Proposal of research subjects for training

group N-Plasmas Reactive: Modelling and Engineering (N-PRiME)
Instituto de Plasmas e Fusão Nuclear (IPFN)
https://www.ipfn.tecnico.ulisboa.pt/nprime/opportunities.html

In case of interest, please email directly the contact person in each proposal

2023

Title: Microscopic simulations of plasma-surface interactions

Supervisors: Pedro Viegas (pedroarsenioviegas@gmail.com), IST/Univ Lisbon, Portugal and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal

Abstract

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, 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.

Goals

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.

Period: School year 2023/2024

Framework: PIC1, PIC2/MSc thesis, internship

Title: Multidimensional modelling of low-temperature plasmas

Supervisors: Pedro Viegas (pedroarsenioviegas@gmail.com), IST/Univ Lisbon, Portugal and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal

Abstract

A sustainable society requires the recycling of greenhouse gases into useful products (e.g. CO_2 into CO and O_2). 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.

Goals

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.

Period: School year 2023/2024

Framework: PIC1, PIC2/MSc thesis, internship

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

Supervisors: Pedro Viegas (pedroarsenioviegas@gmail.com), IST/Univ Lisbon, Portugal and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal

Abstract

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, 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 O_2). 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. O^{2-}) 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.

Goals

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.

Period: School year 2023/2024

Framework: PIC1, PIC2/MSc thesis, internship

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

Supervisors: Pedro Viegas (pedroarsenioviegas@gmail.com), IST/Univ Lisbon, Portugal and Vasco Guerra (vguerra@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal

Abstract

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.

Goals

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.

Period: School year 2023/2024

Framework: PIC1, PIC2/MSc thesis, internship

Title: Electron kinetics with coexistent AC/DC electric fields and DC magnetic fields: the phenomenon of electron-cyclotron resonance

Supervisors: Prof. Vasco Guerra (vguerra@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal and Tiago C. Dias (tiago.cunha.dias@tecnico.ulisboa.pt)

Abstract

Low-temperature plasmas (LTPs) exhibit unique features and advantages that make them invaluable for several applications. These plasmas are characterized by their strong reactivity, featuring a low density of charged particles, high electron temperature (1 eV) and heavy-species translational and internal temperatures ranging from 300 K to 10^4 K. Typically, they are created upon application of a high electric field and, in some cases, a magnetic field. Electrons play a major role in LTPs, since they transmit the energy acquired from the electric field to the heavy species through various collisional channels, thereby sustaining the non-equilibrium and reactivity of these systems.

The behavior of electrons in LTPs 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.

Goals

(i) To include the effect of the magnetic field in LoKI-B;
(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.

Period: 2023/2024

Framework: PIC1, PIC2/MSc thesis

Title: Plasma synthesis of N-graphene for plasmonic antennas applications

Supervisor: Edgar Felizardo (edgar.felizardo@tecnico.ulisboa.pt), IPFN/IST, Portugal

Abstract

Carbon-based antennas are being considered for next generations communications and in wearable smart/medical sensors applications due to their excellent mechanical and chemical stability, high conductivity, lightness, and low-cost. Graphene-based antennas, in particular, could improve miniaturization and efficiency of devices, while also being mechanically flexible and potentially transparent. Furthermore, research efforts have shown that the parallel conductivity of N-doped graphene (N-graphene) at room temperature is considerably higher compared to that of pristine graphene, making N-graphene a better prospect for antennas applications.
In the context of an ongoing collaboration Sofia University, IPFN will make use of its recently developed plasma-based method for the synthesis of carbon nanostructures to produce free-standing flakes of N-graphene to be used in the fabrication of antennas and antenna arrays in the 3-26 GHz frequency range. The properties of the synthetized materials depend strongly on the characteristics of the plasma reactor and the selected operational conditions, with minor variations in the inputs often leading to very dissimilar outputs. Therefore, a careful exploration of the set of available parameters is crucial to unveil the synthesis routes that lead to the sustained production of N-graphene with the desirable properties.

Goals

1) Familiarization with the synthesis methods and materials characterization techniques available at the Plasma Engineering Laboratory (PEL) and collaborating institutions.

3) Operation of the experimental setups available at PEL to produce N-graphene at different Nitrogen doping levels.

3) Characterization of the synthetized materials.

4) Optimization of the synthesis processes and establishment of new production protocols for N-graphene.

Period: 2023/2024

Framework: PIC2/MSc thesis

Title: Plasma enabled synthesis of N-graphene/TiO hybrids for photocatalysis

Supervisor: Edgar Felizardo (edgar.felizardo@tecnico.ulisboa.pt), IPFN/IST, Portugal

Abstract

Photocatalytic materials can be used to generate fuel from CO2 and H2O using solar energy, which can contribute to alleviate societal dependence on fossil fuels. Due to their relatively low environmental impact, TiO_x-based variants are commonly selected for this purpose. Furthermore, the attachment of TiO_x particles onto large-surface-area carbon-based materials, such as carbon nanotubes, has shown to increase the efficiency of the photocatalytic process. The plasma-based technology developed at IPFN allows the synthetises of high-quality free-standing flakes of graphene and graphene derivatives, as well as the possiblity to incorporate metal oxides into those structures. The Plasma Engineering Laboratory has several plasma-based reactors that will be adapted to the production of (N-)graphene/TiO_x hybrids. These devices are highly customizable and can operate in a large interval of operational parameters, which must be explored to produce materials with the desired characteristics.

Goals

1) Literature review and assessment of the state-of-the-art of TiO_x/graphene hybrids synthesis.

2) Familiarization with the synthesis methods and materials characterization techniques available at PEL and in collaborating institutions.

3) Operation of the experimental setups available to produce TiO_x/graphene and TiO_x/N-graphene samples.

4) Characterization of the synthetized materials.

5) Optimization of the synthesis processes and establishment of new production protocols for TiO_x/(N-)graphene.

Period: 2023/2024

Framework: PIC2/MSc thesis

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

Supervisors:
Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal
Vasco Guerra (vguerra@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal

Abstract
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 context, the understanding of the oxygen role in the dissociation process if of special importance. 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). In this work the research efforts will be targeted at investigating the mechanisms that govern the formation of oxygen atoms in the effluent of CO_2 low pressure microwave discharges (see schematic of the setup in figure 1). 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 [2,3]), 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.

Goals:

- Develop a 0D kinetic model for the chemistry of CO_2 plasmas sustained at low-pressure MW discharges.
- Investigate the heating mechanisms of CO_2 discharges, both in the active phase and in the afterglow region of the plasma
- Assess the spatial evolution of oxygen species along the afterglow of the MW discharge (see figure 1).

Period: 2023/2024

Framework: PIC1, PIC2/MSc thesis

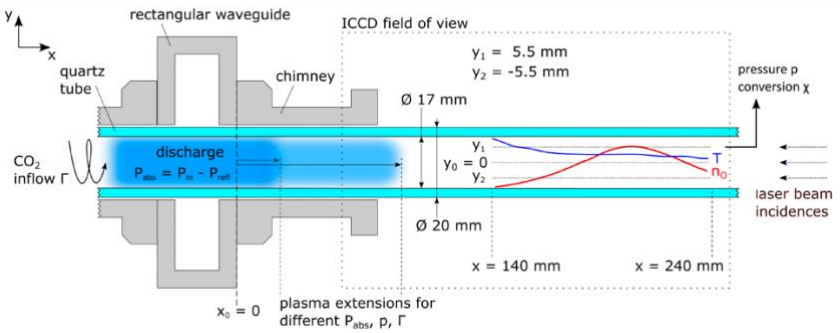

Figure 1.Investigation of atomic oxygen kinetics in the effluent of a CO_2 microwave plasma

References:
[1] T. Silva et al., *Plasma Sources Sci. Technol.* **27(1)** 015019 (2018).
[2] A. Tejero-del-Caz et al., *Plasma Sources Sci. Technol.* **28** (2019) 043001.
[3] A. F. Silva et al., *Plasma Sources Sci. Technol*. **29** (2020) 125020.

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

Supervisors:
Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal
Vasco Guerra (vguerra@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal

Abstract
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.

Goals:

- Describe the time-dependent electron energy distribution function in conditions of interest for atmospheric repetitive He discharge with ns current peaks.
- Develop a chemistry module for a CO_2-He plasma and compare modelling results against experimental data in terms of CO_2 conversion.

Period: 2023/2024

Framework: PIC1, PIC2/MSc thesis

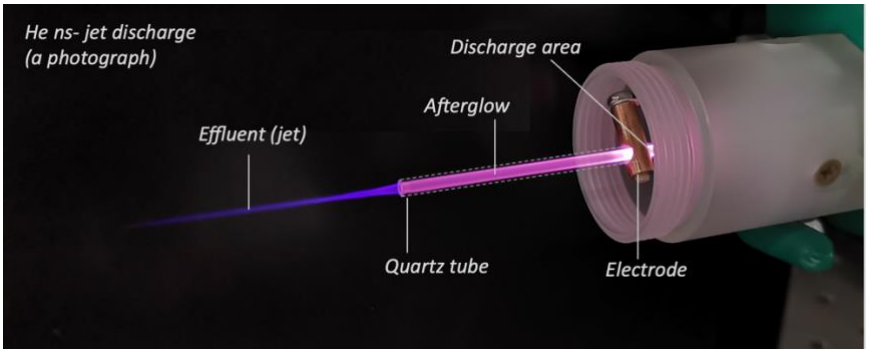

Figure 1. Photograph of a ns jet discharge sustained with Helium at atmospheric pressure.

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.

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

Supervisors:
Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal
Vasco Guerra (vguerra@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal

Abstract
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.

Goals:

- Extend the recently developed low-pressure N_2 plasma description towards atmospheric pressure conditions, thereby providing a comprehensive analysis of N_2 discharges across a broader range of pressure environments.
- Investigate species and radicals formed in the afterglow of a microwave discharge, elucidating their role in the deconstruction of plastic waste into hydrogen and high-value carbons, with applications in sustainable energy and advanced materials.

Period: 2023/2024

Framework: PIC1, PIC2/MSc thesis

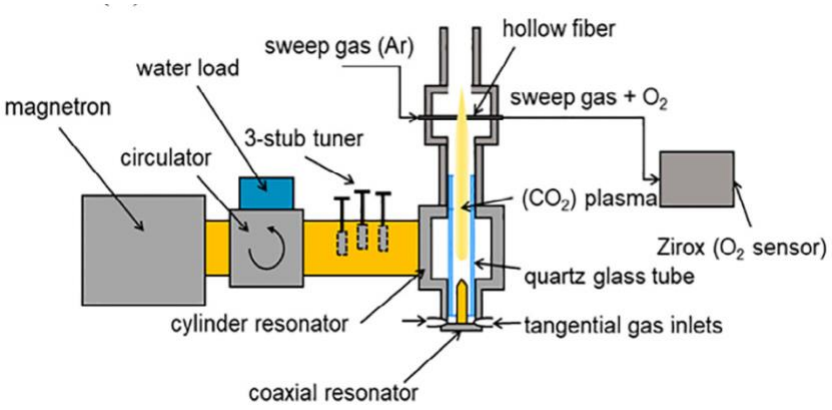

Figure 1. Schematic of a N_2 microwave-sustained discharge used for CO_2 decomposition.

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.

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

Supervisors:
Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal
Vasco Guerra (vguerra@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal

Abstract
Recent experimental work has shown the potential of microwave plasma torches 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 macroscopic parameters (gas temperature and species densities) in CO_2 microwave plasma torch (see figure 1) operated with a solid-state generator. The research efforts will capitalize on recent experimental optical measurements exclusively dedicated to the measurement of fundamental plasma parameters. 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 and the Karlsruhe Institute of Technology (KIT) in Germany where the experimental work will be carried out (see e.g. [1]). First modelling steps will be taken in order to simulate the flow and the heat transfer with the gas/plasma system produced by a microwave-driven injection torch. The study will capitalize on previous works dedicated to the simulation of Navier Stokes equations in He-containing plasmas [2].

Goals:

- Adapt the plasma model originally developed for helium-based plasma torches and apply it to CO_2 discharges, enabling a comprehensive understanding of CO_2 plasma characteristics.
- Investigate macroscopic parameters related with species densities and gas temperature profiles, against experimental data for model validation and refinement in CO_2 discharges.

Period: 2023/2024

Framework: PIC2/MSc thesis

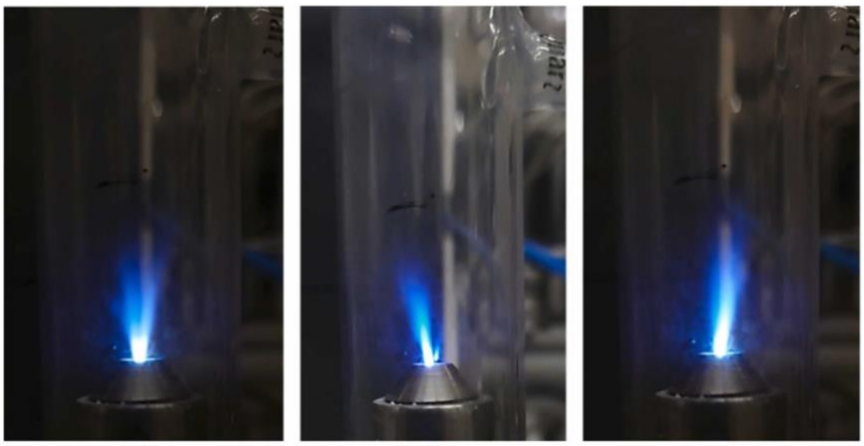

Figure 1. Picture of a CO_2 microwave plasma torch sustained at atmospheric pressure.

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

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

Supervisors:
Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal
Vasco Guerra (vguerra@tecnico.ulisboa.pt), IST/Univ Lisbon, Portugal

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]).

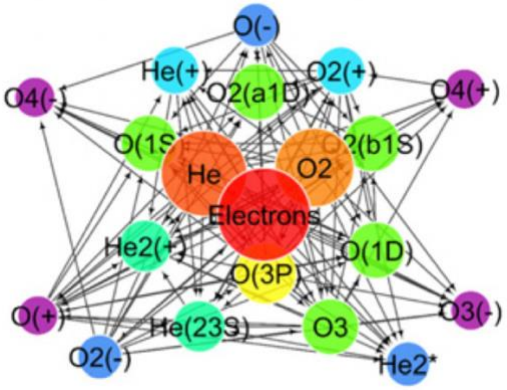

Figure 1. Example of a network diagram using graph-theoretical analysis in O_2-He a discharge taken from [2]

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

Title: Modelling Air-Water Microwave Plasmas for Sustainable Fertilizer Production.

Supervisors: Júlio Henriques (julio.henriques@tecnico.ulisboa.pt), IPFN-IST/Univ. Lisbon, Portugal

Abstract

Traditional nitrogen-based fertilizer (N-fertilizer) production methods are unsustainable due to their substantial energy consumption, representing roughly 2% of global energy usage and approximately 5% of natural gas utilization. Moreover, these practices exert a notable environmental footprint, contributing to approximately 1.4% of the world's CO2 emissions. Finding a viable, long-term sustainable alternative that doesn't depend on natural gas and eliminates greenhouse gas emissions is crucial, aligning with the European Union's objective of achieving carbon neutrality in N-fertilizer production by 2050.

A groundbreaking plasma technology developed at IPFN, utilizes plasma to produce N-fertilizers. This innovative approach involves injecting a mixture containing natural sources of nitrogen, oxygen, and hydrogen through microwave plasmas, where dissociation processes occur, resulting in the formation of reactive species containing atomic nitrogen. After interaction with an aerosol in the post-plasma discharge, a N-fertilizer is produced, namely Ammonium Nitrate (NH_4NO_3). The sole energy source required is electricity, exclusively obtained from renewable sources, promoting energy sustainability. This efficient approach ensures continuous nitrogen nutrient production for plants without environmental harm or resource depletion. To better understand the processes leading to N-fertilizer formation, we have developed a 2D theoretical model based on a self-consistent description of electron kinetics, heavy-species kinetics, gas dynamics, and wave electrodynamics.

Goals

This master's thesis comprises three key elements:

Literature Review: In-depth investigation of existing literature focused on Plasma N-fertilizer production. This review will identify advancements, challenges, and critical research gaps.

Plasma Process Modelling: The development of computational models to simulate the plasma processes involved in N-fertilizer production. These models will analyze nitrogen molecule dissociation processes, reactive species formation within the plasma, and the fertilizer synthesis.

Environmental Impact Assessment: An evaluation of the environmental sustainability of plasma-based nitrogen fertilizer production in comparison to conventional methods.

This master's thesis aims to enhance our understanding of plasma technology's role in sustainable N-fertilizer production. Through research and advanced modelling, we aim to provide valuable insights for future advancements in this field, promoting efficient and eco-friendly N-fertilizer production methods.

Period: Free

Framework: PIC2/MSc thesis

Title: Fitting of Electron Transport Parameters with Optimization Algorithms

Supervisors: Nuno R. Pinhão (npinhao@ctn.tecnico.ulisboa.pt), IST/Univ. Lisboa, Portugal

Abstract

Machine learning algorithms offer innovative solutions to complex problems. One of this problems is the discovery of electron collision cross sections (cs) from the transport parameters of the electrons drifting on a gas under the influence of an electric field. This is a typical “inverse problem” where we aim to retrieve the properties of physical system by interpreting observations of such system.

Solving the electron Boltzmann equation with a set of cs we can obtain transport parameters and compare with experimental values. The difference between them suggests corrections to introduce in the cs, and the process is repeated until the differences are minimized. Unfortunately, while the transport parameters can easily be computed, the fitting of the cs is complex and the conventional approach is labor-intensive.

Evolutionary algorithms are algorithms inspired on the evolution of populations occurring in Nature. The application of these algorithms to complex optimization problems has been successful. In particular genetic algorithms have been applied to this problem but require further study.

Goals

To study the application of a genetic algorithm and an evolution strategy algorithm to the discovery of cs. First a code using a genetic algorithm will be used on a model gas to optimize the convergence of the algorithm. Then the algorithm will be tested both on simple scaling of the cs and to change the cs shape. Finally, an evolution strategy algorithm will be tested and the results of the two algorithms compared.

Period: 2023/2024

Framework: PIC1

Title: Simulation of a Gas Electron Multiplier (GEM) detector for particle physics

Supervisors: Nuno R. Pinhão (npinhao@ctn.tecnico.ulisboa.pt), IST/Univ. Lisboa, Portugal

Abstract

The Gas Electron Multiplier (GEM) [1] based detectors have been widely developed in last years and proposed for many different applications. They are a proven amplification technique for position detection (with resolution < 100 µm) of ionizing radiation such as charged particles, photons, X-rays and neutrons, in gas detectors. The GEM is a detector containing a thin densely pierced polymer foil coated with electrodes on both sides. On application of a difference of potential between the two electrodes, electrons released by radiation in the gas on one side of the structure drift into the holes, multiply and transfer to a collection region. Although their main applications are in high energy physics, they find application in medical imaging, astrophysics, material analysis, and radiation detection and monitoring. E.g., their use on tokamak plasma radiation monitoring/imaging is ongoing research [2]. In order to reach a better understanding and optimization of such kind of detector computer simulation is an important and powerful tool. Tools are available to compute the electric field, gas excitation and ionization, electron and ion transport and simulate the charge collection signal.

Goals

- Define the 3D geometry and optimize the simulation mesh;
- Compare the solution for the electric field using standard FEM or the neBEM (nearly exact Boundary Element Method);
- Select a simplified kinetic model for an Ar – CO_2 mixture;
- Simulate the discharge and study the influence of mixture composition, electric field, etc. on the charge collection signal and resolution.

[1] F. Sauli 1997, Nucl. Instr. and Meth. A 386 531

[2] M. Chernyshova et al 2019, Fusion Eng. and Design 146, Part A, 1039

Period: 2023/2024

Framework: PIC2/Msc thesis

Title: One dimensional modeling of a dielectric barrier discharge

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Abstract

The dielectric barrier discharge (DBD), where at least one electrode is protected by a dielectric, is a very common plasma source. Due to the simplicity and flexibility of construction and the possibility of working at atmospheric pressure, DBD are found not only at laboratories but also in many industrial applications. The applications range from chemical reactors for processing of gases to the treatment of surfaces and liquids.

Due to the presence of the dielectric, at atmospheric pressure, the plasma is produced by filamentary micro-discharges with a very short duration (~20 ns), localized (~1 mm radius) and occupying only a fraction of the discharge volume. The modeling of the discharge is challenging involving different time scales (for the micro-discharge, for the applied voltage and the residence time of the gas). It has been possible, however, to use 0D or 1D model to describe the chemical kinetics in these reactors.

Goals

Develop a 1D model for a cylindrical plug-flow DBD reactor. The goal is to combine the description of the (radially averaged) chemical kinetics occurring in a single filamentary discharge with the effect of the gas flow along the reactor. The model will be applied to study the reactions on a methane-carbon dioxide mixture. The results will be validated comparing with results of composition, conversion and selectivity measured at the exit of the reactor.

Period: 2023/2024

Framework: PIC2/MSc thesis

Title: Plasmas for fertilizers

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Abstract
Understanding the main kinetic paths leading to the synthesis of NH3 in N2-H2 plasmas has topical interest for the large-scale production of fertilizers at low cost and the mitigation of NH3 generation in fusion machines. And tackling this subject opens other research avenues, e.g.

- identifying the main species and the most relevant volume/surface mechanisms controlling the non-equilibrium behaviour of N2-H2 plasmas;
- quantifying the contribution of these mechanisms to the uncertainty in modelling results, using/developing Machine Learning tools;
- exploring the influence of pulsed excitations in the gas/plasma chemistry and energy exchanges, using/developing the LisbOn KInetics (LoKI) simulation tool.

These challenges will be addressed within project PSI.COM (Plasma Surface Interaction (Data and Tools) COupled Modelling) [1] by modelling N2-H2 plasmas with a description of the electron and the heavy-species kinetics in the plasma volume, the transport of species towards the wall and a description of the surface kinetics, accounting for the heterogeneous catalytic formation of ammonia at the wall.
Self-consistent simulations will use the LisbOn KInetics (LoKI) tool suite [1], coupling a Boltzmann solver (LoKI-B) and a Chemistry solver (LoKI-C), to obtain the electron energy distribution function and the densities of the most relevant heavy species with the plasma. LoKI will be further developed and consolidated, aiming the final release of a full time-dependent algorithm, a set of Machine Learning LoKI-tools for sensitivity analysis, and a LoKI-B web-version.
Results will be validated against experimental characterization and diagnostics of N2-H2 discharges (probe, optical/laser spectrometry, mass spectrometry measurements) performed at the Laboratoire de Physique des Plasmas (LPP), Paris, France [3].

[1] https://nprime.tecnico.ulisboa.pt/psi.com/
[2] https://nprime.tecnico.ulisboa.pt/loki/
[3] A Chatain et al, Plasma Sources Sci. Technol. 32 (2023) 035002

Goals

- Update the current N2-H2 Lisbon model (volume and surface), namely with vibrational-translational and vibrational-vibrational processes for the molecular gas mixture extending / reviewing the cross sections data adopted for hydrogen reviewing the surface kinetic mechanisms.
- Development and consolidation of the LoKI tool suite, aiming at full time-dependent description, and including Machine Learning tools for sensitivity analysis.
- Perform experimental characterization and diagnostics of the plasma, for model validation.

Period: 2023/2024

Framework: PIC2/MSc thesis

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The work can include an internship at the Laboratoire de Physique des Plasmas – LPP, Ecole Polytechnique (Paris, France).