from Chinese imported dry wall [36, 38], quantified chemical and particle emissions from office equipment [38, 39] and measured emission profiles under different operational scenarios for coal-fired space heating stoves from Mongolia [40].

Drs. Bennett and Maddalena completed a project for CARB to quantifying the air exchange rates and VOC concentrations indoors and outdoors at 40 small- and medium-sized commercial buildings. The effort from the project resulted in three publications [41-43].

Drs. Bennett, McKone, and Shin have worked together on a number of important modeling projects. Specifically, they worked together on the development of a new approach to estimate indoor residence times of semi-volatile organic compounds, exposure-based prioritization tools of indoor released chemicals, and a comprehensive approach to support that both indoor and outdoor models are needed to capture the source of environmental chemicals [44-46]. Moreover, they recently developed a new approach to estimate source strength of organic compounds from the use of consumer products and diffusive transfers from indoor surface to air by using dust levels and a fugacity-based indoor model [47].

Dr. Hyeong-Moo Shin completed his doctoral degree at the University of California, Irvine, working with Dr. Scott M. Bartell on modeling fate and transport of perfluorooctanoic acid (PFOA) to estimate exposures and serum concentrations for about 50,000 participants in the C8 Health Projects [48, 49]. He has been a post-doctoral researcher working with Dr. Bennett since July 2011. His work has focused on the development and application of environmental fate and transport models for exposure and risk assessment studies. He has also published papers on the spatially-dependent multimedia fate and transport of PFOA [48, 50].

2. SPECIFIC OBJECTIVES

The overall objective is to determine the fraction of LVP-VOCs used in consumer products that is available for potential formation of ozone and/or SOA during daylight hours. In order to achieve this goal, a clear understanding of source, fate, and transport of consumer product chemicals is required from experimental settings and modeling approaches.

Experiments will be done to determine the emission rate of LVP-VOCs from consumer products during use. We will then determine if a model can be developed to predict the emissions from product use based on key physicochemical properties. Next, a modeling framework will be developed that can take emissions into air and the portion entering wastewater treatment facilities when they are disposed down the drain and estimate the resulting percent of the product used that remains in the air. This will be done by developing a multi-function multimedia model.

For LVP-VOCs in wastewater treatment facilities, a wastewater model will be developed and linked to the CalTOX model to predict evaporation rates of LVP-VOCs that may occur at wastewater treatment facilities or in the discharge zone of the facilities as well as partitioning between gas and particle phases.

We will then evaluate the need to integrate the Bennett fugacity-based indoor model to predict the amount of indoor emissions that is available for ozone formation in outdoor environments during daylight hours. We will also evaluate the need to provide a dynamic or multi-box spatial model to correctly determine the fraction of compound in the gas phase and thus available for ozone formation. The goal of all these components is to determine the fraction of LVP-VOC in consumer products that is available for ozone formation reaction.

This project will provide CARB with essential data, including emission profiles of LVP-VOCs used in the consumer products and the impact of the emissions of LVP-VOCs on total ozone formation. The results from this project can be used to determine whether the exemption for LVP-VOCs in the Consumer Products Regulations should continue as is or be modified based on key physicochemical properties and release scenarios.

3. TECHNICAL PLAN

3.1. Experimental Plan and Methods

The final goal of this project is to examine effects of consumer product chemicals on ozone and SOA formation for potential modification of LVP-VOCs in the Consumer Products Regulations. To achieve the goal, this project is designed to determine emissions from products and then understand fate, transport, and distribution among gas and airborne particle phases both through a sewage treatment plant and in multimedia environment. Below we describe each task that will be carried out to determine emission profiles of LVP-VOCs from the experiment and develop, evaluate, and execute the integrated model – including model framework, model revisions, the needed model inputs, and output options.

3.1.1. Determine emission profiles of LVP-VOCs from consumer products

In all tasks, we focus on a set of target compounds. The method for calculating Maximum Incremental Reactivity (MIR) is described in Kwok et al. [11] and updated MIR values¹ are available for all VOCs in Carter [12]. Thus, the scope of this work is to

¹ Compiled on-line at <http://www.arb.ca.gov/consprod/regs/2012/4mirtable50411.pdf>

determine the fraction of LVP-VOCs that are available for atmospheric chemical reactions in the MRI process. Chemicals will be selected in consultation with CARB and industry representatives from a list of exempt LVP-VOCs used in consumer products. A partial list of potential LVP-VOCs is provided in Table 1. Estimation methods for calculating evaporation rate of pure phase compounds are available but uncertainty in these values for compounds in different formulations would be high, particularly for low volatility compounds. Therefore, the experimental measurements of emission profiles for target LVP-VOCs will be determined using specific consumer products selected to represent the product categories listed in Table 2 and used as the source material for the LVP-VOCs.

Table 1. Low-Vapor-Pressure Excluded LVPs used in consumer products (largest volume ingredients are in bold) and maximum incremental reactivity (MIR) [12]

Low-Vapor-Pressure Excluded LVPs	MIR
1. diethanolamine	4.05
2. diethylene glycol ethyl ether (DEGEE)	3.19
3. ethylene glycol	3.01
4. hydrocarbons: normal C13 to C20	
5. hydrocarbons: branched and cyclic C13 to C20	
6. propylene glycol	2.48
7. triethanolamine	2.60
8. 2,2,4-trimethyl-1,3-pentanediolmonoisobutyrate (Texanol)	0.89
9. aminomethylpropanol (AMP)	15.08
10. butoxyethoxyethanol	1.96
11. butylene glycol	-
12. diethylene glycol	3.23
13. dipropylene glycol	2.20
14. dipropylene glycol n-butyl ether (DPNB)	-
15. glycerol	3.50
16. glyceryl triacetate	0.51
17. glycolic acid	2.32
18. hexylene glycol	-
19. isopropyl palmitate	-
20. phenol	2.69
21. polyethylene glycol	-
22. n-tridecane	0.47
ethane (reference chemical)	0.26

Table 2: A list of consumer products potentially containing LVP-VOCs

Automotive fluids (i.e., windshield cleaner fluid)	Coatings (excluding aerosols)
Cleaning solutions	Polishes
Pest management supplies	Adhesives
Personal care products (excluding antiperspirants and deodorants)	Indoor products

Chamber Design: Field measurements of emission rates from consumer product applications would be difficult to control all factors and subsequently have high uncertainty. Therefore, a chamber approach to measuring emission rates during simulated applications is needed. Measurements will be conducted using a medium size chamber constructed from low sorptive materials in a continuous-stirred tank reactor design. The design provides a near ideally mixed system so that exhaust air from the chamber can be sampled as a surrogate for the chamber air concentration. The chamber will be installed in a temperature controlled environment with controlled humidity so that emission rates can be determined as a function of controlled ambient conditions.

Experimental Procedure: A mass balance modeling approach will be used to determine the emission profile based on controlled ventilation rates in the chamber and measured mass of target compounds in the exhaust air over different integrating periods. Real-time measurements using a proton-transfer-reaction mass spectrometry (PTRMS) will be conducted for a subset of the tests to verify the dynamic phase of the mass balance modeling if necessary. The integrated measurements of the LVP-VOCs will be performed by active sampling on multi-sorbent Carbopack tubes analyzed by thermal desorption gas chromatography/mass spectroscopy which will provide both the target chemical results and information on additional product constituents.

Experiments will be conducted by first applying the consumer product to a clean inert surface of standardized dimensions per manufacturer recommended application procedure. The surface will be selected to not interact with the product. The surface matrix will be weighed prior to and immediately following application of the product. The product will be applied to the surface in a fume hood located near the chamber and then after weighing, the sample will be transferred immediately to the chamber to initiate the testing period. The test will continue until steady-state conditions are achieved and tracked for a sufficient period of time to confirm steady-state emissions or until product target chemicals are fully dispersed. The test chamber will be purged prior to each product test.

Pilot tests: A series of pilot tests will be conducted to identify 1) the appropriate ventilation rate per area of emitting surface required to minimize the effect of boundary layer diffusion, 2) the appropriate sampling intervals for the integrated samples, 3) the appropriate sample duration to balance the resolution of the time-series plot and instrumental quantification limits, 4) confirm that emission rates are constant and 5) test whether we can install the sample on a scale inside the test chamber to track total mass loss over time. Real-time measurements with a PTRMS will be conducted concurrently on a limited number of samples to confirm dynamic emission profiles. A limited number of long-term emission tests will be conducted to confirm long term profiles. Preferably the long-term tests will be conducted with a product that contains a number of target LVP-VOCs and VOCs.

Each consumer product will be tested at three different temperatures and the results will be reported along with temperature dependent regression statistics in appropriate units for the different modeling scenarios to be tested. Pure phase emission rates will be determined under identical conditions as the product testing on a subset of compounds for comparison.

Potential model development: We will determine if the emissions from the consumer products correlate with physicochemical properties and the percent of the compound in the product, or if emissions are dependent on other aspects of product composition and application. If it is feasible to develop a predictive emissions model, one will be developed.

3.1.2. Develop a wastewater fate and transport model

When LVP-VOCs are disposed down the drain and enter wastewater treatment facilities, not all of LVP-VOCs are evaporated because there are several competing processes including biodegradation, solid disposal, and discharge to effluents. We need to determine the amount of compounds entering the air from a wastewater treatment facility as well as the amount of compounds in the effluent from a wastewater treatment facility. Once the effluent left the plant, we need to determine the amount of compounds partitioned into the air.

Wastewater Emission Model: To simulate the fate and transport of consumer product chemicals in a wastewater treatment facility, we will first review the WW-TREAT program developed for the fate of chemicals in a primary and activated sludge wastewater treatment plant [51]. For the distribution of a compound's concentration in the discharge zone of wastewater treatment plants and following emissions to ambient environments, we will review the GRiDS model [52] and then update two models for

emission rates of compounds for ozone formation. During this task, we will further review literature for updated parameters and model inputs and develop a new wastewater fate and transport model for improved estimates of evaporation rates of gas phase LVP-VOCs from wastewater treatment facilities.

CalTOX Model: The effluent from a wastewater treatment facility is assumed to enter the surface water. We will model this process through the use of multimedia CalTOX model. The CalTOX model is a mature and widely used multimedia fate and transport and exposure model—with an extensive history of model evaluation exercises and case studies [20]. First issued in 1993 and updated in 1995 and 2002, with continued enhancements ongoing, CalTOX consists of two component models—a multimedia transport and transformation model and a multi-pathway human exposure model. The CalTOX model provides a broad assessment of the partitioning of chemicals between the air, water, soil, and biota, and the resulting total exposure. For this project, we will include a wastewater emission model in the CalTOX model to predict the fate of consumer product chemicals once disposed down the drain and wastewater treatment facilities.

3.1.3. Evaluate existing model components and conditions

Emission rate profiles from Task 1 would include the rate of release, location of release, and time of release. These three factors would dictate whether the LVP-VOCs would contribute to ozone formation locally or regionally because night-time releases would presumably be transferred out of local areas before conditions were present for reaction. There may also be implications of indoor releases causing delayed or off-set source periods. In other words, the emission profiles with above three factors would influence availability of LVP-VOCs for atmospheric reactions leading to ozone and/or SOA formation.

We will use the CalTOX model, discussed above, to determine the amount of compounds in the air in the gas phase. In addition, we will evaluate if using a more detailed model is needed. Specifically, we will evaluate the Bennett indoor fugacity model, a two-box model, and dynamic conditions in atmosphere to see what component is needed in the outdoor multimedia model. We will evaluate these extra components using the target compounds in Table 1 by determining if the outputs from a base model only and a base model with each extra component change by over 10%. If the change is over 10%, we will add the component. If not, we will not.

Each of the extra components is described below.

Indoor Fugacity Model: Some LVP-VOCs have a strong tendency to bind to organic carbon in dust or to indoor surface materials due to the large octanol-air partition coefficient (K_{oa}) and thus removed primarily by surface cleaning [46]. In addition, available LVP-VOCs for ozone formation during daylight hours will be determined depending on the time of consumer product use (day or night) and the air exchange rate of day and night. Thus, the fugacity-based indoor model will be evaluated to see if the indoor model is necessary to be integrated with a multimedia outdoor model [53].

The Bennett indoor model is a dynamic mass-balance model with multiple indoor compartments simultaneously exchanging mass. The room(s) where a compound is released are the source zones, having an air compartment and three surface compartments: carpet, vinyl floor, and walls/ceiling. The source to the model will be determined in Task 1.

The mass in each compartment is the state variable and mass transfer between compartments is defined by mass-transfer rate coefficients accounting for both diffusive and advective transfers. The compartment mass balance is defined by a set of differential equations accounting for all gain and loss processes. Solving these equations determines time varying concentrations in both air (gas and particle phases) and indoor surfaces such as hard flooring and carpets, along with the associated dust. This model will be also evaluated to see if removal pathways of LVP-VOCs are either ventilation or surface cleaning and to determine the fraction of LVP-VOCs in the gas phase.

Two-box models in Southern California: Chen and Luo studied the ozone formation potentials from different emission sources in California's South Coast Air Basin (SoCAB) [2]. Based on the geographic boundary of SoCAB and resulting ozone concentrations depicted in their study, high concentrations of ozone were predicted in downwind areas of the SoCAB, such as Azusa, Rubidoux, and San Bernardino. This indicates that two-box models are needed for areas with downwind effects on ozone formation such as SoCAB.

Dynamic conditions in atmosphere: Forster et al. applied a multimedia mass-balance model to the fate and concentrations of VOCs in the urban atmosphere in both steady-state and dynamic conditions [16]. The dynamic results show that hydroxyl radical (OH) concentrations and advection rate influence and fate and concentrations of a chemical in the atmosphere. This finding supports that dynamic conditions should be used to capture the fate and transport of LVP-VOCs and that the two-box model is necessary in the multimedia model.

3.1.4. Integrate models and develop an estimation tool

Develop integrated model: In Task 4, we will integrate the wastewater model from Task 2 and necessary model components and conditions from Task 3 with the CalTOX model [20]. If we determine that the steady-state integrated model is appropriate, then the model will be programmed in Excel spreadsheet. If the model needs to be dynamic, the model will be programmed in MATLAB. This model can be used by CARB to determine the fraction of compounds in the air.

Develop an estimation tool: As it may be cumbersome to run a model to predict the fraction of compounds in the air, we will try to determine if this value can be predicted in a simple way. We will use two statistical approaches to analyze the input and output of the model above and then determine if a simple method can be used. For both methods, we will first run the above integrated model for a large number of LVP-VOCs, generating a set of chemical properties and the fraction of compounds in the air.

First, a statistical regression model will be tested. This type of approach has been used to relate detailed air pollution models to intake fraction values [54]. Second, we will use the classification and regression tree (CART) analysis [55]. The CART analysis is a non-analytic, computationally intensive, statistical procedure that classifies data by producing a tree structure [55]. The results of the CART approach are concise and easy to understand, which should assist decision making. The CART method has been available for almost 30 years and has been applied in many fields, including engineering, medicine, public health, and economics [56-60]. Drs. Bennett and McKone used this approach to relate chemical properties to persistence in the environment [56].

Hopefully, these two statistical models will provide CARB with a simple estimation tool to determine the impact of the emissions of LVP-VOCs on total ozone formation and to determine whether the exemption for LVP-VOCs in the Consumer Products Regulations should continue as is or be modified based on key physicochemical properties and release scenarios.

3.2. Data Management

The emission testing phase of this study will generate new experimental data. Actual consumer products tested during this study will remain anonymous only reporting category of product and composition of relevant compounds. The raw information from the emission testing will be documented as handwritten notes recorded in laboratory notebooks by researchers, digital photographs, and as electronic output from instruments and data loggers. Laboratory research notebooks will be individually numbered and recorded in an index notebook to be maintained by Dr. Maddalena. At least monthly, backup electronic scans of notebook pages will be created and stored on

the Indoor Environment Group intranet site. Electronic data files generated by the laboratory analytical instruments and data loggers will be backed up on LBNLs automatic secure backup system. Other electronic data files (e.g., online instruments, data acquisition systems) will also be backed up using LBNLs secure system. All other computer files (MS Excel workbooks, Word documents) will be backed up onto a central computer weekly.

All modeling will be done at UC-Davis. Models and data generated will be backed up nightly to a secure, encrypted repository. The backup and recovery scenarios planned are practiced regularly at UC-Davis.

3.3. Quality Assurance and Quality Control (QA/QC)

Plans for quality assurance and quality control (QA/QC) will be developed and submitted to ARB for review and approval as part of a full proposal. Dr. Maddalena will be responsible for all QA/QC aspects of the experimental measurements.

Several steps will be taken to ensure the quality of measurements. Standardized protocols, validated in other studies, will be employed, and thorough training will be conducted with study staff. Sampling equipment will be certified clean or will be pre-cleaned by methods such as thermal desorption and confirmed to have no contamination by periodic analysis of a subset of samplers. All analyses will follow good laboratory practices. Detailed laboratory notebooks will be maintained to record raw data, protocols, and experimental procedures. Raw data will also be recorded and stored on a designated computer and processed using appropriate statistical analysis software. Laboratory quality control procedures will include the use of chamber and laboratory blank and spike samples, calibration curves within the range of expected measurements, evaluation of drift and re-calibration, and, where feasible, the use of laboratory surrogate recovery standards and internal standards. The integrity of samples during storage will be verified through the use of field blank samples, field spike samples, and duplicate samples. Analytical detection and quantification limits will be determined for each target chemical.

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27. Holmes, K. J.; Graham, J. A.; McKone, T.; Whipple, C., Regulatory Models and the Environment: Practice, Pitfalls, and Prospects. *Risk Analysis* **2009**, 29, (2), 159-170.
28. McKone, T. E.; Deshpande, A. W., Can fuzzy logic bring complex environmental problems into focus? *Environmental Science & Technology* **2005**, 39, (2), 42A-47A.
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33. McKone, T. E.; Bennett, D. H., Chemical-specific representation of air-soil exchange and soil penetration in regional multimedia models. *Environmental Science & Technology* **2003**, 37, (14), 3123-3132.
34. Maddalena, R.; McKone, T.; Destalilats, H.; Russell, M.; Hodgson, A.; Perino, C., Quantifying Pollutant Emissions from Office Equipment. California Energy Commission. In Laboratory, L. B. N., Ed. Berkeley, CA, 2010.
35. Bradman, A.; Gaspar, F.; Castorina, R.; Tong-Lin, E.; McKone, T.; Maddalena, R. *Environmental Exposures in Early Childhood Education Environments*; Lawrence Berkeley National Laboratory: 2012.

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37. Parthasarathy, S.; Maddalena, R. L.; Russell, M. L.; Apte, M. G., Effect of Temperature and Humidity on Formaldehyde Emissions in Temporary Housing Units. *Journal of the Air & Waste Management Association* **2011**, 61, (6), 689-695.
38. Maddalena, R., Effect of Environmental Factors on Sulfur Gas Emissions from Problem Drywall. In Laboratory, L. B. N., Ed. Berkeley, CA, 2011.
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40. Maddalena, R.; Lunden, M.; Wilson, D.; Ceballos, C.; Kirchstetter, T.; Slack, J.; Dale, L., Quantifying Stove Emissions Related to Different Use Patterns for the Silver-mini (Small Turkish) Space Heating Stove. In Laboratory, L. B. N., Ed. Berkeley, CA, 2012.
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42. Bennett, D. H.; Fisk, W.; Apte, M. G.; Wu, X.; Trout, A.; Faulkner, D.; Sullivan, D., Ventilation, temperature, and HVAC characteristics in small and medium commercial buildings in California. *Indoor Air* **2012**, 22, (4), 309-320.
43. Wu, X.; Apte, M. G.; Bennett, D. H., Indoor Particle Levels in Small- and Medium-Sized Commercial Buildings in California. *Environmental Science & Technology* **2012**, 46, (22), 12355-12363.
44. Shin, H.-M.; McKone, T. E.; Bennett, D. H., Intake Fraction for the Indoor Environment: A Tool for Prioritizing Indoor Chemical Sources. *Environmental Science & Technology* **2012**, 46, (18), 10063-10072.
45. Shin, H.-M.; McKone, T. E.; Bennett, D. H., Evaluating environmental modeling and sampling data with biomarker data to identify sources and routes of exposure. *Atmospheric Environment* **2013**, 69, (0), 148-155.
46. Shin, H.-M.; McKone, T. E.; Tulse, N. S.; Clifton, M. S.; Bennett, D. H., Indoor Residence Times of Semivolatile Organic Compounds: Model Estimation and Field Evaluation. *Environmental Science & Technology* **2012**, 47, (2), 859-867.
47. Shin, H.-M.; McKone, T.; Nishioka, M.; Daniele, F. M.; Croen, L.; Hertz-Piccioto, I.; Newschaffer, C.; Bennett, D. H., Tracking Source Strength of Semivolatile Organic Compounds from Indoor Dust. **submitted**.
48. Shin, H.-M.; Vieira, V. M.; Ryan, P. B.; Detwiler, R.; Sanders, B.; Steenland, K.; Bartell, S. M., Environmental Fate and Transport Modeling for Perfluorooctanoic Acid Emitted from the Washington Works Facility in West Virginia. *Environmental Science & Technology* **2011**, 45, (4), 1435-1442.
49. Shin, H.-M.; Vieira, V. M.; Ryan, P. B.; Steenland, K.; Bartell, S. M., Retrospective Exposure Estimation and Predicted versus Observed Serum Perfluorooctanoic Acid Concentrations for Participants in the C8 Health Project. *Environmental Health Perspectives* **2011**, 119, (12), 1760-1765.
50. Shin, H.-M.; Ryan, P. B.; Vieira, V. M.; Bartell, S. M., Modeling the air-soil transport pathway of perfluorooctanoic acid in the mid-Ohio Valley using linked air dispersion and vadose zone models. *Atmospheric Environment* **2012**, 51, 67-74.
51. Cowan, C. E.; Larson, R. J.; Feijtel, T. C. J.; Rapaport, R. A., An improved model for predicting the fate of consumer product chemicals in waste-water treatment plants. *Water Research* **1993**, 27, (4), 561-573.

52. Rapaport, R. A., Prediction of consumer product chemical concentrations as a function of publicly owned treatment works treatment type and riverine dilution. *Environmental Toxicology and Chemistry* **1988**, 7, (2), 107-115.
53. Bennett, D. H.; Furtaw, E. J., Fugacity-based indoor residential pesticide fate model. *Environmental Science & Technology* **2004**, 38, (7), 2142-2152.
54. Levy, J. I.; Wolff, S. K.; Evans, J. S., A regression-based approach for estimating primary and secondary particulate matter intake fractions. *Risk Analysis* **2002**, 22, (5), 895-904.
55. Breiman, L.; Friedman, J.; Olshen, R.; Stone, C., *Classification and Regression Trees*. Wadsworth Publishing: Monterey, CA, 1984.
56. Bennett, D. H.; McKone, T. E.; Kastenbergh, W. E., Evaluating multimedia chemical persistence: Classification and regression tree analysis. *Environmental Toxicology and Chemistry* **2000**, 19, (4), 810-819.
57. Eisenberg, J. N.; Seto, E. Y. W.; Olivieri, A. W.; Spear, R. C., Quantifying water pathogen risk in an epidemiological framework. *Risk Analysis* **1996**, 16, (4), 549-563.
58. Eisenberg, J. N. S.; McKone, T. E., Decision tree method for the classification of chemical pollutants: Incorporation of across-chemical variability and within-chemical uncertainty. *Environmental Science & Technology* **1998**, 32, (21), 3396-3404.
59. Spear, R. C.; Bois, F. Y.; Woodruff, T.; Auslander, D.; Parker, J.; Selvin, S., Modeling benzene pharmacokinetics across 3 sets of animal data - parametric sensitivity and risk implications. *Risk Analysis* **1991**, 11, (4), 641-654.
60. Spear, R. C.; Grieb, T. M.; Shang, N., Parameter uncertainty and interaction in complex environmental-models. *Water Resources Research* **1994**, 30, (11), 3159-3169.

4. PROJECT SCHEDULE

Task 1: Conduct experiments to measure emission rates from consumer products

Task 2: Develop a wastewater fate and transport model

Task 3: Evaluate existing model components for the outdoor multimedia model

Task 4: Integrate all multimedia models and develop a predictive model of ozone formation potential

Task 5: Draft final report

Task 6: Amend final report

		Year 1												Year 2											
	Month	1	2	3	4	5	6	7	8	9	10	11	12	1	2	3	4	5	6	7	8	9	10	11	12
Task																									
1																									
2																									
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4																									
5																									
6																									
		m	p			m	p			m	p		p	dm		p			p			m	p		f

p = quarterly progress report

d = deliver draft final report (to be submitted 6 months prior to contract expiration)

f = deliver final report

m = meeting with ARB staff

5. CURRICULA VITAE

BIOGRAPHICAL SKETCH

NAME Deborah Hall Bennett	POSITION TITLE Associate Professor		
eRA COMMONS USER NAME DHBENNETT			
EDUCATION/TRAINING <i>(Begin with baccalaureate or other initial professional education, such as</i>			
INSTITUTION AND LOCATION	DEGREE <i>(if applicable)</i>	YEAR(s)	FIELD OF STUDY
University of California, Los Angeles	B.S.	1993	Mechanical Engineering
University of California, Berkeley	M.S.	1996	Mechanical Engineering
University of California, Berkeley	Ph.D.	1999	Mechanical Engineering

A. Positions and Honors.

1993- 1995	Member of Technical Staff, Hughes Aircraft Company, El Segundo, California
1999-2000	Postdoctoral Researcher, Lawrence Berkeley Lab, Environmental Energy Technology Division, Berkeley, CA
2000-2001	Scientist, Lawrence Berkeley Lab, Environmental Energy Technology Division, Berkeley, CA
2001-2004	Assistant Professor of Environmental Health and Risk Assessment, Harvard School of Public Health, Environmental Health Department and Center for Risk Assessment, Boston, MA
2005-2009	Assistant Professor, Department of Public Health Sciences, UC Davis, Davis, CA
2009-	Associate Professor, Department of Public Health Sciences, UC Davis, Davis CA

Honors

EPA STAR Fellow, 1997 – 1999; ISEA Early Career Award, 2002-2005; Journal of Exposure Science and Environmental Epidemiology, Associate Editor

B. Selected Publications (selected out of over 60 publications)

1. Eisenberg, JNS, Bennett, DH, McKone, TE. Chemical Dynamics of Persistent Organic Pollutants: A Sensitivity Analysis Relating Soil Concentration Levels to Atmospheric Emissions. *Environ Sci and Technol* 1998; 32:115-123.
2. Bennett, DH, McKone, TE, Kastenber, WE, Matthies, M. General Formulation of Characteristic Travel Distance for Semi-Volatile Organic Chemicals in a Multi-media Environment, *Environ Sci and Technol* 1998; 32:4023-4030.
3. Bennett, DH, Kastenber, WE, McKone, TE. A Multimedia, Multiple Pathway Risk Assessment of Atrazine: The Impact of Age Differentiated Exposure Including Joint Uncertainty and Variability. *Reliability Eng and System Safety* 1999; 63:185-198.
4. Bennett, DH, Kastenber, WE, McKone, TE. General Formulation of Characteristic Time for Persistent Chemicals in a Multimedia Environment. *Environmental Sci and Technology* 1999; 33:503-509.
5. Bennett, DH, McKone, TE, Kastenber, WE. Evaluating Multimedia Chemical Persistence: A CART Analysis. *Environ Tox and Chem* 2000; 19:810-819.
6. Bennett, D.H., Scheringer, M., McKone, T.E., and Hünigbuhler, K., The Scientific Basis for Predicting Long Range Transport: A Systematic Evaluation of Two Multimedia Transport Models, *Environmental Science and Technology*, 2001, 35, 1181-1189.

7. MacLeod, M, Woodfine, D, Mackay, D.; McKone, T., Bennett, D., and Maddalena, R., BETR North America: A Regionally Segmented Multimedia Contaminant Fate Model for North America, *Environmental Science and Pollution Research*, 2001, 8, 156-163.
8. Bennett, D.H., McKone, T.E., Evans, J.S., Nazaroff, W.W., Margni, M.D., and Jolliet, O., Defining Intake Fraction, *Environmental Science and Technology*, 2002, 36: 206A-211A.
9. Deborah H. Bennett and Edwin J. Furtaw, Jr., A Fugacity-Based Indoor Residential Pesticide Fate Model, *Environmental Science and Technology*, 2004, 38, 2142-2152.
10. MacLeod, M., Bennett, D.H., Perem, M., Maddalena, R.L., McKone, T.E., and Mackay D. Dependence of Intake Fraction on Release Location in a Multi-media Framework: A Case Study of Four Contaminants in North America, *Industrial Ecology*, 2004 8(3):89-102.
11. Bennett DH, Furtaw Jr. EJ. Fugacity-Based Indoor Residential Pesticide Fate Model *Environmental Science and Technology*, 38: 2142-2152. 2004.
12. Bennett DH and Koutrakis, P. Determining the Infiltration of Outdoor Particles in the Indoor Environment Using a Dynamic Model. *Journal of Aerosol Science*. 2005
13. Nishioka Y, Levy JI, Norris GA, Bennett DH, Spengler JD. *A risk-based approach to health impact assessment for input-output analysis – Part 2: Case study of insulation*. Submitted to *International Journal of Life Cycle Analysis*. 2006
14. Loh MM, Houseman EA, Gray GM, Levy JI, Spengler JD, Bennett DH. Measured concentrations of VOC's in Non-residential microenvironments. *Environmental Science and Technology*, 40: 6903-6911. 2006.
15. Sonja N. Sax, Deborah H. Bennett, Steven N. Chillrud, James Ross, Patrick. Kinney, John D. Spengler, A CANCER RISK ASSESSMENT OF INNER-CITY TEENAGERS LIVING IN NEW YORK CITY AND LOS ANGELES, *EHP*, 2006; 114 (10): 1558-1566.
16. Loh MM, Levy JI, Spengler JD, Houseman EA, Bennett DH. Ranking Cancer Risks of Organic Hazardous Air Pollutants in the United States. *Environmental Health Perspectives*. 2007;115(8):1160-1168.
17. Dodson RE, Levy JI, Shine JP, Spengler JD, Bennett DH. Multi-zonal air flow rates in residences in Boston, Massachusetts. *Atmos Environ*, 2007; 41 (17): 3722-3727.
18. Vincent Y. Seaman, Deborah H. Bennett, Thomas M. Cahill. Origin, Occurrence, and Source Emission Rate of Acrolein in Residential Indoor Air. *Environ Sci Technol*. 2007 Oct 15;41(20):6940-6.
19. Robin E. Dodson, E. Andres Houseman, Jonathan I. Levy, John D. Spengler, James P. Shine, and Deborah H. Bennett, Measured and Modeled Personal Exposures to and Risks from Volatile Organic Compounds. *Environ Sci Technol*. 2007 Dec 15;41(24):8498-505.
20. Dodson RE, Levy JI, Houseman EA, Spengler JD, Bennett DH. Evaluating methods for predicting indoor residential volatile organic compound concentration distributions. *J Expo Sci Environ Epidemiol*. 2009 Nov;19(7):682-93.
21. Loh MM, Houseman EA, Levy JI, Spengler JD, Bennett DH. Contribution to volatile organic compound exposures from time spent in stores and restaurants and bars. *J Expo Sci Environ Epidemiol*. 2009 Nov;19(7):660-73.
22. Rose M, Bennett DH, Bergman A, Fångström B, Pessah IN, Hertz-Picciotto I. PBDEs in 2-5 year-old children from California and associations with diet and indoor environment. *Environ Sci Technol*. 2010 Apr 1;44(7):2648-53.
23. Shin HM, McKone TE, Bennett DH. (2012). Intake Fractions for Releases into Indoor Environment: A Tool for Chemical Prioritization. *Environmental Science & Technology* 46(18): 10063-10072. PMID: 22920860.
24. Shin HM, McKone TE, Tulve NS, Clifton MS, Bennett DH. 2012. Indoor Residence Times of Semivolatile Organic Compounds: Model Estimation and Field Evaluation. *Environmental Science & Technology* 47:859-867. PMID: 23244175.
25. Shin HM, McKone TE, Bennett DH. (2013). Evaluating Environmental Modeling and Sampling Data with Biomarker Data to Identify Sources and Routes of Exposure. *Atmospheric Environment* 69:148-155

BIOGRAPHICAL SKETCH

NAME	POSITION TITLES		
McKone, Thomas E.	Adjunct Professor of Public Health, UC Berkeley Senior Scientist, Deputy Department Head, Group Leader, Lawrence Berkeley National Laboratory.		
eRA COMMONS USER NAME TEMCKONE			
EDUCATION/TRAINING (Begin with baccalaureate or other initial professional education, such as			
INSTITUTION AND LOCATION	DEGREE (if applicable)	YEAR(s)	FIELD OF STUDY
University of St. Thomas (St. Paul, MN)	B.A.	1972	Chemistry
University of California, Los Angeles	M.S.	1977	Engineering
University of California, Los Angeles	Ph.D.	1981	Engineering

A. Positions and Honors.**Positions and Employment**

1981 – 1983	Post-Graduate Fellowship with the Advisory Committee on Reactor Safeguards, U.S. Nuclear Regulatory Commission, Washington, DC
1983 – 1995	Lawrence Livermore National Laboratory, Health & Ecological Assessments
1987 – 1988	Visiting Scientist, School of Public Health, Harvard University, Boston, MA
1992 – 1995	Lecturer and Research Environmental Engineer, Environmental Toxicology Department, University of California, Davis, CA
1996 – present	Senior Scientist, Deputy Department Head, Environmental Energy Technologies Division, Lawrence Berkeley National Laboratory, Berkeley, CA
1996 – present	Adjunct Professor and Researcher, Environmental Health Sciences, School of Public Health, University of California, Berkeley, CA

Honors

1984-1985	National Lecturer, North American Association for Environmental Education
2001	Fellow, Society for Risk Analysis
2003	Constance L. Mehlman Award for "outstanding contributions in exposure analysis research that helped shape a National or State policy and provided new approaches for reduction or prevention of exposure".
2007	Selected by Governor Arnold Schwarzenegger as one of his five appointments to the Scientific Guidance Panel of the California Environmental Contaminant Biomonitoring Program
2008	International Society of Exposure Science Jerome J. Wesolowski award for outstanding contributions to the field of exposure assessment.

Other Experience and Professional Memberships (Selected)

1994 – 2000	Science Advisory Board, U.S. Environmental Protection Agency
1995 – 2001	National Research Council, National Academy of Sciences, Committee on Toxicology,
1998 – 2000	Principal Investigator, Study on Strategies to Protect the Health of Deployed U.S. Forces, National Research Council, Institute of Medicine, National Academy of Sciences.
2002 – 2003	Member, Expert Working Group, California Environmental Health Tracking Planning Project, Environmental Health Investigations Branch, California Department of Health Services.
2002 – present	Member, International Life Cycle Board, United Nations Environment Program.
2004 – 2006	Member, Committee on EPA's Exposure and Human Health Reassessment of TCDD and Related Compounds National Research Council, National Academy of Sciences,
2004 – 2007	Member, Committee on the Selection and Use of Models in the Regulatory Decision Process, National Research Council, National Academy of Sciences

- 2004 – present Member, Uncertainty in Exposure Assessment Working Group, International Program in Chemical Safety (IPCS), World Health Organization.
- 2006 – 2008 Member, Committee on Improving Risk Analysis Approaches Used by the US EPA, National Research Council, National Academy of Sciences
- 2007 – present Scientific Guidance Panel, California Environmental Contaminant Biomonitoring Program
- 2010 – present Member, Committee on Exposure Science for the 21st Century, National Research Council, National Academy of Sciences.

B. Selected peer-reviewed publications (selected from 160 publications)

(Publications selected from 160 peer-reviewed publications)

1. Bennett, D.H., T.E. McKone, J.S. Evans, W.W. Nazaroff, M.D. Margni, O. Jolliet, and K.R. Smith "Defining Intake Fraction," *Environmental Science & Technology*, **36**:207A-211A, 2002.
2. Bennett, D.H., M.D. Margni, T.E. McKone, O. Jolliet, "Intake Fraction for Multimedia Pollutants: A Tool for Life Cycle Analysis and Comparative Risk Assessment," *Risk Analysis* **22**(5):903-916, 2002.
3. McKone, T.E., D.H. Bennett, "Chemical-Specific Representation of Air-Soil Exchange and Soil Penetration in Regional Multimedia Models, *Environmental Science & Technology*, **33**(14):2123-2132, 2003.
4. Castorina, R., A. Bradman, T.E. McKone, D. Barr, B. Eskenazi "Cumulative Organophosphate Pesticide Exposure and Risk Assessment Among Pregnant Women Living in an Agricultural Community: A Case Study from the CHAMACOS Cohort," *Environmental Health Perspectives*, **111**(13):1640-1648, 2003.
5. Sohn, M.D., T.E. McKone, M.L. Rigas, J.N. Blancato, "Reconstructing Population-scale Exposures from Dose Biomarkers: An Integrated Bayesian Statistical Framework" *Journal of Exposure Analysis and Environmental Epidemiology*, **14**(3):204-213, 2004.
6. McKone, T.E., R. Castorina, Y. Kuwabara, M.E. Harnly, B. Eskenazi, and A. Bradman, "Merging Models and Biomonitoring Data to Characterize Sources and Pathways of Human Exposure to Organophosphorous Pesticides in the Salinas Valley of California", *Environmental Science and Technology*, **41**:3233-3240, 2007.
7. Lobscheid, A.B., T.E. McKone, and D. Vallero, "Exploring relationships between outdoor air particulate-associated polycyclic aromatic hydrocarbon and PM2.5: A case study of benzo(a)pyrene in California metropolitan regions," *Atmospheric Environment*, **41**:5659–5672, 2007.
8. Destailats, H., R.L. Maddalena, B.C. Singer, A.T. Hodgson, and T.E. McKone. "Indoor pollutants emitted by office equipment: A review of reported data and information needs," *Atmospheric Environment* **42**:1371–1388, 2008.
9. Rosenbaum, R.K., T.M. Bachmann, L.S. Gold, M.Z. Hauschild, M.A.J. Huijbregts, O. Jolliet, R. Juraske, A. Köhler, H.F. Larsen, M. MacLeod, M. Margni, T.E. McKone, J. Payet, M. Schuhmacher, D. van de Meent, "USEtox - The UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in Life Cycle Impact Assessment," *The International Journal of Life Cycle Assessment*, **13**(7):532-546, 2008.
10. McKone, T.E., P. B. Ryan, and H. Ozkaynak "Exposure Information for Ozone, PM and Toxic Air Pollutants in Environmental Health Research: Current Opportunities and Future Directions," *Journal of Exposure Science and Environmental Epidemiology*, **19**:30-44, 2009.
11. Holmes, K.J., J. Graham, T.E. McKone, and C. Whipple, "Regulatory Models and the Environment: Practice, Pitfalls, and Prospects," *Risk Analysis*, **29**(2):159-170, 2009.
12. Hellweg, S., E. Demou, R. Bruzzi, A. Meijer, R.K. Rosenbaum, M.A.J. Huijbregts, and T.E. McKone, "Integrating Indoor Air Pollutant Exposure within Life Cycle Impact Assessment" *Environmental Science and Technology*, **43**(6):1670–1679, 2009.
13. C. Cowan-Ellsberry, M. McLachlan, J. Arnot, M. MacLeod, T.E. McKone, F. Wania. "Modeling Exposure to Persistent Chemicals in Hazard and Risk Assessment," *Integrated Environmental Assessment and Management (IEAM)* **5**(4):662-679, 2009.
14. Shin HM, McKone TE, Bennett DH. (2012). Intake Fractions for Releases into Indoor Environment: A Tool for Chemical Prioritization. *Environmental Science & Technology* 46(18): 10063-10072. PMID: 22920860.

BIOGRAPHICAL SKETCH

NAME Maddalena, Randy L.	POSITION TITLE Physicist Research Scientist/Engineer		
eRA COMMONS USER NAME			
EDUCATION/TRAINING <i>(Begin with baccalaureate or other initial professional education, such as</i>			
INSTITUTION AND LOCATION	DEGREE <i>(if applicable)</i>	YEAR(s)	FIELD OF STUDY
University of California, Davis	B.S.	1992	Environmental Toxicology
University of California, Davis	Ph.D.	1998	Agricultural and Environmental Chemistry

A. Positions and Honors.**Positions and Employment**

1988 – 1992 General Building Contractor, Maddalena General Contracting, Winters CA
 1992 Staff Toxicologist, EMCON Associates, 1433 North Market Blvd., Sacramento, CA
 1992 – 1997 Post Graduate Researcher, Risk Science Program, Department of Environmental Toxicology, University of California, Davis, CA
 1996 – 1998 Graduate Student Research Associate, Energy and Environment Division, Ernest Orlando Lawrence Berkeley National Laboratory, University of California, Berkeley, CA 94720
 1998 – present Scientist, Lawrence Berkeley Lab, Environmental Energy Technology Division, Berkeley, CA

Honors

The Honors Society of Phi Kappa Phi (1992-) by election of the Chapter at University of California, Davis; Graduate Student Representative, Graduate Group in Agricultural and Environmental Chemistry, University of California, Davis (June 1995-June 1996)

B. Selected Publications

1. Srinandini Parthasarathy, Randy L. Maddalena, Marion L. Russell, and Michael G. Apte (2011) "Effect of Temperature and Humidity on Formaldehyde Emissions in Temporary Housing Units" Journal of Air and Waste Management Association. 61:689-695.
2. Xiangmei (May) Wu, Michael G. Apte, Randy Maddalena, and Deborah H. Bennett (2011) "Volatile Organic Compounds in Small- and Medium-Sized commercial Building in California" Environmental Science & Technology 45(20), 9075–9083
3. Maddalena R, M. Russell, DP Sullivan and MG Apte (2009) "Formaldehyde and other volatile organic chemical emissions in four FEMA temporary housing units" Environmental Science & Technology 43 (15), 5626-32.
4. Urs Schenker, Martin Scheringer, Michael D. Sohn, Randy L. Maddalena, Thomas E. McKone, Konrad Hungerbühler (2009) "Using Information on Uncertainty to Improve Environmental Fate Modeling: A Case Study on DDT" Environmental Science & Technology 43 (1), 128-134
5. Sleiman, M., R. L. Maddalena, L.A. Gundel, H. Destailats (2009). "Rapid and sensitive gas chromatography ion-trap mass spectrometry method for the determination of tobacco-specific N-nitrosamines in secondhand smoke". J. Chromatography A, 1216: 7899-7905.

6. Hugo Destailats, Randy L. Maddalena, Brett C. Singer, Alfred T. Hodgson and Thomas E. McKone (2008) "Indoor pollutants emitted by office equipment: A review of reported data and information needs" *Atmospheric Environment* 42 (7), 1371-1388.
7. Reiko Kobayashia, Robert A. Okamoto, Randy L. Maddalena, Norman Y. Kado. (2008) "Polycyclic aromatic hydrocarbons in edible grain: A pilot study of agricultural crops as a human exposure pathway for environmental contaminants using wheat as a model crop". *Environmental Research*, 107 (2) 145-151.
8. Reiko Kobayashi, Thomas M. Cahill, Robert A. Okamoto, Randy L. Maddalena, and Norman Y. Kado (2007) "Controlled Exposure Chamber Study of Uptake and Clearance of Airborne Polycyclic Aromatic Hydrocarbons by Wheat Grain" *Environmental Science & Technology* 41 (22), 7934 -7940.
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15. Maddalena R.L. McKone T.E. Riley W.J. (2003) "Is There a "Forest Filter Effect for Organic Pollutants?" *Stochastic Environmental Research and Risk Assessment (SERRA)*. 17(4): 231-234
16. Maddalena, R.L., T.E. McKone and N.Y. Kado (2002) "Exposure Chamber Measurements of Mass Transfer and Partitioning at the Plant/Air Interface" *Environmental Science and Technology*. 36 3577-3585
17. MacLeod, M., D. Woodfine, D. Mackay, T. McKone, D. Bennett and R. Maddalena (2001) "BETER North America: A regionally segmented multimedia contaminant fate model for North America". *Environmental Science and Pollution Research*. 8 156-163.
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19. Maddalena, R.L., T.E. McKone and N.Y. Kado (1998) "Simple and Rapid Extraction of Polycyclic Aromatic Hydrocarbons Collected on Polyurethane Foam Adsorbent" *Atmospheric Environment*, 32 2497-2503
20. McKone, T.E. and R.L. Maddalena, (1997) "Soil Contamination and Human Exposure: A Comprehensive Assessment of Exposure Analysis Methodology" *International Journal of Toxicology*, 16 319-337.

BIOGRAPHICAL SKETCH

NAME Shin, Hyeong-Moo		POSITION TITLE Post-doctoral Researcher	
eRA COMMONS USER NAME HMSHIN			
EDUCATION/TRAINING <i>(Begin with baccalaureate or other initial professional education, such as</i>			
INSTITUTION AND LOCATION	DEGREE <i>(if applicable)</i>	Year(s)	FIELD OF STUDY
Yonsei University, Seoul	B.S.	2005	Environmental Engineering
Carnegie Mellon University, Pittsburgh	M.S.	2007	Environmental Engineering
University of California, Irvine	Ph.D.	2011	Environmental Health Sciences
University of California, Davis	Postdoctoral	2013	Environmental Health Sciences

A. Positions and Honors.**Positions and Employment**

2007-2011	Graduate Research Assistant, School of Social Ecology with a concentration in Epidemiology and Public Health, University of California, Irvine, CA
2011-2013	Postdoctoral Researcher, Department of Public Health Sciences, University of California, Davis, CA

Honors

2005	Korea Research Found Scholarship Award
2006-2007	Korea Science Engineering Foundation Scholarship Award

B. Selected Peer-reviewed Publications

1. Shin HM, Vieira VM, Ryan PB, Detwiler RL, Sanders BF, Steenland K, Bartell SM. (2011). Environmental fate and transport modeling for perfluorooctanoic acid emitted from the Washington Works Facility in West Virginia. *Environmental Science & Technology* 45(4): 1435-1442. PMID: 21226527.
2. Shin HM, Vieira VM, Ryan PB, Steenland K, Bartell SM. (2011). Retrospective Exposure Estimation for Perfluorooctanoic Acid in the C8 Health Project. *Environmental Health Perspective* 119(12): 1760-1765. PMC3261988.
3. Shin HM, Ryan PB, Vieira VM, Bartell SM. (2012). Modeling the air-soil transport pathway of perfluorooctanoic acid in the mid-Ohio Valley using linked air dispersion and vadose zone models. *Atmospheric Environment* 51:67-74
4. Savitz DA, Stein CR, Bartell SM, Elston E, Gong J, Shin HM, Wellenius G. (2012). Perfluorooctanoic Acid Exposure and Pregnancy Outcome in a Highly Exposed Community. *Epidemiology* 23(3): 386-392. PMC3321117.
5. Savitz DA, Stein CR, Elston E, Wellenius G, Bartell SM, Shin HM, Vieira VM, Fletcher T. (2012). Relationship of perfluorooctanoic acid exposure to pregnancy outcome based on birth records in the mid-Ohio Valley. *Environmental Health Perspective* 120(8): 1201-1207. PMID: 22450153.
6. Shin HM, McKone TE, Bennett DH. (2012). Intake Fractions for Releases into Indoor Environment: A Tool for Chemical Prioritization. *Environmental Science & Technology* 46(18): 10063-10072. PMID: 22920860.

7. Shin HM, McKone TE, Tulse NS, Clifton MS, Bennett DH. 2012. Indoor Residence Times of Semivolatile Organic Compounds: Model Estimation and Field Evaluation. *Environmental Science & Technology* 47:859-867. PMID: 23244175.
8. Shin HM, McKone TE, Bennett DH. (2013). Evaluating Environmental Modeling and Sampling Data with Biomarker Data to Identify Sources and Routes of Exposure. *Atmospheric Environment* 69:148-155
9. Vieira VM, Hoffman K, Shin HM, Weinberg, J, Webster TF, Fletcher T. (2013). Association of perfluorooctanoic acid exposure and cancer in a contaminated community: a geographic analysis. *Environmental Health Perspectives* (In press) DOI:10.1289/ehp.1205829
10. Watkins DJ, Josson J, Elston B, Bartell SM, Shin HM, Vieira VM, Savitz DA, Fletcher T, Wellenius GA. 2013. Exposure to perfluoroalkyl acids and markers of kidney function in children and adolescents living near a chemical plant. *Environmental Health Perspectives* (Accepted)

6. ESTIMATED COST BY TASK

Task	Labor	Employee Fringe Benefits	Subs, Consultants	Travel Subsist	Copy Print	Materials and Supplies	Overhead	Total
1			\$180,600	\$100		\$10,000	\$3,510	\$194,210
2	\$42,100	\$10,525	\$16,000	\$50			\$5,268	\$73,943
3	\$35,100	\$8,775	\$10,000				\$4,388	\$58,263
4	\$40,100	\$10,025	\$11,000				\$5,013	\$66,138
5	\$34,113	\$8,528	\$13,000	\$2,000			\$4,464	\$62,105
6	\$20,000	\$5,000	\$6,359	\$100	\$50		\$2,515	\$34,024
Total	\$171,413	\$42,853	\$236,959	\$2,250	\$50	\$10,000	\$21,647	\$488,683

Note: We are also planning to submit a proposal to the Consumer Specialty Products Association and Allied Industry Associations that includes some of the work proposed here in Tasks 3 and 4. If we are funded by both organizations, a portion of the costs will be shared between the two funders.