Computational Fluid Dynamics based design of steam cracking reactors

David Van Cauwenberge, Kevin M. Van Geem, Jens Floré, Guy B. Marin

Laboratory for Chemical Technology
Technologiepark 914, 9052 Ghent, Belgium
http://www.lct.UGent.be E-mail: David.VanCauwenberge@UGent.be

Coke formation in steam cracking tubes

A carbonaceous layer on the inner wall of the reactor tubes, formed through secondary reactions, inhibits conductive heat transfer to the process gas.

- Rise in Tube Metal Temperature (TMT)
- The pressure drop increases due to the reduction of the cross-sectional flow area.
- Loss of selectivity to ethylene and propylene
- Frequent decoking of industrial reactors is required.

Reducing coking rates is possible with 3D reactor geometries

- Improved convective heat transfer
- Enhanced radial mixing → more uniform profiles
- Increased pressure drop

Effect on product selectivity?

Simulation of 3D reactor designs

Evaluation on industrial scale or up-scaling of pilot plant data is not straightforward

- Olefin yield losses may be difficult to measure but very significant due to the economy of scale
- Typical 1D and 2D simulation tools can only account for these geometries to a limited extent
- Deviation from plug flow behavior

Multiscale approach combining 3D Computational Fluid Dynamics (CFD) with reaction kinetics obtained using quantum chemistry methods

Fully first principles-based reactor simulation

Computational setup

Based on open source CFD toolbox OpenFOAM

- “Easy” implementation of different boundary conditions, turbulence models, thermophysical models, production rate calculation routines, ...
- No license fee restrictions and excellent scaling down to 20,000 cells/CPU
- Structured or unstructured grids generated using built-in mesher snappyHexMesh or commercial packages such as Pointwise®
- Open source post-processor ParaView

- Transient solver for incompressible flow
- SIMPLE-algorithm for pressure-velocity coupling
- Generic turbulence modeling, i.e. laminar, RANS, LES or DNS can be selected
- Periodic boundary conditions in order to limit the extent of the computational domain
  - Splitting of temperature and pressure field into a fluctuating periodic part and a non-periodic gradient
  - Non-periodic part appears in momentum and temperature equation as driving force
- Methodology validated with DNS data
  - Cold flow design evaluation and optimization tool
  - RANS model validation

- Steady state solver for compressible reacting flow
- SIMPLE-algorithm for pressure-velocity coupling
- Wall-resolved or wall-modeled RANS turbulence models
- Conjugated heat transfer between metal-cokes-gas
- Efficient implementation of large kinetic networks containing up to 165 species and 3200 reactions
- Pseudo-steady state assumption applied a priori for all μ-radicals, during simulation for selected β-radicals
- Dynamic zoning method for fast initial convergence

- Industrial-scale simulations allowing quantitative yield predictions

Dynamic run length estimation

Non-uniform coke layer formation will affect reactor geometry and hence fluid dynamics, product yields and successive coke formation.

Coke formation needs to be incorporated in the simulation to correctly simulate a run length of a steam cracking reactor.

<table>
<thead>
<tr>
<th>Time (h)</th>
<th>Coke Layer</th>
<th>Temperature (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1180</td>
</tr>
<tr>
<td>12</td>
<td>1290</td>
<td>213</td>
</tr>
</tbody>
</table>

The need for mesh creation in each iteration makes the procedure time consuming.

Automatic mesh generation is necessary to apply the technique to full-scale simulations

Octree-based mesh generation using snappyHexMesh

I. Generation of Cartesian grid around object
II. Local grid refinement at all surface intersections
III. Removal of cells outside the desired computational domain
IV. Slicing of cells by the surface in order to conform to the boundary
V. Extrusion of a boundary layer from the snapped surface grid

Prospects and future work

- Patent application for novel reactor design in cooperation with BASF SE
- Cold flow geometry optimization through mesh deformation and cost function minimization techniques
- Implementation of in-situ adaptive tabulation or operator splitting methods for further reduction in computational cost
- Experimental validation of the performed simulations in cooperation with the von Karman Institute for Fluid Dynamics using 3D PIV and liquid crystal thermography
- 3D-3D coupled furnace-reactor simulations for reliable heat flux profiles
- Adaptation of existing RANS models from results obtained using LES
- Benchmarking of the OpenFOAM code with other LES codes such as AVBP and CharlesX

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