Editorial: Special Issue on Numerical Modelling of Low-temperature Plasmas for Various Applications – Part II: Research papers on numerical modelling for various plasma applications

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We present here part II of the special issue on "Numerical Modeling of Low-temperature Plasmas for Various Applications", which was divided in two parts, with each part organized as a double issue. The first double issue contained review and tutorial papers on the various modelling approaches and closely related topics, like model verification and validation, plasma-surface interaction modelling and input data for modelling. In the present double issue, we give illustrations of the different modelling approaches for various applications.

Low-temperature plasmas are extensively used for microelectronics applications. The two main plasma sources used for this purpose are inductively coupled plasmas (ICP) and capacitively coupled plasmas (CCP). This special issue contains a number of papers, describing these two different plasma sources. Wen and colleagues from Dalian University of Technology, University of California and University of Antwerp apply a global (i.e., volume-averaged) bulk plasma model, coupled bi-directionally with a Monte Carlo (MC) / fluid sheath model for an ICP operating in Ar/O_2 gas mixtures [1]. The model calculates the ion energy and angular distribution functions bombarding the rf-biased electrode for different bias voltages, pressures and coil powers. Mouchtouris and Kokkoris (National Center for Scientific Research (NCSR) "Demokritos" in Attica) present a multi-scale model for a low pressure ICP in Ar, based on a reactor scale model for describing the plasma behaviour, a MC particle tracing model to calculate the ion energy and angular distributions, and a MC surface model to calculate the evolution of surface morphology during the etching of a polymeric substrate [2]. This model allows linking the operating parameters of the plasma reactor with the evolution of the surface roughness. Stratakos, Zeniou and Gogolides, also working at NCSR "Demokritos", perform a full-wave 3D electromagnetic analysis in vacuum, to calculate and compare the electric/magnetic field components of different helical and helicon antennas used to generate ICPs [3]. This is important to select the appropriate antenna type for a plasma source.

Large scale CCPs, operating at high frequencies, are studied by Eremin, Brinkmann and Mussenbrock (Ruhr-University Bochum) by means of 2d3v particle-in-cell / Monte Carlo collision (PIC/MCC) simulations, focusing on the effect of the self-bias surface mode on the plasma uniformity [4]. The authors demonstrate that the self-bias mode leads to a non-uniform plasma density profile, attributed to heating of high- and low-energy electrons. Voloshin et al. from Lomonosov Moscow State University apply a 1D hybrid PIC/MCC – fluid model to describe both single frequency (SF) and dual frequency (DF) CCPs in H_2/Ar mixtures [5]. In the SF discharge the effect of the H_2 dilution is studied, while in the DF discharge the effect of the low-frequency voltage is investigated for both low and high pressures. Finally, Schüngel et al., in a collaboration between West Virginia University, the Institute for Solid State Physics and Optics in Budapest and Ruhr-University Bochum, present a model to calculate ion energy distribution functions (IEDFs) in CCPs, operating at single and multiple radio-frequencies in both symmetric and asymmetric configurations, for various gases, pressures and voltage waveforms [6]. The model is based on a simplified ion density profile and a quadratic charge voltage relation for the plasma sheaths. The calculated IEDFs are compared with results obtained from PIC/MCC simulations and from retarding field energy analyser measurements.

One of the fastest growing application fields of low-temperature plasmas is in plasma medicine. As the tissue or cells to be treated are usually covered by liquid, it is important to understand the chemistry of plasma-liquid interaction. Furthermore, plasma-activated liquids are gaining increasing interest for various applications in plasma medicine, and most prominently for cancer treatment applications. Liu and colleagues from Xi'an Jiaotong University and Old Dominion University present a model for understanding the chemistry in plasma-activated solutions [7], namely normal saline and deionized water solutions. The model consists of three modules: a 0D chemical kinetics model for the plasma region, a 1D model describing diffusion and chemical reactions in the air gap between plasma and liquid, treating only neutral species, and a 1D fluid model for the liquid phase, based on continuity equations, drift-diffusion and Poisson's equation.

Another topic of growing interest for low-temperature plasmas is CO_2 conversion into value-added chemicals. Koelman and colleagues from Eindhoven University of Technology, including their spin-off company "Plasma Matters", University of Antwerp and University of West Bohemia present an extensive chemical kinetics model for CO_2 splitting in a dielectric barrier discharge (DBD) [8]. The input data set (available for downloading) is critically assessed and the correctness of the implementation of the model is carefully benchmarked using two independent codes, i.e., Plasimo and ZDPlaskin. A normal DBD has quite limited energy efficiency for CO_2 conversion, but this can be improved by inserting a (dielectric) packing inside the DBD reactor, yielding a so-called packed bed DBD reactor. Van Laer and Bogaerts (University of Antwerp) apply a two-dimensional (2D) fluid model to describe a packed bed DBD reactor in helium, focussing on the effect of the dielectric constant of the packing material, in a comparison between mm-gap and microgap reactors [9]. The results demonstrate that the microgap reactor leads to an increase in the electric field strength, which can be further enhanced by increasing the dielectric constant, but only up to a certain value. The same effect was observed for the electron temperature, but the electron density exhibits the opposite trend. Finally, the effect of this behaviour on the CO_2 dissociation rate is estimated.

Gliding arc and microwave plasmas are also known to yield energy efficiencies for CO_2 conversion higher than a DBD reactor. Kolev (University of Sofia), together with colleagues from the University of Antwerp, present a quasi-neutral model for a gliding arc discharge in argon, in two different, complementary 2D geometries [10]. The validity of this model is first verified by comparison with a non-quasi-neutral model. Subsequently, the advantages of this fast modelling approach are demonstrated for two complex cases, which typically require longer calculation times, i.e., a reverse vortex flow gliding arc and a gliding arc operating in CO_2. Finally, a consortium of researchers from Université Libre de Bruxelles, University of Antwerp, University of Mons, Sofia University and Eindhoven University of Technology compare two different 2D fluid-modelling approaches, as well as experiments, for a microwave surface-wave-sustained argon plasma at intermediate pressure, with the purpose to later extend the models to CO_2 [11]. The first model describes the plasma bulk – sheath interaction, by solving Poisson's equation, while the second model uses a quasi-neutral approach, applying the ambipolar diffusion approximation. The paper also discusses the transformation of the fluid equations from a local frame of reference to a laboratory frame of reference, to account for the gas flow.

A related, environmental topic is the conversion of biomass, for which microwave plasmas can again be utilized. Tsyganov (Brest State Technical University) and colleagues from the University of Lisbon develop a model for the pyrolytic conversion of biomass in a microwave plasma operating at atmospheric pressure [12]. The model includes the thermal balance equations for the gas and biomass particles and the kinetic rate balance equations for stable and intermediate compounds of biomass decomposition. The model is solved for both the assumption of thermal equilibrium and non-equilibrium, demonstrating that the former is acceptable given the high temperature of the environment.

This special issue also contains a few other papers related to thermal plasmas. Almeida et al. (University of Madeira and University of Lisbon) critically evaluate some time-dependent solvers for studying DC glow and high-pressure arc discharges, including different modes of current transfer with different patterns of spots on the cathode [13]. The work uses the plasma module of COMSOL Multiphysics and the authors conclude that time-dependent modelling often gives incomplete solutions, and that the numerical stability of the time-dependent solver is not equivalent to physical stability. Furthermore, Traldi and colleagues from University of Bologna adopt a combined modelling and experimental approach for the design and optimization of atmospheric-pressure low-power RF thermal plasmas [14]. The authors use the ANSYS FLUENT environment to develop a 2D axisymmetric fluid dynamics model for the plasma generation region, and a 3D model for the downstream region, studying the effect of the interaction of the RF torch effluent with a substrate placed downstream. The modelling results are compared with several experimental data.

Some papers also present models for non-thermal plasma jets. Sigeneger and colleagues from INP Greifswald investigate a non-thermal RF-driven atmospheric-pressure plasma jet used for plasma enhanced chemical vapour deposition, by means of fluid modelling [15]. The model describes the gas flow and heating, the plasma generation, the interaction of plasma species with precursor molecules and the transport of the precursor fragments to the substrate. Naidis (Joint Institute for High Temperatures in Moscow) describes streamer propagation along an atmospheric-pressure air plasma jet, formed by pulsed discharges in a thin dielectric tube, by means of a 2D axisymmetric fluid model [16]. He concludes that the jet is characterized by substantial gas heating from the discharge, and that the hot gas is cooled when mixing with surrounding air.

Babaeva (also Joint Institute for High Temperatures in Moscow) applies both hybrid and fluid modelling, using the nonPDPSIM modelling platform, to study the intersection of plasma filaments in a DBD with small polymer particulates, either suspended in air or residing on surfaces [17]. The study might be relevant for applications in plasma medicine as well as plasma-based surface treatment. She shows that the energy and flux of the ions arriving at the particulate depend on the dielectric properties of the underlying substrate materials. Furthermore, the relative location of the particulate with respect to the filament axis determines the asymmetry of treatment.

Verma and colleagues (University of California Merced) compare fluid modelling, based on the full-momentum equations, with PIC/MCC simulations for moderate pd microplasmas driven by cathodes with high secondary electron emission coefficients [18]. The authors conclude that significant discrepancies exist between both modelling approaches, and they point out the need to calibrate fluid simulation parameters based on kinetic simulations.

Finally, part II of the special issue also contains one paper related to elementary data, which are indispensable for accurate modelling as discussed also in the first double issue. More specifically, Laricchiuta and colleagues, from PLASMI Lab in Bari, present calculated electron-scattering cross sections for optically allowed excitations to the B $^2\Pi$ and C $^2\Pi$ states in NO, of interest for hypersonic plasma modelling [19]. A similarity approach is adopted, accounting for the nonadiabatic vibronic coupling perturbing the vibrational progression in the excited states, to generate both state-to-state and total cross sections that are compared with available experimental data.

It is clear from the variety of papers in this second double issue that low-temperature plasma modelling is a very broad and also very active field of research, with many collaborations among different universities worldwide. Plasma is used in a wide range of applications, resorting to a variety of different plasma sources. This implies that different types of modelling approaches need to be used, depending on the type of plasma source, the application and the kind of information to extract from the model. It was our intention to illustrate this diversity, by showing examples of different modelling approaches for different types of plasma sources and applications. We hope to have succeeded in our mission.

As guest editors, we would like to thank all the authors for their interesting contributions, and the reviewers for their useful feedback on these papers. Last but not least, we would also like to thank Michael Wertheimer and Ricardo D'Agostino, as the editors-in-chief responsible for this special issue, as well as Renate Forsch and Regina Hagen, for the smooth collaboration, in bringing this special issue to a good end. We hope that you, as a reader, will be as satisfied as we are with the result.

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