Machine Learning for optimizing plasma resource utilization on Mars

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Plasma technologies for *in situ* resource utilization (ISRU) on Mars have been proposed recently, in particular to decompose CO_2 from the Martian atmosphere and extract the oxygen for life-support, fuels and agriculture (V. Guerra et al., 2022). On top of that, control and optimisation of plasma chemistry is dependent on accurate modelling of the associated kinetics. The reaction scheme of low-temperature plasmas can be described with a set of reactions and rate coefficients. However, the underlying plasma chemistry is very complex and efficient prediction of the plasma properties is mandatory. Moreover, some of the reaction constants of the plasma are not yet well determined or have a significant uncertainty associated. In such situations this lack of knowledge is made up to some extent by the experience and intuition of an expert. Due to this required expertise and the time-consuming nature of this trial-and-error approach, it is of major relevance to find automated methods to determine these constants. In this study, we use machine learning to predict and optimize the set of rate coefficients used in the kinetic schemes that describe CO_2 conversion. An artificial neural network is trained to learn and optimize the rate constants of the reactions given a set of plasma parameters that can be measured experimentally. Furthermore, the complexity of plasma chemistry models is increasing rapidly, where they may comprise several hundreds of reactions and over a hundred different species (L. Terraz et al., 2020), and it can become difficult, while crucial, to identify which mechanisms are the most influential on the results. Thus, we explore the use of automated processes to identify the most relevant features of the reaction set, eliminating minor species and less important elementary reactions. Additionally, we investigate different methods to model uncertainties in the neural network and provide an estimate of confidence for the model output (J. Gawlikowski et al., 2022). This solution is of great relevance as it enables the successful development of precise low-temperature plasma simulations, while enabling the determination of simpler models through the use of dimensionality reduction techniques for the assessment of the completeness of the reaction scheme, potentially providing information on the lack of relevant species and/or reaction mechanisms on the current scheme.

What original discovery problem did you want to solve?

Our aim is to utilize deep learning techniques to address the challenge of determining rate coefficients that describe the kinetics of low-temperature plasma, using data-driven machine learning models.

How did you formulate the problem in computational terms?

We have formulated the problem as an optimization task that involves predicting the optimal set of rate coefficients using a neural network. Specifically, the network takes in the densities of the species present in the plasma as inputs and outputs the corresponding set of rate coefficients.

What data and knowledge did you provide as system inputs?

The inputs for the model comprise the plasma's final state densities, acquired through simulations utilizing a self-consistent and well-established physics model.

What types of models did your system produce as outputs?

The system produces a model that performs the inverse problem of mapping the non-linear function between the final plasma densities and the corresponding set of rate coefficients used in the simulations.

What criteria did you use to evaluate candidate models?

In our preliminary results, we evaluate the model's performance by comparing the results against the physics model simulations.

How did you interpret results that the system generated?

As anticipated, the inverse problem we are addressing is ill-posed, meaning that there are multiple possible sets of rate coefficient values, $\boldsymbol{k}$, that can result in the same final plasma densities. Our ongoing investigation aims to improve the model's accuracy in predicting the exact set of $\boldsymbol{k}$ values used in the simulations, by developing methods to deal with the rank deficit of the forward problem and improve the stability and uniqueness of our results.

References:

V. Guerra et al. "Plasmas for in situ resource utilization on Mars: Fuels, life support, and agriculture". In: Journal of Applied Physics 132 (7 Aug. 2022), p. 070902.

L. Terraz et al. "Sensitivity Analysis in Plasma Chemistry: Application to Oxygen Cold Plasmas and the LoKI Simulation Tool". In: Journal of Physical Chemistry A (10 May. 2020), pages 4354-4366

J. Gawlikowski et al. "A Survey of Uncertainty in Deep Neural Networks". (18 Jan. 2022) http://arxiv.org/abs/2107.03342

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