Development of a numerical modeling strategy for joint experimental/simulation analysis of plasma/catalysis interactions

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The transition towards a bioeconomy requires the development of novel technologies capable of efficiently and flexibly utilizing resources. Within this context, the conversion of biogas into chemical compounds that are valuable to industry during periods of decreased heat or electricity demand is a method of effectively storing chemical energy. The synthesis of methanol from biogas emerges as a promising alternative to the conventional process reliant on fossil carbon. Nonetheless, existing methanol production systems are characterized by their large size, utilization of rare or costly materials, and operation at high pressures and temperatures. An alternative and promising technology is non-thermal plasma-assisted catalysis. This process operates at atmospheric pressure and room temperature in ''on/off'' mode. However, there is still a need to improve its energy efficiency and the selectivity of the target product to facilitate effective industrial development. Despite recent advancements in the field of plasma/catalysis research [1], a deeper comprehension of the interaction between the active species generated in the gas phase and the catalyst's surface can only be achieved by combining experimental and simulation results. This study focused on developing a dedicated numerical tool for simulating a DBD catalytic reactor [2] with flexible structural configurations and operating conditions, enabling progressive validation of the simulation strategy, kinetic schemes, and physical models. The catalyst may be placed on the inner wall of the DBD reactor or within a ceramic foam with controlled pores; however, the initial validations was conducted with bare walls. A 1-D simulation of methane oxidation was first considered using a coupled Boltzmann/kinetic solver [3] based on two open-source libraries Cantera and Bolos. Subsequently, the numerical parameters of the 1-D model were set incorporating experimental data.

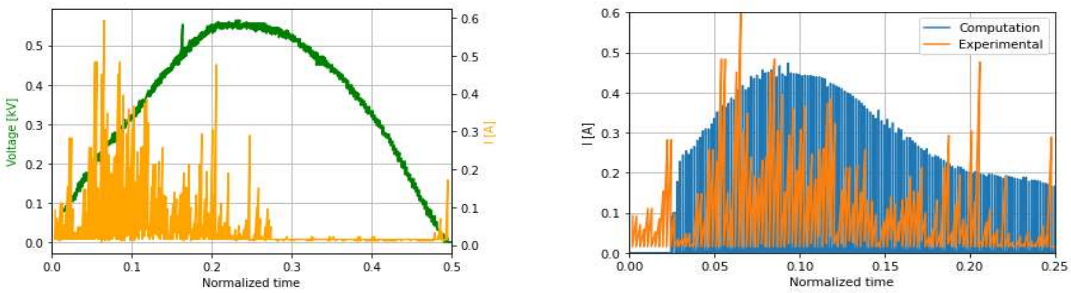

Figure 1 : *Experimental voltage-current waveforms for DBD reactor (left). Experimental and computed current waveforms comparison (right).*

Références

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