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Low-order modeling of non-oxidative Coupling of Methane (NOCM) in a plasma catalytic reactor

Aim

Low-dimensional, real-time prediction of the output of a multifunctional catalytic nanosecond-pulsed discharge (NPD) plasma reactor, employed for methane (CH_4) conversion to ethylene (C_2H_4).

Justification

Ethylene production via steam cracking is the second-largest GHG emitter in the chemical industry after NH_3 synthesis, and the largest without stoichiometric CO_2 production. The growing efforts to decarbonize the chemical industry require the development of alternative, electrified routes. The non-oxidative coupling of methane (NOCM) is an excellent candidate pathway for natural gas valorization:

$$2CH_4 \rightarrow C_2H_4 + 2H_2 \tag{1}$$

Within this scope, a novel reactor concept has been developed in our past work, coupling nanosecond-pulsed discharge plasma technology (NPD) and 3D-printed catalysts. The assembly has achieved remarkably high C_2H_4 yields [1](34.4%), demonstrating potential for scalability and broader application. Concurrently, the reactor design, including the catalyst geometry, has been based solely on a heuristic approach, underscoring the need for a predictive model and a rational design procedure. As noted in previous work [2], radial segregation and axial dispersion can play an important role in this type of application. For this reason, the scope of the project lies in the development and integration of two low-order simplified models that can describe the entire reactor assembly. The coupling of the two is aimed at a single interface that can predict the time-dependent output of the plasma reactor in terms of outlet composition and temperature, with the broader aim of optimizing and further developing the reactor.

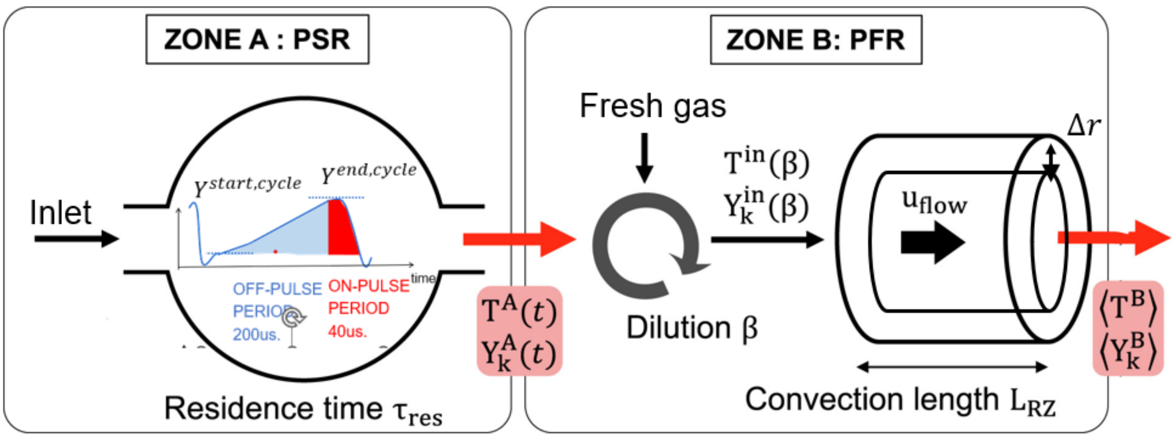

Figure 1 Low-oder model of an NPD+catalyst system with a perfectly stirred reactor (PSR) model coupled with a downstream PFR catalytic model with radial compartments.

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Program

- 0-D plasma model simulations with a tailored solver within the Python Cantera framework. Fitting of parameters to previously gathered experimental data.
- PFR radial compartment simulations of a post-plasma catalyst and comparison with experiments
- Coupling of the plasma and catalytic models within a single Python interface to predict the time-varying output of the plasma+catalyst system.

Bibliography
[1] Cameli, F., et al., *Electrified methane upgrading via non-thermal plasma: Intensified single-pass ethylene yield through structured bimetallic catalyst.* Chemical Engineering and Processing - Process Intensification, 2024. **204**: p. 109946.
[2] Mastroianni, L., et al., *DLP 3D printing of alumina catalyst architectures: Design, kinetics and modeling of structure effects on catalyst performance.* Chemical Engineering Journal, 2024. **501**: p. 157691.