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Multi-scale mapping between the control parameter space and a cold atmospheric plasma chemical space

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Cold atmospheric plasma (CAP) is a low-temperature plasma exposed to open air without thermal equilibrium, and it is currently widely used for plasma-based biomedical applications, relying on a unique chemical system [1]. Based on the air species such as N_2, O_2, and H_2O, CAP can synthesize the reactive oxygen species (ROS) and reactive nitrogen species (RNS) including O, OH, HO_2, and NxOy [1]. ROS can lead to cell cycle arrest and apoptosis for cancer therapy, while NO and other reactive species can assist tissue regeneration, and the ozone and UV generated by CAP can deactivate microorganisms for sterilization [2]. However, the plasma chemistry in the open air is thus too complicated to be manually controlled [3]. There are more than 100 chemical species with 1000 chemical reactions occurring at the same time [4]. Each reaction has a unique and highly dynamic rate coefficient. Meanwhile, there are many different types of CAP generators such as plasma jet and dielectric barrier discharge (DBD). Each generator can also work at different hardware setups such as discharge voltage, discharge frequency, gas flow rate, etc. Any one of those hardware setup and control parameters can change the entire chemical system, including all the species concentrations.

Therefore, it is urgent to investigate and understand the complicated relationship between the control inputs and the complete concentrations of CAP chemistry. Several experimental diagnostics have been well-developed and widely used, such as laser-induced fluorescence (LIF), optical emission spectroscopy (OES), mass spectroscopy (MS), etc. However, these measurement methods have limits. For example, LIF relies on the specific species' energy levels and thus it can only give access to OH-related species. OES, however, merely provides the excited species information and indirectly provides other information such as the electron temperature by assuming a simplified chemical kinetic scheme. MS can measure a relatively full picture of the species spectrum, but it is not sensitive to low-concentration species, such as those at about 1 ppm and lower.

Numerical simulations, on the other hand, can overcome these experimental difficulties. One needs a temporal resolution at sub-nanosecond to ensure an accurate simulation of both the chemistry and the dynamic discharge process, such as the streamer propagation of CAP jets. However, the actual biomedical applications usually require CAP chemistry applied to targeting cells and tissues for several minutes. On the other hand, the spatial resolution of the simulation is usually set at a sub-micrometer scale while the actual hardware is at a centimeter scale with a dynamic CAP gas flow field. Therefore, this is a multi-scale problem for both time and space, which is challenging to simulate.

In this work, a machine learning (ML) assisted method is developed to solve such a problem. Physics-informed data-driven modeling is a mapping between the two mathematical spaces: the space of control parameters of the plasma generator and the space of chemical species compositions in the plasma. Fourier-transform infrared spectroscopy (FTIR) is used to measure the concentrations of NO, NO_2, and N_2O. Like LIF, FTIR can merely provide limited species concentrations. Along with other physical laws such as mass and charge conservations, this physical information will be the constraint to training a physics-informed neural network (PINN). The input of PINN is a randomly selected control parameter while the output of it will be the full picture of all species concentrations. They will then be sent to a 0D chemical simulation to verify if all the species are at a steady state. Any changes of them will be an error, while the violation of physics laws and experimental observations of NO, NO_2, and N_2O will also increase the error. The total error will be used in an evolutionary algorithm to update the weights of PINN and complete an iteration of the training loop. Finally, the total error will converge to an acceptable low value. This means that no matter what control parameters are input to the PINN, it can always provide the full picture of all the species concentrations at steady state, agree with the conservation laws, and agree with the experimental observations for those species available to measure. Such a multi-scale problem is thus solved.

References

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