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## Power-to-olefins: the analysis of unsteady flow behaviour and secondary losses via Computational Fluid Dynamic studies.

### Aim

Computational assessment of the occurrence and impact of unsteady flow behaviour and secondary flows in a novel power-to-heat reactor design for olefin production.

### Justification

Anno 2020, the petrochemical industry is heavily based upon the production of olefins, as these components are the building blocks of a large variety of products like packing applications, solvent, fibers, or resins. Ethylene and propylene are the most important olefins and are produced in large amounts ( $1.5 \times 10^8$  and  $8 \times 10^7$  tonnes, respectively, and increasing at a rate of 5% per year) by steam cracking. Being the most important petrochemical process, it is consuming large amounts of energy causing it to be one of the major contributors to CO<sub>2</sub> emissions in Flanders. It contributes 50% of the total CO<sub>2</sub> emitted by the chemical industry, some 5 million tonnes/year of CO<sub>2</sub> equivalents. Combustion of fossil fuels, to produce the required heat, amounts to 75-93% of the CO<sub>2</sub> produced by steam cracking. As the Belgian government committed itself to the Paris Agreement, Flanders aims to reduce its greenhouse gas emissions by 30% by 2030 and 80-95% by 2050. Reducing CO<sub>2</sub> emissions related to olefin production will be crucial to accomplish this goal. In this respect, the electrification of steam cracking is a promising and future-proof concept that is strongly supported by the industry.

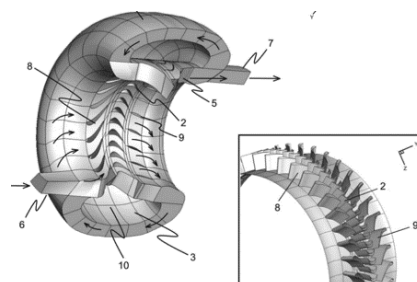


Figure 1: Electrified rotor stator reactor.

The current idea of the power-to-heat reactor combines aerospace engineering with chemical reactor engineering yielding a reactor that applies the dynamic action of rotating blades to transfer energy to the fluid (see Figure 1). This type of reactor only works because of the unsteady flow phenomena that are taking place within them. However, the occurring periodically encountered flow distortions have a significant impact on the stage efficiency, blade loading, metal fatigue, heat transfer, and noise generation of this reactor. Also, the complex 3D geometry of this reactor is prone to the occurrence of 'loss factors'. These loss factors are historically divided into profile, end wall, and secondary losses (recognizing that losses are seldom independent). The latter is what sparks the interest since losses in work added to the fluid reduces the potential diffusion into internal energy, which negatively impacts the chemical reaction rate and yield. Equally, the streamwise vortices associated with secondary flows (negatively?) influence the aerodynamics and mixing in downstream blade rows.

### Program

- Literature survey on the unsteady behaviour and loss factors within a traditional turbomachine. The main focus should be on how to accurately grasp these phenomena during CFD-simulations given the large difference in length and frequency scale.
- Implementation of secondary flow losses in a validation case
- Analysing the effects of the unsteady behaviour and secondary losses in the electrified rotor-stator reactor.
- Adapting reactor geometry to reduce the negative impact of unsteady behaviour and losses.