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

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Coke reduction methods

- Feed additives
- Metal surface technologies
- 3D reactor technology
3D reactor technology | The Good, the Bad & the Ugly

Enhanced heat transfer & mixing → Less cokes?

Increased pressure drop
Lower olefin selectivity?

Long term performance and stability?
Where are we?

- **Short term performance**
  - Reactor residence time
  - Product yields, selectivities

- **Intermediate term performance**
  - Reactor run length
  - Coking rate, pressure drop, TMT

- **Long term performance**
  - Reactor stability & lifetime
  - Deterioration of reactor material
1D Reactor performance

- Does the improved coking rate outweigh the loss of selectivity?
- In a 1D world...

<table>
<thead>
<tr>
<th>1D Simulation</th>
<th>Bare</th>
<th>Straight fins</th>
<th>Rifled</th>
<th>MERT</th>
<th>SFT</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta P/\Delta P_{\text{Bare}}$</td>
<td>1.00</td>
<td>1.22</td>
<td>1.67</td>
<td>2.17</td>
<td>1.26</td>
</tr>
<tr>
<td>$U/U_{\text{Bare}}$</td>
<td>1.00</td>
<td>1.21</td>
<td>1.58</td>
<td>1.50</td>
<td>1.19</td>
</tr>
<tr>
<td>$T_{\text{gas/cokes}} [\text{K}]$</td>
<td>1079.4</td>
<td>1066.4</td>
<td>1050.2</td>
<td>1054.5</td>
<td>1066.9</td>
</tr>
<tr>
<td>Rel. $r_{\text{coke}}$</td>
<td>-</td>
<td>-4.8%</td>
<td>-34.9%</td>
<td>-43.1%</td>
<td>-24.1%</td>
</tr>
<tr>
<td>Rel. yield $C_2H_4$</td>
<td>-</td>
<td>-0.27%</td>
<td>-0.83%</td>
<td>-1.47%</td>
<td>-0.32%</td>
</tr>
<tr>
<td>Rel. yield $C_3H_6$</td>
<td>-</td>
<td>+0.03%</td>
<td>+0.08%</td>
<td>+0.13%</td>
<td>+0.03%</td>
</tr>
</tbody>
</table>

~ seconds

3D CFD simulations are computationally very expensive

~ 1000 CPU hours
Spatial vs. streamwise periodic

Full-scale reactor simulation

~ 10,000 time steps
~ 10 million cells

Trick: streamwise periodicity

Computational domain can be limited by using streamwise periodic boundary conditions
Periodic reactive simulations

- Assume **velocity fully-developed** over the short computational volume
- Use transient velocity field to evaluate **species and enthalpy radial mixing**
- Translate transient results back to the true steady-state by reconstructing the position from the bulk velocity:

\[
\Delta z = U_{bulk} \Delta t = \frac{\int \rho u_z dA}{\int \rho dA} \Delta t
\]

**Transformation: Time → Position**

Speedup factors of 200+
Periodic reactive | 3D Product yields

<table>
<thead>
<tr>
<th></th>
<th>Bare tube</th>
<th>Finned tube</th>
<th>Ribbed tube</th>
</tr>
</thead>
<tbody>
<tr>
<td>COT [K]</td>
<td>1152.6</td>
<td>1151.6</td>
<td>1155.2</td>
</tr>
<tr>
<td>TMT [K]</td>
<td>1230.6</td>
<td>1222.7</td>
<td>1177.2</td>
</tr>
<tr>
<td>ΔP [Pa]</td>
<td>27682</td>
<td>29061</td>
<td>110001</td>
</tr>
<tr>
<td>Conversion</td>
<td>74.96%</td>
<td>74.99%</td>
<td>76.18%</td>
</tr>
<tr>
<td>CH4</td>
<td>13.96%</td>
<td>14.04%</td>
<td>14.54%</td>
</tr>
<tr>
<td>C2H2</td>
<td>1.64%</td>
<td>1.69%</td>
<td>1.55%</td>
</tr>
<tr>
<td>C2H4</td>
<td>27.60%</td>
<td>27.87%</td>
<td>27.74%</td>
</tr>
<tr>
<td>C2H6</td>
<td>1.23%</td>
<td>1.27%</td>
<td>1.32%</td>
</tr>
<tr>
<td>C3H6</td>
<td>22.91%</td>
<td>22.50%</td>
<td>23.52%</td>
</tr>
<tr>
<td>1,3-C4H6</td>
<td>2.91%</td>
<td>2.97%</td>
<td>2.88%</td>
</tr>
</tbody>
</table>

Spatial: 10 hrs
Periodic: 0.04 hrs

Spatial: 3000 hrs
Periodic: 20 hrs

Spatial: 800 hrs
Periodic: 50 hrs
Evaluation of 3D reactor technologies requires tracking coke layer growth.

**NO** streamwise periodicity
**NO** limitation of computational domain
**NO** fast periodic simulation approach

Tracking coke formation requires simulation of the entire geometry and is **computationally very expensive**
Dynamic modeling of coke formation

- $t_0 = 0$
- Run simulation $t_{sim}$ time steps
- $t_i = t_{i-1} + t_{sim}$
- $TMT \geq TMT_{max}$
- $\Delta p \geq \Delta p_{max}$
- Coke layer growth
- Mesh update

- $t_i = t_{i-1} + 1$
- YES
- END

- NO
- Read $T$ & $Y_k$ on gas / cokes interface
- Calculate coking rate*
- Calculate growth of coke layer
- Create new mesh

$\Rightarrow$ New library of extrusion models in OpenFOAM, including a variety of 3D steam cracking reactor geometries

*P.M. Plehiers, Laboratorium voor Petrochemische Techniek, Rijksuniversiteit Gent, 1989
Extrusion of 3D reactor geometries

Internally finned tube

1. Start from core cylindrical geometry
2. Extrusion to 3D surface

R: inner radius
e: fin height
t: minimum wall thickness

Coke layer growth

Extrusion of gas and cokes region from core cylinder wall to specified surface geometry, while taking into account calculated coke layer thickness
Test case | Millisecond propane cracker

- Feedstock: 118.5 kg/h propane
- Propane conversion: 80% (± 0.05%)
- Steam dilution: 0.326 kg/kg
- CIT: 903.7 °C
- COP: 170 kPa

Two geometries were simulated
- Same reactor volume
- Same axial length
- Same minimal wall thickness

Bare | Straight fin
• Two mesh updates, each corresponding to 48 hours of coke layer growth
• Heat flux updated to keep propane conversion constant
Heat flux correction

Scaling factor [-]

Run length [hrs]

0 48 96

bare finned

0.98 1 1.02
Turbulence modeling
• RANS: $k-\omega$ SST model (Menter, 2001)

Numerical setup
• Steady-state
• SIMPLE algorithm
• 2nd order central differencing spatial discretization scheme

Chemistry model
• Full single-event microkinetic CRACKSIM model reduced to core for propane cracking:
  o 151 reactions
  o 29 species (13 radicals)

Meshing
• Structured grids for improved grid spacing control and cell orthogonality
• 1/8th of the tube’s cross section
• Near wall grid resolution satisfying $y^+ < 1$
Max. TMT finned: 30 K lower
Max. coking rate: 32.5% lower

Increased run length?
Minor effect on \textit{total} olefin selectivity

Radial mixing effects cannot be predicted based on 1D simulations only
Coke layer growth

Bare tube: velocity magnitude contours @ z= 6 m

SOR 48 hrs 96 hrs

Finned tube: velocity magnitude contours @ z= 6 m

SOR 48 hrs 96 hrs
Coke layer growth

**z = 6 m**

- Large difference in coke layer thickness BUT greater internal surface area
- Small difference in effective coke volume

Coke volume at $z = 6$ m [cm³ m⁻¹]

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<th>Finned</th>
</tr>
</thead>
<tbody>
<tr>
<td>48 hrs</td>
<td>12.98</td>
<td>11.84</td>
</tr>
<tr>
<td>96 hrs</td>
<td>23.59</td>
<td>23.24</td>
</tr>
</tbody>
</table>

Total coke volume for finned tube still smaller than for bare tube
Pressure drop increases for bare tube almost 2x faster than for finned tube.
Tube metal temperature

Thermal resistance coke layer

Max. TMT increases

TMT increase for bare tube 4x faster than for finned tube
Conclusions & future work

• 3D computational fluid dynamic simulations allow optimization of industrial steam cracking reactors

• New method to perform yield & run length simulations of industrial steam crackers was developed
  – Combination with streamwise periodic simulations not possible

• Proof-of-concept reactive simulation of industrial propane cracker: bare vs. finned tubes
  – Strongly non-uniform formation of cokes in fins
  – Pressure drop increases faster in bare tube
  – TMT increases faster in bare tube

• Advantages of other 3D geometries (e.g. MERT) over finned tubes to be evaluated
Acknowledgements

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Thank you for your attention!

Questions ?