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# Accelerating steam cracking electrification: unsteady computational fluid dynamics reactor design

## Aim

Computational assessment of the occurrence and impact of unsteady flow behaviour in a novel and revolutionizing Power-2-Heat reactor design for olefin production with net-zero $CO_2$ emissions.

## Justification

Ethylene and propylene are the most important olefins and are produced in large amounts by steam cracking. As the most important petrochemical process, this pathway consumes large amounts of energy causing it to be one of the major $CO_2$ emitters in Flanders with some 5 million tonnes/year of $CO_2$ equivalents. Fossil fuel combustion, to generate the required heat, amounts to 75-93% of the $CO_2$ produced by steam cracking. As the Belgian government committed itself to the Paris Agreement, Flanders aims to reduce its greenhouse gas emissions by 80-95% by 2050. Reducing $CO_2$ emissions related to olefin production will be crucial for accomplishing this goal. In this respect, a Power-2-Heat steam cracking reactor is a promising and future-proof concept.

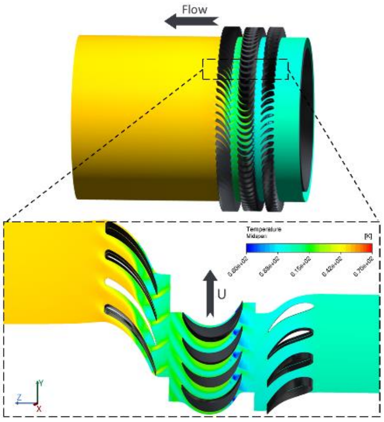

*Figure 1: Power-2-Heat reactor.*

The current idea of the Power-2-Heat reactor can be described, in layman's terms, as a 'bad' compressor that causes an increase in temperature but not in pressure via the dynamic action of rotating blades and strategically located stationary blades. Combining this with a factor 10 reduction in residence time, this revolutionizing reactor can carb the $CO_2$ emissions with 90% while drastically increasing the olefin yield compared to conventional steam cracking furnaces. Despite the novelty of this reactor, the large resemblance with traditional turbomachines gives us a preliminary overview of the occurring phenomena within this reactor. One of these phenomena is the inherent unsteadiness due to the rotating rotor. Even though this is a chemical reactor, the emphasis of this thesis will be on the investigation of the unsteady non-reactive flow field. This results in two major objectives. Firstly, the impact of the stator and rotor wake on each other needs to be investigated and mapped for different operating conditions. This will provide us with the well-needed insights for the reactor operation. Additionally, this thesis aims to identify the occurring secondary flow structures (i.e. flow streams that deviate from the main flow path), as these cause a reduction in work added to the fluid. Hence, they reduce the potential to increase the temperature, which leads to larger reactor design and smaller economic benefits. Consequently, the second objective is to study these structures and identify potential techniques to reduce their effect.

## Program

- Literature survey on the unsteady behaviour within a traditional turbomachine.
- Analysing the effects of the unsteady behaviour and secondary losses in the electrified rotor-stator reactor through CFD simulations.
- Mapping the unsteady behaviour for different operational conditions.
- Modifying reactor geometry to reduce the negative impact of secondary flow losses.
- Investigate the influence of the modifications on the product yields via 1D simulations.