

Comparison of the relative importance of the gas-phase and the aqueous-phase pathways for H_2SO_4 is difficult due to the different parameters that control each. The instantaneous rate expressions given in Table 4.1 must be integrated over periods of events if either the SO_2 or oxidizing agent is depleted. For example, if SO_2 and HO_2 enter a convective cloud, the formation of H_2SO_4 through their reaction will cease if either reactant is totally consumed. Such a reactant is called the "limiting reactant" since its concentration governs the net amount of product formed.

4.4 Chemical Knowledge and LRT Models

To date, the detailed chemical knowledge presented above has not been incorporated into regional transport models. The MOI LRT models only use linearized approximations of the non-linear H_2SO_4 and HNO_3 formation rates. Regional Eulerian grid models are capable of employing non-linear chemistry, but they are presently insufficiently developed for assessment use.

Rodhe et al.¹² have formulated a simple non-linear chemistry box model for atmospheric acidification. Their work is useful in demonstrating the influence of non-linearity on acid formation and removal rates, but the model possesses serious deficiencies which limit its usefulness for assessment applications. Specifically, its major deficiencies are:

- (a) The use of ethylene as a surrogate for VOC in polluted atmospheres is not sufficient to represent the variety of reactive VOC present in polluted atmospheres;
- (b) The chemical mechanism does not provide an adequate representation of VOC- NO_x oxidation cycle as presently understood for polluted atmospheres; and