Simu-tech Mid Term Report

Dijkstra’s algorithm on plasma chemical reaction

The things I understand is that this paper explores how graph theory can be applied to plasma chemical reaction engineering. It mainly focuses on constructing a weighted directional graph that includes reaction nodes based on existing air reaction data. The graph visualizes the reaction network and identifies potentially useful or problematic reaction pathways. The paper uses Dijkstra’s algorithm to analyse species connectivity and suggests that certain conditions, reactions, or species can be enhanced or suppressed to achieve targeted chemical formation. The authors introduce a graph analysis algorithm, OCARINA, to optimize conditions for specific chemical formation. The algorithm's predictions align with known conditions for optimal ozone production in air. Time-dependent simulations show preferential formation of O and O3 using conditions from the algorithm.

One more benefit is Visualisation of graphs can be especially useful as a means of comparing pathways. The visual representation of the data arranged in graph format has the advantage of being able to show the relationships between data entities

Whilst the concentration of species changes over time, the rate coefficients are constant for a given set of conditions and can be used as a measure of each reaction as a fast or slow step in the whole network.

In summary, the paper presents an innovative approach to plasma chemical reaction engineering by applying graph theory. This method allows researchers to identify and optimize pathways for targeted chemical production in plasmas. By using Dijkstra's algorithm and OCARINA, the study successfully demonstrates the potential of graph theory to guide the optimization of plasma chemistry processes.

**Findings:** Visualization of the graph revealed insights into potential reaction pathways for ozone formation and the influence of different conditions (e.g., temperature and electron energy) on reaction rates. OCARINA algorithm predictions aligned with known optimal electric field strength regimes for ozone production, suggesting its potential in identifying promising simulations and experiments.

**Limitations:** The research paper primarily focuses on a specific dataset for air plasma, which may limit the generalizability of the findings to other plasma chemical systems. The visualization and algorithmic approaches may require significant computational resources and could become cumbersome with larger, more complex reaction networks. Further validation of the OCARINA algorithm and other proposed methods in real-world scenarios and with diverse plasma systems is necessary to establish their efficacy. The study does not extensively address the impact of varying initial conditions (e.g., species concentrations) on the graph analysis results.