Special Issue on Numerical Modelling of Low-Temperature Plasmas for Various Applications – Part I: Review and Tutorial Papers on Numerical Modelling Approaches

Low-temperature plasmas are used for a growing number of applications. To improve these applications, a good insight in the underlying plasma processes is indispensable. This insight can be obtained by experimental research, but also by computer modelling. Several different modelling approaches exist in literature for describing low-temperature plasmas, and the type of modelling approach that is most suitable for a certain application will depend on the plasma operating conditions (e.g., pressure, power, dimensions, gas temperature) and the type of information requested (e.g., information on the breakdown and maintenance of the discharge, on the non-equilibrium behaviour of electrons / ions or on the detailed chemical kinetics of the heavy species). This special issue of Plasma Processes and Polymers aims to give an overview of the various modelling approaches that can be used to describe the plasma behaviour, as well as of closely related topics, such as model verification and validation, modelling of plasma-surface interactions and input data for the models. Furthermore, several examples of modelling efforts in various application fields are demonstrated.

The special issue contains 31 papers in total, divided in two parts, with each part organized as a double issue. Part I, presented here, contains all review and tutorial papers. It was indeed our intention to cover the different modelling approaches in tutorial-like review papers that provide a good introduction to the field for starting PhD students. Roughly speaking, two major groups of numerical modelling approaches to describe the plasma behaviour can be distinguished: (i) kinetic approaches, such as particle-in-cell / Monte Carlo collision (PIC-MCC) and direct simulation Monte Carlo (DSMC) approaches, describing the microscopic non-equilibrium behaviour of the various plasma species, and (ii) fluid models and global models, focusing more on the description of the energy-averaged continuum properties of the plasma. The first approach is typically very accurate, as it follows an *ab-initio* methodology, but in order to obtain statistically valid results it is computationally quite expensive, certainly for more complicated plasma chemistries. The second approach uses more approximations, and therefore is less computationally demanding. This applies especially to global models which adopt an average description in both energy and configuration spaces, usually providing only the time evolution of plasma species densities. Conversely, this allows using more complicated plasma chemistries in such models.

In part I, the PIC-MCC and DSMC approaches are presented by Trieschmann, Schmidt and Mussenbrock (Ruhr University Bochum), for the kinetic simulation of sputtering transport.[1] This tutorial review paper explains when a kinetic approach is needed, and it provides the fundamentals of the applied MC methods and their conceptual details. Next, Hurlbatt and colleagues, from University of York and Ecole Polytechnique in Palaiseau, give an overview on the global modelling approach, including development and techniques, as well as a discussion on the issues and pitfalls.[2] Furthermore, the authors also explain how to bridge the gap between global models and fluid models by discussing methods of extending global modelling techniques to include variations in either time or space. Capitelli and colleagues, from PLASMI Lab in Bari and Université Paris 13, present the coupling of plasma chemistry, vibrational kinetics, collisional-radiative models and the electron energy distribution function at non-equilibrium conditions, for two case studies, i.e., atomic hydrogen and CO_2.[3] Finally, as the kinetic and continuum approaches both have their advantages and limitations, a third option exists in combining these methods into a hybrid approach. In the latter case, a kinetic approach (e.g., Monte Carlo) can be used to treat the plasma species that are not in equilibrium with the applied electric field, such as the high-energy electrons or the ions submitted to strong electric fields in the sheaths, while other plasma species in thermal equilibrium can be treated with a fluid-type approach. The basic principles and some applications of the hybrid approach are outlined by Economou (University of Houston).[4] Whenever possible, he also compares the hybrid modelling results to kinetic and/or fluid simulations, as well as experimental data.

Although this special issue focuses mainly on models for low-temperature non-equilibrium plasmas, we also wanted to give a somewhat broader overview, presenting some modelling approaches for thermal plasmas as well, as many concepts and challenges are similar. Trelles (University of Massachusetts Lowell) gives an overview on finite element methods for arc discharges, to cope with several

challenges associated with this type of plasmas, such as the resolution of multiscale features, multiphysics coupling and the robustness in case of large gradients.[5] Another review paper, by Murphy and Park (CSIRO Manufacturing) discusses the importance of two-way interactions between the plasma and surfaces in modelling thermal plasma processes.[6] Several examples are presented, like for arc welding, plasma cutting and various plasma-particle interactions.

The modelling of plasma-surface interactions is indeed indispensable for many plasma applications. For this reason, we also have two review papers dedicated to this topic. First, Neyts and Brault (University of Antwerp and Université d'Orléans) explain the current capabilities and limitations of molecular dynamics simulations, describing the interactions at the atomic scale.[7] Attention is paid to typical fundamental processes occurring in low-temperature plasmas, including sputtering, etching, implantation and deposition, and to what extent the typical plasma components, such as excited species, electric fields, ions, photons and electrons, can be accounted for. Subsequently, Marinov, Teixeira and Guerra (Ecole Polytechnique in Palaiseau, imec and University of Lisbon) discuss two mesoscopic approaches for describing plasma-surface interactions, i.e., coarse-grained deterministic models, which are computationally effective and can readily be coupled to reactor-scale plasma simulations, and the kinetic MC approach, which is computationally more demanding but bridges the gap between atomic scale and macroscale simulations.[8]

Essential for accurate modelling predictions is the verification and validation of the modelling results. This is carefully analysed by Turner (Dublin City University) who gives an overview of various techniques for this purpose and discusses their application to improvements of the simulation capability for low-temperature plasmas.[9] Furthermore, the accuracy of the models does not only depend on the modelling approach but also on the input data, like collision cross sections, reaction rate coefficients and transport coefficients of the plasma species. The latter can be obtained by swarm models, for most collision-dominated non-equilibrium plasmas, as explained by Petrovic and colleagues from the University of Belgrade.[10] The authors give several examples of ionized gases where swarm models can be employed to provide a full description of the discharge. In addition, electron and ion scattering cross sections and swarm/transport parameters, ion-neutral interaction potentials, and optical oscillator strengths can be obtained from the LXCat database, which is an open-access platform for curating data needed for plasma modelling. An overview of this joint initiative is presented by Pitchford (University of Toulouse) and colleagues from more than 20 different groups all around the world.[11] Collision cross sections can be experimentally measured, but they can also be generated from quantum-mechanical calculations, e.g., for electron scattering. The latter is explained by Bartschat, Tennyson and Zatsarinny (Drake University and University College London) who present an overview of various quantum-mechanical methods, with special focus on the time-independent close-coupling approach.[12] Examples are shown for electron collisions with both atoms (Ar) and molecules (CH_4).

In part II of this special issue, we will present illustrations of the different modelling approaches for various applications. This second double issue will be published in April.

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