Utilizing a Global Model to Identify Relevant Reactions in Chemically Complicated Plasma Systems*

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Plasma chemistry mechanisms in gaseous breakdown, such as plasma assisted combustion (PAC) systems, involve many species, reactions, and spatially dependent system variables, e.g. species' densities and temperatures, which become prohibitively computationally expensive. Global models can be used to prioritize and thereby reduce the number of reactions and species, where variables of interest show little spatial dependence, and where plasma sheath and surface processes can be either simplified or neglected.

We present a kinetic global model framework (KGMf [1]) that employs spatially-averaged energy and particle balance equations, chemical reactions in bulk plasma, and takes into account time-dependent power absorption via Joule heating, to identify the impact of relevant reactions on temperatures and species' densities. The electron energy distribution function (EEDF) can be either predefined (e.g. Maxwellian) or self-consistently computed with coupled Boltzmann equation solver. The sensitivity analysis is performed to evaluate the uncertainty of simulation results based on uncertainty of input parameters, which can be performed completely with the KGMf. The uncertainty of input parameters is specified in a single input text file and the resulting sensitivities of the variables of interest are saved into HDF5 formatted file for easy retrieval. PumpKin [2] and the KGMf's results, i.e., the stoichiometric matrix and the temporal evolutions of species densities and reaction rates, are used to reduce the reaction set, which can still capture the time evolution of selected system variable (e.g., temperature and density of target species).

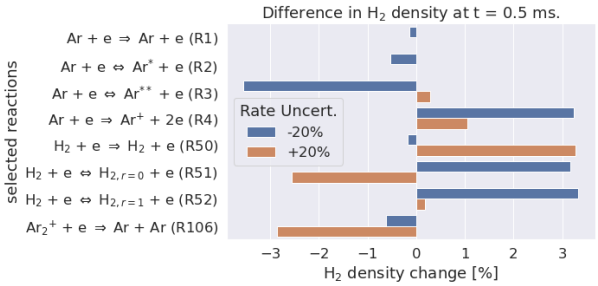

Figure 1 – Sensitivity analysis of H_2 density: H_2 density change after 10 pulses (t=0.5 ms) due to ±20% change of reaction rate coefficient of selected reactions in nanosecond pulse discharge in 1% H_2 - 0.15% O_2 - Ar mixture.

The sensitivity analysis and the determination of dominant pathways are performed in 1% H_2 - 0.15% O_2 - Ar mixture at p = 300 Torr and gas temperature T_g = 500 K, excited by nanosecond pulse plasma with a repetition frequency ν = 20 kHz and coupled discharge energy of 2.6 mJ/pulse [3].

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References

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