

# ISSUES IN OXIDANT MODELING

*Joel L. Horowitz, Office of Policy Analysis, U.S. Environmental Protection Agency*

Since 1969 a variety of legal requirements have been established that make it necessary to forecast the effects of changes in transportation systems on atmospheric oxidant concentrations. Such forecasts are needed in connection with the environmental impact statements required by the National Environmental Policy Act, the state implementation plans required by the Clean Air Act, and the certification process carried out under the Federal-Aid Highway Act.

The development of legal requirements for oxidant forecasting has been accompanied by the development of numerous techniques that planners might use to predict the effects of transportation changes on oxidant concentrations. These techniques range in complexity from the almost trivial to the almost incomprehensible. Some of the techniques require minimal skills and data to use, but others require large quantities of data, sophisticated computing facilities, and highly skilled users. Moreover, the accuracy of all the techniques is known poorly, if at all. Given these factors, it is not surprising considerable uncertainty and confusion exist as to the technical procedures that should be used to forecast the oxidant impacts of transportation system changes.

The proliferation of oxidant forecasting techniques and the confusion surrounding their use reflect the extreme difficulty of modeling the relation between the emissions of air pollutants by motor vehicles and other sources and the concentrations of oxidant in the atmosphere. The principal reason for this difficulty is that oxidant is not emitted into the atmosphere by any emissions source. Rather, it is the product of chemical reactions in the atmosphere involving a wide variety of organic compounds and oxides of nitrogen. The organics and nitrogen oxides are emitted by motor vehicles, various industrial and commercial operations, and certain natural processes. In forecasting oxidant levels or changes in oxidant levels, one must consider not only atmospheric dispersion and transport, as must be done with any air pollutant, but also a complex set of chemical reactions.

One of the consequences of the involvement of atmospheric chemical reactions in oxidant formation is that it is not possible to state a priori whether oxidant concentrations will decrease if emissions of oxidant precursors (organic compounds and nitrogen oxides) decrease. In the case of an inert pollutant, such as carbon monoxide, a decrease in emissions is likely to cause a decrease in concentrations, other things being equal. However, under certain conditions decreasing either organic or nitrogen oxide emissions can cause oxidant concentrations to increase. This observation leads to what might be the most basic questions about oxidant control from the point of view of transportation planners and others responsible for formulating and implementing public policy options: What kinds of emissions should be reduced in order to reduce oxidant concentrations? Can it be said with reasonable confidence that reducing emissions of organics or nitrogen oxides or both in some suitable proportion will reduce oxidant concentrations?

These questions are addressed in the papers by Dimitriades and by Myrabo, Wilson, and Trijonis, who conclude that achieving the ambient air quality standard for oxidant in urban areas requires substantial reductions of emissions of hydrocarbons and other

reactive organics in the source areas. The situation with respect to nitrogen oxide emissions is more delicate. In some urban areas reductions of nitrogen oxide emissions are needed to attain or maintain the ambient air quality standard for nitrogen dioxide. Moreover, reductions in urban area nitrogen oxide emissions may be needed to control oxidant concentrations in rural areas. However, excessive reduction of nitrogen oxide emissions may increase the difficulty of controlling urban oxidant concentrations.

The question of the directionality of oxidant changes leads to the problem of estimating the magnitudes of these changes. The papers in this report describe 4 techniques that might be used to estimate the changes in oxidant concentrations resulting from changes in precursor emissions:

1. Linear or nonlinear rollback methods, by Dimitriades and by Myrabo, Wilson, and Trijonis;
2. Smog chamber models, by Dimitriades;
3. Statistical models, by Myrabo, Wilson, and Trijonis; and
4. Diffusion models, by Demerjian and by Ranzieri and Shirley.

These techniques also are addressed by Seinfeld and Eschenroeder.

Rollback is the simplest of the 4 approaches and the one that has received the most widespread use to date. Its drawbacks are well known. These include failure to incorporate explicitly the effects of nitrogen oxide emissions, lack of spatial and temporal disaggregation, and lack of a clear statistical meaning.

Diffusion models are the most sophisticated of the various modeling approaches and provide the most detailed (and, presumably, most realistic) description of the oxidant formation and dispersion process. These models offer the possibility of providing spatially and temporally disaggregated descriptions of the relation between oxidant and its precursors. However, the models have not yet reached a stage of development and verification such that the authors of papers in this report would advise an agency that does not already have access to a diffusion model to go to the expense and difficulty of acquiring one. On the other hand, agencies that have access to diffusion models probably should use them, preferably in parallel with other techniques and in connection with a program to monitor their validity.

Even when the current developmental problems have been solved, the cost and difficulty of using diffusion models will prohibit their use in many situations. Thus, there will remain a need for modeling techniques that are simpler than diffusion models but more sophisticated (and, presumably, more accurate) than rollback methods. Smog chamber models and statistical models estimated from aerometric data or, possibly, from data obtained through numerical experiments with diffusion models offer promising approaches to fulfilling this need. Both modeling approaches can incorporate nitrogen oxide effects explicitly, and statistical models may be capable of achieving spatial disaggregation. Each of the approaches has certain problems, the most notable being that they are at relatively primitive stages of development and of unknown validity. However, they are sufficiently easy and inexpensive to use that the authors of papers in this report suggest that planning agencies consider making use of smog chamber and statistical methods in parallel with rollback methods and, when available, diffusion models. The widespread use of smog chamber and statistical models, in parallel with other models and in connection with programs to monitor their validity, is likely to be the best way to acquire the information needed to assess the value of these techniques.

All of the applications of models to date have been based on the assumption that oxidant concentrations in a region are attributable to precursor emissions in the same region. Recently, however, it has been discovered that oxidant can be transported over distances of at least 30 miles (48 km) and that high oxidant concentrations exist in rural areas. These findings lead to several significant questions for urban-based oxidant models and oxidant control strategies.

1. To what extent are elevated rural oxidant concentrations caused by natural

sources and, therefore, uncontrollable?

2. To what extent does rural oxidant, whatever its source, contribute to urban oxidant concentrations?

3. To what extent are urban areas polluting rural areas?

4. Do the rural oxidant and transport phenomena imply that oxidant modeling and control can be carried out meaningfully only on a multiregional or multistate basis?

These questions are addressed in the paper by Angus and Martinez, who conclude that elevated rural oxidant concentrations are attributable largely to man-made emission sources. However, it was suggested in the workshop that this conclusion may be premature and that there is a possibility of significant natural contribution. It was also suggested that, based on chemical considerations, the transport of oxidant from rural areas into urban areas may have relatively little effect on urban oxidant concentrations but that the transport of oxidant precursors from rural areas into urban areas may be capable of affecting urban oxidant levels. All the authors agree that more research is needed before a satisfactory understanding of rural oxidants and transport and their implications for urban oxidant control is achieved.

It is clear from the papers in this report that the field of oxidant modeling contains many ambiguities and few unqualified conclusions. However, it is also clear that a variety of potentially promising modeling approaches exist. It is likely that the validity and usefulness of these approaches cannot be determined until there has been widespread experience with them. I hope that the papers in this report encourage potential users of the modeling techniques to become users and, thereby, contribute to the needed experience.

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