Prediction of Reaction Rates with Machine Learning in a CCP

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Abstract: In this contribution, we report a new method for calculating reaction rates within a capacitively coupled system. Using a 1D simulation of a radiofrequency (RF) argon capacitively coupled plasma (CCP), ionization rates are extracted and used to train an artificial neural network based on local parameters. Findings demonstrate the validity of this method for the tested operating conditions.

1. Introduction

Production of ions and excited species within a plasma are integral to sustaining that plasma, and understanding the mechanisms by which these species are produced is invaluable. The primary way to quantify the production of these species is using reaction rates, which detail the rate of production of an individual species through some mechanism. Having accurate reaction rates is integral to describing the chemistry of a plasma system.

Here, machine learning is used to predict the reaction rates within a CCP, with the goal of showing that local information extracted from a particle-in-cell code is sufficient to predict these rates.

2. Methods

A particle-in-cell (PIC) code eduPIC [1] is used to extract data regarding the operation of an argon CCP, including electron density, electric field and potential, mean energy and ionization rates. An artificial neural network is then trained using Keras [2], with this data to predict ionization rates across the CCP based on the other plasma parameters listed. Model operating conditions are 13.56 MHz, 50 Pa, 2.5 cm gap, 350 K background gas temperature. The data is then averaged over 1/10th of the cycle to reduce noise, and multiple cycles are taken to be used as training and testing data. Each location in space and time provides a data point on the relationship between the ionization rates and other plasma parameters. This approach incorporated the impact of non-Maxwellian electron energy distribution functions on these reaction rates.

3. Results and Discussion

The directly measured ionization source term from PIC is compared to the source term predicted by the machine learning model in Figure 1. The machine learning (ML) model performs well over a majority of the domain, faltering mainly at the replication of the peak of the source term. This is likely due to sparse data on the conditions in that region, as the peaks have far less data points associated with them than the other regions. Some smaller features are also slightly misrepresented by the model, such as the minor peak between 1-1.5 cm. These small features can be difficult to capture with machine learning, so particular care needs to go into data selection and hyperparameter tuning to ensure they can be properly represented. This analysis can be performed for each 1/10th of the cycle, where the peak region of the source term is seen to shift across the domain, due to the variation of the applied voltage across the cycle.

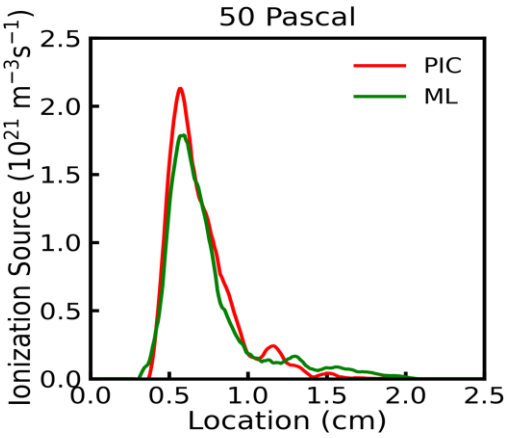

Fig. 1. Comparison of directly measured ionization rates from a PIC simulation compared to the values predicted with machine learning based on local plasma conditions.

4. Conclusion

Exploration of the applications of ML to predicting reaction rates has shown that ionization rates can be predicted using local information extracted from a PIC simulation. The trends of the rates are preserved within the ML model, although the peaks and edges of the curves do not perfectly align. Increasing the amount of training data may assist with increasing the accuracy of the trends, as well as increasing the number of inputs being considered by the neural network. In particular, including a neighborhood of plasma conditions can provide non-local information that may be critical at lower pressures. Additionally, a similar exploration of excitation rates will also be performed and its accuracy quantified.

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References

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