Dynamic Graphical Interface for Online Analysis of Chemical Kinetic Pathways in Complex Kinetic Mechanisms

Detailed chemical kinetic mechanisms are often employed in the analysis of complex chemical reaction systems. The simulations with detailed mechanisms provide concentration of species – molecules and free radicals – involved in hundreds or even thousands of simultaneous chemical reactions. The simulation results, however, do not directly indicate which of the multitude of parallel reaction pathways dominates the process. In order to improve the process, for example, minimizing the formation of by-products, knowledge of the reactions sequence and the dominant pathway is essential. We found that there is sufficient information within the simulation results to generate reaction pathway diagrams.

To facilitate automatic generation of pathway diagrams, a series of software Fennimore, 1970). Recently published studies have indicated the importance of N2 + H? NNH channel, but attributed to it only a third of NO emissions. In contrast our study suggests that the NNH channel is the dominant NO production path.

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