LA-UR-97- 2248

Approved for public release;
distribution is unlimited

Title: **A New Model to Estimate Regional
Emissions Inventories**

Author(s): Michael Williams, Michael Brown, Gerald Streit, and
Gary Thayer, TSA-4
Scott Elliott, EES-8
Ron Henry, Univ. of S. Cal.

Submitted to: DOE Office of Scientific and Technical Information (OSTI)

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

Los Alamos
NATIONAL LABORATORY

hg
MASTER

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the University of California for the U.S. Department of Energy under contract W-7405-ENG-36. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

DISCLAIMER

**Portions of this document may be illegible
in electronic image products. Images are
produced from the best available original
document.**

A New Model to Estimate Regional Emissions Inventories

Michael Williams*, Michael Brown, Scott Elliott, Gerald Streit, and Gary Thayer
Los Alamos National Laboratory

Ron Henry
University of Southern California

Abstract

This is the final report of a one-year, Laboratory-Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). The project objective was to develop new techniques that employ models and measurements to estimate air pollution emissions at a grid-cell level. Our ultimate objective is to construct a new model for computing gridded air pollution emissions by integrating meteorological, photochemical, and hybrid receptor models. We considered the simpler case of nonreactive emissions and have produced one month of synthetic meteorological data using the HOTMAC mesoscale meteorological model. This required analysis and reformatting of one month's worth of rawinsonde meteorological data, modification of the HOTMAC model to allow for time-varying upper-level wind input, and the associated data analysis of the model output. The emissions model has been successfully tested against synthetic data and data collected from a field experiment in the El Paso/Juarez area.

Background and Research Objectives

Robust estimation of emissions inventories is a prerequisite to useful air quality modeling, whether urban, regional, or global. Current emissions estimation techniques are often lacking in the amount and accuracy of information they provide. A case in point is Juarez, Mexico, where the US Environmental Protection Agency (EPA) has been working for years to acquire an emissions inventory to accurately model the El Paso/Juarez basin. EPA has met with limited success, yet a recent model of the region suggested that El Paso would be within EPA's attainment standards if Juarez's emissions were to disappear. While one may assume emissions from Juarez have some (possibly great) impact on El Paso's air quality, without a good emissions inventory this assertion remains only an assumption. Los Alamos and the University of Southern California (USC) have the

*Principal Investigator, E-mail: mdw@lanl.gov

expertise to develop a method for more accurately estimating emissions, even in regions that have no emissions inventory at all. Our objective is to construct a new model for computing gridded air pollution by integrating meteorological, photochemical, and hybrid receptor models. The model works by taking existing ambient concentration measurements and then runs "backwards" using statistical and prognostic models to obtain gridded emissions.

Importance to LANL's Science and Technology Base and the Nation's R&D Needs

This LDRD project supports the following core technical competencies at the Laboratory: 1) earth and environmental science, 2) analysis and assessment, 3) theory, modeling, high-performance computing, and 4) complex experiments and measurements. The project supports LANL's *Integrated Environmental Assessment and Modeling, Simulation, and High-Performance Computing* tactical goals. In addition, the tool developed by this project strengthens the Laboratory's suite of air quality assessment capabilities; EPA Region-6 has already expressed interest in this expanded capability.

Emissions inventories are critical to any valid assessment of urban air quality; our model provides a competitive advantage when compared to other approaches. We have the opportunity to integrate emissions estimates with forthcoming species-specific lidar capability. The potential combination of species-specific lidar and modeling is unmatched, and it addresses a significant national need.

Scientific Approach and Accomplishments

With collaborators from USC, we are optimizing a new model for computing gridded air-pollution emissions by integrating meteorological, photochemical, and hybrid receptor models. At present, estimating gridded emissions inventories is seen as the weakest link in air-quality evaluations. Our model, called SITEOF for Source Identification through Empirical Orthogonal Functions, uses existing ambient concentration measurements of pollutants and then runs "backwards" to derive the pollutants' source location and strengths. By applying a statistical empirical-orthogonal-eigenfunction approach [1], SITEOF produces emissions inventories over an entire city on 1-km² grids (see Fig. 1).

Since emissions inventories are not known with any certainty in the real world, we have tested our new model with synthetic concentration fields (see Fig. 2). These fields are produced by a Laboratory-developed air-quality modeling system [2]—the higher-order

turbulence model for atmospheric circulation (HOTMAC) and the random particle transport and dispersion (RAPTAD) model—with user-specified emissions inventories.

We produced one month of synthetic meteorological data using the HOTMAC mesoscale meteorological model. This effort required analysis and reformatting of one month's worth of rawinsonde meteorological data, modification of the HOTMAC model to allow for time-varying upper-level wind input, and the associated data analysis of the model output. The model-produced meteorological fields extend over several hundred kilometers on three nested grids and include three-dimensional winds, temperature, relative humidity, turbulence parameters, as well as two-dimensional fields of surface radiation parameters and mixing height.

These meteorological fields were used to drive the RAPTAD random-walk/puff dispersion model to produce 30 days of synthetic concentration fields from assumed emissions inventories. The RAPTAD dispersion model was modified to allow for a restart capability, which is necessary for extended simulation times.

Using the 30 days of model-computed synthetic hourly concentration fields, we are investigating the most effective ways to construct gridded emissions from the assumed inventories. With our USC collaborators, we are also determining the optimum location and number of measurement sites needed to calculate an emissions inventory. In this phase, the hybrid receptor model may be modified from two to three dimensions to accurately account for vertical wind shear and to fully take advantage of the meteorological model integration.

We initially addressed the simpler case of nonreactive pollutants (e.g., carbon monoxide). As a prelude to the next step in developing our SITEOF model, we coordinated an extensive volatile organic compounds (VOCs) canister study as part of a larger field experiment in the El Paso/Ciudad Juarez region. The field experiment was a joint effort with the Texas Natural Resource Conservation Commission and the US Environmental Protection Agency. Measurements show significant correlation between carbon monoxide and both acetylene and *trans*-2-butene (see Fig. 3), indicating that routinely measured CO might be used as a surrogate for other VOCs and thus be used as an input parameter to the SITEOF model when studying reactive species.

References

- [1] Henry, R., Y. Wang, and K. Gebhart, "*The relationship between empirical orthogonal functions and sources of air pollution*," *At. Env.*, **25A**, p 503 (1991).
- [2] Williams, M. and T. Yamada, "*A microcomputer-based forecasting model: potential applications for emergency response plans and air quality studies*," *J. Air Waste Manage. Assoc.*, **40**, p 1266 (1990).

Figure 1. Example of gridded emissions fields generated with SITEOF from synthetic concentration fields produced by a simple Gaussian dispersion model. The gray box represents an emissions source of 8 units strength; the contours depict the computed emissions inventory. Agreement is good for this simple case; we are using HOTMAC and RAPTAD data to optimize the SITEOF model for more realistic (complicated) scenarios.

Sept. 2, 0300 1st

Figure 2. A one-hour average concentration field computed with the HOTMAC/RAPTAD modeling system for a 1-km² area source of a nonreactive pollutant (CO) in the El Paso/Ciudad Juarez region. Near the source, the plume travels close to the ground and is transported to the south-southeast by low-level winds; as the plume mixes upwards, it bends to the south-southwest and is carried along by upper-level winds. Thirty days of hourly synthetic concentration, wind, and boundary-layer-depth fields were produced and fed into the SITEOF statistical model. The computed emissions inventory was then compared with the known emissions inventory that was input into HOTMAC/RAPTAD. The white dots in the figure are monitoring stations.

Figure 3. Gas chromatograph measurements of carbon monoxide (a nonreactive air pollutant) and *trans*-2-butene (a highly reactive ozone precursor) taken in El Paso during an extensive field experiment. The high correlation between the two sets of measurements indicates that the routinely measured CO can be used as a surrogate for VOCs like *trans*-2-butene, which are seldom measured for thirty consecutive days at multiple locations. From the data collected, we will determine statistical relationships between CO and relevant VOCs.