Deep Learning for Low-Temperature Oxygen-Based Plasmas Modelling

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Low-temperature plasmas (LTPs) are versatile in their applications, finding uses in areas ranging from plasma medicine to CO_2 conversion for *in-situ* resource utilisation [1,2]. While experimental studies provide valuable physical parameters for these systems, a comprehensive understanding of LTPs necessitates a synergy of experimental and modelling efforts. Models can access crucial information unattainable by experiments alone. However, plasma simulations, while essential, can often be computationally intensive [3]. Surrogate models mitigate this limitation by offering quick approximations of complex systems, crucial for optimisation, real-time decision-making, and analysing large-scale problems [4]. Conversely, accurate modelling of LTPs presents challenges due to the complex plasma chemistry and uncertainties in input parameters. A key aspect of LTP modelling is developing an accurate kinetic scheme, which involves identifying relevant reactions and determining their rate coefficients. This task is complicated by the limited available knowledge of rate coefficients [5], often derived through time-consuming trial-and-error methods.

In this work, we apply deep learning to tackle both the modelling and parameter recovery challenges in plasma physics, illustrating the benefits of merging physical insights with machine learning to improve the accuracy and efficiency of models. The system under study is an oxygen plasma created by a DC glow discharge at gas pressures of $p = 0.2 - 10$ Torr and discharge currents of $I = 10 - 40$ mA. The reason for this choice is twofold. On the one hand, this system exhibits a high degree of complexity, as its properties depend on the interplay between electron, vibration, chemical, ion and surface kinetics. On the other hand, a detailed reaction mechanism was recently developed [3], providing an ideal test bed for the proposed novel approaches.

Surrogate models can be designed to predict steady-state species concentrations, temperature, and transport coefficients as a function of the reactor's relevant operating conditions. Since data collection can be costly, encoding prior physics knowledge into the neural network (NN) can be helpful as it amplifies the available information. Modern physics-informed machine learning methods include a penalty term in the loss function, discouraging deviations from physical constraints and efficiently guiding the model toward the correct solution [6]. However, these models do not guarantee that, after training, the outputs for unseen inputs will satisfy such constraints. Here, we propose a novel approach for integrating physical information into the deep learning model. Our method involves projecting the model's predictions onto a manifold defined by the constraint $g(x, y) = 0$, where x is the model's input, y is the model's output and $g(x, y)$ is a vector-valued constraint function that is zero if, and only if, those physical laws are satisfied. To that aim, through sequential quadratic programming, we formulate the projection operation as a constrained optimisation problem

$$minimise\ ||p - f(x;\Theta)||_W^2\ ,\quad s.t.\ g(x,p) = 0 \qquad (1)$$

where W is a symmetric positive definite weighting matrix, i.e. $||v||_W^2 = v^T W v$, $f(x;\Theta)$ is the machine learning parametric model and Θ is the model parameter vector [7]. This projection is pivotal in guiding the network to adhere to the physical laws governing plasma behaviour, enhancing the model's accuracy and minimising the dataset's training size. We have developed a surrogate model to the reaction mechanism developed in [3]. The physical laws included in the constraint function are the ideal gas law, the quasi-neutrality condition, and the relation between the discharge current and electron density. Fig. 1 compares the NN modelling and target simulation values of the concentration of ground state positive ions O_2^+, denoted as O2(+, X), as a function of pressure and for $I = 30$ mA. It evidences the method's

ability to improve the pressure-related trend, yielding predictions that closely match those observed in the simulation. The mean error in predicting this species is reduced from 1.2% to 0.5%. Moreover, this technique reduces the error of compliance with physical laws to below 0.50% of its original value, ensuring adherence to the imposed physical laws.

We carried out an additional study to extend the use of deep NNs to automate the prediction of a selected set of rate coefficients within this oxygen-based plasma scheme. Our framework comprises data generation using the LoKI-B+C modules [8] of the LisbOn KInetics (LoKI) simulation tool, data processing, architecture search, and hyperparameter tuning. This deep learning model is trained on artificial data generated by LoKI-B+C with sampled reaction rate coefficients around their established reference values. The aim is for the model to accurately recover these coefficients. The NN, receiving the steady-state densities of species as input, under various experimental conditions, learns to inversely map the simulations, thereby determining the reaction rate coefficients. We consider the prediction of seven rate coefficients based on heavy-species densities under diverse pressure and current conditions. The model effectively predicts rate coefficients with a mean relative error of 2.00% across predictions, showcasing its reliability as a proof-of-concept.

Future work will broaden the scope of the study to include more reactions, rate coefficients, and plasma systems and operating conditions. This expansion will also incorporate experimental data and explore diverse chemistries (*e.g.* CO_2, CH_4, N_2-H_2) and plasma-surface interactions, enriching the model's applicability and accuracy.

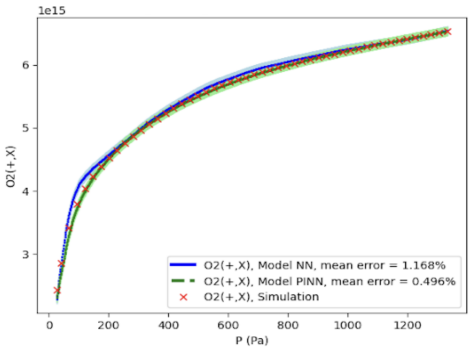

Fig. 1: Comparison between NN predictions and simulation values of the concentration of O_2^+ as a function of pressure, for a reactor radius of 12 mm and $I = 30$ mA, before projecting the model's predictions and after projecting the model's predictions.

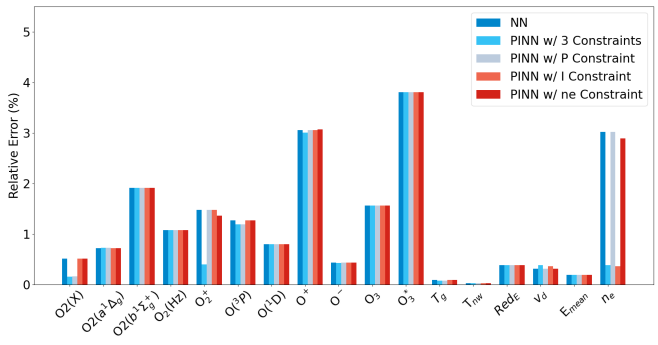

Fig. 2: For each output, comparison of the relative errors of the standard NN model; NN with each of the physical constraints applied individually; and NN with the three constraints applied simultaneously.

This work was partially supported by the Portuguese FCT-Fundação para a Ciência e a Tecnologia, under funding to IPFN (DOI: 10.54499/LA/P/0061/2020, 10.54499/UIDB/50010/2020, 10.54499/UIDP/50010/2020, and 10.54499/PTDC/FIS-PLA/1616/2021); and to LARSyS (DOI: 10.54499/LA/P/0083/2020, 10.54499/UIDP/50009/2020 and 10.54499/UIDB/50009/2020).

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