Opening chemical reaction paths in a plasma global model: an uncertainty quantification approach

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As iodine is establishing itself as an alternative to xenon for electric propulsion in space, different global models are published to characterize the plasma formed by molecular iodine [2, 3]. The model by Grondein et al. [2] is derived from the xenon version by Chabert et al. [1]. This model is constructed around a particle balance and a power balance. A differential system is composed of an equation of temporal evolution per chemical species (2 for the xenon model [1] and 6 for the iodine model [2]), an equation for the temporal evolution of the electron energy (or electron temperature) and one for the neutral energy (or neutral gas temperature). This differential system is solved until a steady state is reached.

Ten volume or surface reactions are considered by Grondein et al. [2], with I, I_2, I^+, I_2^+ or I^- in reactants or products. Some of these reactions are poorly characterized due to lack of data, and many reactions are missing because assumed negligible. The uncertainty quantification is used to answer two questions:

- How does the poor understanding of some reactions affect the error of the code output?
- Among the reactions currently in the code and others that could be added, where should the effort to better characterize the reactions be focused?

The first question is addressed using a Monte-Carlo approach, generating one hundred thousand configurations with reaction coefficients drawn from a log-normal distribution around their usual value and solving the differential system each time. This gives an absolute uncertainty on the outputs, and we also calculate Sobol indices to determine the sensitivity to each parameters. This allowed to determine that for the xenon model, the electron density and temperature are additive functions of the uncertain parameters, and can be modeled using a polynomial regression on these coefficients, greatly reducing the computation time required to compute the uncertainties.

The second question is answered by opening reaction paths in the code with a 'guessed' reaction rate associated to a large uncertainty. It is then observed 1) if the reaction has an effect on the final output and 2) if the uncertainty of the reaction has an effect on the uncertainty of the final output. If the reaction changes the results without increasing the uncertainty too much, it can be added to the reaction scheme with no further effort. If it also affects the uncertainty, this reaction can be listed as prioritary in the list of reactions to investigate.

References

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