1. INTRODUCTION
The development of new reactors and burners for non-catalytic partial oxidation of natural gas as well as the optimization of in-operation plants can be rapidly accelerated by the use of numerical models. However, CFD calculations require high computational effort and time. Alternatively, reduced order models can provide necessary information for the process development in a fast way. In the present work, a reduced order model is developed, which is based on a detailed CFD reactor model, and which is the first step towards an accelerated and fully automated process optimization.

2. CFD MODEL BASED ON VIRTUHCON BENCHMARK

![Residence time distribution](image)

<table>
<thead>
<tr>
<th>Zone Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flame Zone</td>
<td>(short residence time)</td>
</tr>
<tr>
<td>Post-Flame Zone</td>
<td>(short residence time)</td>
</tr>
<tr>
<td>Recirculation Zone</td>
<td>(highest residence time)</td>
</tr>
</tbody>
</table>

**Fig 1. Residence time distribution [1, 2]**

**Fig 2. Reduced order scheme**

**Modeling Approach**
- ChemkinPro 17.2
- ATR mechanism (reduced GRI 3.0)
- All zones modeled as PSRs
- Residence time taken from CFD

**Optimization Potential**
- Residence time:
  \[ \tau = \sum_{i} \frac{m_i x_i r_i}{m_i} \]
  where: \( m_i \) is the mass flux to the \( i \)th zone; \( x_i \) is the gas fraction; \( r_i \) is the local residence time
- Flow field: volume of recirculation and post-flame zones can be optimized
- Flame Zone: improved mixing at the burner

3. REDUCED ORDER MODEL

**Modeling Approach**
- ChemkinPro 17.2
- ATR mechanism (reduced GRI 3.0)
- All zones modeled as PSRs
- Residence time taken from CFD

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  \[ \tau = \sum_{i} \frac{m_i x_i r_i}{m_i} \]
  where: \( m_i \) is the mass flux to the \( i \)th zone; \( x_i \) is the gas fraction; \( r_i \) is the local residence time
- Flow field: volume of recirculation and post-flame zones can be optimized
- Flame Zone: improved mixing at the burner

4. RESULTS

**Fuel Slip**

The graph shows the dominant dependency of the \( \text{CH}_4 \) conversion on the fuel slip from the burner to the downstream section and the recirculation zone. The bigger fuel slip the higher \( \text{CH}_4 \) content at the outlet, however, \( \text{H}_2/\text{CO} \) ratio remains stable in almost all reactor zones.

**Post-Flame Zone**

The influence of the post-flame zone on the conversion is significant. However, the temperature drops and the amount of \( \text{CH}_4 \) at the outlet strongly depends on the flame zone.

**Reforming Zone**

Conversion of \( \text{CH}_4 \) is shifted towards equilibrium with increase of reforming zone volume. However, the changes in species concentration and temperature are minor.

**Fig 3. Influence of the fuel slip**

**Fig 4. Influence of the post-flame zone**

**Fig 5. Influence of the reforming zone**

**Table 1. Reactor operation conditions**

<table>
<thead>
<tr>
<th>Reactor zone</th>
<th>T, K</th>
<th>( \text{H}_2 ), mol%</th>
<th>( \text{H}_2\text{O} ), mol%</th>
<th>( \text{CH}_4 ), mol%</th>
<th>( \text{CO} ), mol%</th>
<th>( \text{CO}_2 ), mol%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flame</td>
<td>2538.54</td>
<td>31.52</td>
<td>39.61</td>
<td>0.03</td>
<td>23.41</td>
<td>4.67</td>
</tr>
<tr>
<td>Post-flame zone</td>
<td>1603.70</td>
<td>46.07</td>
<td>21.05</td>
<td>4.81</td>
<td>23.89</td>
<td>3.62</td>
</tr>
<tr>
<td>Recirculation zone</td>
<td>1455.45</td>
<td>40.19</td>
<td>20.00</td>
<td>15.08</td>
<td>19.89</td>
<td>4.13</td>
</tr>
<tr>
<td>Outlet pipe</td>
<td>1495.08</td>
<td>46.12</td>
<td>20.98</td>
<td>4.85</td>
<td>23.82</td>
<td>3.69</td>
</tr>
<tr>
<td>Outlet CFD</td>
<td>1480.18</td>
<td>47.19</td>
<td>19.91</td>
<td>4.90</td>
<td>23.85</td>
<td>4.01</td>
</tr>
</tbody>
</table>

5. SUMMARY AND OUTLOOK

- The reactor network model allows for a rapid analysis of the interaction between different reactor zones, fast parameter studies for different sections, and the analysis of different operating modes.
- Since the computational effort is moderate, reduced order modeling allows for the calculation of a large number of configurations, which is the basis for a fully automated reactor optimization [3].

REFERENCES