Final Report

Award Number: DE-SC0018230
Title: Nonequilibrium Phenomena in Plasmas in Contact with Liquids
Principal Investigator: Trelles, Juan
Institution: University of Massachusetts Lowell, Lowell, MA

Accomplishments

1. Major goals of the project

The project's objective was to determine the properties of dissipative (macroscopic) and kinetic (microscopic) nonequilibrium phenomena, and the interrelation between them, in low-temperature atmospheric-pressure plasmas in contact with liquid electrodes.

Plasma-liquid interaction is a low-temperature plasma science frontier involving fundamental issues in plasma-materials interaction, multiphase kinetics, and collective effects. Plasmas in contact with liquids present two distinctive types of nonequilibrium: kinetic - across the interface - involving complex physical and chemical kinetics; and dissipative - along the interface - comprising superficial transport that is often conducive to instabilities and the formation of dissipative structures such as spot patterns. The project investigated dissipative and kinetic nonequilibrium phenomena concurrently in plasmas in contact with liquid water electrodes.

Two major goals were pursued:

Goal 1: Establish a computational simulation methodology for plasmas in contact with liquids for the analysis of application-relevant three-dimensional configurations with detailed kinetics models.

Goal 2: Identify the parameters controlling the stability and the emergence of collective behavior at the plasma-liquid interface (dissipative nonequilibrium) and characterize their role and interrelation with the rate of plasma-driven electrolysis (kinetic nonequilibrium).

2. Accomplishments under these goals

Towards Goal 1:

(1) Atmospheric pressure glow discharge model. A self-consistent model of atmospheric pressure glow discharge in helium has been developed, validated, and used to investigate the occurrence of dissipative nonequilibrium. The model has been implemented in the TransPORT solver (TPORT), developed by the PI's group and the main computational platform for the project. The model encompasses chemical and thermal nonequilibrium and is aimed towards time-dependent three-dimensional (3D) simulations of normal glow discharges sustained by electric currents ranging from milli-amperes to amperes. Time-dependent 3D simulations are required to computationally capture the occurrence of pattern formation (dissipative nonequilibrium). Distinct accomplishments include:

- Chemical kinetics model of atmospheric pressure helium discharges. The development of the chemical kinetics model included: (1) comparisons against a wide set of reactions in the literature (values of reaction rate constants, assessment of the most appropriate data for atmospheric pressure conditions); (2) determination of the range of validity of cross sections obtained from BOLSIG+ (i.e., minimum values of reduced electric field for reliable data); and (3) determination of the most appropriate functional dependency of cross sections and/or reaction rate constants (i.e., ratio of electron to gas temperatures instead of electron temperature and reduced electric field for low values of electric field).

- External circuit model. The modeling of glow discharges requires an external circuit model for the evaluation of boundary conditions over the electrodes. An external circuit model implies that the boundary conditions are nonlinear, as they dependent on the solution (i.e., integral of current density distribution over the electrode surface). This task involved the implementation of the boundary condition over the cathode using a Resistive-Capacitive circuit model in TPORT. The implementation involved the integration over the faces of the discretization elements along the boundary (in the context of the Finite Element Method, FEM) such to ensure continuity of the imposed external electric circuit (target value of total current for user-specified values of resistance and capacitance).

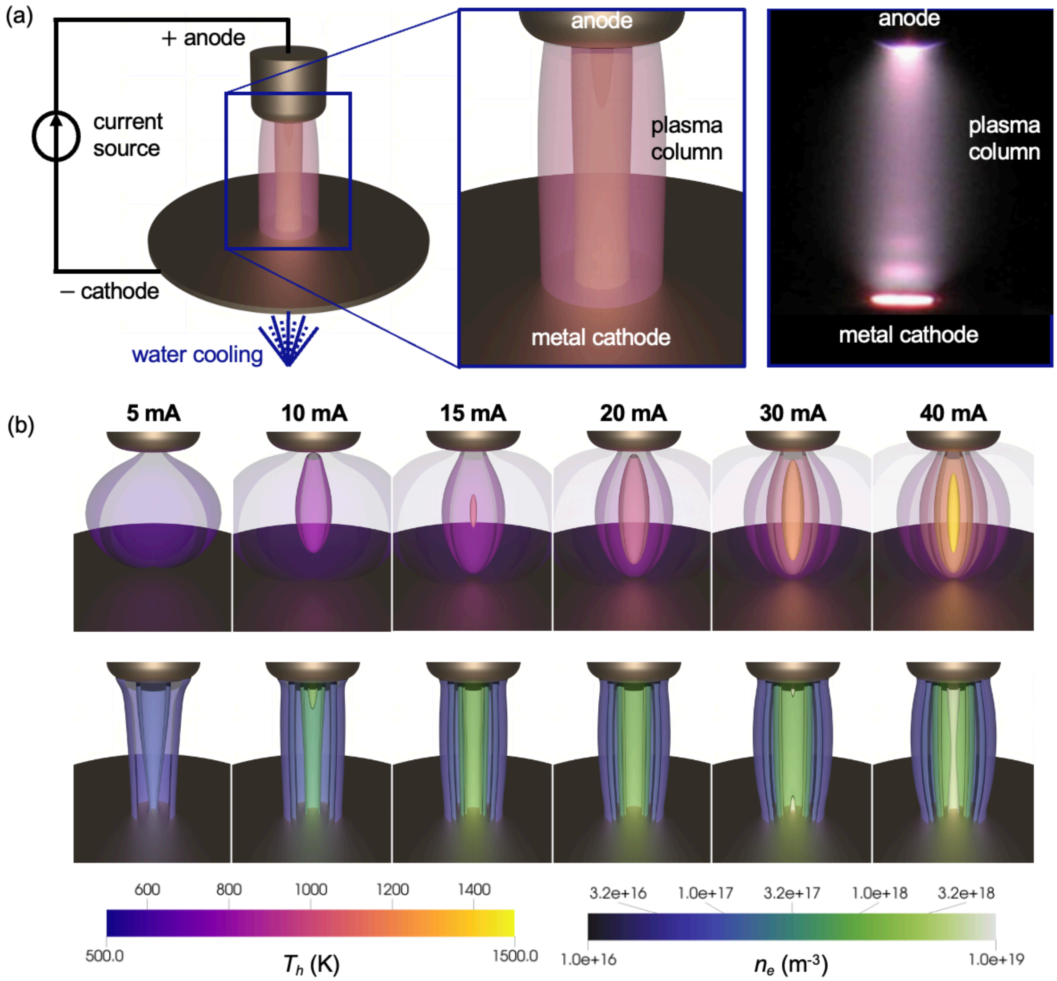

Figure 1. Atmospheric pressure glow discharge model. (a) Self-sustained atmospheric pressure glow discharge together with an experimental image from [Arkhipenko et al., Plasma Sources Sci. Technol. (2009) 18 045013]. (b) Effect of total current on positive column characteristics. [V. D. Boutrouche, J. P. Trelles, "Three-dimensional Modelling of a Self-Sustained Atmospheric Pressure Glow Discharge", Journal of Physics D: Applied Physics (2022), Vol. 55, No. 48, 485201]

- Glow discharge model verification and validation. The complete glow discharge model described above is being validated with data from [V. I. Arkhipenko, A. A. Kirillov, Y. A. Safronau, L. V. Simonchik, and S. M. Zgirouski, "Self-sustained dc atmospheric pressure normal glow discharge in helium: from microamps to amps", Plasma Sources Sci. Technol. (2009) , Vol. 18 , No. 045013]. This publication describes a detailed assessment of a normal glow discharge with copper electrodes comprised of a plate cathode and a pin anode. The model validation encompassed the comparison of simulation results against the experimental results for range of currents relevant to technological applications of atmospheric pressure glow discharges. The model is depicted in **Figure 1a** and representative results of three-dimensional simulations in **Figure 1b**. Validation results are shown in **Figure 2a**.

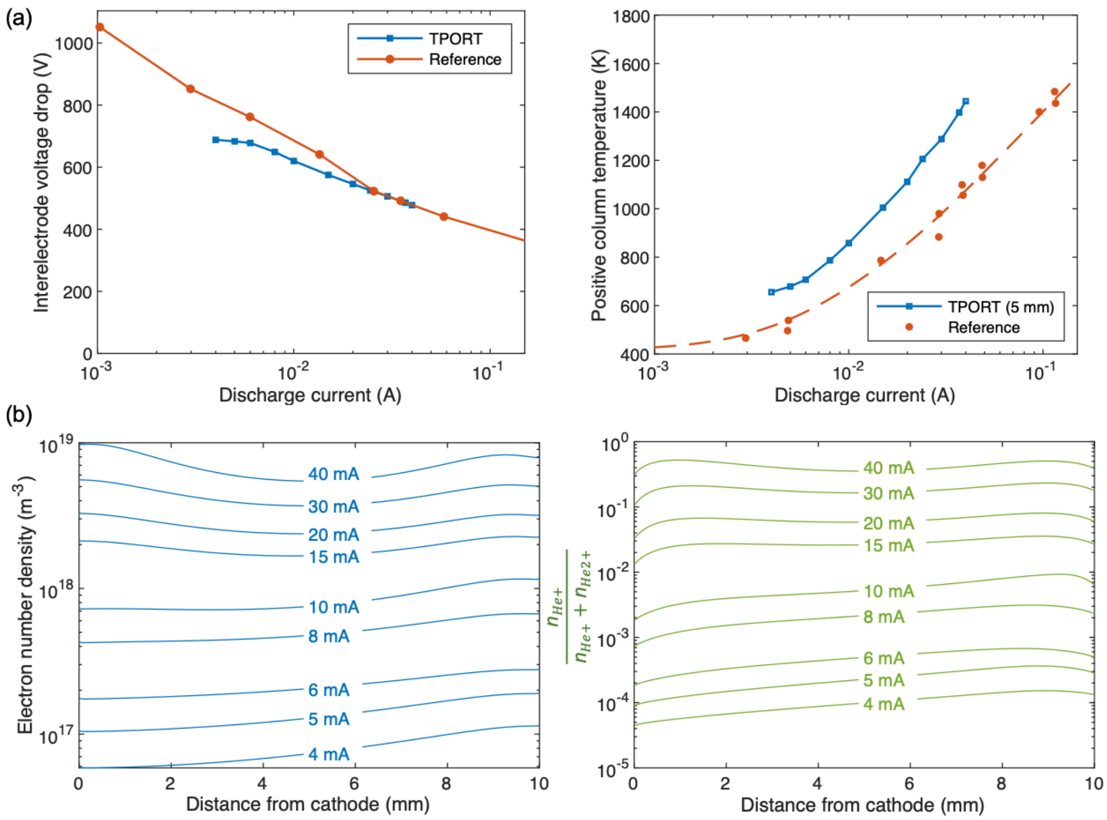

Figure 2. Glow discharge characteristics. (a) Validation of the glow discharge model against experimental data in [Arkhipenko et al., Plasma Sources Sci. Technol. (2009) 18 045013], (left) voltage drop across the plasma column and (right) positive column temperature. (b) The structure of the positive column transitions from being monotonically increasing away of the cathode to depicting nearly flat around 10 to 15 mA, (left) electron number density and (right) relative dominance of helium ions. [V. D. Boutrouche, J. P. Trelles, "Three-dimensional Modelling of a Self-Sustained Atmospheric Pressure Glow Discharge", Journal of Physics D: Applied Physics (2022), Vol. 55, No. 48, 485201]

- Regime transition in positive column structure. The validated model was used to investigate dissipative nonequilibrium manifested by a change in structure of the positive column of an atmospheric pressure glow discharge. The specific change of regime investigated is driven by the discharge current and it manifest as a transition in the distribution of electron number density - from monotonically increasing away from the cathode to flat and depicting a minimum towards the center of the column – for a critical current value neat 12 mA. Representative results of this behavior unveiled by the glow discharge model are depicted in **Figure 2b**.

(2) Interfacial plasma-on-liquid transport. A plasma-liquid interfacial transport model was developed and validated. Distinct accomplishments include:

- Interfacial plasma-on-liquid transport model. The model is composed of constitutive equations describing: (1) fluid flow motion, (2) energy conservation, (3) species transport and chemical kinetics (in the gas/plasma and liquid domains), (4) electrostatics (Poisson's equation through the gas/plasma and liquid domains, and charge accumulation along the interface), (4) interfacial transport (Henry's law), and (5) interphase dynamics. Importantly, as an advancement to the state-of-the-science, the inclusion multiphase transport using a Volume-Of-Fluid (VOF) method will allow the description of the dynamics of the gas-liquid interface due to inertial and electrostatic stresses. The model was implemented in the open-source platform OpenFOAM.

- Evaluation of interphase transport. A single-field approach based on the volume-of-fluid (VoF) method together with conditional volume averaging (CVA), were used to consistently describe the dynamics of the interface together with interfacial reactive mass transfer. Three CVA-based interface species transport models, based on arithmetic, harmonic, and unified mixture species diffusivities, were evaluated. The results revealed the relative strengths and weaknesses of each approach, and that the harmonic interface diffusivity model, given its accuracy and low computational overhead, is the most appropriate for the simulation of general plasma-on-liquid systems.

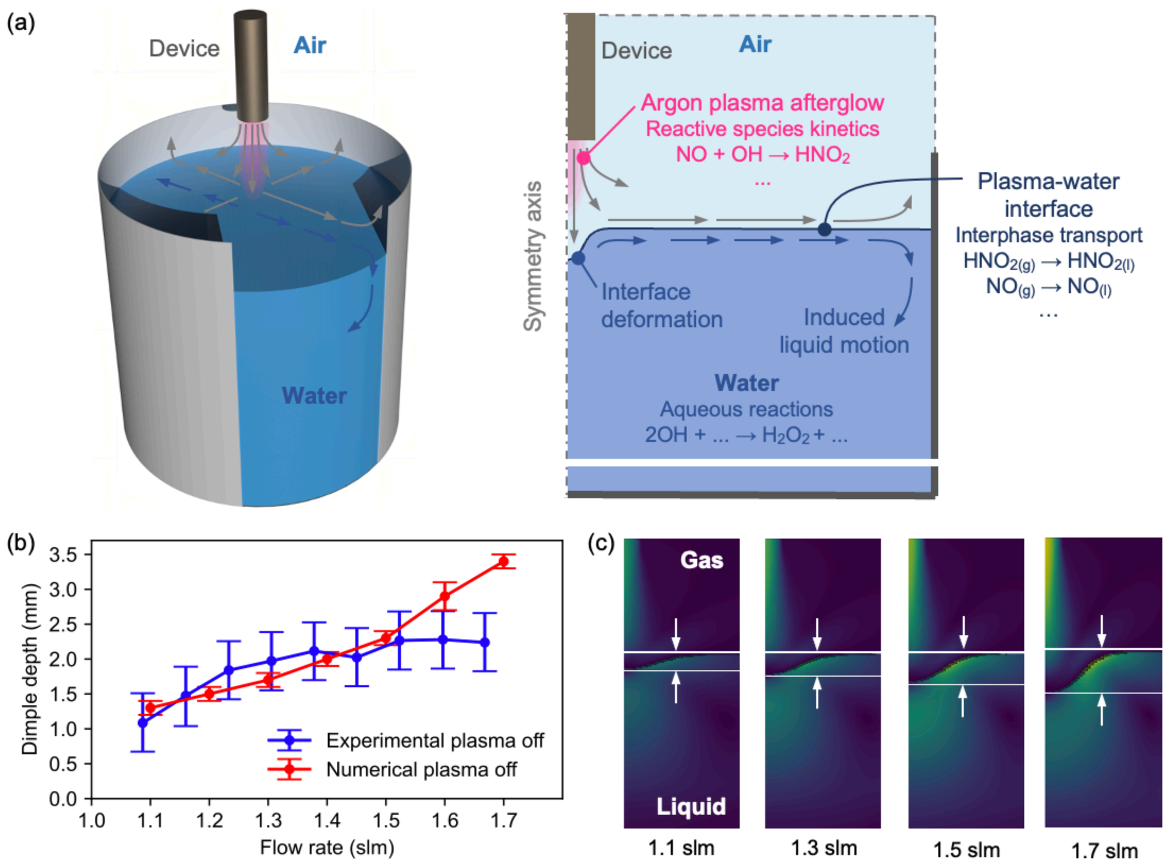

Figure 3. Model of air plasma impinging on water. (a) Air plasma jet impinging water confined in a cylindrical container and cross-sectional view of the system and its representative components. (b) (Left) Validation of the model with experimental data of dimple depth from [Winter et al., J. Phys. D: Appl. Phys. (2014) 47 285401] and (right) cross-sectional plots of velocity magnitude distribution depicted the dimple depth. [T. Kamidollayev, **J. P. Trelles**, *"Modeling of Reactive Species Interphase Transport in Plasma Jet Impinging on Water*", Journal of Physics D: Applied Physics (2023), Vol. 56, 505203]

- Interfacial plasma-on-liquid model verification and validation. The computational model was verified against four benchmark tests: immiscible multiphase transport (parallel shear flow), species transport across a static interface (problem with an analytical solution), chemical kinetics (three-species global model), and transient interfacial species transport (evolution of species concentration along the gas and liquid domains). Validation encompassed comparisons simulation results of an argon plasma jet on ambient air impinging on liquid water against the experimental data on surface deformation and H_2O_2 concentration reported in from [Winter et al., J. Phys. D: Appl. Phys. (2014) 47 285401]. The model is summarized in **Figure 3a**, and **Figure 3b** shows representative validation results.

- Kinetic nonequilibrium in multiphase gas/plasma-liquid water systems. The model was used to investigate the dynamic coupling between the deformation of the plasma-water interface and the transport of reactive species across the interface. The computational studies focused on the interaction between a kINPen®-generated argon APPJ with water 10 mm away from the device and contained in a cylindrical container. Representative results of the effect of jet flow rate on the induced motion in the water are depicted in **Figure 4**. These results shows the formation and evolution of recirculation regions in the gas and liquid domains. The formation of such dissipative structures has a primary role on the driving of species across the gas-liquid interface. Such primary role is clearly depicted in the results in **Figure 5**, which show the distribution of different reactive species through the gas and liquid domains. The extent of interface deformation, primarily quantified by the depth of the dimple, is directly correlated with the initial uptake of reactive species by the water. The presence of recirculation regions changes such initial rate of species uptake by causing local saturation or depletion of species concentration leading to reduced or increased species uptake, respectively.

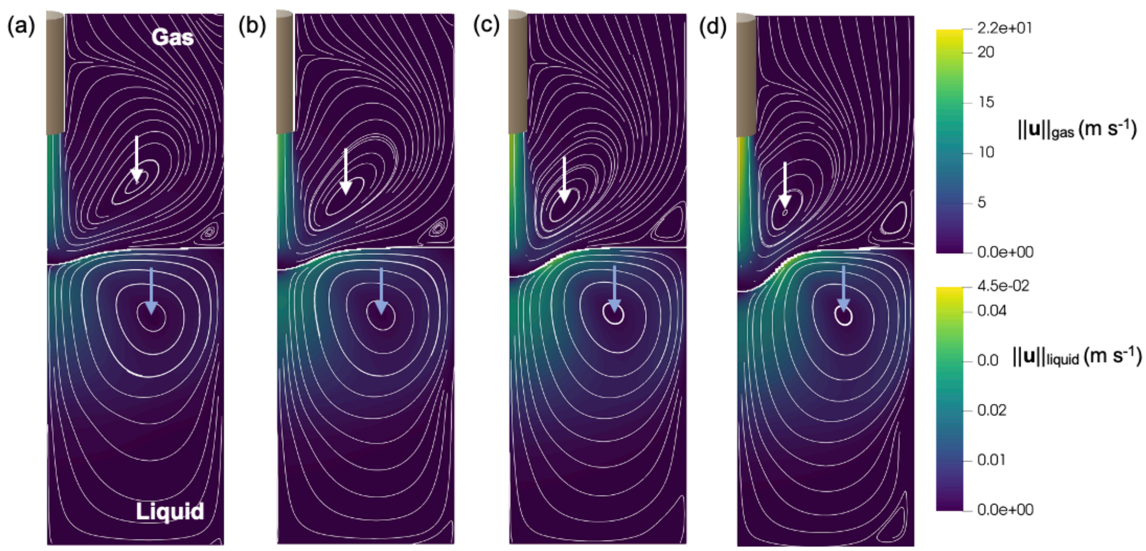

Figure 4. Evolution of the plasma gas-liquid interface. Evolution of the gas-liquid interface given by the distribution of velocity magnitude and streamlines for increasing jet flow rates (from left to right). The results show the progressive increase of the dimple depth formation and the formation of recirculation regions in the gas and liquid domains. The occurrence of such dissipative structures has a primary role on maintaining kinetic nonequilibrium across the plasma-liquid interface and consequently on the update of plasma-produced reactive species by the water. [T. Kamidollayev, **J. P. Trelles**, *"Modeling of Reactive Species Interphase Transport in Plasma Jet Impinging on Water*", Journal of Physics D: Applied Physics (2023), Vol. 56, 505203]

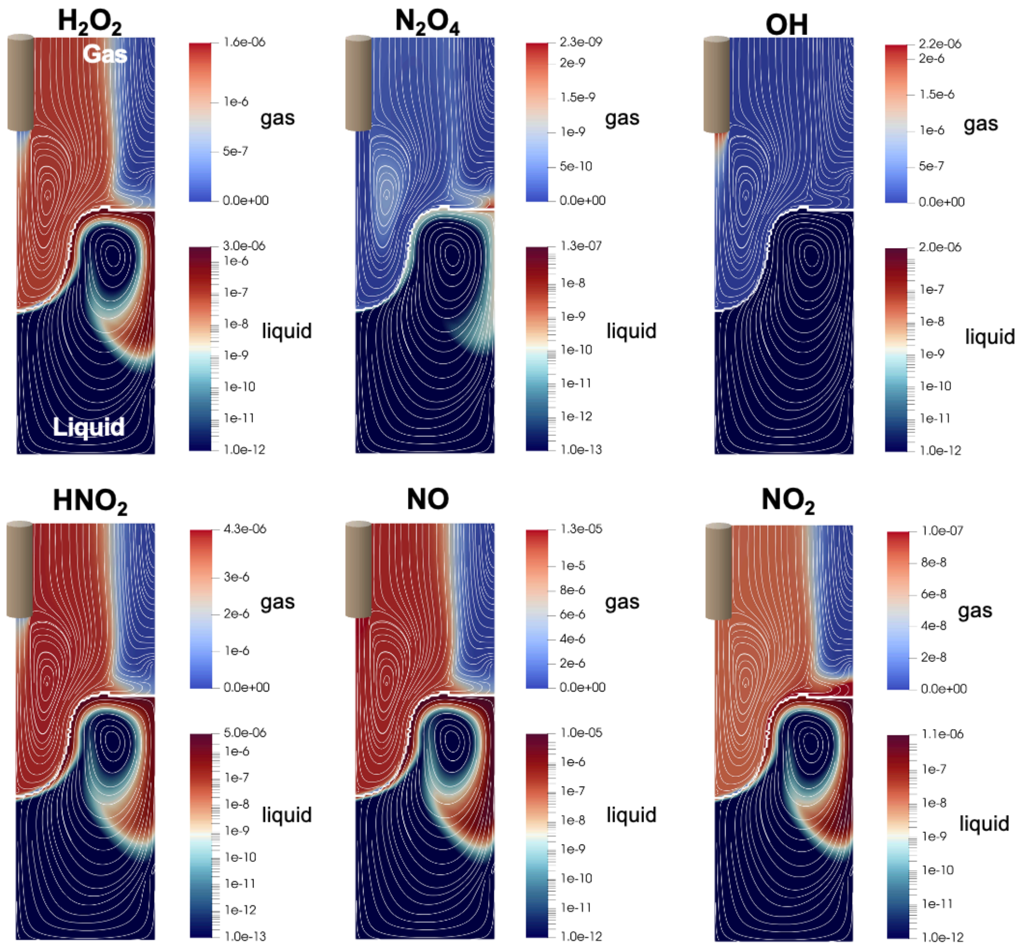

Figure 5. Kinetic nonequilibrium through air plasma-water interface. Distribution of reactive species through the gas and liquid domains. The occurrence of dissipative structures (recirculation regions) has a primary role in the update of reactive species by the liquid water. [T. Kamidollayev, **J. P. Trelles**, *"Modeling of Reactive Species Interphase Transport in Plasma Jet Impinging on Water*", Journal of Physics D: Applied Physics (2023), Vol. 56, 505203]

Towards Goal 2:

(3) Air plasma water electrolysis. The occurrence of coupled kinetic and dissipative nonequilibrium in a plasma-on-liquid system was investigated experimentally. Distinct accomplishments in this area include:

- Digitally-manufactured plasma reactor. The interaction of air plasma-generated reactive oxygen and nitrogen species with water produces nitrate (NO_3^-) and related species, which are a form of fixed-nitrogen essential to plants. The design, implementation, and characterization of a digitally manufactured air plasma-on-water reactor (POWR) for the synthesis of nitrate as green nitrogen fertilizer were accomplished. The mild conditions of the operation of the POWR were exploited for its fabrication using plastics, particularly through digital manufacturing strategies such as 3D-printing. A pin-to-plate reactor configuration powered by high-voltage alternating power was chosen due to its simplicity and efficacy. A computational thermal-fluid model was used to evaluate the design and attain expected operational characteristics. The fabricated reactor together with the mechanisms leading to the formation of nitrates are schematically depicted in **Figure 6a**.

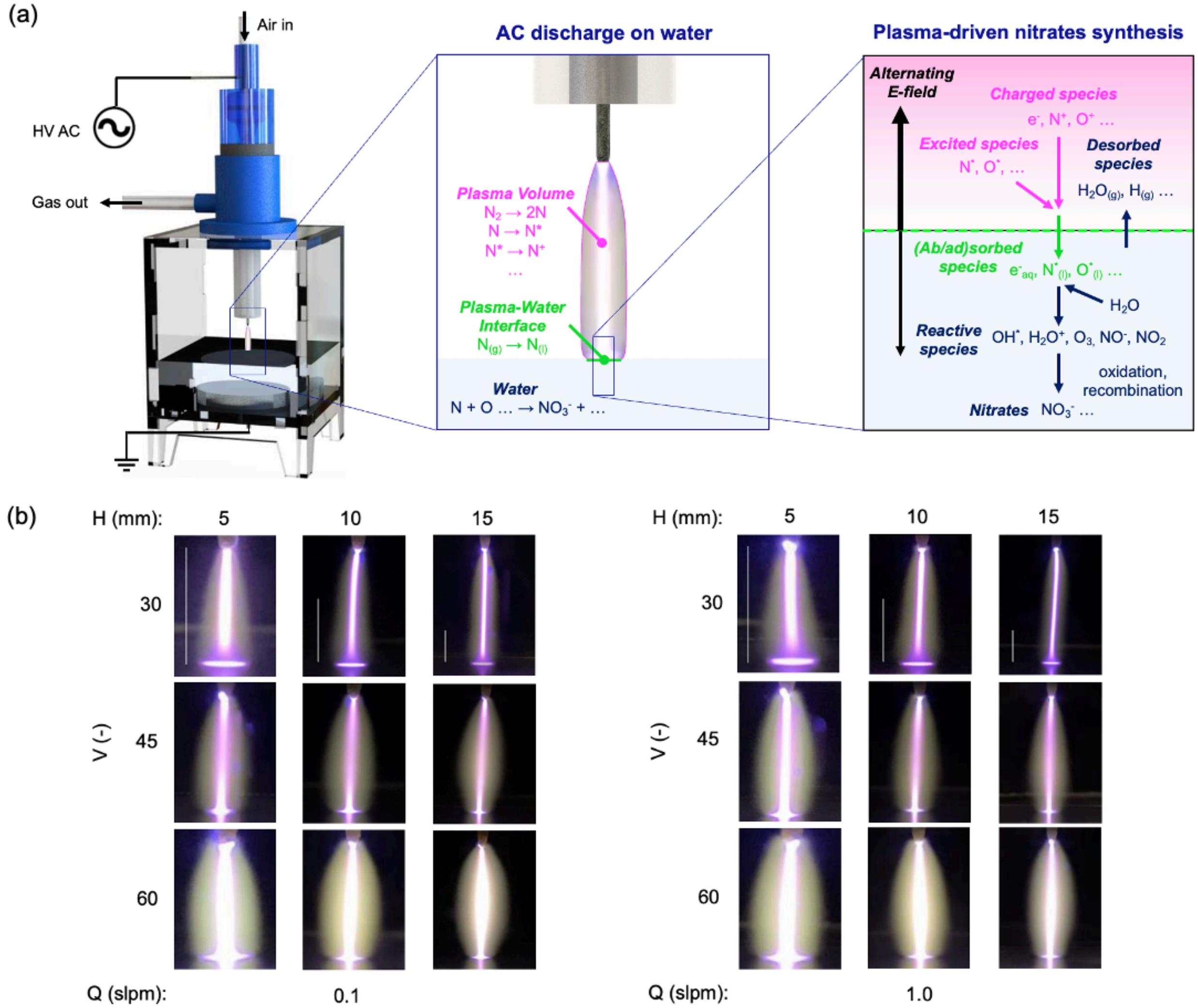

Figure 6. Kinetic nonequilibrium in air plasma contact with liquid water. (a) Self-sustained atmospheric pressure glow discharge together with an experimental optical image depicting the occurrence of dissipative nonequilibrium (image from Arkhipenko et al., Plasma Sources Sci. Technol. (2009) 18 045013). (b) Representative results of three-dimensional simulations of the glow discharge depicting the distributions of heavy-species temperature (T_h), electron temperature (T_e), and electron number density (n_e). [T. B. Nieduzak, V. Veng, C. N. Prees, V. D. Boutrouche, **J. P. Trelles**, *"Digitally Manufactured Air Plasma-On-Water Reactor for Nitrate Production*", Plasma Sources Science and Technology (2022), Vol. 31, No. 3, 035016]

- Experimental characterization of an alternating current glow discharge on water. The experimental characterization of the POWR encompassed design and operation parameters, namely electrode-water spacing, air flow rate, and voltage level. A machine learning approach is implemented to extract and quantify characteristic features of the plasma–water interaction, such plasma volume and plasma–water interface area. Representative results are presented in **Figure 6b**.
- Plasma regime transition and enhanced reactivity in water. The experimental results indicate the occurrence of a change in operating regime between low and mid voltage levels. This change in operating regime is manifested by large changes in plasma characteristics (approximately doubling of plasma frequency, drastic drop in rms voltage, etc.), and particularly in the rate of nitrate production. Results of the electrical signals from the discharge depicting the change in regime as a doubling of frequency are shown in **Figure 7a**. The POWR performance metric given by a dimensionless plasma

volume (i.e., plasma volume divided by electrode-water spacing squared times a reference length) was found to vary linearly with nitrate production rate (within the high voltage level regime). **Figure 7b** shows results of the correlation between dimensionless interface area and plasma volume, and between the plasma volume and nitrate production rate. The unveiling of the threshold for a regime change can be exploited to control and/or optimize plasma-on-liquid systems, for example, to maximize the production rate of target species or to maximize the energy efficiency of the system (amount of target species produced per unit energy spent).

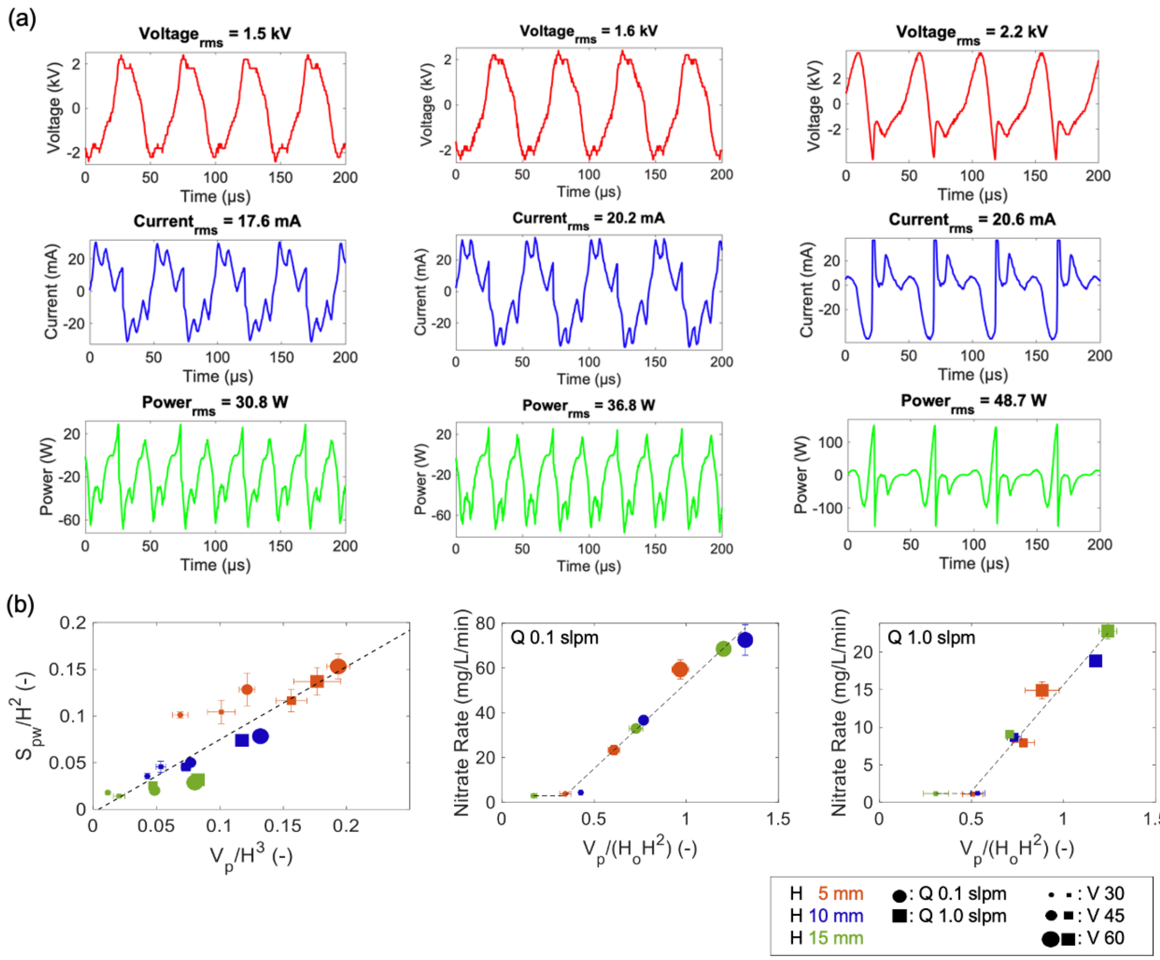

Figure 7. Kinetic and dissipative nonequilibrium across air plasma – liquid water interface. (a) Representative voltage, current, and power signals, showing that a change of regime characterized by an approximately doubling of dominant frequency occurs between V_{rms} = 1.6 and 2.2 kV. (b) (Left) correlation between dimensionless plasma-water interface area (S_{pw}) and plasma volume (V_p) normalized with the electrode-interface gap (H) and (center and right) nitrate rate for gas flow rate Q equal to 0.1 and 1.0 slpm as function of the dimensionless plasma volume normalized using H and the reference distance H_o. The change from flat to linearly increasing is correlated with the doubling of frequency. [T. B. Nieduzak, V. Veng, C. N. Prees, V. D. Boutrouche, **J. P. Trelles**, *"Digitally Manufactured Air Plasma-On-Water Reactor for Nitrate Production*", Plasma Sources Science and Technology (2022), Vol. 31, No. 3, 035016]

(4) Pattern formation over electrodes in glow discharges. The Atmospheric Pressure Glow Discharge (APGD) is a relatively simple and versatile plasma source with diverse applications in diagnostics, lighting, materials processing, and particularly, plasma-liquid systems. Stable APGD operation at high currents is challenging because instabilities lead to glow-to-arc transition. However, controlled cathode cooling is an effective approach to circumvent such a transition. Moreover, APGDs depict the formation of self-organized patterns over the electrodes, which can affect discharge performance. Distinct accomplishments in this area include:

- Three-dimensional time-dependent computational glow discharge model. The verified and validated glow discharge model developed towards Objective 1 was extended and enhanced with a higher fidelity species diffusion model and model of the near-cathode region – these aimed at enabling the capturing the spontaneous formation of patterns. The target system for the simulations, including an image depicting dissipative nonequilibrium along the cathode of a glow discharge, is shown in **Figure 8a**. Representative results of the enhanced model are presented in **Figure 8b**.

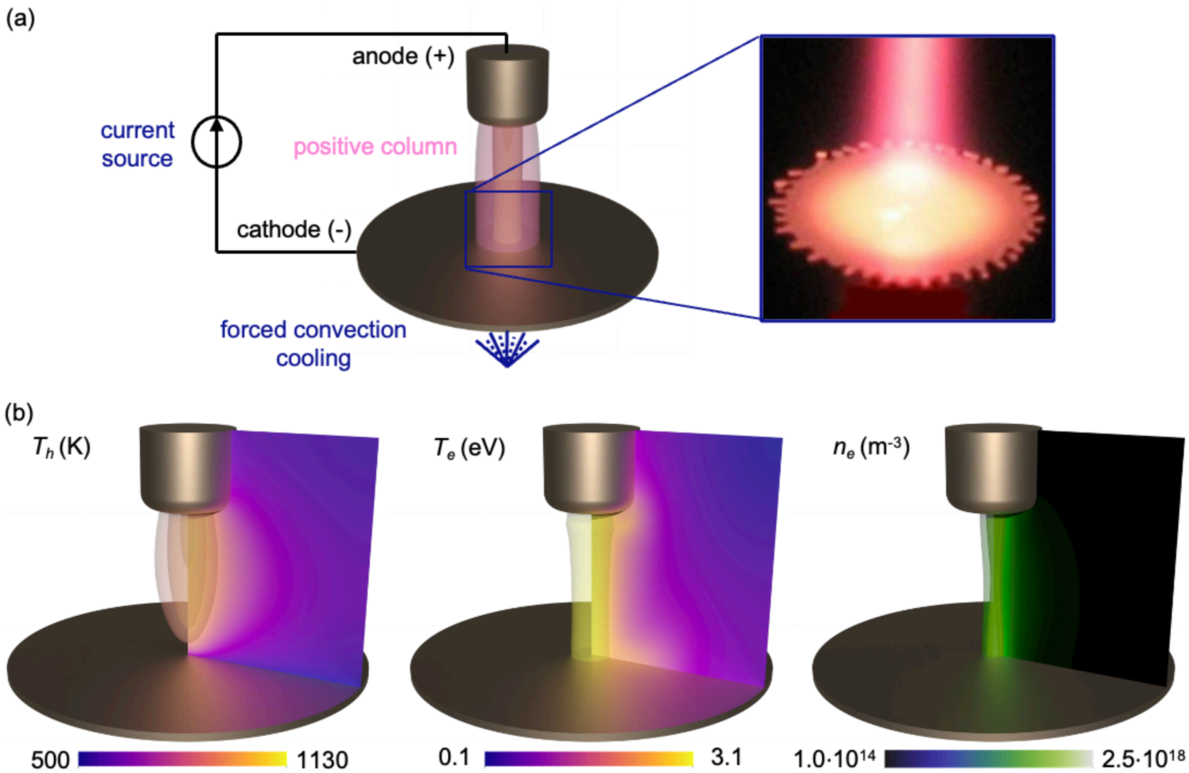

Figure 8. Dissipative nonequilibrium in atmospheric pressure glow discharge. (a) Self-sustained atmospheric pressure glow discharge together with an experimental optical image from [Arkhipenko et al., Plasma Sources Sci. Technol. (2009) 18 045013] depicting the occurrence of dissipative nonequilibrium. (b) Representative results of three-dimensional simulations of the glow discharge depicting the distributions of heavy-species temperature (T_h), electron temperature (T_e), and electron number density (n_e).

- Effect of current and cooling on APGD characteristics. The capabilities of the enhanced model to reproduce actual APGD behavior were assessed with validation against the experimental data by [Arkhipenko et al., Plasma Sources Sci. Technol. (2009) 18 045013]. Representative results of this validation are shown in **Figure 9a** depicting the variation of voltage drop and positive column temperature versus discharge current for different degrees of cathode cooling. Subsequently, the model was used to investigate the effect of thermal energy dissipation on the structure of the APGD. Illustrative results of this study are shown in **Figure 9b**. The results show the distribution of electron number density n_e for different values of current I_{tot} and levels of cathode cooling h_c. In our previous study (associated to Objective 1), the electron number density for the lowest current cases showed a monotonically increasing trend with increasing the distance from the cathode. In contrast, the higher current cases displayed a local minimum in the center of the discharge and a higher number density at the anode and cathode. Nevertheless, in this study the global trend of the discharge is still monotonically increasing with increasing the distance from the cathode. The slight difference in this trend is explained by the change in the plasma characteristics as being a marker of competing phenomena during the progressive thermalization of the discharge. Competing transport phenomena are usually seen as triggering mechanisms for pattern formation. This aspect is investigated next.

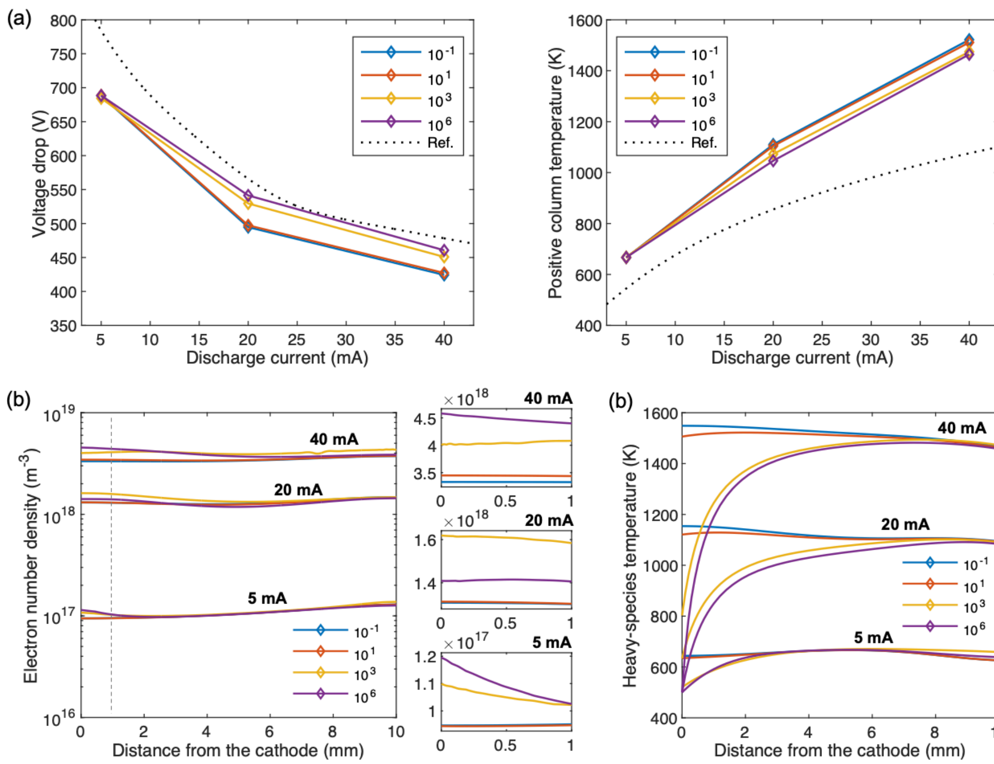

Figure 9. Effect of thermal energy dissipation on discharge structure. (a) Validation of the enhanced glow discharge model against experimental data by [Arkhipenko et al., Plasma Sources Sci. Technol. (2009) 18 045013], depicting the variation of voltage drop and positive column temperature versus discharge current for different degrees of cathode cooling as characterized by the value of the convective heat transfer coefficient indicated in the legends. (b) Effect of cathode cooling (value of convective heat transfer coefficient in the legends) on discharge characteristics - electron number density and heavy-species temperature – for different values of discharge current.

- Formation of cathodic pattern formation in an APGD. The occurrence of patterns is generally associated with the existence of multiple solutions of the model equations, as well as to instabilities. In the context of the present study, the occurrence of instabilities is of primary importance given their predominance in APGDs operating at high currents. Particularly, AGPDs are known to be prone to thermal instabilities in the cathode region fall, to tend to stabilize with the use of strong cathode cooling. The enhanced APGD model was used to investigate the spontaneous formation of cathode patterns using total current I_{tot} and level of cathode cooling characterized by the convective heat transfer coefficient h_c as control parameters. A summary of the results is presented in **Figure 10**. **Figure 10a** shows the distribution of electron number density n_e and heavy-species temperature T_h over the cathode, and **Figure 10b** the distribution of the electric field magnitude $||\mathbf{E}||$. The patterns appeared spontaneously and demonstrate dependency on the level of cooling and total current. These results show that pattern formation can occur due to the competition between electrical and energy transport in the region near the cathode. The findings related to this accomplishment are going to be reported in an upcoming publication.

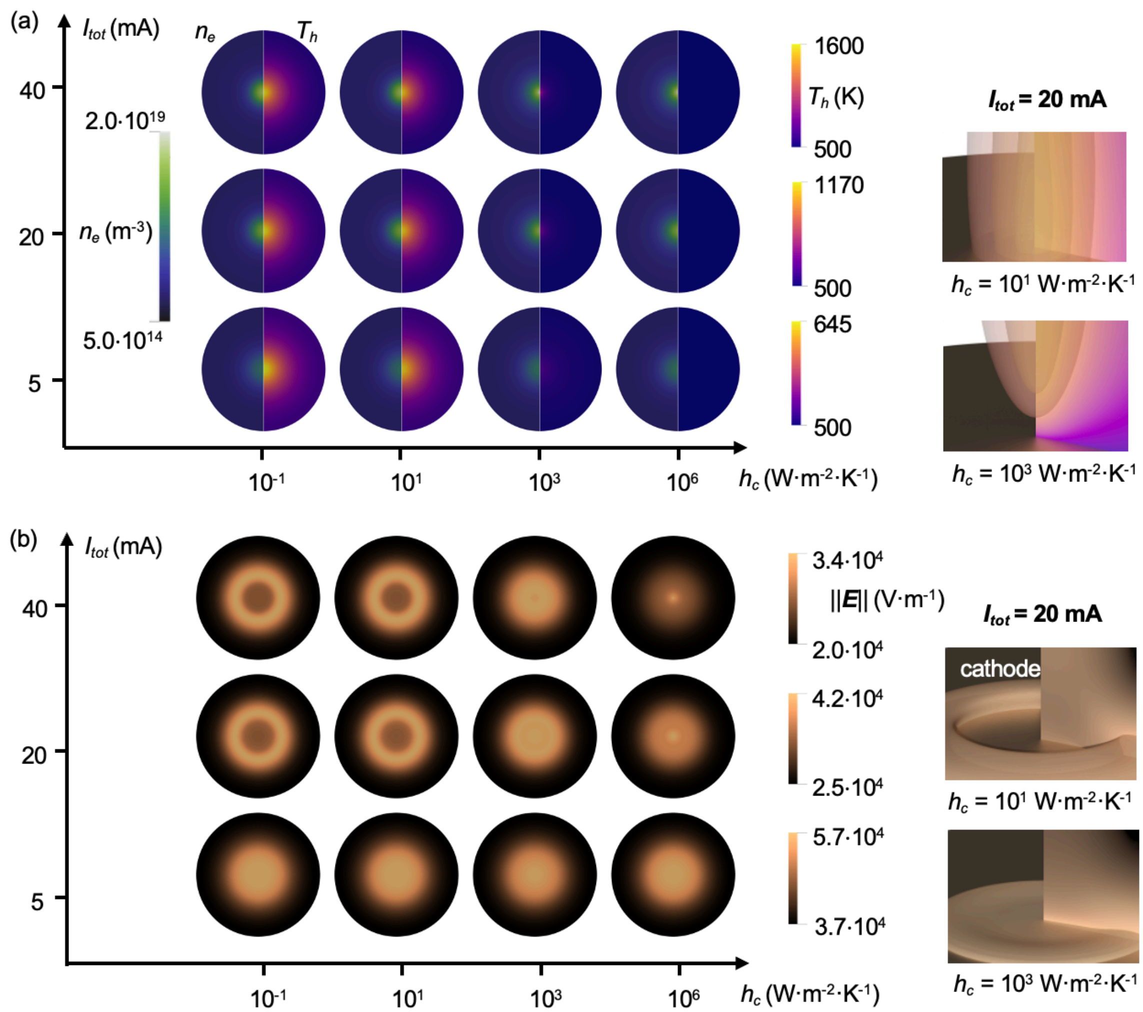

Figure 10. Pattern formation. (a) Distribution of electron number density (n_e) and heavy-species temperature (T_h) over the cathode as function of current (I_{tot}) and level of cathode cooling characterized by the convective heat transfer coefficient (h_c). The distributions appear axisymmetric and show a gradual decrease in magnitude with either decreasing or increasing. The right-side images show 3D renderings of the distribution of T_h for two values of h_c. (b) Formation of annular patterns in the distribution of electric field magnitude $\|\mathbf{E}\|$ for low levels of cooling and high currents. The right-side images show 3D renderings of the distribution of $\|\mathbf{E}\|$ corresponding to the same conditions in the plots in (a). These results show that pattern formation can occur due to the competition between electrical and energy transport in the region near the cathode.

3. Training and professional development by the project

The project trained four doctoral students and one post-doctoral research scholar. The project participants were trained in diverse areas of low-temperature plasma science and engineering, including nonequilibrium physical and chemical kinetics, electrode phenomena, interphase transport, coherent structures, among others. Their training also encompasses computational plasma physics, numerical methods for transport problems, and High-Performance Computing.

4. Dissemination of results

Journal articles:

V. D. Boutrouche, J. P. Trelles, *"Three-dimensional Modelling of a Self-Sustained Atmospheric Pressure Glow Discharge*", Journal of Physics D: Applied Physics (2022), Vol. 55, No. 48, 485201. DOI: 10.1088/1361-6463/ac9536

T. Kamidollayev, J. P. Trelles, *"Modeling of Reactive Species Interphase Transport in Plasma Jet Impinging on Water*", Journal of Physics D: Applied Physics (2023), Vol. 56, 505203. DOI: 10.1088/1361-6463/acf86a

T. B. Nieduzak, V. Veng, C. N. Prees, V. D. Boutrouche, J. P. Trelles, *"Digitally Manufactured Air Plasma-On-Water Reactor for Nitrate Production*", Plasma Sources Science and Technology (2022), Vol. 31, No. 3, 035016. DOI: 10.1088/1361-6595/ac56ee

S. M. Modirkhazeni, V. Bhigamudre, J. P. Trelles, *"Evaluation of a Nonlinear Variational Multiscale Method for Fluid Transport Problems*", Computers and Fluids (2020), No. 209, 104531. DOI: 10.1016/j.compfluid.2020.104531

V. Bhigamudre, J. P. Trelles, *"Investigation of Flow Regimes in Arc Plasma - Gas Interactions Using a Two-Temperature Arc in Crossflow Model*", Physics of Plasmas (2020), Vol. 27, 022305. DOI: 10.1063/1.5113772

J. P. Trelles, *"Nonequilibrium Phenomena in (Quasi-) Thermal Plasma Flows*", Plasma Chemistry and Plasma Processes (2019) Vol. 40, No. 3, pp. 727-748. DOI: 10.1007/s11090-019-10046-1

P. Liang, J. P. Trelles, *"3D Numerical Investigation of a Free-Burning Argon Arc with Metal Electrodes Using a Novel Sheath Coupling Procedure*", Plasma Sources Science and Technology (2019), Vol. 28, 115012. DOI: 10.1088/1361-6595/ab4bb6

V. G. Bhigamudre, J. P. Trelles, *"Characterization of the Arc in Crossflow Using a Two-Temperature Nonequilibrium Plasma Flow Model*", Journal of Physics D: Applied Physics (2019), Vol. 52, 015205. DOI: 10.1088/1361-6463/aae643

Conference proceedings:

E. Simasiku, J. P. Trelles, "*Three-dimensional Modelling of an Atmospheric Pressure Glow Discharge with Liquid Anode*", IEEE 50th International Conference on Plasma Science (ICOPS), Santa Fe, New Mexico, May 21-25, 2023.

J. P. Trelles, "*Advances and Challenges in Computational Fluid Dynamics of Atmospheric Pressure Plasma*", 38th Annual Meeting of the Japan Society of Plasma Science and Fusion - Plasma Generation at Near Atmospheric Pressure and Its Applications, Virtual, Nov. 22-25, 2021.

V. Boutrouche, J. P. Trelles, "*Computational Study of Current-Voltage Characteristics of a DC Atmospheric Pressure Glow Discharge Using a 3D Model*", 2021 APS Gaseous Electronics Conference (GEC), Virtual, Oct. 4-8, 2021.

V. Boutrouche, J. P. Trelles, "*Machine Learning Approach for Plasma Image Processing: Application to Plasma-On Water Characterization*", 2021 APS Gaseous Electronics Conference (GEC), Virtual, Oct. 4-8, 2021.

V. Boutrouche, J. P. Trelles, "*Computational 3D Modeling and Simulation of DD Atmospheric Pressure Glow Discharge in Helium*", IEEE 48th International Conference on Plasma Science (ICOPS), Virtual, Sept. 12-16, 2021.

J. P. Trelles, "*Nonequilibrium Phenomena in Thermal Plasmas*", 24th International Symposium on Plasma Chemistry (ISPC 24), Naples, Italy, June 9 – 14, 2019.

V. G. Bhigamudre, J. P. Trelles, "*Computational Investigation of Regimes of the Arc in Crossflow*", 24th International Symposium on Plasma Chemistry (ISPC 24), Naples, Italy, June 9 – 14, 2019.

P. Liang, V. D. Boutrouche, J. P. Trelles, "*Coupled Plasma-Electrode Simulation of the Free-Burning Arc using a Chemical and Thermal Non-Equilibrium Model*", 24th International Symposium on Plasma Chemistry (ISPC 24), Naples, Italy, June 9 – 14, 2019.

J. P. Trelles, "*Advances and Challenges in Modeling and Simulation of Thermal Plasma Flows*", 15th International High-Tech Plasma Processes Conference (HTPP15), Toulouse, France, July 2 – 6, 2018.

V. G. Bhigamudre, J. P. Trelles, "*Thermodynamic Nonequilibrium Effects in the Arc in Crossflow*", 15th International High-Tech Plasma Processes Conference (HTPP15), Toulouse, France, July 2 – 6, 2018.

J. P. Trelles, "*Nonequilibrium Plasma Flows Simulations: Kinetics, Patterns, and Turbulence*", 10th International Symposium on Advanced Plasma Science and its Applications for Nitrides and Nanomaterials / 11th International Conference on Plasma-Nano Technology & Science (ISPlasma / IC-PLANTS), Meijo University, Aichi, Japan, March 4 – 8, 2018.

S. M. Modir Khazeni, V. G, Bhigamudre, J. P. Trelles, "*Stability and Turbulence in Nonequilibrium Plasma Flow Simulations*", 10th International Symposium on Advanced Plasma Science and its Applications for Nitrides and Nanomaterials / 11th International Conference on Plasma-Nano Technology & Science (ISPlasma / IC-PLANTS), Meijo University, Aichi, Japan, March 4 – 8, 2018.

Impacts

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1. Impact on the development of the principal discipline(s) of the project

The principal discipline of the project is Plasma Science and Engineering. The project's impacts on its principal disciplines are:

- **Understanding of the plasma state:** The project brought novel understanding of plasma-on-liquid interactions, particularly of the interrelation among kinetic and dissipative nonequilibrium phenomena, which will impact other multi-phase plasma systems, such as plasmas-within-liquids, plasma aerosols, and discharges in bubbles.

- **Advancing computational plasma physics:** The project brought state-of-the-science approaches in other fields to plasma physics. The methods being developed, encompassing detailed physical models (detailed chemical kinetics, interphase dynamics and transport) within 3D time-dependent computational implementations, advance the state-of-the-science in computational low-temperature plasma science and engineering.

- **Improved and novel technological applications:** The project's outcomes contribute towards achieving methods for generating, controlling, and optimizing plasma in contact with liquid systems founded on fundamental science principles. These methods will impact established technologies (welding, metallurgy) and emerging applications (water treatment, nanoparticle synthesis, biomaterial processing, medicine).

2. Impact on other disciplines

- The methods developed in the project enable computational analyses with a high level of physical fidelity suitable for simulation-based scientific discovery. These methods can be applied to other technological energy-related fields, such as combustion, electrochemistry, pyrolysis and gasification, chemical processing, particle synthesis, among others.

- The project's outcomes, by enabling simulation-based analyses founded on fundamental science principles, has the potential to impact diverse established and emerging plasma-on-liquid applications, from metallurgy and metal processing to water treatment, liquid functionalization, nanoparticle synthesis, biomaterials processing, and medicine.

3. Impact on the development of human resources

- The project has trained four doctoral students and one post-doctoral research scholar in plasma science and engineering, advanced transport phenomena applied to energy systems, computational science and engineering, and high-performance computing.

- The project participants were also trained in professional communication skills through structured interactions in research group meetings and individual guidance from the PI.

- The postdoctoral associate has been mentored on establishing independent research, such as identifying relevant research topics, formulating a research program, programming of tasks and deliverables, and managing personnel.

4. Impact on society beyond science and technology

- The fundamental understanding of the plasma state and the computational analysis methods attained by the project can assist the development of controlled fusion as the ultimate source virtually unlimited, safe, clean energy.

- The understanding of plasma-on-liquids obtained by the project can help the development of novel processes for the synthesis of materials and particles, the treatment of liquids, agriculture, medicine, among others. These processes can lead to the inception of new industries and opportunities for economic growth, assist on remediating and mitigating environmental impacts, help improve food production, security, and safety, and improve human health.