Claus Process Reactor Simulation

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The Claus process is the largest volume gas desulfurizing process and is used to recover elemental sulfur from hydrogen sulfide.

H₂S is burned and then reduced to form elemental sulfur. Often ammonia is present in the feed and needs to be converted to N₂.

Originally developed as a term project for an Advanced Chemical Reactor Design course.

\[ 8\text{H}_2\text{S} + 5\text{O}_2 \rightarrow \text{SO}_2 + 7\text{S} + 8\text{H}_2\text{O} \]
Claus Process Reactor

- Claus reactors contain a checkerwall to protect a downstream heat exchanger from the furnace and help mixing.
- Project was the first stage of a process designed to model a Claus reactor and determine the effects of introducing a static mixing element, a Vectorwall™, into the reactor.
  - Preliminary data suggests the Vectorwall™ provides > 40% improvement in throughput and yield.
### Claus Process Reactions

<table>
<thead>
<tr>
<th>Reactions and Rate Laws</th>
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<tbody>
<tr>
<td>$H_2S + \frac{3}{2}O_2 \xrightarrow{k_1} SO_2 + H_2O$</td>
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<tr>
<td>$r_1 = k_1P_{H_2S}P_{O_2}^{0.5}$</td>
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<tr>
<td>$NH_3 + \frac{3}{4}O_2 \xrightarrow{k_2} \frac{3}{2}H_2O + \frac{1}{2}N_2$</td>
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<tr>
<td>$r_2 = k_2P_{NH_3}P_{O_2}^{0.75}$</td>
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<tr>
<td>$H_2 + \frac{1}{2}O_2 \xrightarrow{k_3} H_2O$</td>
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<tr>
<td>$r_3 = k_3C_{H_2}C_{O_2}$</td>
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<tr>
<td>$CO + \frac{1}{2}O_2 \xrightarrow{k_4} CO_2$</td>
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<tr>
<td>$r_4 = k_4C_{O_2}^{0.25}C_{CO}C_{H_2O}^{0.5}$</td>
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- The basic model was chosen to consist of 7 non-elementary reactions with 11 separate species. Reactions are very fast and highly exothermic.
- The model was designed to solve the fluid mechanics, heat transfer, reaction kinetics, and mass transfer processes governing the behavior of the reactor.
- Thermodynamic properties – NASA polynomial format.
- Transport properties – kinetic theory approximations.
• The model coupled the Chemical Engineering, CFD, and Heat Transfer modules together and assumed compressible flow.
• Used simplified 1-D and eventually 2-D geometries. Adaptive meshing was required (~700,000 – 1,000,000 degrees of freedom).
• Class project solved the kinetics in ideal continuous stirred tank and plug flow reactors.
• COMSOL had trouble with reaction rates containing fractional orders.
  • Express the rate laws in logarithmic form and reconvert.
  • Penalty functions were required to insure that all concentrations remained in bounds.
  • A solution could not be obtained unless the heat generation was slowly ramped up to its ultimate value.

**Claus Process Reactor**
**Comsol Implementation**

**Gas Velocity**

**Heat Generation Rate**
• Implemented a 2-D formation to provide the first approximation to Vectorwall™ formulations.
• Great differences in rates and distribution of species depending on the insert geometry. All geometries have same open area for flow.
• Sulfur conversion is greater in the Vectorwall™ reactor.

Hydrogen Sulfide Concentration Profiles
Claus Process Reactor
Comsol Implementation

- Reactions actually take place in a flame. Comsol simulation was able to show the flame front.
- Look at different Vectorwall™ configurations. Specifically, whether it is better to have a central opening or central obstruction.

Flame Fronts
(heat generation rate)
Conclusions and Future Work

• We successfully simulated the Claus process in ideal chemical reactors, in a dispersed, plug flow reactor, and a two-dimensional flow reactor with checkerwall and VectorWall™, static mixing configurations.

• The 2-D simulations showed where problem spots may lie and where the enhanced mixing of the static mixing element may be put to best use.

• The next steps will be:
  – To apply this kind of modeling effort to incinerators, coal combustors, or fertilizer operations.
  – To develop full 3-D simulations using the supercomputer resources at RPI’s Computational Center for Nanoscale Innovations.
  – Goal: To define the optimal arrangement of Vectorwall™ elements.

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  New York State Pollution Prevention Institute