Machine learning for optimization of plasma-assisted conversion of CO_2

Unite! Fellowship Call: PhD Proposal Submission

Abstract:

Plasma technologies are very promising for green conversion of CO_2 into value-added products and energy storage in liquid fuels. However, accurately predicting plasma properties presents a significant challenge, given the inherent complexity of the underlying chemistry models and the uncertainties surrounding several input parameters. In particular, the predictions critically depend on reaction rate coefficients that are often poorly known and are tuned with time-consuming trial-and-error approaches. This thesis aims at using machine learning to optimize a model for plasma-assisted conversion of CO_2 and to find the corresponding reaction rate coefficients. Additionally, automated processes will be explored to identify the most relevant features of the reaction set and to model uncertainties in deep learning models, as to identify influential mechanisms and to provide an estimate of confidence for the model outputs. Experimental data for model validation will also be obtained.

Supervisors:

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Research goals:

- Use deep learning models to learn and optimize the set of reaction rate coefficients in predictive plasma models
- Use dimensionality reduction techniques to identify the most relevant species and mechanisms
- Model uncertainties in the neural network and estimate confidence intervals for the outputs
- Obtain experimental data for model validation

State-of-the-art

In recent years, the rising levels of CO_2 in the atmosphere, primarily caused by the consumption of fossil fuels, has brought a growing need to re-examine the economic technologies on which we rely. To address the issue, significant effort is being invested in the development of carbon capture, utilization, and storage strategies, which involve using renewable energy sources to convert carbon dioxide into high-value products such as liquid fuels [1].

Among other solutions, the use of low-temperature plasmas for CO_2 utilization is very attractive [1]. However, detailed kinetic models are necessary for plasma control and optimization, which critically depend on reaction rate coefficients that are often poorly known and require time-intensive trial-and-error methods for calibration.

In this context, the utilization of Machine Learning (ML) in low-temperature plasmas is a multidisciplinary and highly novel topic, with the potential to bring a significant breakthrough in the development of plasma technologies in general, and their application to plasma-assisted CO_2 conversion to produce solar fuels. Machine Learning techniques remain substantially under-explored in the field of low-temperature plasmas. As they become more prevalent, it is increasingly important to be able to critically analyse and assess the concepts and techniques behind data-driven approaches, and their potentially substantial impact on complex plasma modelling [2].

Building on the very recent advances in the field, the primary goal of this research is to use ML to accurately estimate poorly known plasma parameters or parameters for which state-of-the-art methods are unable to provide precise estimates.

[1] Pietanza, L. D, Silva, T. *et al* (2021). Advances in non-equilibrium CO2 plasma kinetics: a theoretical and experimental review. The European Physical Journal D 2021 75:9, 75(9), 1–55. https://doi.org/10.1140/EPJD/S10053-021-00226-0
[2] Bonzanini, A. D., Shao, K., Graves, D. B., Hamaguchi, S., & Mesbah, A. (2023). Foundations of machine learning for low-temperature plasmas: methods and case studies. Plasma Sources Science and Technology, 32(2), 024003. https://doi.org/10.1088/1361-6595/ACB28C

Research Environment

Research areas:

- The incorporation of machine learning in plasma physics is an emerging idea and a highly novel topic. It aligns well with the objectives of Unite!, bridging two main priority areas: **Energy conversion** and **Artificial Intelligence**.

Laboratories:

- The thesis will benefit from the competences of **two** Portuguese **Associated Laboratories**, Instituto de Plasmas e Fusão Nuclear (IPFN) and the Laboratory of Robotics and Engineering Systems (LARSyS) of IST, and of the vast experience in Interpretable Machine Learning from the Helsinki Institute for Information Technology (HIIT)
- The resources available at both the affiliated and partnered laboratories offer exclusive access to highly specialized software and hardware, ensuring the project's computational needs are adequately met.

Ongoing relevant projects:

- PARADiSE, the PlasmA RoAD to Solar fuEls, that investigates plasma decomposition of CO_2 using only renewable electricity. Funding source: FCT
- Neuraspace, AI flights space debris, that focuses the use of AI and ML models to predict and compute the probability of collision between satellites and space debris. Funding source: PRR/IAPMEI