

2.178 Determination of pathways in chemical reaction systems: an algorithm and applications to atmospheric chemistry.

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Abstract:

When a complex chemical system is analysed, a typical question is: How, i.e. via which reaction sequences (= pathways), is a certain species of interest produced or destroyed? An algorithm for the automatic determination of such reaction sequences is presented. Under the assumption that a chemical reaction system is given and reaction rates are known (from a chemical model run), the algorithm constructs all significant pathways and calculates a rate for each of them. Up to now the algorithm has been applied to analyse the chemistry in the stratosphere (ozone formation and destruction, methane oxidation, maintenance of elevated active chlorine levels through HCl null cycles), the mesosphere (HNO_3 formation by ion chemistry), the atmosphere of Mars (CO_2 formation), and the atmospheres of potential extra-solar planets.