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Application of graph theory for argon plasma chemistry with excited level transitions

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We aim to understand the chemical reaction system of argon plasma and to identify the primary chemical species and reaction processes by applying graph theory. Multidimensional numerical simulations of plasma discharges and chemistry often require enormous computational time due to the large number of particles and the variety of chemical reactions involved. One way to reduce computational costs is to simplify the reaction system. Applying graph theory may enable us to extract key elements while preserving the system's fundamental properties.

Argon is employed in this study due to its prevalence as a plasma gas and its role in influencing vacuum chamber chemistry through excited states, facilitated by its low ionization potential. These excited states can influence the chemistry of other molecules in vacuum chambers through its exciting states. Argon-based plasmas find applications in diverse areas such as microplasmas [1], jet plasmas [2], and plasma metamaterials [3].

Plasma chemistry is inherently collision-driven, where each collision event corresponds to a distinct chemical reaction. Our research group specializes in numerical plasma modelling and has successfully applied graph-theoretic methods to reduce complex reaction systems, such as He–humid air mixtures [4]. Validation against numerical simulations has demonstrated the efficacy of this approach, and graph theory further enables identification of key molecular species governing dominant processes [5].

Several graph typologies exist [6], each posing unique construction challenges. For this work, we adopt a *directed multigraph* framework, as illustrated in Figure 1, where:

- Edges encode directional relationships (reactants → products)
- Nodes permit self-loops and multiple edges
- Edge weights correspond to reaction rates (K)

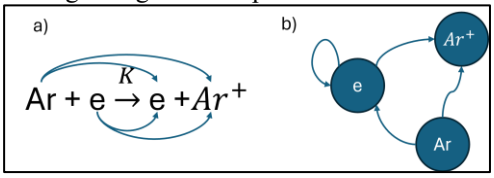

Figure 1 : (a) Schematic link from reactive species to products species of a collision reaction. (b) Directed edge diagram of previous equation (a).

Species in the reaction set are mapped to nodes, with edges constructed from reactants to products, weighted by their respective reaction rates. Figure 2 illustrates a graph for argon–electron species, with edge coloration quantitatively representing reaction rates (dark purple = high, light yellow = low).
We systematically evaluate how graph topology affects the power law's capacity to streamline the reaction network while preserving critical dynamics.

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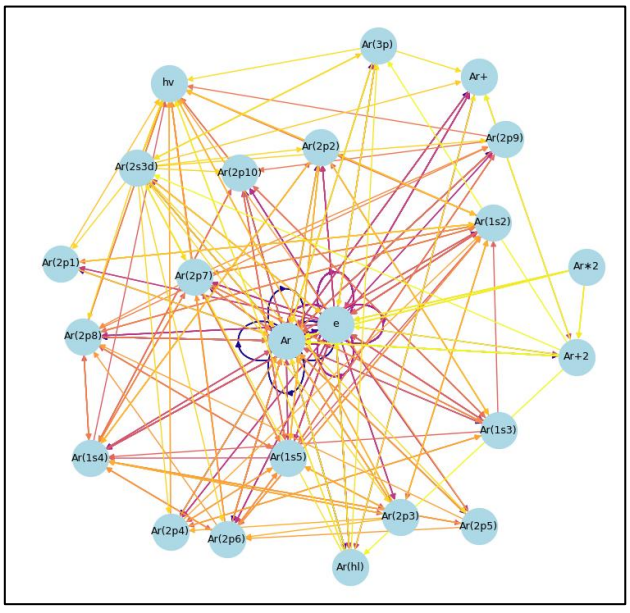

Figure 2 : Graph of Argon plasma.