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**Type of Organization:** College or University

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**Project Title:** Emission Inventories for Atmospheric PCBs: Model/Calibration

**Project Category:** Pollution Prevention and Reduction - BNS

**Rank by Organization (if applicable):** 0

**Total Funding Requested (\$):** 282,000 **Project Duration:** 2 Years

**Abstract:**

The two pronged strategy of air quality (NAAQS) and emission standards (NESHAP, NSPS) has not been effective in improving air quality for many POPs/PBTs, especially in their deposition to Great Waters including the Great Lakes. Organic compounds in this group include PCBs, PAHs, DDTs, and PCDDFs that may have large volatilization/emission sources from water, vegetation, soils, and urban/industrial areas. Use only of stack emissions or even links to mobile sources will underestimate air concentrations. We propose a novel strategy for estimating emission inventories for gas-phase PCBs. This strategy is based initially on correlations between measured air PCB concentrations and regional land-use and climate factors to construct a calibration function for predicting emission inventories for areas or regions. The emission factor will contain predictors for mass releases of gas-phase PCBs such as surface temperature (seasonal), mean mixing height, population, number or size of criteria industries, number or size of Brownfield's, and date of major industrial expansion. The calibration initially will be based on the data set derived from the LMMB and AEOLOS studies in 1994-95 in Lake Michigan. Second, we will compare predicted PCB concentrations based on the LM calibration data set with PCBs measured elsewhere (e.g., CB and NY Bight). Third we will conduct intensive mini-field campaigns to cover areas where no measurements exist and to test our emission function. This will involve air sampling, analysis and modeling of air-borne PCB concentrations. Lastly, we will use area source dispersion models to predict the emissions of PCBs over areas of the US and Canada that may influence deposition to the Great Lakes. The lack of emission inventories for PCBs and other banned compounds is the major limitation to atmospheric transport and deposition modeling. This approach may also provide ground-truth for those compounds for which candidate emission inventories exist.

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**Geographic Areas Affected by the Project**

**States:**

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|-------------------------------------|-----------|-------------------------------------|--------------|
| <input checked="" type="checkbox"/> | Illinois  | <input checked="" type="checkbox"/> | New York     |
| <input checked="" type="checkbox"/> | Indiana   | <input checked="" type="checkbox"/> | Pennsylvania |
| <input checked="" type="checkbox"/> | Michigan  | <input checked="" type="checkbox"/> | Wisconsin    |
| <input checked="" type="checkbox"/> | Minnesota | <input checked="" type="checkbox"/> | Ohio         |

**Lakes:**

|                          |          |                                     |           |
|--------------------------|----------|-------------------------------------|-----------|
| <input type="checkbox"/> | Superior | <input type="checkbox"/>            | Erie      |
| <input type="checkbox"/> | Huron    | <input type="checkbox"/>            | Ontario   |
| <input type="checkbox"/> | Michigan | <input checked="" type="checkbox"/> | All Lakes |

**Geographic Initiatives:**

Greater Chicago    NE Ohio    NW Indiana    SE Michigan    Lake St. Clair

**Primary Affected Area of Concern:** Not Applicable

**Other Affected Areas of Concern:**

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***For Habitat Projects Only:***

**Primary Affected Biodiversity Investment Area:** Not Applicable

**Other Affected Biodiversity Investment Areas:**

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**Problem Statement:**

The two pronged strategy of air quality (NAAQS) and emission standards (NESHAP, NSPS) has not been effective in improving air quality for many POPs/PBTs, especially in their deposition to Great Waters including the Great Lakes. Organic compounds in this group include PCBs, PAHs, DDTs, toxaphene, chlordanes, and PCDD/Fs that may have large volatilization/emission sources from water, vegetation, soils, and urban/industrial areas. Volatilization from urban, industrial or "natural" surfaces is well known to be important sources of these compounds. This is a critical determination since air pollution controls by industry will not improve this situation. It is likely that current industrial operations are small sources of these materials. Industrial brownfields, urban surfaces, land fills and even remote pristine surfaces are likely more important. Use only of stack emissions or even links to mobile sources will underestimate air concentrations. We propose a novel strategy for estimating emission inventories for gas-phase PCBs.

With the exception of the Lake Superior region, atmospheric PCBs appear to be decreasing in the other lakes with estimated half-lives of about 2-6 years, comparable to the response times of PCBs in the water and fish species. Given that PCBs are primarily removed by OH-radical attack with atmospheric half-lives of 2-14 days, the difference must reflect the extent to which PCBs and other POPs concentrations are "buffered" by emission from surface sources. In fact, atmospheric PCBs are now apparently close to equilibrium with the waters of the Great Lakes and future responses of water and biota will be determined largely by atmospheric deposition. Thus it is critical that models be developed to link PCB emissions with transport and deposition. This cannot be done without knowledge of PCB emission inventories.

This project will be a collaboration between Dr. Keri Hornbuckle of the University of Iowa and Dr. Steven J. Eisenreich of Rutgers University, both experienced researchers in the environmental fate and transport of PCBs and other semi-volatile organic compounds, and especially experienced in atmospheric processes.



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### Proposed Work Outcome:

We propose a novel strategy for estimating emission inventories for gas-phase PCBs. This strategy is based initially on correlations between measured air PCB concentrations and regional land-use and climate factors to construct a calibration function for predicting emission inventories for areas or regions. The emission factor will contain predictors for mass releases of gas-phase PCBs such as surface temperature (seasonal), mean mixing height, population, number or size of criteria industries, number or size of Brownfield's, and date of major industrial expansion. The calibration initially will be based on the data set derived from the LMMB and AEOLOS studies in 1994-95 in Lake Michigan. Second, we will compare predicted PCB concentrations based on the LM calibration data set with PCBs measured elsewhere (e.g., CB and NY Bight). Third we will conduct intensive mini-field campaigns to cover areas where no measurements exist and to test our emission function. This will involve air sampling, analysis and modeling of air-borne PCB concentrations. Lastly, we will use area source dispersion models to predict the emissions of PCBs over areas of the US and Canada that may influence deposition to the Great Lakes. The lack of emission inventories for PCBs and other banned compounds is the major limitation to atmospheric transport and deposition modeling. This approach may also provide ground-truth for those compounds for which candidate emission inventories exist.

Thus a predictive model for PCB emissions via volatilization/evasion will be constructed from chemical, meteorological, climatological and land-use/geographic data. While these data are generally available, robust data sets of PCB air concentrations are more sparse. We will use data primarily from two of the largest data sets generated in North America: The LMMB atmospheric PCB data set tied to IADN, and the New Jersey Atmospheric Deposition data set (S. Eisenreich). These data sets are robust and evaluated for data quality. The data sets have not been fully published or otherwise available to outside investigators.

We have constructed a preliminary calibration model to illustrate this approach using the LMMB data set as calibration. The most appropriate predictive factors in determining the atmospheric concentrations were air temperature (effect of T in mobilizing the surface-associated PCBs) and 1970 population (period of maximum PCB sales in the US with population density a surrogate for the size of the environmentally-mobile PCB inventory. In this correlation, T describes 31% of the variability in the  $\ln$  [PCB-air] while 1970 population describes 60% of the variability. The correlation with population has not been previously described although urban areas are the major sources of PCBs in our environment. The calibration data set was applied to predicting the atmospheric PCB concentration in three sites in NJ (urban/industrial; coastal; suburban) and even one in Riga, Latvia. The regression expression of actual to predicted was:  $[\text{PCB-measured}] = 1.00 [\text{PCB-predicted}] + 0.0$  with  $r^2 = 0.740$ . That is, 74% of the variability in the measured PCB concentrations can be explained by the calibration model with no bias (intercept = 0). The very good fit using only two predictors is surprising but, in retrospect, not unexpected. It was surprising since total PCBs rather than PCB congeners were used in the calibration model and the effect of T on individual congeners varies. We will create a calibration model based on individual congeners. The strength of the fit was surprising since the only meteorological parameter employed was T. We will, in the proposed project, introduce mean mixing height, and wind speed and direction. Using dispersion models the concentrations can be converted to emission inventories.

Overall Hypothesis: Atmospheric emission of semivolatile organic compounds can be predicted as a function of climate factors and census data.

#### Specific Objectives:

1. Construct a calibration model for a select set of PCB congeners (~80) analyzed in the LMMB and NJADN studies.
2. PCB concentrations at several sites will be predicted using the calibration model. This will provide measured and predicted data for diverse environments of the US. The model will be designed to provide predictions at the county level.
3. PCB gas-phase concentrations will be measured in a series of mini-intensive field campaigns for some of the areas identified in (2) above.
4. We will evaluate the use of available area source dispersion models (EPA's Industrial Source Complex Model or Urban

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Air Toxics Model; NOAA's HYSPLIT-HYBRID Single Particle-Lagrangian Integrated Trajectory Model) to improve the prediction.

5. Quantify the uncertainty of the model by comparing measured to predicted atmospheric PCB concentrations, and by propagated error where appropriate.

**Project Milestones:**

**Dates:**

|  |         |
|--|---------|
| Project Start                            | 09/2000 |
| Submit QA Project Plan                   | 10/2000 |
| Report- Models, Calibration, Data QA     | 10/2001 |
| Calibration Model Complete               | 10/2001 |
| Field Campaign-Air PCB Measurement-Begin | 11/2000 |
| Field Campaign-Air PCB Measurement-End   | 10/2001 |
| Report on PCB Emission Factors/Invent.   | 08/2002 |
| Project End                              | 08/2002 |

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Project Addresses Environmental Justice

**If So, Description of How:**

Project Addresses Education/Outreach

**If So, Description of How:**

**Project Budget:**

|                            | <b>Federal Share Requested (\$)</b> | <b>Applicant's Share (\$)</b> |
|----------------------------|-------------------------------------|-------------------------------|
| <b>Personnel:</b>          | 55,000                              | 8,000                         |
| <b>Fringe:</b>             | 7,000                               | 0                             |
| <b>Travel:</b>             | 5,000                               | 0                             |
| <b>Equipment:</b>          | 1,000                               | 0                             |
| <b>Supplies:</b>           | 12,000                              | 0                             |
| <b>Contracts:</b>          | 135,000                             | 8,000                         |
| <b>Construction:</b>       | 0                                   | 0                             |
| <b>Other:</b>              | 2,000                               | 0                             |
| <b>Total Direct Costs:</b> | 217,000                             | 16,000                        |
| <b>Indirect Costs:</b>     | 65,000                              | 0                             |
| <b>Total:</b>              | 282,000                             | 16,000                        |
| <b>Projected Income:</b>   | 0                                   | 0                             |

**Funding by Other Organizations (Names, Amounts, Description of Commitments):**

**Hornbuckle:**

-U.S. Environmental Protection Agency, Great Lakes National Program Office. "Study of Organic Contaminants in Air and Water in Conjunction with Episodic Events - Great Lakes Experiment." Jan. 1, 1998 to Feb 4, 2001: \$364,000.

-U.S. Environmental Protection Agency, Great Lakes National Program Office. "Atmospheric Loading of PCBs, Trans-nonaclor, Atrazine, Nitrogen and Phosphorous to Lake Michigan." Oct. 1, 1996 to Sept 30, 1999: \$251,000. (with J.V. DePinto - Co-PI)

-National Science Foundation Faculty Early Career Development (CAREER) Program. "Dynamics of Gas-Phase Persistent Organic Chemicals: An Investigation of the Effect of Climate using a Controlled Chamber." Sept. 1, 1997 through Aug. 30, 2001: \$200,000.

-Center for Global and Regional Environmental Research (CGRER). "Design and Installation of the Iowa Atmospheric Measurement Station (IA-AMS)." August 1999 - August, 2000. \$20,000. (with W.E. Eichinger Co-PI)

-University of Iowa Carver Scientific Research Initiative Grant Program. "Stage I Planning For a Trinational Atmospheric Deposition Network for Persistent Organic Pollutants." May, 1999 - May 2000. \$15,000.

**Eisenreich:**

-Hudson River Foundation, Air-Water Exchange Supports Bioaccumulation of Organic Contaminants in Phytoplankton in the Hudson River Estuary, 1999-2001, \$172 K (with J. Reinfelder).

-New Jersey Marine Science Consortium/NJ DoCommerce. PCB Air Emissions in Sites Receiving Stabilized Harbor Sediment. 1999-2001. \$238K.

-NJ Dept. of Environmental Protection/US EPA. Atmospheric Deposition Network - New Jersey. 1999-2002, \$646K.

-Hudson River Foundation, Atmospheric Concentrations and Deposition of PCBs, PAHs, and Hg to the Hudson River Harbor Estuary. 1998-2000. \$238K.

**Description of Collaboration/Community Based Support:**

Dr. Hornbuckle is an active member of the International Joint Commission's (IJC) Science Advisory Board and a liaison to the IJC's International Air Quality Advisory Board. Through these activities, Dr. Hornbuckle remains abreast of current measurement and modeling efforts in the Great Lakes region and beyond. Dr. Hornbuckle is the PI for the atmospheric modeling component of the Lake Michigan Mass Balance project. Four papers have been submitted to peer-review journals (2 are accepted by Environ. Sci. Technol.) on the LMMB. She is also the PI for the EPA-sponsored portion of the EEGLE study, an investigation of physical-chemical-biological effects of episodic events.

This project is expected to include collaboration with Mr. Orlando Cabrera-Rivera (Wisconsin DNR). Mr. Cabrera is currently assembling emission inventory estimates for organic chemical emissions from major sources, area sources, and mobile sources (point sources) in Wisconsin. The results of Mr. Cabrera's efforts are expected to result in large

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underestimation of PCB emissions, since he cannot include estimates from volatilization. Mr. Cabrera has also indicated a willingness to assist us in developing these point source emission inventories for other states.

S.J. Eisenreich's Collaboration with the New Jersey Dept. of Environmental Protection and the Hudson River Foundation relative to the development of atmospheric concentration data sets in the Mid-Atlantic States. These data will constitute one of the main calibration and model evaluation data sets for the emission inventory model. S.J. Eisenreich was PI on the AEOLUS Study that has described the emission of PCBs and PAHs into the Chicago and Baltimore atmospheres and subsequent transport and deposition to proximate Lake Michigan and Chesapeake Bay, respectively.