INCORPORATING UNCERTAINTY INTO AIR QUALITY MODELING AND PLANNING – A CASE STUDY FOR GEORGIA

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1. INTRODUCTION

Accuracy of Air Quality Model (AQM) results and sensitivity of atmospheric pollutants to changes in emission is of serious concern in air quality planning and formulation of policies involving the selection of control strategies for multiple pollutants. Proper air quality assessment requires accurate estimation of the uncertainty in photochemical sensitivities. Many studies so far have tried to find out the sensitivity of atmospheric pollutant concentrations to precursor emissions due to uncertain model input parameters. However, the uncertainty of these sensitivities to uncertain photochemical model input parameters remains largely unexplored. We intend to focus on this grey area of research and present a direct way of gauging the accuracy of the photochemical sensitivities of ozone and particulate matter (PM) to precursor emissions. We also present some preliminary results supporting the efficacy of our approach by applying it to a case study for ozone and PM attainment planning in Georgia using High-order Decoupled Method (HDDM) in the Community Multi-scale Air Quality (CMAQ) model.

2. MOTIVATION

This work is done as a part of the project funded by U.S. EPA STAR grant program # R833665. The state of Georgia pioneered an integrated approach for linking photochemical models with economic and health benefit analyses in its recent State Implementation Plan (SIP) development efforts for ozone and fine particulate matter ($PM_{2.5}$) (Cohan et al., 2006). This integrated approach aimed at satisfying three major criteria's (***Figure 1***):

(1) Air Quality – to bring down the multiple criteria pollutants by the help of a advanced atmospheric sensitivity analysis technique like HDDM (Hakami et. al., 2003; Boylan et al., 2006) in conjunction with CMAQ (Byun and Schere, 2006);

(2) Estimation of cost of control strategies and emission reduction using cost assessment tools at worst monitor (specially power plants and specific anthropogenic sources); and

(3) Assessment of health benefits (Marmur, 2006) using BENMAP for a given population exposure (Abt Associates, 2003)

Although these major improvements were done with respect to the previous SIP development, all analyses were conducted in a deterministic sense, with no formal efforts to quantify uncertainty. Our work in this overall project would be estimating this uncertainty. Here, we will present the detailed methodology for part (1) of the 3 sectors discussed above and present some preliminary results. In the future, results from this study will be used to find a cross-linkage between the 3 broad areas and come up with best suitable and optimum control strategies for Georgia.

3. BACKGROUND

Secondary pollutants have a nonlinear response to their precursor emissions, as a result of which the sensitivity of these secondary species is not always constant. For example, ozone may

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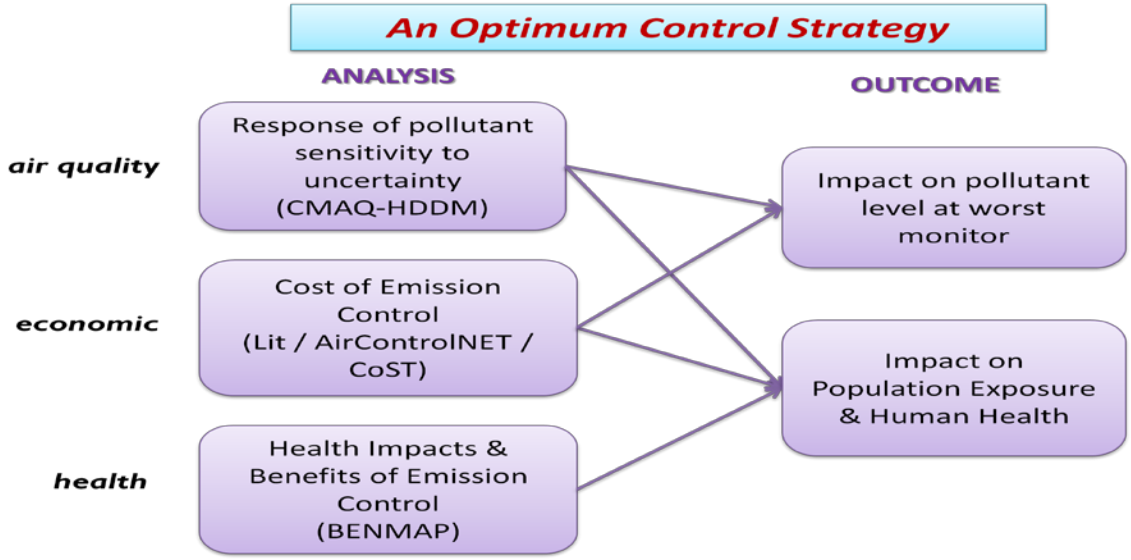

Figure 1. Linked models applied in previous Georgia ozone and $PM_{2.5}$ planning to assess the impacts of potential control measures on attainment and health (Cohan et al., 2006).

respond differently to reductions in nitrogen oxides or volatile organic compounds emissions depending on the base levels of these emissions and the size of reductions. Therefore, it becomes very important to accurately determine the nonlinear responses of these photochemical sensitivities. In 2003, Hakami *et. al.* introduced High-order Decoupled Direct method (HDDM) as an evaluation tool for CMAQ which is capable of efficiently determining the nonlinearities in AQM. HDDM estimates the high-order sensitivity coefficients by calculating the local derivatives. This method is used here to find out the response of the sensitivity of secondary pollutants to precursor emissions due to uncertainty in the emission inventories (high-order self sensitivity) or due to perturbed meteorological/chemical conditions like reaction rates, deposition velocities or other precursor emissions (cross-sensitivities).

4. METHODOLOGY

Sensitivity coefficient is evaluated by calculating the response of a secondary pollutant, ozone and fine particulate matter in this case, to any perturbation in the precursor emission. Let us assume that atmospheric concentration of a secondary pollutant is ***C***, then the first order sensitivity (slope) of this pollutant to any perturbation ***p*** in the ***j***th parameter is given by (Cohan *et. al,* 2005)

$$S_j^{(1)} = \frac{\partial C}{\partial \varepsilon_j} \qquad (1)$$

where ε_j is the scaling variable with a nominal value of 1. Since ***C*** is a non-linear function of ***j***, $S_j^{(1)}$ will not be a constant term for all points of the response function. Therefore, it becomes necessary to calculate this non-linear variability (curvature) which is estimated by the second-order sensitivity coefficient (high-order self sensitivity),

$$S_j^{(2)} = \frac{\partial^2 C}{\partial \varepsilon_j^2} \qquad (2)$$

Similarly, the second-order sensitivity of C to ***j***th parameter when parameter $k \neq j$ is perturbed is given by (cross-sensitivities),

$$S_{j,k}^{(2)} = \frac{\partial^2 C}{\partial \varepsilon_j \partial \varepsilon_k} \qquad (3)$$

These local derivatives calculate accurately the sensitivities for small degree of uncertainty, say within 30% of nominal value, which is most often encountered in practice.

Now, when we have additional condition where any parameter P_j is uncertain by $\Delta\varphi_j$. Then, following the same logic as above we have,

$$u_j = \varphi_j P_j = (1 + \Delta\varphi_j) P_j \qquad (4)$$

where u_j is the perturbation due to the uncertain scaling variable φ_j with a nominal value of 1. Due to this uncertain parameter, the modeled sensitivity values will be different from actual sensitivities as we are now calculating derivatives at a point different from the earlier point on the response function (***Figure 2***).

Hence, the actual first-order sensitivity of a secondary pollutant to j^{th} emission $S_j^{(1)*}$ when j is uncertain by u_j will be given by,

$$S_j^{(1)*} = \left(1 + \Delta\varphi_j\right)\left(S_j^{(1)} + \Delta\varphi_j S_{j.j}^{(2)}\right) \quad (5)$$

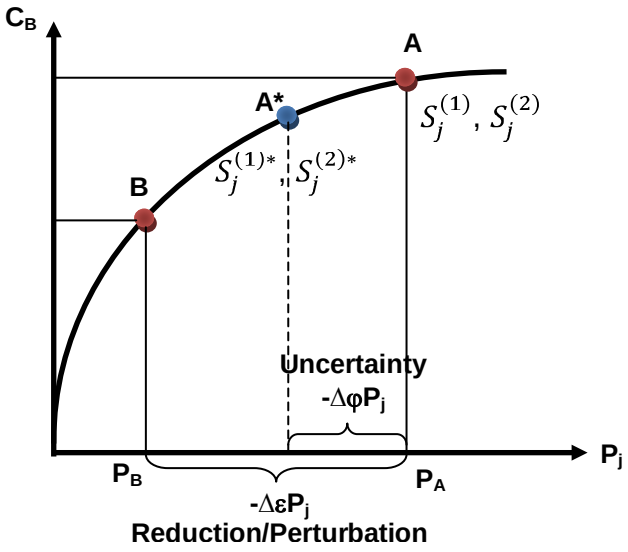

Figure 2. Pollutant response to model input parameter due to perturbation and uncertainty within the model values. [Figure illustrates the response of ***C*** due to perturbation in jth parameter P_j when P_j is uncertain by $-\Delta\varphi P_j$. Modeled response is expressed as the sensitivity coefficients $S_j^{(1)}$ and $S_j^{(2)}$ and actual sensitivities due to uncertainty are $S_j^{(1)*}$ and $S_j^{(2)*}$].

Similarly, actual sensitivity of a secondary pollutant to j^{th} emission $S_j^{(1)*}$ when parameter $k \neq j$ is uncertain by u_k will be given by,

$$S_j^{(1)*} = S_j^{(1)} + \Delta\varphi_k S_{j.k}^{(2)} \quad (6)$$

Extending this to our current goal, we step forward to venture into the real world where multiple input parameters to a given AQM are uncertain at the same time. The recipe to analyze a situation like this is quite straight-forward. The actual sensitivity of a secondary pollutant to j^{th} emission $S_j^{(1)*}$ when both parameters j and $k \neq j$ are uncertain can be given by,

$$S_j^{(1)*} = \left(1 + \Delta\varphi_j\right)\left(S_j^{(1)} + \Delta\varphi_j S_{j.j}^{(2)} + \sum_{k \neq j} \Delta\varphi_k S_{j.k}^{(2)}\right) \quad (7)$$

In the above equation, $S_j^{(1)}$, $S_{j.j}^{(2)}$, $S_{j.k}^{(2)}$ can be calculated using CMAQ-HDDM based on equations 1, 2 and 3 respectively. $\Delta\varphi_j$ and $\Delta\varphi_k$ are the scaling factors for uncertainty in input parameters j and k respectively.

Many studies have been conducted to determine the uncertain nature of input parameters used in an air quality model like CMAQ (Gao et. al. 1996, Bergin et. al. 1999, Hanna et. al. 2001, Deguillaume et. al. 2007 & 2008). For each input parameter, probability distribution functions can be developed specifying the upper and lower bounds within which the parameter values can vary (e.g. L-N function with ± 1.3σ values, where σ is the standard deviation from the mean, μ). To generate values for uncertainty scaling factors in equation 7, $\Delta\varphi_j$ and $\Delta\varphi_k$, we limit ourselves to these distributions that are available from literature.

Therefore, $S_j^{(1)*}$ can be evaluated using equation 7 for all values of $\Delta\varphi_j$ and $\Delta\varphi_k$ within the PDFs and running HDDM over and over again for all cases. However this would require inordinate number of runs which become very expensive to be carried out and thus would be computationally inefficient. Instead we can adopt a surrogate model approach where we can randomly sample out $\Delta\varphi_j$ and $\Delta\varphi_k$ values from these input PDFs and plug them into equation 7 to solve for the output actual sensitivity $S_j^{(1)*}$ using simple/Bayesian Monte Carlo analysis.

The output sensitivity $S_j^{(1)*}$ will also have a random distribution which will be a non-linear function of input variables representing the randomness of the modeled sensitivity. This uncertainty can be characterized by curve-fitting techniques using these random Monte Carlo

outputs. Thus, this method will help us to probe the uncertainty associated with modeled sensitivities when multiple model input parameters are uncertain.

4. CASE STUDY - GEORGIA

A 12 km modeling domain for the region of Alabama-Georgia (ALGA) was selected and our focus was specially based on Georgia and CMAQ version 4.6 was use. HDDM was used to calculate the first and high-order sensitivities. A summer episode ranging from May 30 – June 06, 2009 has been chosen as the test case period. Analysis was carried out to probe the effect of single uncertain input parameter on ozone sensitivity to its precursor emissions. Results for multiple uncertainties are not presented here.

Uncertain AQM input parameters are prioritized and selected based on literature (Gao et. al. 1996, Bergin et. al. 1999, Hanna et. al. 2001, Beekman & Derognat 2003, Deguillaume et. al. 2007 & 2008). Results have been presented here for 2 scenarios: (1) Uncertain emission inventory and (2) Uncertain reaction rate. For the first scenario emission of NOx was considered as an example case and for the latter case reaction rate for HNO_3 formation was selected.

5. PRELIMINARY RESULTS

5.1 Uncertain Emission Inventory

As an example case for this study, the impact of a ±30% change (uncertainty) in modeled NOx emission inventory on ozone sensitivity to NOx and VOC emission is analyzed (***Figure 3***).

Ozone sensitivity to Atlanta NOx generally increases when the actual NOx emission is greater than the modeled inventory value; however some locations observe NOx disbenefit ***(Figure 3a & 3b)***. On the other hand, sensitivity of ozone to Atlanta VOC shows slight increment when modeled NOx inventory is smaller than the actual emission ***(Figure 3c & 3d)***.

5.2 Uncertain Reaction Rate

To study the response of ozone sensitivity to NOx emission when there is an uncertainty in the photochemical reaction rates, an example case of ±30% change (uncertainty) in the rate constant for $NO_2 + OH \rightarrow HNO_3$ is selected. It is found that the sensitivity of ozone to Atlanta NOx gradually decreases when the NOx emission is actually greater than the reported value (Fig 3e & 3f).

5.3 Conclusion

From the above results we find that uncertainty plays a vital role in the selection of control strategies for a given region. For example, in section 5.1 ***(Figure 3a & 3b)***, if we did not consider the uncertainty in NOx emission then we might end up saying that in order to reduce O_3 levels we have to bring down Atlanta NOx, which is actually not going to happen if NOx emission is greater than the inventoried value. Similarly if reaction rate of $NO_2 + OH \rightarrow HNO_3$ is larger than expected then the response of ozone reduction to emission control actually decreases.

6. SUMMARY

A unique method of estimating the uncertainty of ozone sensitivity to precursor emissions due to multiple uncertain air quality model input parameters is presented here. A model has been introduced which involves Monte Carlo analysis as a post-processor alongwith CMAQ-HDDM. In the selection process for an overall State Implementation Plan (SIP) for ozone attainment, it must be ensured that the ensemble of individual controls is effective in the overall attainment of the National Ambient Air Quality Standard (NAAQS). To demonstrate this generally Brute Force is conducted to estimate the response of pollutant sensitivity to the ensemble of separate emission controls due to multiple parametric uncertainties. However, the computational burden and numerical noise makes this process unfavorable. A surrogate inexpensive model development like this can be used in place of the traditional Brute-Force method to bridge these gaps by averting numerical noises and saving computational time.

However CMAQ-HDDM is not presently capable of calculating high-order PM sensitivities; hence brute force will be used for such cases.

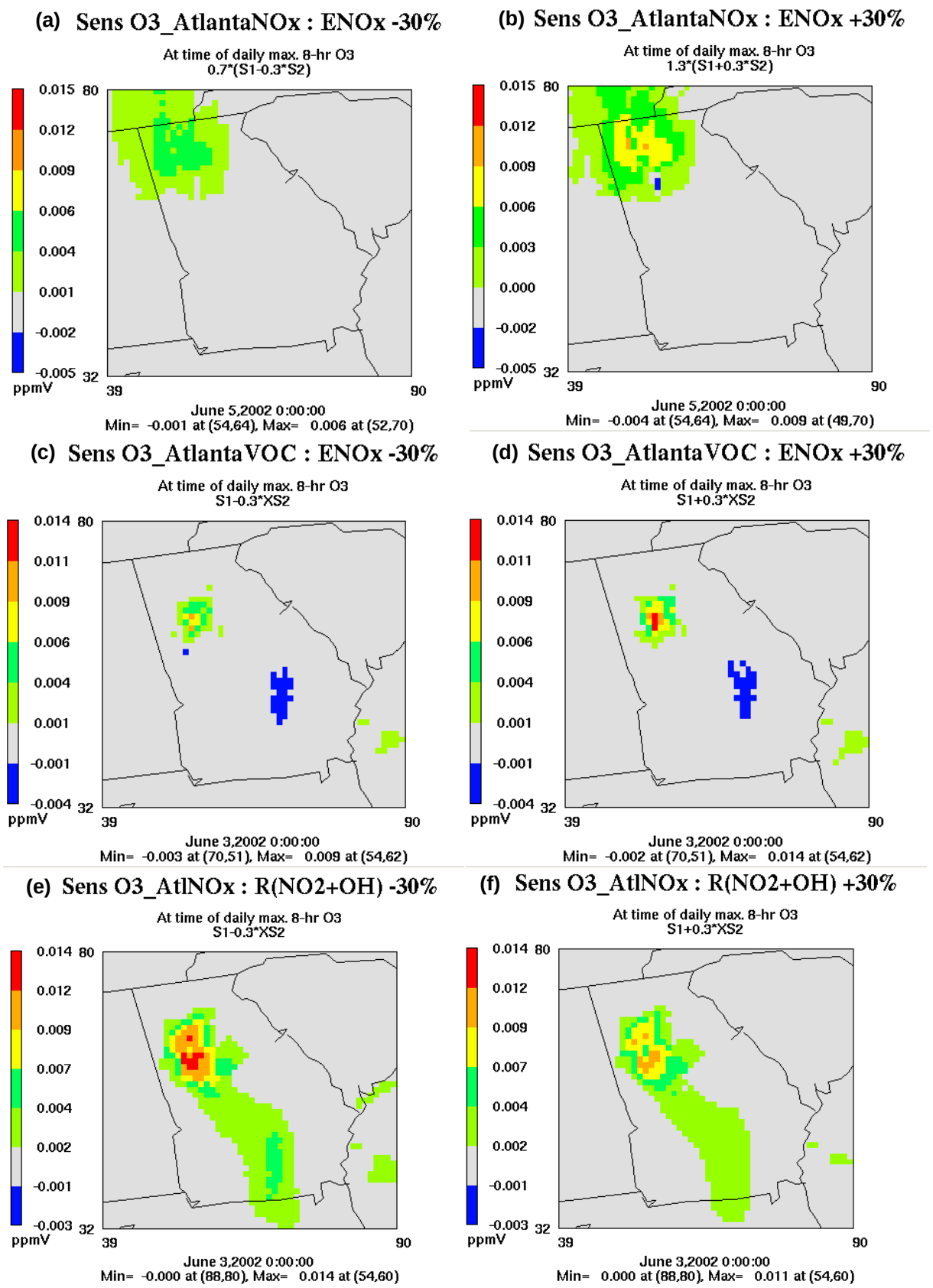

Figure 3. Response of ozone sensitivity to NOx (a, b, e & f) and VOC (c & d) emission at time of daily maximum 8-hr ozone when NOx emission (a, b, c & d) and Reaction rate for NO_2+OH → HNO_3 (e & f) is actually (left) -30% less and (right) +30% more than the inventoried value used in Air Quality Models.

7. FUTURE WORK

In the future we intend to extend our work to inform the selection of control strategies that satisfy the three criteria discussed in Figure 1. Control costs for effective mitigation measure will be estimated using available control cost software and health assessment will be carried out for different population exposures. These analyses will be linked to re-examine control strategy for ozone and $PM_{2.5}$ attainment in Georgia.

8. ACKNOWLEDGEMENT

Our project is funded by U.S. Environmental Protection Agency (EPA) as a Science To Achieve Results (STAR) program under research grant #R833665. We thank Georgia Environmental Protection Division (GA EPD) for providing us with the emission inventory data and their sincere help all through our research.

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