Abstract. Photochemical air quality models provide the most defensible method for relating future air quality to changes in emission, and hence are the foundation for determining the effectiveness of proposed control strategies. However, strategies, based primarily on controlling reactive organic gas emissions, have not provided the expected benefits. This raises the question of what have been the deficiencies in previous studies utilizing these tools? Furthermore, what changes are necessary, and desired, to improve upon past efforts? The current generation of models have matured within their original frameworks to represent, relatively accurately, the important physical and chemical processes affecting pollutant dynamics in urban atmospheres. The ability to follow regional dynamics is less well demonstrated. Current regional models have a single horizontal resolution scale. Multiscale models will enable detailed treatment of urban chemistry, and also effectively follow long range transport and chemistry. Improved computational capabilities will allow more detailed chemistry and heterogeneous processes to be followed within the models. The practice of photochemical modeling will benefit greatly from recent and future intensive field studies. The advancements in both the model framework and practice will allow much more accurate evaluation of proposed control strategies, and lead to a much improved understanding of pollutant dynamics.

1. Introduction

Over $40 billion dollars is spent annually on air pollution control in the United States; revisions to the Clean Air Act could double that. A central element in designing strategies to best allocate those resources has been air quality modeling (Figure 1). Use of models is necessary because of the complexities of pollutant formation and transport in the atmosphere. This is especially true when chemical transformation is involved, such as in photochemical oxidant models used to design \( \text{O}_3 \) control strategies. Future requirements likely will put an even greater reliance on air quality models.

The increased demand for and dependence upon models calls for an analysis of the present state of air quality modeling. In particular, the interest here is in oxidant models and the future directions in photochemical air quality modeling. Those directions can be classified in two areas: (1) advancements in air quality models, and (2) future developments in the practice of air quality modeling. As discussed below, much of the progress will be in the practice as well as new model formulations. Before delving into the future, however, it is appropriate to assess the current situation and the state-of-the-science. Two issues are of direct relevance. First, why have strategies, based primarily on controlling reactive organic gas (ROG) emissions, not provided the expected benefits? It is only recently that \( \text{NO}_x \) control has become widely accepted as the key to reducing \( \text{O}_3 \) in many areas. Likewise,
what were the deficiencies in previous studies (that led to an ROG only path), and what changes are necessary to improve upon past efforts?

2. Current Photochemical Air Quality Models

The current generation of photochemical models used for research and regulatory purposes are relatively mature within the frameworks that were adapted when they originated. They are composed of descriptions of the major processes affecting air quality: emissions, atmospheric chemical dynamics, and pollutant transport mechanisms along with a mathematical solution procedure. The description of the processes is further broken down into specific processes (Figure 2). The intent has been to include the best available information within the detailed descriptions (or modules), and in this way keep the model up to date. Thus, air quality models serve two very immediate purposes. They are the most scientifically defensible methods for designing control strategies by relating future air quality to emission changes. Also, they serve to integrate and expand our knowledge of how pollutants behave in the atmosphere. As such, they are both regulatory and research tools.

There are two standard classes of models used in regulatory analysis of $O_3$ control requirements. First, there are those based primarily on following the chemical dynamics of a pollutant system with a rather minimal (if any) description of the co-occurring physics (e.g., deposition, convection, wind shear, etc.). The classic