

## 8.4 MODELING FRAMEWORK TO EVALUATE SAMPLING STRATEGIES AND ESTIMATE SURFACE EMISSIONS OF TRACE GASES IN MESOSCALE

Marek Uliasz  
Colorado State University, Fort Collins, Colorado

### 1. INTRODUCTION

The Bayesian inversion method is commonly used to estimate surface emissions of CO<sub>2</sub> and other trace gases in a global scale (Kasibhatla et al., 2000). The application of this approach to limited domains used in mesoscale or regional scale modeling is more challenging. In addition to estimation of the surface tracer flux it is necessary to evaluate unknown fluxes through model lateral boundaries. The inflow flux of CO<sub>2</sub> may be several orders of magnitude larger than the CO<sub>2</sub> flux from the surface of regional modeling domain. In addition, the CO<sub>2</sub> flux from the land surface shows a strong diurnal cycle related to the uptake of CO<sub>2</sub> by photosynthesizing plants and the release of CO<sub>2</sub> by microbial decomposition in the soil.

The proposed modeling framework is based on a Lagrangian Particle Dispersion Model (LPDM) linked to CSU RAMS (Regional Atmospheric Modeling System) (Uliasz, 2000). The LPDM is used in a receptor-oriented mode (tracing particles backward in time) to derive influence functions for each concentration sample. The influence function provides information on potential contributions from surface sources and inflow fluxes through the modeling domain boundaries into tracer concentration sampled at the receptor. Then the Bayesian inversion technique is applied in an attempt to estimate unknown surface emissions.

### 2. INFLUENCE FUNCTIONS

The concentration sample,  $\Phi[C]$ , from any measurement system can be represented in a general way as an integral of concentration field,  $C$ , over the entire domain and time of simulation:

$$\Phi(C) = \int_T \iiint_V RC dx dy dz dt$$

The weight function,  $R$ , defines a location, geometry and time characteristic of the receptor. It also can take into account any processing (e.g., averaging) of real concentration data.

It is assumed that trace gases under consideration may be treated as passive tracers. Therefore, the

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*Corresponding author address:* Marek Uliasz  
Department of Atmospheric Science, Colorado State University, Fort Collins, CO 80523  
e-mail: marek@atmos.colostate.edu

concentration sample can be expressed in an alternative way directly through the emission field,  $q$ , inflow concentration,  $C_w$ , and initial concentration,  $C_0$ , with the aid of influence function,  $C^*$ , (Uliasz and Pielke, 1991):

$$\Phi(C) = \underbrace{\int_0^T \int_0^{L_x} \int_0^{L_y} C^* \Big|_{z=0} q dx dy dt}_{\Phi_1} + \underbrace{\int_0^T \int_0^{L_x} \int_0^H C^* \Big|_{t=0} C_0 dx dy dz}_{\Phi_2} + \underbrace{\int_0^T \int_0^{L_y} \int_0^H C^* \Big|_{x=0} C_w dy dz dt dx dz dt}_{\Phi_3}$$

The influence function,  $C^*$ , characterizes atmospheric transport from the point of view of a receptor (Uliasz, 1994). The influence functions can be derived in a more or less efficient way from any atmospheric transport model. In particular, they are calculated as a solution of adjoint equations in the case of an Eulerian model governed by partial differential equations. In our study, we apply a Lagrangian particle model (Uliasz, 1994) which can be run both forward and backward in time.

The first term,  $\Phi_1$ , in the above expression represents the contribution from the area surface sources,  $q$ . It describes what source area is influencing the tracer concentration measured at the receptor. In general, this term depends on the source location and time of tracer release. The second term,  $\Phi_2$ , is the contribution from the initial concentration,  $C_0$ , at the start of simulation. It depends on the sampling time of concentration and the residence time of tracer within the modeling domain. It is always possible to choose the simulation period long enough that this term becomes negligible. Finally, the third term,  $\Phi_3$ , represents the contributions from the distant sources outside the modeling domain characterized by a background concentration,  $C_w$ , at the lateral boundaries of the modeling domain. For simplicity only a term for the western boundary is shown.

### 3. CURRENT RESEARCH

The current research using the proposed framework has been focused on evaluating area averaged surface fluxes and inflow fluxes for different sizes of mesoscale domains for a tracer with constant in time emission and CO<sub>2</sub> like tracer with a strong diurnal cycle. The explored sampling strategies included air-

craft sampling and concentration time series from a tall (400m) tower.

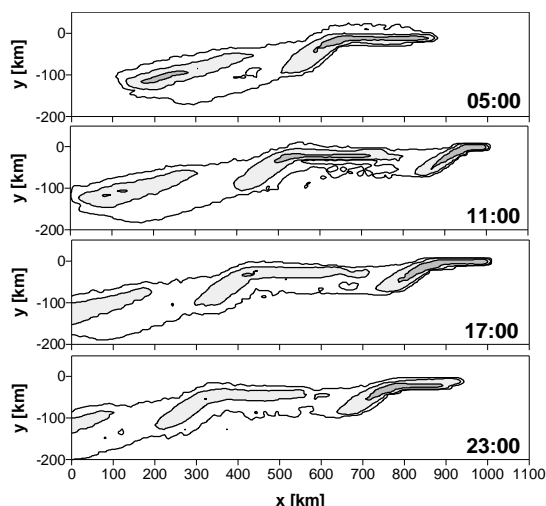


Figure 1: Surface influence functions for samples at different time of day taken at 1050m

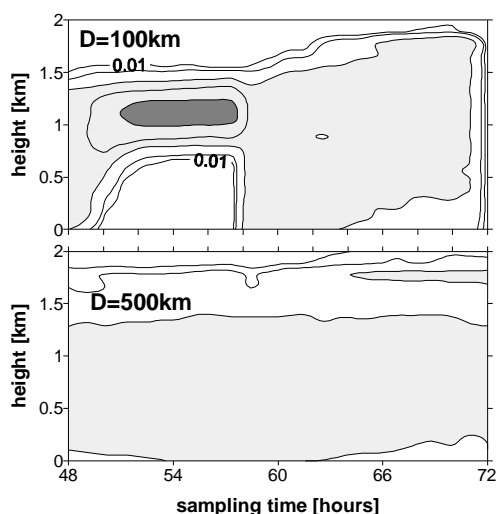


Figure 2: Upwind boundary influence functions for two domains D and different sampling times at z=1050m

Examples presented here were derived from the idealized PBL simulation over homogenous terrain for a tracer with constant in time surface flux. Figure 1 shows the surface influence functions calculated for a sample taken at 1050m at different times of day. The corresponding inflow boundary influence functions for two domain sizes are shown in Figure 2. Some results of surface flux estimations from aircraft profiles and tower time series data are presented in Figure 3.

The developed modeling framework for evaluating atmospheric sampling strategies is general and can be applied to other problems involving trace gases or air pollution. Further developing work will use pseudo-data from regional RAMS/LPDM simulations as well as real CO<sub>2</sub> concentration data collected during the

COBRA project in August 2000 in Wisconsin and the LBA project in August 2001 at Santarem in Amazonia.

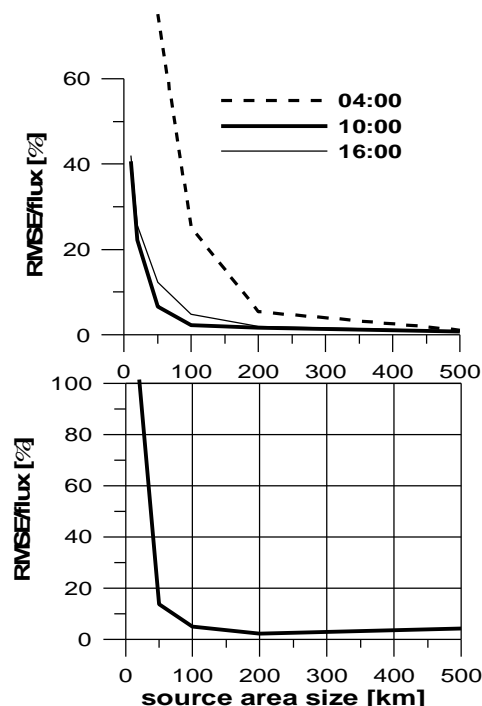


Figure 3: Estimation error for the area averaged flux for different source size using single aircraft profiles without estimation of the inflow flux (top) and 24 hour time series from a 400 m tower with the estimation of the inflow flux for the 500 km domain (bottom)

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