Computations in chemical engineering

This document is regarding my understanding of the research paper on the topic Graph Theory Applied to Plasma Chemical Reaction Engineering.

An abstract idea on this topic is how graph theory is useful to plasma chemical reaction engineering , running Dijkstra’s algorithm between all species reaction nodes. A connectivity matrix of Dijkstra’s algorithm between each two species gave a measure of the relative potential of species to be created and destroyed under specific conditions.

There is a new development of a graph analysis algorithm to quantify demand for conditions for targeted chemical reactions:- this is the Optimal Condition Approaching via Reaction-In-Network Analysis (OCARINA).

From what I understand, plasma used in such reactions need to be at atmospheric pressure which is called as Atmospheric pressure plasmas(APP) and regular plasmas have plenty of uses in the industry like electrolysis cells, biomass treatment and packed bed reactors. But there are certain limitations as well like their inherent lack of selectivity at atmospheric pressure . The energy supplied to the plasma manifests in the movement of charged particles, but where these particles move, and which other particles they collide with and when, is not trivial to control at the particle densities encountered at atmospheric pressure.

There are some solutions to it such as plasma catalysis and tailored waveform yet one problem that each solution must encounter, however, is the ever-expanding complexity of plasma chemical reaction schemes.

For the graph theory to work we could draw upon an exhaustive dataset to answer some questions and a complete experimental characterisation over all the combinations of variable values. There has been some work done by Sakai et al, which analysed the centrality index of a methane plasma chemical reaction system and also proposed the use of the reaction rate coefficients as edge weights, and Mizui et al who conducted more complex numerical analysis of the roles of the chemical species in the plasma chemical reaction network.

Next is the methodology, building the graph of a plasma chemical reaction system as well as variation of rate coefficients with electron temperature and gas temperature and then the visualization.

As mentioned earlier about the use of dataset, it contains the data required for plasma chemical reaction engineering generally consists of a list of reactions with their corresponding reactants and products, along with the rate coefficients of such reactions which are generally constants. Then a simulation is run with changing concentrations of the species over time.

The rate of reaction is a major factor in plasma chemistry which is affected by electron energy. Therefore, the values of the rate coefficients change if these variables change. Comparing with the DBD plasma which has the range of 1-10 eV shows that the vast majority of the rate coefficients simply increase or decrease over this range. A matrix of rate constants was computed using a range of different electron energies and the maximum and minimum values were found from this.

The next part is of visualization, how can large amounts of key information be visualized simultaneously. Gephi is used for it, it generates a directional weighted graph from an existing plasma chemical reaction system which breaks down into the thickness of each edge was used to show the rate of reaction, the fastest rates having the thickest edges. As the rate constants ranged over more than 30 orders of magnitude, log values of the rate constants were taken to create a visual logarithmic scale. Other attributes of each reaction and species were weighted as other visual properties of the edges and nodes and the weighting factors. Using the filtering functions of Gephi, information relevant to single or small numbers of species of interest can be viewed in increasing levels of complexity.

Then, it mentioned an example of such visualization and what all information is gathered from it (Ozone formation)

And then Dijkstra’s shortest path algorithm is applied which takes in consideration all the different parameters. The resulting chart gives us an indication of which other species have the highest potential to be formed from a given species