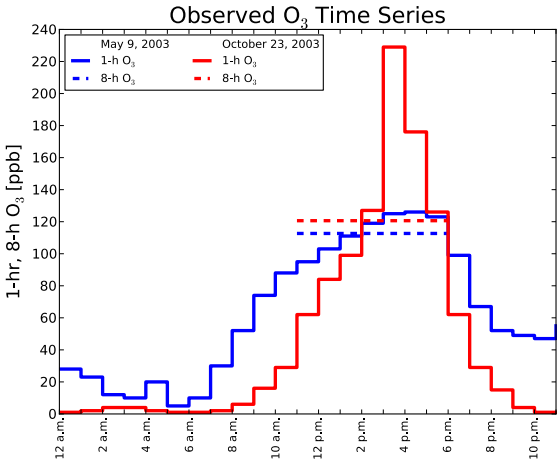

Lies, Damned Lies, and Photochemical Models

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Abstract

Since time immemorial, the modeling community has debated the nature and purpose of numerical models in a way that would make Plato smile. Are models real or just shadows on the wall? Must models maintain strict fidelity to natural laws or can they make pragmatic assumptions? Air quality managers and regulatory agencies don't have the luxury of debating modeling philosophy, virtuous though it is. They need decision-making tools today and cannot wait for the body of science to be completed tomorrow. Hence, regulatory photochemical modeling takes the pragmatic approach. These models, many of them developed and evaluated for use in Houston, Texas, incorporate the atmospheric community's current understanding of environmental principles and best guesses at input parameters (e.g. emissions, meteorological fields, boundary conditions). The process of model formulation necessarily introduces error and uncertainty because models *cannot* be identical to an open environmental system. Remaining cognizant of this fact is paramount to a responsible and justifiable use of model predictions. In the right hands, regulatory photochemical models are powerful predictive tools that assist in the development of pollution control strategies.

In this work, we look at factors that contribute to Houston's highest measured ozone (O_3) concentrations and deficiencies in the regulatory modeling that has been developed to test control strategies and, ultimately, show future attainment of the federal O_3 standard. Some of the highest O_3 peaks are characterized by sudden increases in observed concentrations of at least 40 parts per billion (ppb) in one hour, or 60 ppb in two hours – a phenomenon that is unique to Houston. Measurements show that these large hourly changes appear at only a few monitors and span a narrow geographic area suggesting a spatially heterogeneous field of O_3 concentrations. Regulatory air quality modeling was unable to reproduce the magnitude or location of some of the highest observed hourly O_3 changes, and it also failed to capture the limited spatial extent. There is a growing body of evidence that inculpates large releases of volatile organic compounds associated with the vast network of petrochemical facilities in Houston. Understanding why these O_3 events occur is critical to developing an effective and defensible regulatory air quality management policy in Houston.