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Fouling in the High Pressure LDPE Process

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Experimental and Computational Investigation Approach

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What is LDPE Fouling?

- low-density polyethylene (LDPE) is produced under high temperatures (140°C – 330°C) and pressures (1000 bar – 3500 bar)
- fouling mechanisms still not understood
- fouling impacts:

  - productivity
  - operating safety
  - product quality
  - insulating effect
  - MWD tailing
Investigation Strategy

experiments

validation

classification

modeling

1D model

radial model

compartment model

understanding fouling formation

application of countermeasures
Experiments: Preliminary Considerations

- MWD tailing pronounced at higher surface-to-volume ratios and even existent at technical scales
  - fouling formation within the laminar boundary layer reasonable
  - idea: lab-scale reactor with as much laminar flow as possible
Experiments: Setup

- combined autoclave and tubular reactor setup
- autoclave
  - 100 mL
  - premixing, preheating
  - $p = 2000$ bar
- tubular reactor
  - laminar flow
  - heated
  - $L = 2$ m, $d = 4.8$ mm
  - ~ 30 sec residence time
Experiments: Results

- fouling material strongly branched
  - indication for polymer-rich environment

- pronounced MWD tailing with increasing running time
Modeling: Model Family

1D module
- plug flow (ODEs)
- complex reaction network with primary and secondary radicals
- rigorous MWD

radial module
- radial profiles (PDEs)
- laminar velocity profile
- wall temperature from 1D module (boundary condition)
- simplified kinetic scheme

compartment module
- two ideally mixed compartments for center and wall layer (ODEs)
- temperatures and velocities from radial module
- rigorous MWD
Modeling: Model Family

1D module

radial module

compartment module

increasing information about polymeric microstructure near the wall
Modeling: 1D Module

- slow heating due to laminar flow

- satisfying agreement of modeled distribution with main MWD
Modeling: Radial Module

- temperature contour plot
  - faster heat transport in the outer area

- $M_n$ contour plot
  - slightly lower $M_n$ at the wall $\rightarrow$ more transfer to CTA
Modeling: Radial Module

\[ D_{\text{polymer}} = D_{\text{monomer}} \]
\[ X_{\text{wall}} = 5.4\% \]
\[ X_{\text{avg}} = 2.7\% \]

\[ D_{\text{polymer}} = \frac{1}{10} D_{\text{monomer}} \]
\[ X_{\text{wall}} = 11.9\% \]
\[ X_{\text{avg}} = 1.9\% \]

\[ D_{\text{polymer}} = \frac{1}{20} D_{\text{monomer}} \]
\[ X_{\text{wall}} = 15.7\% \]
\[ X_{\text{avg}} = 1.8\% \]
Modeling: Radial Module

- viscosity gradient influences velocity profile
- description via Stokes law possible

\[
\frac{dw}{dr} = -\frac{1}{2\eta} \frac{dp}{dL} \quad r
\]
Modeling: Radial Module

- higher friction leads to lower wall speeds
- fouling as a self-accelerating process as proposed by Krasnyk et al.
- implementation in radial module follows

Modeling: Compartment Module

- \( D_{\text{polymer}} = D_{\text{monomer}} \)
- \( \dot{m}_{\text{shell}} = 1/100 \dot{m}_{\text{total}} \)
- significant broadening even for fast diffusing polymer
- same prediction as radial module regarding \( M_n \)

<table>
<thead>
<tr>
<th></th>
<th>core</th>
<th>shell</th>
</tr>
</thead>
<tbody>
<tr>
<td>( M_n ) (kg/mol)</td>
<td>13.6</td>
<td>13.4</td>
</tr>
<tr>
<td>( M_w ) (kg/mol)</td>
<td>31.4</td>
<td>81.0</td>
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</tbody>
</table>
Summary

- generating of tailed distributions with the chosen experimental setup possible
- fouling material highly branched
- model family delivers coherent results
- polymer diffusion speed crucial for buildup of higher polymer concentrations close to the wall
- indication that fouling is the result of a self-accelerating process; effects are to be investigated
Acknowledgements

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