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Modeling of Non-oxidative Coupling of Methane (NOCM) in a multifunctional 3D printed plasma reactor

Aim

Low-dimensional, real-time prediction of the output of a multifunctional catalytic nanosecond-pulsed discharge (NPD) plasma reactor, employed for methane conversion to ethylene.

Justification

Ethylene production via steam cracking is the second largest GHG emitter in the chemical industry after ammonia synthesis, and the largest one without stoichiometric CO2 production. The increasing efforts to decarbonize the chemical industry lead to the necessary elaboration of alternative, electrified routes. The NOCM reaction is an excellent candidate starting from future's expected feedstocks, i.e. greenhouse gases (methane), and blue or green hydrogen. Within this scope, a novel reactor based on nanosecond-pulsed discharge plasma technology (NPD) and a 3D printed catalyst support has been developed and optimized at LCT in the past years, reaching remarkably high ethylene production efficiency at 1000kJ/mol. Recently, accurate predictive models have been developed for the plasma and the downstream catalytic sections separately, with the larger scope of proposing an optimal heat integration geometry for the two. The scope of this master thesis lies in the integration of these two models in a single interface, capable of predicting the time-dependent output of the plasma reactor, with a larger aim of reactor optimization and further development.

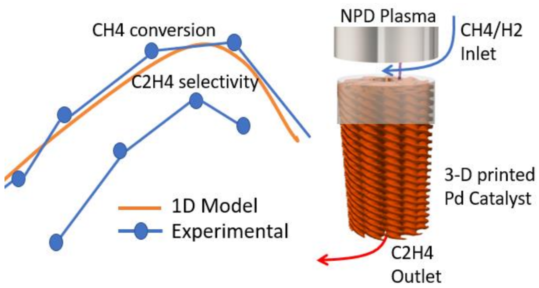

Figure 1 Representation of the NPD catalytic reactor setup and its action through a computational model.

Program

- 0-D plasma model simulations on ZDPlasKin with the model developed by LCT and partners at UAntwerp. Comparison of results with experiments, and development of a Python script to reproduce the same routine.
- Fine tuning of parameters for non-ideal reactor Cantera(Python) models, inclusive of surface reactions, to match experimentally validated RTD curves and reactive CFD results obtained by LCT.
- Coupling of the plasma and catalytic models within a single Python interface to predict the time-varying output of the catalyst-coupled plasma reactor.
- Further optimization of the plasma reactor based on validated modelling results.

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