Proposal of Research subjects for PIC2 within project PARADiSE

group N-Plasmas Reactive: Modelling and Engineering (N-PRiME)
Instituto de Plasmas e Fusão Nuclear (IPFN)

https://www.ipfn.tecnico.ulisboa.pt/paradise/opportunities.html

In case of interest, please email Vasco Guerra (vguerra@tecnico.ulisboa.pt) or the contact person in each proposal

2023

Título: Microscopic simulations of plasma-surface interactions

Supervisor:
Pedro Viegas (pedroarsenioviegas@gmail.com), IST/Univ Lisbon, Portugal

A sustainable economy requires the recycling of greenhouse gases into useful products (e.g. CO2 into CO and O2). For this conversion process, low-temperature plasmas are essential, in interaction with solid-state catalysts, electrolysers and other surfaces. Low-temperature plasmas are electrically-powered reactive gases with ideal conditions for gaseous conversion, while solid-state materials can promote specific reactions and be highly selective to certain species. To merge the two technologies is a novel approach with increasing attention, but the interaction between plasma species and surface materials is still mainly unknown. In this project, a software package will be used to perform Density Functional Theory calculations, based on the quantum mechanical description of the electronic structure of many-body systems. These will focus on specific reactions of interest of plasma-surface systems for gaseous conversion, which have never been studied. The project will be supervised by DFT experts and plasma researchers together, within the cadre of wider international projects developing technologies for gaseous conversion.

Título: Multidimensional modelling of low-temperature plasmas

Supervisor:
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A sustainable society requires the recycling of greenhouse gases into useful products (e.g. CO2 into CO and O2). Low-temperature plasmas, electrically-powered reactive gases, are essential for this process due to the possibility of reaching ideal conditions for gas conversion. The physics of low-temperature plasma reactors comes across different temporal and spatial scales and involves the interplay between different branches of physics: electromagnetism, fluid mechanics, statistical physics and gaseous and surface reactivities. An accurate description of these media that allows predictive modelling and reactor optimization requires the development of multidimensional numerical models. The goal of this work is to engage in multidimensional continuum simulations of low-temperature plasmas. The first step is to carry out an assessment of available numerical plasma CFD (computational Fluid Dynamics) codes (e.g., SOMAFOAM, FEniCSx, SPARK), in order to choose the one most suited for the simulation of microwave, RF, DC, and nanosecond pulsed discharges or choose the development of an in-house code. Subsequently, a simplified system will be defined to be used as a test-bed to study the capabilities and performance of the code. Depending on the available time, the model can be further developed to study more complex systems. The project will be supervised by plasma modelers, within the cadre of wider projects developing technologies for sustainable gaseous conversion, such as Project PARADiSE - the PlasmA RoAD to Solar fuEls. International collaborations are in place and research stays at laboratories in France, The Netherlands, Czech Republic, Italy, Japan and the USA, among other countries, are possible.

Título: Modelling the interaction between low-temperature plasmas and separation membranes

Supervisor:
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A sustainable economy requires the recycling of greenhouse gases into useful products (e.g. CO2 into CO and O2). For this conversion process, low-temperature plasmas are essential, in interaction with solid-state electrolyzer separation membranes. Low-temperature plasmas are electrically-powered reactive gases with ideal conditions for gaseous conversion, while solid-state membranes can promote specific reactions and selectively induce the transport of certain species, thus potentially separating conversion products (e.g. CO and O2). The merge of the two technologies is a novel approach with increasing attention, but the interaction between the plasma and these surface materials is still widely unknown. In this project, the student will develop a numerical model to self-consistently describe the plasma, the adsorption of plasma species (e.g. O) onto the surface, the formation of ions to be conducted at the surface (e.g. O2-) and the transport of ions within the material, for different operating conditions of practical interest. Such a model will allow to study the interdependence between plasma and membrane parameters and analyse the fundamental interactions between plasma species and surface materials. The numerical model will start from an existing code of the research team for plasma kinetics and plasma-surface interactions and will be further developed to study the new phenomena of interest concerning the separation membranes and their interaction with the plasma. Depending on the student’s specific interest and the available time, the model may be developed within a global modelling approach or in a multidimensional fluid/kinetic framework. The project will be supervised by plasma researchers in close contact with surface experts, within the cadre of wider projects developing technologies for sustainable gaseous conversion, such as Project PARADiSE - the PlasmA RoAD to Solar fuEls. International collaborations are in place and research stays at laboratories in France, The Netherlands, Italy, Japan and the USA, among other countries, are possible.

Título: Modelling plasma-surface interactions in plasmas for CO_2 conversion

Supervisor:
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A sustainable economy requires the recycling of greenhouse gases into useful products (e.g. CO_2 into CO and O_2). For this conversion process, low-temperature plasmas are essential. Low-temperature plasmas are electrically powered reactive gases that can have ideal conditions for CO_2 conversion. In plasma reactors, the interaction of the plasma with surfaces is of crucial importance. In order to predict plasma reactor performance and optimize it to reach ideal conditions for CO_2 conversion, it is essential to describe plasma-surface interactions, and in particular to model the fluxes of species between the two media. The aim of this work is to develop a numerical model to describe the formation of molecules as a result of the interaction between the reactive species created in a plasma and silica-based surfaces. In particular, the investigation will focus on the formation of molecules such as O_2, O_3 and CO_2 in oxygen and CO_2 plasmas, of interest for re-entry studies on Earth and Mars, as well as for CO_2 conversion on Earth and In-situ Resource Utilization on Mars.

The model development will start from existing models of the research team that separately describe the plasma production and maintenance and the surface processes. An important part of the work will consist on self-consistently coupling the two separate models, significantly increasing the potential for understanding of plasma reactor systems as a whole. The surface kinetics model will account for the elementary steps of physisorption, thermal desorption, chemisorption, and both Eley-Rideal and Langmuir-Hinshelwood recombination of O. Surface modifications due to the impingement of fast particles from the plasma, an area of novelty and increasing interest, will also be considered. The simulations will be carried out with numerical codes available for pure oxygen, that shall be modified to account for new elementary processes in CO_2 plasmas. The project will be supervised by plasma researchers in close contact with surface experts, within the cadre of wider projects developing technologies for sustainable gaseous conversion, such as Project PARADiSE - the PlasmA RoAD to Solar fuEls. International collaborations are in place and research stays at laboratories in France, The Netherlands, Russia, Italy, Japan and the USA, among other countries, are possible.

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N PRiME

Título: Modeling of atomic oxygen in the effluent of a CO_2 microwave discharges

Supervisor:
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The goal of zero net emissions by 2050 requires new technologies capable of solving the unpredictable nature of renewable energy sources. One promising and environmentally friendly solution relies on CO_2 recycling towards high-energy-density chemicals, using the excess of renewable power along the transformation process. To this purpose, microwave plasma technology has gained much attention due to its potential to activate CO_2 at reduced energy cost while exciting molecular vibrations to overcome the dissociation barrier [1]. In this work we aim at investigating the mechanisms that govern the formation of oxygen atoms in CO_2 microwave discharges sustained at low pressure conditions (see schematic of the setup in figure 1). Note that the dissociation of CO_2 produces O atoms, which will then undergo further reactions that can have beneficial impact in the final conversion (via collisions with vibrationally excited CO_2 increasing the dissociation) or detrimental effect for the overall CO_2 conversion (due to oxidation of CO that recombines back to CO_2). The work will be developed in the framework of a collaboration between the Instituto Superior Técnico, where the models will be developed (based on the LisbOn KInetics (LoKI) simulation tool [1,2]), and the Max Planck Institute in Germany where the experimental work will be carried out. The research will capitalize on recent 1D-resolved ground state atomic oxygen measurements obtained in microwave discharges through ns pulsed dye laser diagnostics (see fig.1). The experimental campaign will be supervised by Dr. Arne Meindl from the Plasma for Gas conversion (P4G) group – ITED at the Max Planck Institute for Plasma Physics.

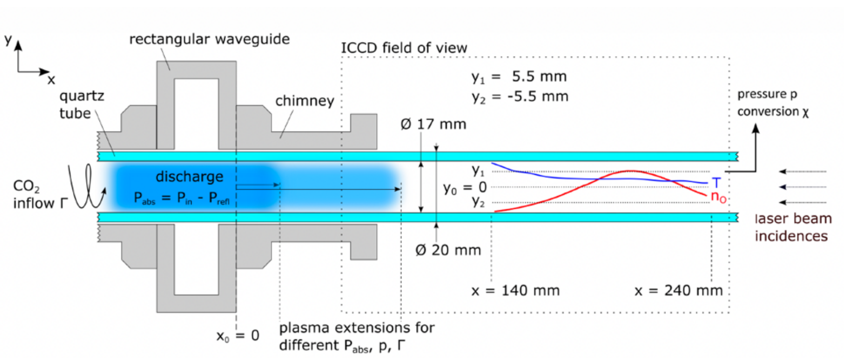

Figure 1.Investigation of atomic oxygen kinetics in the effluent of a CO_2 microwave plasma

References:
[1] A. Tejero-del-Caz et al., *Plasma Sources Sci. Technol.* **28** (2019) 043001.
[2] A. F. Silva et al., Plasma Sources Sci. Technol. **29** (2020) 125020.

Título: Electron dynamics and heavy-particle kinetics in atmospheric pressure air plasmas

Supervisor:
Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal

Atmospheric pressure plasmas are of great interest due to their simple operation, reduced processing cost, and the possibility of the application of plasma to samples that are not compatible with low-pressure conditions, in particular in the rapidly growing fields of plasma medicine and plasma agriculture. This work proposes a joint modeling and experimental study of air-containing atmospheric discharges aiming at a precise determination of the plasma parameters, namely electron density and electron temperature. Research efforts will be targeted at developing a plasma-based kinetic scheme for ns pulse jet discharges (see figure 1) sustained at atmospheric pressure and with gases mixtures containing Helium with small admixtures of CO_2. The work will be developed in the framework of a collaboration between the Instituto Superior Técnico, where the models will be developed (based on the LisbOn KInetics (LoKI) simulation tool [1,2]), and the Nagoya University where the experimental work (see e.g. [3]) will be carried out. The experimental campaign will be supervised by Dr. Nikolay Britun.

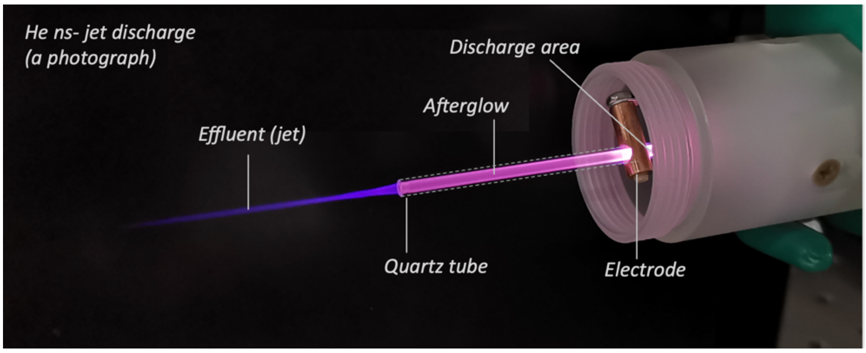

Figure 1. Photograph of a ns jet discharge sustained with Helium at atmospheric pressure

References:
[1] A. Tejero-del-Caz et al., *Plasma Sources Sci. Technol.* **28** (2019) 043001.
[2] A. Tejero-del-Caz et al., Plasma Sources Sci. Technol. **30** (2021) 065008.
[3] N. Britun et al., Plasma Sources Sci. Technol. **31** (2021) 125012.

Título: Development of N_2 plasma chemistry for microwave discharges sustained at atmospheric pressure conditions.

Supervisor:
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Atmospheric-pressure plasma have attracted growing interest over the last decades owing to their efficiency in converting ordinary gas content into diverse reactive species for a wide range of purposes, including as air pollution control, surface treatment, or plasma synthesis. In this work, the research efforts will be targeted at developing a N_2 plasma chemistry for microwave discharges sustained at atmospheric pressure conditions (see schematic in figure 1). This subject is motivated by recent experimental campaigns carried out at the Fraunhofer IWKS institute in Germany related to microwave-initiated catalytic deconstruction of plastic waste into hydrogen and high-value carbons. The work will be developed in the framework of a collaboration between the Instituto Superior Técnico, where the models will be developed (based on the LisbOn KInetics (LoKI) simulation tool [1,2]), and the Fraunhofer IWKS institute in Germany where the experimental work (see e.g. [3]) will be carried out. The experimental campaign will be supervised by Dr. Guoxing Chen.

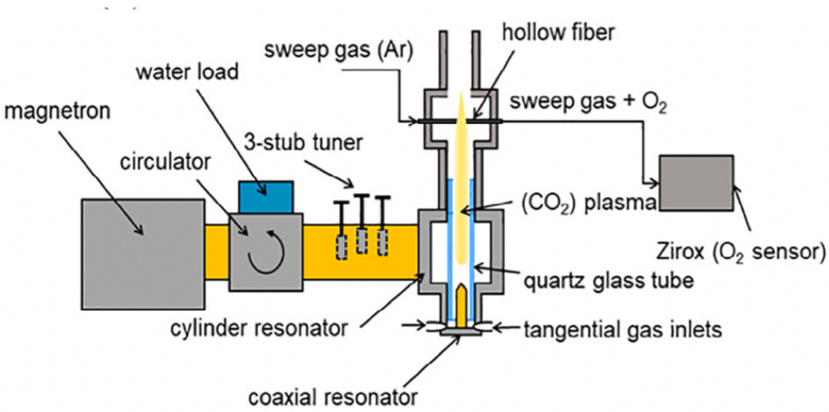

Figure 1. Schematic of a N_2 microwave-sustained discharge used for CO_2 decomposition.

References:
[1] A. Tejero-del-Caz et al., *Plasma Sources Sci. Technol.* **28** (2019) 043001.
[2] A. Tejero-del-Caz et al., Plasma Sources Sci. Technol. **30** (2021) 065008.
[3] G. Chen et al., Nature Reviews Materials **7** (2022) 333-34.

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N PRiME

Título: Modelling of a CO_2 coaxial plasma torch driven by microwave power pulsing.

Supervisor:
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Recent experimental work has shown the potential of microwave discharges (sustained with ultrafast pulsations) at decomposing CO_2 into CO and O_2 [1]. This is a fundamental and required step to achieve plasma-based renewable energy storage, while mitigating greenhouse gases emissions. In this work the research efforts will be directed at describing a CO_2 microwave plasma torch (see figure 1) connected to a solid-state generator. The work will be developed in the framework of a collaboration between the Instituto Superior Técnico, where the models dedicated to the description of the plasma torch will be developed (based on the simulation of the Navier Stokes equations for the gas/plasma system – see [1] for more details) and the Karlsruhe Institute of Technology (KIT) in Germany where the experimental work will be carried out (see e.g. [2]).

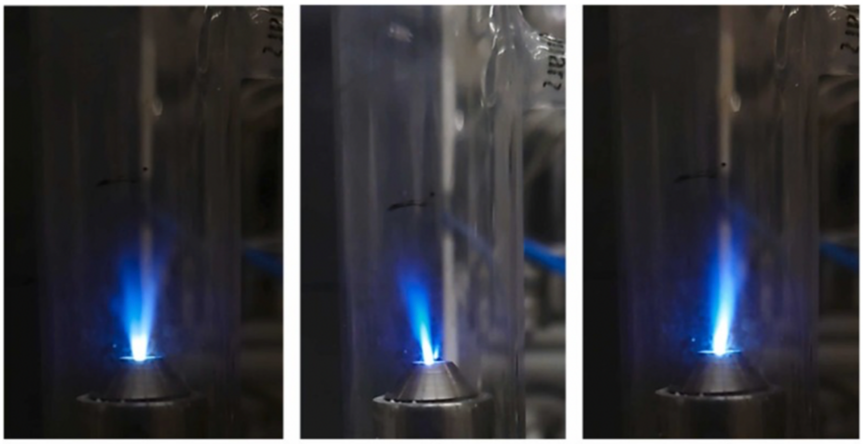

Figure 1. Picture of a CO_2 microwave plasma torch sustained at atmospheric pressure.

References:
[1] K. Gadonna et al., Eur. Phys. J. Appl. Phys. **2** (2011) 24008.
[2] S. Soldatov et al., J. CO2 Util., 58 (2022) 101916

Title: Development of a graph-theoretical approach for understanding of plasmas.

Supervisors:
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Abstract
Plasmas play a critical role in a wide range of industrial, environmental, and technological applications. In order to gain insight into the intricate chemistry of plasmas, it becomes imperative to construct precise yet simplified kinetic models. Within this context, the research team at N-PRiME of IPFN has focused on the development of sensitivity analysis methods to better understand the pivotal mechanisms that elucidate plasma behavior [1]. To establish a more comprehensive and versatile platform for the study, reduction, and simplification of kinetic plasma schemes, the incorporation of innovative approaches becomes imperative. In this study, we propose the utilization of graph-theoretical analysis as a novel method to extract essential information from complex plasma chemistry (see figure 1). By leveraging the inherent structure of chemical networks, this approach promises to streamline and enhance our understanding of plasma reactions. To showcase its potential, this work will target the developing a graph-theoretical approach to a well-established kinetic chemistry model developed for CO_2 plasmas. The work will capitalize on a collaboration between Instituto Superior Técnico and Seikei University via Dr. Tomoyuki Murakami (author of the article in [2]).

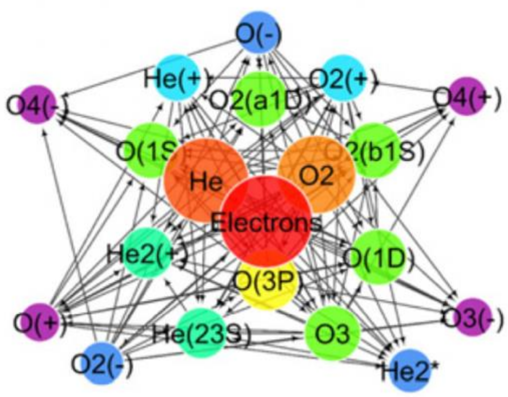

Figure 1. Example of a network diagram using graph-theoretical analysis in O_2-He a discharge taken from [2]

Goals:

- Develop a graph-theoretical analysis method tailored to the CO_2 kinetic scheme, facilitating a systematic and efficient understanding of reaction rates in plasmas.
- Explore the complex chemistry underlying CO_2 plasmas via graph-theoretical analysis.

Period: 2023/2024

Framework: PIC1, PIC2/MSc thesis

References:
[1] L. Terraz et al., *J. Phys. Chem.* A 124 4354 (2020)
[2] T. Murakami and O. Sakai, *Plasma Sources Sci. Technol.* 29 (2020) 115018

Título: Electron kinetics with coexistent AC/DC electric fields and DC magnetic fields

Supervisor:
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The behavior of electrons in low-temperature plasmas is governed by the electron Boltzmann equation. The LoKI-B code was developed in Lisbon and solves the electron Boltzmann equation under the two-term approximation. However, the code does not allow to study configurations with a magnetic field. The aim of this work is twofold: (i) to include the effect of the magnetic field in LoKI-B and (ii) to explore the physics behind the interaction between AC/DC electric fields and DC magnetic fields, with a special focus on the phenomenon of electron-cyclotron resonance.