Challenges in the modeling and the simulation of low-temperature plasmas

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The modeling and simulation of the multiple physical and chemical phenomena occurring over a large range of time and length scales in low-temperature plasmas remains a challenge. Recent advances and bottlenecks are discussed with a focus on two applications at atmospheric pressure: plasma jets and plasma assisted combustion and also on low-pressure magnetized plasmas for electric propulsion

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1. Introduction

Low-temperature plasmas are used for a large range of applications including material processing, chemical synthesis, bio-medical or electric propulsion applications.
Many different physical and chemical phenomena occur in these discharges as multi-species nonequilibrium gas chemistry and transport, electrostatics or electromagnetic, fluid mechanics, and coupling with surfaces and interfaces. In the last decade, advances have been obtained on the mathematical modeling and high performance computing of low-temperature plasmas. In particular, the possibility to use multi-scale coupling methods, structured, unstructured, and adaptive mesh techniques, new algebraic equation solvers and parallel computing have opened a large range of new simulation possibilities. More recently, the need of a more systematic benchmarking of low-temperature plasma simulation tools [1] and the importance of uncertainty quantification [2] has also appeared. To present some recent developments in the field of modeling and simulation of low-temperature plasma discharges, two examples are discussed in this paper: fluid simulations of atmospheric pressure plasma jets for biomedical applications and plasma assisted combustion and PIC and fluid simulations of low-pressure magnetized plasmas for electric propulsion.

2. Fluid simulations of low-temperature plasmas at atmospheric pressure for plasma jet applications and plasma assisted combustion applications

In the study of plasma jets for biomedical applications and in the study of nanosecond pulsed plasmas for plasma assisted combustion, the coupling of the discharge with the flow is of key importance.
In plasma jets, the discharge is ignited usually in helium and the helium flow mixes with air at the tube exit. The timescales of the helium flow are much slower than those of the fast ionization fronts of the discharge [3,4]. Therefore, generally, the flow is pre-calculated and the local mixture composition is used in the discharge simulation. Nevertheless, in some conditions, the flow is significantly modified by the discharge and currently two hypotheses have been proposed: either an ionic wind effect or a local gas heating. More experimental and modeling work is still required to clearly address this complex plasma-flow coupling. In this work, we will focus on plasma jets impacting targets [5,6,7], as it is a key issue for biomedical applications. Even if the flow is chosen to be laminar, its spreading on the target has to be accurately modelled to simulate the discharge interaction with the target. Recently, different techniques (optical in the jet, with an electro-optic probe outside of the jet and using Mueller polarimetry on a dielectric surface impacted by the plasma jet) have been developed to measure the electric filed in atmospheric pressure discharges. These new measurements open the possibility to carry out, for the first time, quantitative comparisons with simulations, on the spatiotemporal evolution of the electric field, a key quantity for the discharge and for the applications.
For plasma jet applications, there is also the need to efficiently simulate multi-pulsed multi-jet configurations. The current limitations and challenges to develop more efficient simulation tools of plasma jets will be discussed.

In plasma assisted combustion applications, with nanosecond spark discharges, the key issue is to be able to accurately simulate the spatial distribution of radicals and active species produced and of the fast gas heated gas [8,9]. The coupling of the nanosecond discharge with a compressible flow is necessary to accurately simulate the pressure waves generated by the local fast gas heating. The combustion ignition occurs only after. The current limitations and challenges to develop more efficient simulation tools for plasma assisted combustion applications will be discussed.

3. PIC and fluid simulations of low-pressure magnetized plasmas for electric propulsion

Electric thrusters use electrical power to ionize and accelerate a propellant to velocities up to twenty times larger than those of chemical thrusters. Among the different electric thrusters, Hall thrusters have been studied since their invention in the 1960s. However, the physics of magnetized plasmas in these thrusters is very complex; many plasma processes that have direct relevance to the thruster performance and lifetime are still poorly understood [10]. Today, the design and development of Hall Thrusters remains semi empirical with long and expensive life tests. The physics of Hall thrusters has been the subject of many research efforts, including experimental, theoretical, and numerical studies (using fluid, hybrid and particle-based models). However, important plasma processes are still far from being fully understood: plasma-wall interaction phenomena, and electron transport and related instabilities. Their better understanding is crucial as these processes have direct relevance to the thruster performance and lifetime. Therefore, in spite of the long experience on Hall effect thrusters, a fully self-consistent model to accurately predict the operating conditions of Hall effect thrusters and to help in designing new thrusters is not yet available. New theoretical insights [11,12] have allowed to reconsider the issue of electron transport in Hall thruster discharges. The recent development of massively parallel PIC codes [13,14] allow to carry out parametric studies that were out of reach a few years ago to compare simulation results with theory [14,15] and experimental results. Recent results on the comparison of PIC and fluid code predictions with theoretical results on electron transport for different propellants will be presented. Finally, the steps to develop an efficient computer-aided engineering design tool for electric propulsion will be discussed.

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