Oxidative Coupling of Methane: a heterogeneously catalysed gas phase reaction

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Catalytic reactions network

Simulated reaction conditions and catalyst properties derived from RUB experiments

<table>
<thead>
<tr>
<th>Pressure (kPa)</th>
<th>Temperature (K)</th>
<th>CH₂/O₂ molar</th>
<th>W/F (mg s⁻¹)</th>
<th>Porosity</th>
<th>Density (kg m⁻³)</th>
<th>SiC dilution weight (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>190.0</td>
<td>990.0 - 1180.0</td>
<td>2.0 - 4.0</td>
<td>2.0 - 11.0</td>
<td>0.27</td>
<td>2300.0</td>
<td>1.0 10⁻²</td>
</tr>
</tbody>
</table>

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Oxidative Coupling of Methane (OCM) is one of the most attractive methods to utilize natural gas as chemical feedstock for the production of higher hydrocarbons.

OCM process occurs through a mechanism in which catalytic reactions interact with gas phase reactions.

CH₃ radicals, produced on the catalyst surface, either couple in the gas phase to produce the desired C₂ hydrocarbons or are oxidized forming undesired carbon oxides.

CH₂ radicals are highly reactive. In order to account for the irreducible mass transport limitations, an one-dimensional heterogeneous reactor model is employed (coordinate z), which distinguishes between a solid-intraparticle phase (coordinate ξ) and a fluid-interstitial phase (coordinate r).

The microkinetic model contains 39 reversible gas phase reactions (adopted from Chen et al.) and 26 reversible catalytic reactions; 24 gas phase and 11 surface species are involved.

Gas phase reactions couple with the catalytic reactions via the reactor model equations.

25 catalyst descriptors are incorporated in the microkinetic model.