Machine Learning for Optimizing Plasma Resource Utilization on Mars

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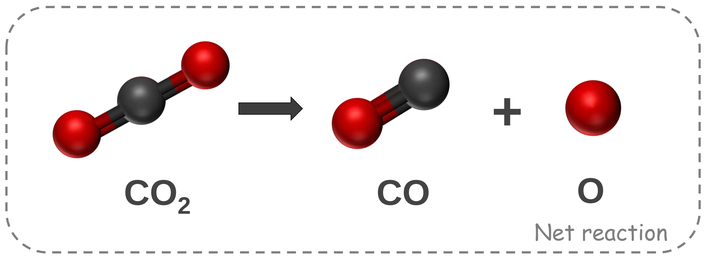
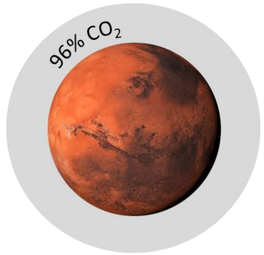
Motivation

On Mars, the atmosphere is very thin and is composed mainly of CO_2, with a small percentage of other gases. The **conversion of CO_2** could play a crucial role in supporting human exploration beyond our planet, by enabling the production of both fuel and breathable oxygen on Mars [1].





To account for the dissociation of CO_2 in plasma, various reactions including direct electron collisions and stepwise processes must be considered. The reaction scheme of **low-temperature plasmas** can be described with a set of reactions and **rate coefficients**. However, some of these coefficients **are not yet well determined** or have a significant uncertainty associated.

Objectives

Primary Goal: determine rate coefficients that describe the kinetics of low-temperature plasma.

Other aims:

- improve reaction scheme completeness, by utilizing dimensionality reduction techniques to eliminate less relevant reactions and minor species, and potentially uncover new reaction mechanisms and species not included in the current scheme.
- investigate methods for modelling uncertainties in the neural network.

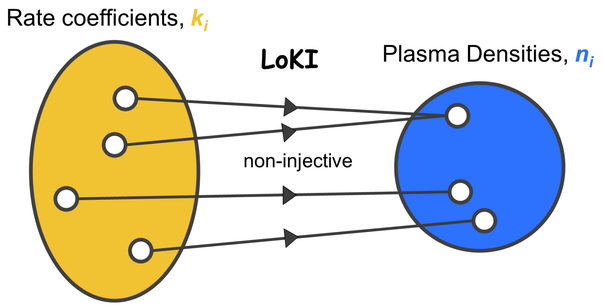
Simplified Oxygen Model

When dissociating CO_2, atomic oxygen is also produced, which can in turn influence the overall dissociation. We start this research by studying a simplified oxygen kinetic model, comprising a total of 9 reactions and 3 different heavy species. For the first results we choose to predict the rate coefficients for the **first 3 reactions**:

$$\begin{array}{l|l} e + O_2(X) \rightarrow e + O_2(a) & k_1 \\ e + O_2(a) \rightarrow e + O_2(X) & k_2 \\ e + O_2(X) \rightarrow e + 2O(^3P) & k_3 \end{array}$$

$$O_2(a) + O(^3P) \rightarrow O_2(X) + O(^3P)$$
$$O_2(a) + O(^3P) + O_2(X) \rightarrow O_2(X) + O(^3P) + O_2(X)$$
$$2O(^3P) + O_2(X) \rightarrow 2O_2(X)$$
$$O_2(a) + \text{wall} \rightarrow O_2(X) + \text{wall}$$
$$O_{2(^3P)} + \text{wall} \rightarrow 1/2\ O_2(X) + \text{wall}$$

Methodology



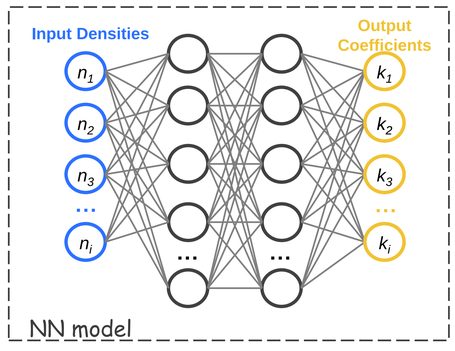
The simulations are performed using the **LoKI** (LisbOn KInetics) simulation tool [2], which provides a self-consistent description of both electron and heavy species kinetics in the plasma. Overall LoKI can provide large datasets for different user-defined working conditions, making possible the use of supervised learning ML models.

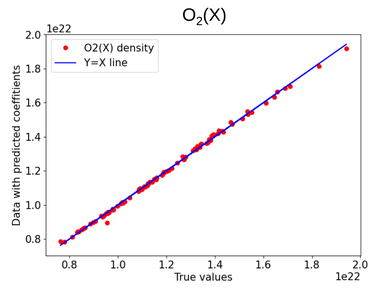
The forward mapping given by the simulation tool suffers from a rank deficit, making the problem more challenging. We are tackling a non-linear and ill-posed problem by seeking a machine learning model to solve the inverse mapping problem. Specifically, we aim to determine the rate coefficients, ***k***, given the steady-state plasma densities.

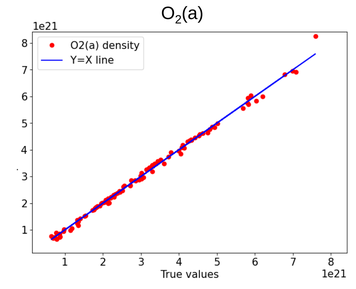
Deep Learning Model / First Results

Fully-connected neural network:

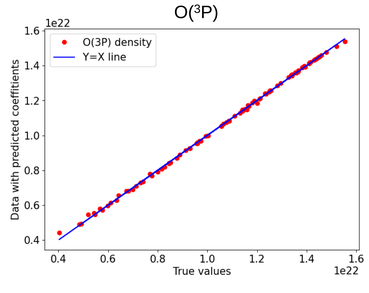
- 2 Hidden layers
- Tanh activation
- ADAM Optimizer
- MSE loss function







By inserting the predicted ***k*** back into the physical model (LoKI), we compare the resulting densities with their true value.



References

[1]- 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.
[2]- A. Tejero-Del-Caz et al. “The LisbOn KInetics Boltzmann solver”. In: Plasma Sources Science and Technology 28 (4 Apr. 2019), p. 043001