Computational Fluid Dynamics design of steam cracking reactors: extrusion method for simulation of dynamic coke layer growth

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Steam cracking of hydrocarbons is the predominant commercial process for producing many platform chemicals such as light olefins (i.e. ethene, propene, and butadiene) and aromatics (i.e. benzene, toluene, and xylenes). A major factor for the process efficiency is the formation of a coke layer on the inner surface of the tubular shaped reactors. Due to this insulating carbonaceous layer, heat transfer to the process gas is hampered, leading to excessively high tube metal temperatures. Additionally, the cross sectional area for flow is reduced and the reactor pressure drop increases, resulting in a loss of olefin selectivity. Decoking of industrial reactors is thus inevitable. In consideration of this energetic and economic drawback, many efforts have been made towards the development of technologies to reduce coke formation. Three-dimensional coil geometries are often introduced to enhance radial mixing resulting in lower coking rates and longer run lengths.

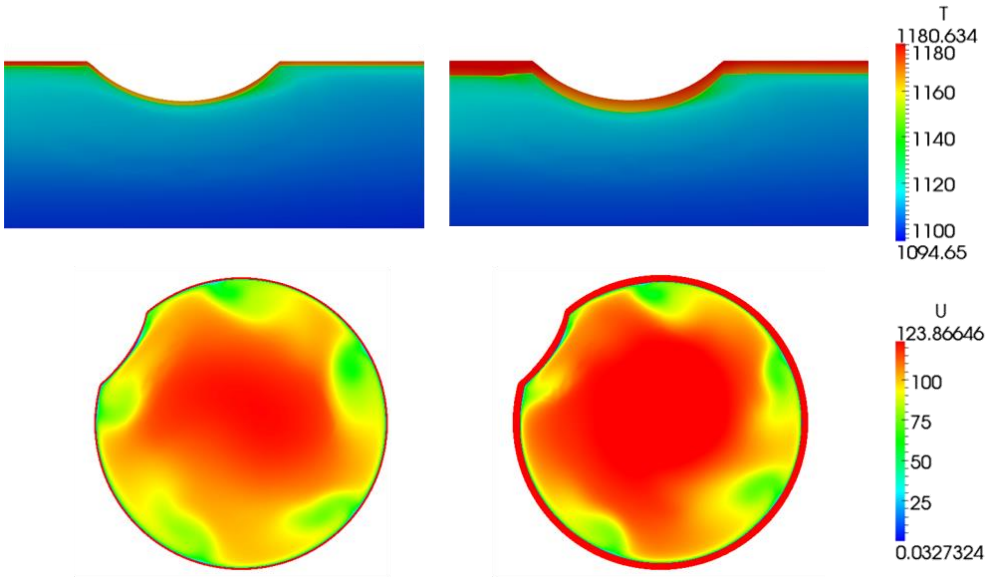

Figure 1: Coke layer growth in a slit-MERT 3D reactor geometry. The temperature profile and the velocity profile in a cross section of the reactor are shown for start-of-run conditions (left) and after 5 days of coke layer growth (right).

Our group has successfully applied computational fluid dynamics (CFD) for the evaluation of the effect of 3D reactor geometries on pressure drop, coking rates and product yields [1, 2]. These studies however focused on start-of-run performance,

whereas the most attractive characteristic of the enhanced reactor designs is the extension of the run length. Determining the full economic potential of a coil hence involves tracking its performance throughout the run, i.e. as function of the time on stream. In the case of enhanced tubular geometries or reactors with a strongly non-uniform heat flux profile (e.g. due to shadow effects), the growth of the coke layer will generally not be uniform. Because of this, the reactor geometry will change in time, which will in turn influence the fluid dynamics, product yields and successive coke formation. To take this into account, the coke layer growth needs to be incorporated in the CFD simulations. An algorithm based on dynamic meshing was therefore developed for simulating coke formation on the 3D reactor geometry and tracking the geometry deformation caused by the growing coke layer. In this algorithm, the reactor mesh is updated on a regular basis as coke deposits on the reactor wall until an end-of-run constraint is met, indicating that decoking is required.

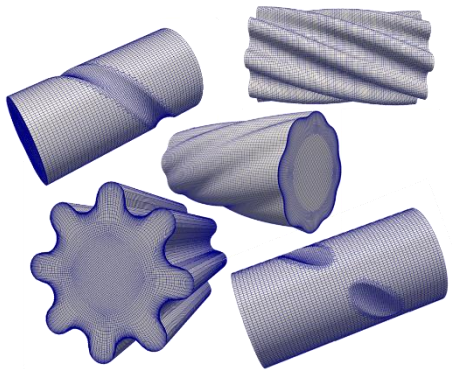

Figure 2: Structured meshes of complex 3D reactor geometries.

The open source CFD package OpenFOAM has been extended with a module for dynamically simulating the growing coke layer. The module includes a new library of extrusion models which makes it possible to automatically generate structured meshes of high quality on several complex 3D reactor geometries, see Figure 2. The module can be used in a post-processing step to simulate the growth of the coke layer based on the temperature and species concentrations at the gas-cokes interface.

As a proof-of-concept, a Millisecond propane cracker was simulated over the first days of its run length for a bare, a classically applied finned tube and a MERT reactor design.

References

[1] C.M. Schietekat, D.J. Van Cauwenberge, K.M. Van Geem, G.B. Marin, Computational fluid dynamics-based design of finned steam cracking reactors, AIChE Journal 60 (2014) 794-808.
[2] P.A. Reyniers, C.M. Schietekat, D.J. Van Cauwenberge, L.A. Vandewalle, K.M. Van Geem, G.B. Marin, Necessity and Feasibility of 3D Simulations of Steam Cracking Reactors, Industrial & Engineering Chemistry Research (2015).

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