Simulation and design of novel steam cracking reactors

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Cokes formation during steam cracking
Carbonaceous layer on the internal tube metal surface causing:
- Less efficient convective heat transfer to the process gas
- Drastic rise in tube metal temperatures (TMT) over time
- Increased pressure drop due to narrowed cross-section
- Loss of product selectivity
Decoking needs to be performed at regular intervals
Several methods to reduce coking rates:
- Metal surface technologies
- Feed additives
- 3D reactor technologies
- Increased internal surface
- Turbulence-promoting structures

Fluid dynamics and heat transfer
- Experimental data of Albano et al. (1988)
- Reynolds Stress Model
- No wall functions
- QUICK discretization scheme
- Rotationally periodic boundary conditions
- Prismatic grid of 8x10^3 cells/m
- Kinetic network extensively validated with pilot plant and industrial data
- Pyrolytic coking model of Pleihiers for light feedstocks

Re = f(C_{C_{H_2}}, C_{C_2H_6}, T_{in})

Model validation

Simulation of 3D reactors
Evaluation on industrial scale or up-scaling of pilot plant data is not straightforward
- Additional pressure drop can cause small but significant losses in olefin selectivity
- Typical 1D and 2D simulation tools can only account for these geometries to a limited extent
- Deviations from plug flow behavior
- Computational Fluid Dynamics (CFD) can offer reliable predictions using validated models for heat transfer, turbulence, kinetics and cokes formation
- Simulations performed using the commercial software package Ansys FLUENT 13.0

4 distinct geometries were simulated with the same:
- Reactor volume
- Minimal metal thickness
- Total heat input profile

- Kellogg Millisecond propane cracker (KBR)
- Feedstock: 118.54 kg/s C_{3}H_{8}
- Steam dilution: 0.326 kg/kg
- Residence time: ±0.1 s
- XOT: 903 K
- COP: 1190 K
- Coil length: 10.5 m
- Internal diameter: 30.2 mm
- Metal thickness: 6.75 mm

Radial cracking network
- 26 components
- 13 radical species
- 2/2 reactions

Minor effect on total olefin selectivity!

Coking considerations
Non-uniform coking on the fin surface
Due to the increased surface area, the total cok yield is in fact greater for a finned tube -> shorter run lengths?

Future work
- Move towards open-source CFD packages
- Implementation of larger, automatically generated reaction networks to allow simulation of naphtha feedstocks
- Dynamic mesh deformation to account for non-uniform coking rates
- Coupled reactor-furnace simulations
- Model validation for state-of-the-art reactor designs such as X-MERT and SFT

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