Proposal of Research Subjects

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

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

2021 (version 2)

Proposal of Research Subject to develop at

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https://www.ipfn.tecnico.ulisboa.pt/nprime/

Title: Large scale synthesis of graphene and N-graphene using surface-wave plasmas

Supervisors:
Luís L. Alves (llalves@tecnico.ulisboa.pt), IST/Univ. Lisbon, Portugal
Edgar Felizardo (edgar.felizardo@tecnico.ulisboa.pt), IST/Univ. Lisbon, Portugal

Abstract
Graphene and its derivatives (e.g. N-graphene) have electronic and structural properties that make them very useful in a large spectrum of established and emerging applications. However, producing these materials at high yields while maintaining their desirable properties is challenging. As a leading research institution in the production of high-quality free-standing graphene flakes, IPFN is developing a microwave-based plasma prototype that aims at significantly improve the production rates obtained from previously developed proof-of-concept setups.

During the development of the MSc thesis, the student will have the opportunity to work with Plasma Engineering Laboratory researchers of N-PRiME/IPFN (https://www.ipfn.tecnico.ulisboa.pt/nprime/pel/team.html), exploring the wide range of operational parameters of the prototype, developing new features and improving/creating production protocols for the researched nanomaterials.

Framework: MSc thesis.

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Title: Plasma techniques applied to the synthesis of graphene-metal-based nanocomposites

Supervisors:
Luís L. Alves (llalves@tecnico.ulisboa.pt), IST/Univ. Lisbon, Portugal
Ana Inês Dias (ines.vieitas@tecnico.ulisboa.pt), IST/Univ. Lisbon, Portugal

Abstract
Graphene has been extensively explored to enhance mechanical and functional properties of metal-matrix composites for a wide range of applications, being very promising for energy storage devices, since they exhibit extra-ordinary properties unlike conventional materials. However, one of the major challenges in the field lies in the complexity and sensitivity of the synthesis processes. Plasmas are an alternative and sustainable strategy to synthesize disruptive nanostructures since they allow the effective control over the nucleation and assembling mechanisms at atomic scale level. In the present proposal a novel, single-step microwave plasma-enabled technique will be used to synthetize customized graphene-metal-based nanocomposites at high-yield. To better understand the nucleation processes several plasma characterization techniques will be used, including optical emission and FTIR spectroscopy. For nanomaterials characterization TEM, SEM, XRD, FTIR, XPS and Raman spectroscopy technologies will be employed.

During the development of the MSc thesis, the student will have the opportunity to work with Plasma Engineering Laboratory researchers of N-PRiME/IPFN (https://www.ipfn.tecnico.ulisboa.pt/nprime/pel/team.html), exploring the wide range of operational parameters of the plasma-based method and characterization techniques, developing new features, and establishing production protocols for the synthesised materials.

Framework: MSc thesis.

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Title: Modelling of N_2-H_2 plasmas, including the catalytic formation of ammonia

Supervisors:
Luís L. Alves (llalves@tecnico.ulisboa.pt), IST/Univ. Lisbon, Portugal
Luís Marques, CF/Univ Minho and Porto, Portugal

Abstract
Understanding the main kinetic paths leading to the synthesis of NH_3 in N_2-H_2 plasmas has topical interest for the large-scale production of fertilizers at low cost and the mitigation of NH_3 generation in fusion machines. And tackling this subject opens other research avenues, e.g.
- identifying the main species and the most relevant creation/destruction mechanisms in N_2-H_2 plasmas;
- clarifying the influence of surface mechanisms in the non-equilibrium plasma behaviour;
- optimizing the plasma-assisted production of ammonia.
These challenging topics will be addressed by modelling N_2-H_2 plasmas, considering a description of the electron and the heavy-species kinetics in the plasma volume, the transport of species towards the wall and the surface kinetics, accounting for the heterogeneous catalytic formation of ammonia at the wall. Self-consistent simulations will use the LisbOn KInetics (LoKI) tool [1], coupling a Boltzmann solver and a Chemistry solver, to obtain the electron energy distribution function and the densities of the most relevant heavy species with the plasma. Results will be validated against experimental characterization and diagnostics of N_2-H_2 RF discharges, obtained in a cylindrical metal-free chamber at the University of Basel [2], using the following techniques: mass spectrometry, Temperature-Programmed Desorption, Langmuir probe measurements and Optical Emission Spectroscopy.
[1] https://nprime.tecnico.ulisboa.pt/loki/
[2] M. B. Yaala et al. 2019 *Phys.Chem.Chem.Phys.* **21** 16623

Goals
- Update the current N_2-H_2 Lisbon model, with vibrational-translational and vibrational-vibrational processes for the molecular gas mixture.
- Extend the model kinetics and review the cross sections data adopted for hydrogen.
- Extend the model kinetics to surface mechanisms.
- Perform experimental characterization and diagnostics of the plasma, for model validation

Framework: MSc thesis or internship.

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Title: Testing the QDB for air plasma

Supervisors:
Luís Lemos Alves (llalves@tecnico.ulisboa.pt), IST, University of Lisbon, Portugal
Jonathan Tennyson, Dept. Physics and Astronomy, UCL and Quantemol Ltd, UK

Abstract
There are countless applications of models of plasmas formed in air (here taken to be a mixture of nitrogen and oxygen molecules). Such models require an accurate validation of the various processes (electron collisions, chemical reactions etc) which can occur in the plasma. The Quantemol Data Base (QDB) [1], is new database that aims not only to provide data on the individual atomic and molecular processes important in a plasma but to also aggregate them into so-called chemistries which consider all the important processes that occur in the given plasma mixture. The model chemistries are then validated by comparison with available experiments for the plasma.

Goals
The aim of this project is to construct an air chemistry from the data available in QDB and use this chemistry in plasma models to give results that can be compared with the observed air plasma behaviour. Models will be performed using either the LisbOn KInetics code (LoKI) [2] after initial tests using the zero-dimensional plasma model that is integrated in the QDB database. The study will be performed in collaboration with scientists from Quantemol Ltd (London, UK) who are spin out company from University College London.

[1] https://www.quantemol.com/
[2] https://nprime.tecnico.ulisboa.pt/loki/

Period: 2021/2022

Framework: MSc thesis; short-term mission to UCL is envisaged

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Title: Nonequilibrium excitation, dissociation, and ionization processes in high-speed (>10km/s) shockwaves

Supervisors: Mario Lino da Silva (mlinodasilva@tecnico.ulisboa.pt)

Abstract
The development of accurate heavy-impact kinetic schemes is an important technology driver for the development of high-temperature plasma torches (arcjets or Inductively-Coupled Plasmas) used for high-temperature materials testing, but also for the improvement of the design of atmospheric entry spacecraft. Currently very little is known about heavy-impact processes at extremely high temperatures (from 5,000K to 100,000K), and there is the potential for significant improvements of current state-of-the art approaches, if new and improved models (such as the ones that have been developed at IPFN over the last 10 years) are properly deployed.

Goals
The objective of this work is to update the STELLAR database of vibrationally-specific state-to-state rates for excitation and dissociation of air species (N_2, O_2, NO, N, O).

The work is subdivided in several work-packages:
1) Calculation of the potential curves for the ground and electronic states of N2, O2 and NO using an extrapolated RKR method and determination of vibrational and rotational dissociation limits, for all the relevant electronic states. A list of electronic-vibrational-rotational levels will be produced, and the corresponding internal partition functions will be compared against other results in the literature, up to 50,000K.

2) Update of the calculated vibration-translation (V-T) and vibration-dissociation (V-D) rates using the Forced Harmonic Oscillator approach and comparison against experimentally-determined dissociation rates

3) Update of the calculated vibration-electronic (V-D) rates using a Landau-Zener or Rosen-Zener approach to estimate for the first-time the excitation of molecular radiative states through heavy-impact collisions

4) Application of the developed thermochemical models in 1D and 2D Computational-Fluid Dynamics simulations using the in-house CFD code SPARK to reproduce experimental data issued from shock-tubes applications or from flight-test data from Spacecraft entries. The obtained results will allow calibrating the models obtained in work-packages 1, 2, 3 and determine the needs for future improvements

Period: Free

Framework: MSc thesis or internship

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Title: European Shock-Tube for High Enthalpy Research

Supervisors: Mario Lino da Silva (mlinodasilva@tecnico.ulisboa.pt)

Abstract
The ESTHER (European Shock-Tube for High Enthalpy Research) shock-tube is a research facility currently being deployed in the premises of IPFN, in the IST Campus of Sacavém. This research infrastructure is being developed in the scope of three contracts awarded by the European Space Agency (ESA) to an international consortium led by IST-IPFN. The overall budget for the facility (including the hosting building funded by IST) amounts to over 2.5M€. The primary mission of ESTHER is to support future planetary exploration missions through the reproduction of atmospheric entry plasmas at the ground level. Indeed, as a spacecraft enters the upper layers of a planetary atmosphere at velocities of several km/s, a strong shock wave is created upstream of the spacecraft, heating and ionizing the surrounding gas and ultimately creating a so-called atmospheric entry plasma. This low-pressure, high-temperature non-equilibrium plasma strongly heats the spacecraft thermal protections through convective and radiative heating. It is therefore important to properly characterize and model the physical-chemical properties of such plasma, with a strong emphasis on the adequate quantitative reproduction of non-equilibrium processes (departure of the internal states from a Boltzmann equilibrium distribution).

Goals
The student will participate in the setup of the shock-tube facility and will assist in the preparation, execution, and postprocessing of the facility shots.

Other tasks include the preparation of the spectroscopy setup for the tests execution (arrays of fast intensified cameras and VUV, visible and IR spectrometers), and numerical reproduction of the obtained shockwave data against numerical models developed and maintained at IPFN/N-PRiME.

Period: Free

Framework: MSc thesis or internship

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Title: Implementation of the CASL approach in the SPARK code

Supervisors: Mario Lino da Silva (mlinodasilva@tecnico.ulisboa.pt)

Abstract

The modeling of High-speed reentry flows is one of the most challenging tasks at contemporary level, alongside with turbulence modeling. The necessity to account for a large array of physical-chemical processes occurring downstream of the strong hypersonic shockwave means that fluid descriptions have to account for multicomponent flow models for the difference chemical species of the flow (N2, O2, NO, N, O, N2+, O2+ NO+, N+, O+, e-), and deploy complex transport models valid up to higher temperatures. In addition, chemistry has to be accounted for owing to the endothermical dissociation and ionization reactions favored by the steep rise in the shocked flow. This means that the amount of calculations to be carried out in each cell of a computational grid can sometimes be daunting, and it is therefore necessary to develop simplified geometries to allow for fast and efficient testing of such advanced models, while retaining an affordable spatial computational grid.

One very attractive approach is the so-called "Computation along a stagnation line" or CASL approach, also called as a "1.5D" model. Here the evolution of the flow along the stagnation streamline may be modeled along the r coordinate of the stagnation line, including a boundary condition on the derivative of the cylindrical angle theta, allowing for the evacuation of the flow near the wall boundary. The Navier-Stokes equations can be rewritten for such a geometry, and a complex hypersonic flow model can henceforth be tested along a grid of about 100points before being deployed in more complex 2D and 3D descriptions with tens to hundreds of thousands cells and calculation times that may take several weeks.

The SPARK code is a CFD code for hypersonic and reentry applications maintained at IPFN. The code has been applied to past and future exploration missions (Galileo 1995 Jupiter entry, Huygens 2004 entry in Titan, EXOMARS 2016 entry in Mars, and future Neptune entry missions).

Goals

The objective of this work is to implement the CASL approach in the SPARK code and couple the resulting Navier-Sokes equations to the detailed transport solvers sported by the code. A few testcases will be carried out in 1.5D and compared to a more detailed (and lengthy 2D axysimmetric solution). The code speed-up will be determined.

Period: Free

Framework: MSc thesis or internship

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Title: 3D Monte Carlo electron Boltzmann solver

Supervisors: Vasco Guerra (vguerra@tecnico.ulisboa.pt)

Abstract
The basic problem in the kinetic theory of dilute charged particles in a neutral gas is to solve the Boltzmann equation for the charged particle velocity distribution function. In low-temperature plasmas, such as those found in space shuttle re-entry or created for technological applications as diverse as production of synthetic fuels, pollution abatement or biomedical treatments, this problem is of paramount importance. Indeed, the electrons exhibit a distinctive non-equilibrium behaviour and must be dealt-with in terms of the full velocity distribution function and Boltzmann equation analyses or Monte Carlo simulations are mandatory.

The N-PRiME team at IPFN developed recently an open-source tool to solve the homogeneous (0-Dimensional) electron Boltzmann equation in the two-term expansion in Legendre polynomials [1,2]. However, the validity of this approach is limited to small anisotropies in the distribution function (i.e., relatively low values of the electric field) and is not easy to generalise to non-homogeneous fields. The aim of this project is to develop a general 3D Monte Carlo code to obtain the electron velocity distribution function.

Goals
Develop a numerical code to perform time-resolved 3-D Monte Carlo simulations of the electron kinetics in crossed electric and magnetic fields, and in the presence of nonconservative collisions, ionization, and attachment. This is a very ambitious project, suited for a MSc thesis. However, it can be divided in sub-tasks appropriated for shorter internships.

[1] A Tejero-del-Caz et al 2019, *Plasma Sources Sci. Technol.* **28** 043001
[2] https://github.com/IST-Lisbon/LoKI

Period: 2021/2022

Framework: MSc thesis, internship (3+ months)

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

Supervisors: Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt) and Vasco Guerra, IST, University of Lisbon, Portugal
Nikolay Britun and Masaru Hori, Nagoya University, Japan

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 which are not compatible with low-pressure conditions, in particular in the rapidly growing fields of plasma medicine and plasma agriculture. The non-equilibrium nature of the plasma, where the temperature of electrons is much higher than the temperature of gas, allows the creation of reactive species without excessive heat of the gas and the treatment of targets which are sensitive to overheating, such as polymers, plants, and tissues. However, maintaining low gas temperature at atmospheric pressure and tailoring the plasma to the desired application is not an easy task, requiring and a deep understanding of the system at a fundamental level.

Goals
This work proposes a joint modelling and experimental study of air-containing atmospheric discharges aiming at a precise determination of the plasma parameters, namely electron density and electron temperature. The additional plasma parameters necessary as an input for modelling, such as gas temperature and electric field, will be obtained via experiment, including optical emission-based and as laser-based plasma spectroscopy.

The work will be developed in the framework of a collaboration between Instituto Superior Técnico, where the models will be developed, and the Nagoya University, where the experimental work will be carried out.

Period: 2021/2022

Framework: MSc thesis, including internship (3+ months) at Nagoya University.

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Title: Plasma-based production of oxygen on Mars

Supervisors: Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt) and Vasco Guerra, IST, University of Lisbon, Portugal

Abstract

The achievement of a manned mission to Mars will mark the next frontier of discovery and the dawn of a new age in planetary exploration. Among the many scientific and technical challenges required to make this journey a reality, the harvesting of local resources at the site of exploration is of a special and mandatory importance. This approach is known as in situ resource utilization (ISRU) and it has the potential to enable humans to thrive beyond Earth, in a self-sufficient way, for extended periods of time. ISRU becomes particularly interesting when considering the possibility of oxygen production directly from the CO_2-enriched Martian atmosphere. A local production of oxygen would reduce the logistics and costs of missions, while providing a breathable environment for future human outposts and a source of rocket propellant.

The N-PRiME team at IPFN has been deeply involved in the study of plasma-based CO_2 decomposition, while investigating the potential of plasmas for oxygen production on Mars [1,2]. This project goes beyond the state-of-the-art by providing the first steps towards the development of a proof-of-concept plasma-based system for oxygen production under Martian environment, validated in laboratory. This will enable to study new and promising conditions for CO_2 valorization, explore the differences between Earth and Mars in terms of CO_2 plasma-based decomposition and test the potential integration of plasma reactors in future missions to Mars.

Goals

The students will integrate the research team of the recently funded FCT project ROADMARS and participate in the installation of a plasma setup targeted at producing oxygen from CO2 decomposition under Martian environment. Other tasks will be focused on the: (i) analysis/study of plasma parameters that influence the production of oxygen under Martian environment and (ii) development of a kinetic model to describe the heavy particle collisions of Martian plasmas.

[1] V. Guerra et al 2017, *Plasma Sources Sci. Technol.* **26** 11LT01.
[2] P. Ogloblina et al 2021, *Plasma Sources Sci. Technol.* **30** 065005.

Period: 2021/2022

Framework: MSc thesis with scholarship

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Title: Computational and Experimental Validation of Laser Induced Fluorescence (LIF) Model

Supervisors: Tiago Silva (tiago.p.silva@tecnico.ulisboa.pt) and Vasco Guerra, IST, University of Lisbon, Portugal
João Vargas, CCRC/KAUST (Saudi Arabia)

Abstract
Due to both the population and economic growth, the world energy demand is expected to rise by 25% in the coming 20 years. This growth emphasizes that drastic changes are required to meet our CO2 emission objectives from the Paris Conference of the Parties (COP 21). Even considering this objective, the main scenarios proposed by international agencies (e.g., the World Energy Outlook) evidenced that combustion will remain the main energy source for the next decades. Thus, the most promising strategies to reach our emissions objectives are the ones based on circular carbon economy (so-called 4Rs: reduce, reuse, recycle, and remove). Thus, the use of highly efficient combustion processes combined to low-carbon/carbon-free fuel is one of the most promising approach to effectively reduce our carbon emissions and meet the energy demand. Such ideal conditions may be achieved by using detonation engines fueled with green hydrogen (i.e., obtained from renewable sources). However, the development of efficient and reliable detonation engines is still challenging and a deeper understanding of the detonation phenomena is required. One strategy to bridge the current knowledge gaps of the detonation phenomena is to employ laser diagnostics to characterize detonation waves.

While laser diagnostics are of common practice in conventional (subsonic) combustion processes, the experimental characterization of detonation historically relies on the determination of macroscopic parameters such as the mean detonation velocity, global pressure, and density gradient structure. The laser-induced fluorescence of OH radical (OH-LIF) is a powerful technique that induces specific molecules emission from laser light excitation. When employed with a laser sheet, this technique can provide spatially-resolved measurements and is called OH-PLIF. Despite the previous usages of the OH-PLIF in detonation, several limitations prevented quantitative measurements or direct

experimental-numerical comparisons. To overcome this, post-processing of numerical simulation results with spectroscopic codes are currently a common practice. The recent works conducted in the Plasmas and Flames (PaF) group, on simulating the OH-LIF process and the non-equilibrium effects, revealed that additional challenges may need to be considered before reaching quantitative measurements by OH-PLIF in detonations.

Goals

The goal of the project is to further develop an existing LIF code, KAT-LIF, that is able to simulate radiative signals of molecules of interest in a range of conditions relevant for detonation experiments. Firstly, the student will have to become familiar with the preexisting KAT-LIF code and the physics of the LIF diagnostic. Secondly, the code will need to be transferred to a more adequate software framework along the development of some new features. Thirdly, an ensemble of experimental measurements will be employed to validate the developments. The candidate could either perform these experimental measurements himself or they could be provided to him by another team member, depending on his interests. The candidate will be supervised at KAUST by Dr. João Vargas.

This remunerated M.Sc. thesis/internship can be done fully remote or partially/fully executed at KAUST, depending on the pandemic situation and candidate. Based on the progress, the candidate will have the opportunity to present his research work in local/international conferences, as well as applying for a Ph.D. position at KAUST.

Period: 2021/2022

Framework: MSc thesis with scholarship

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Title: Fast multipole method for plasma physics

Supervisor: Vasco Guerra (vguerra@tecnico.ulisboa.pt) and Tiago Dias

Abstract
The numerical solution to N-body problems in gravitation or electrostatics has traditionally been obtained via particle-in-cell methods (PIC), since direct evaluation of all pairwise interparticle forces requires O(N^2) operations and is computationally too expensive. An alternative to PIC are hierarchical solvers, which use tree data structures and lumped-force approximations, making simulations feasible in O(N log N) operations.

Goals
The purpose of this work is to explore the use of the fast multipole method (FMM) in electrostatic particle simulations in plasma physics and compared FMM with the PIC methodology.

Period: 2021/2022

Framework: MSc thesis

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

Supervisor: Nuno Pinhão (npinhao@ctn.tecnico.ulisboa.pt)

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 – CO2 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: 2021/2022

Framework: MSc thesis

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Title: Implementation of the HDF5 data format in the LoKI software suite

Supervisor: Nuno Pinhão (npinhao@ctn.tecnico.ulisboa.pt)

Abstract

LoKI is a suite of MATLAB solvers to study the chemical processes in a plasma. This requires the computation of the energy distribution of electrons in the plasma, of the reaction coefficients for electron-molecule processes and the study of the chemical kinetics.

The data produced in these studies is miscellaneous and large. The data recorded for later processing may include the electron energy distribution, the values of electron transport parameters, of the rate coefficients for each reaction considered and the density of several species. And these values may be studied as function of the electric field, time or space. The data format for writing, and later read, these values needs to be sufficiently flexible to handle this diversity.

The HDF5 data format has been developed to address similar problems occurring in multiple scientific and technical field. It is cross-platform, developed to work with heterogeneous data and to handle big volume of data in a fast and efficient way.

Goals

The goal of this project is to implement the HDF5 data format on the LoKI software suite for data output. The task involves a) the analysis of the required data and structure; b) a proposal of data organization; c) the code implementation and, d) the development of tests and examples

Period: 2021/2022

Framework: Internship / UC Introdução à Investigação