COMSOL CONFERENCE BOSTON 2013

Claus Process Reactor Simulation

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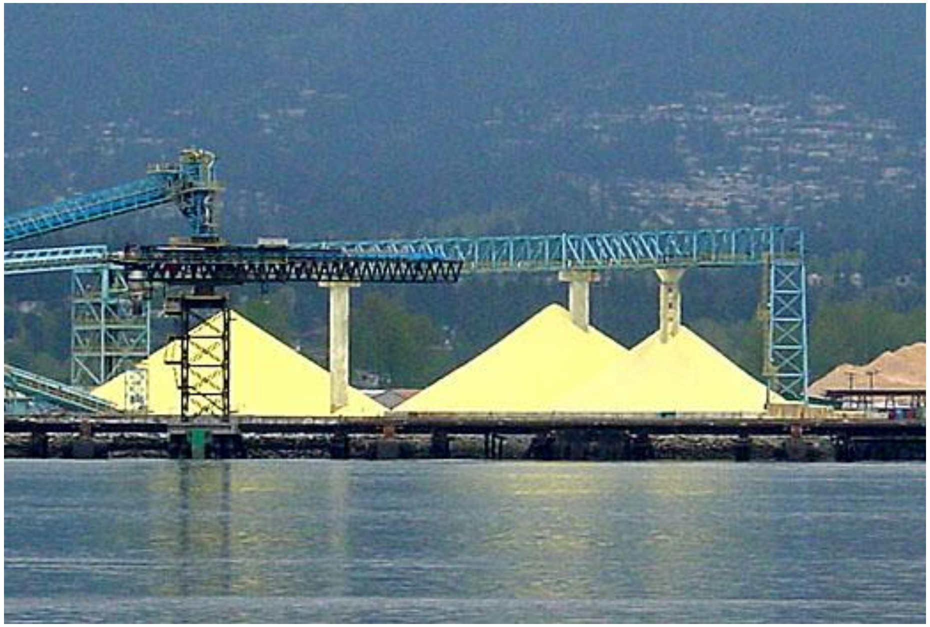
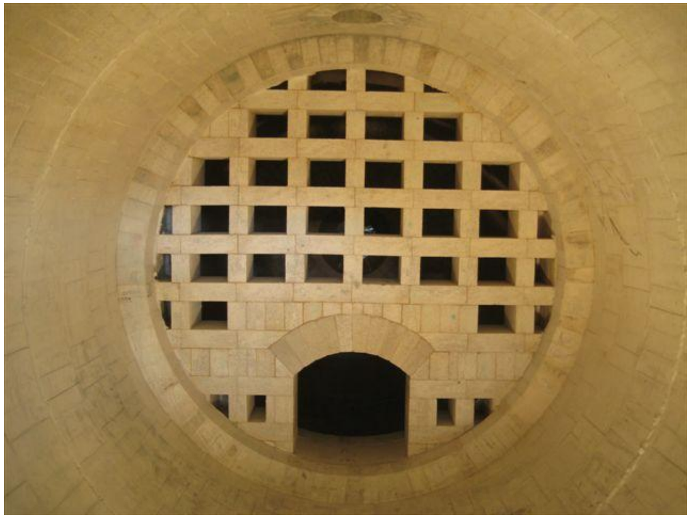
Claus Process



$$8H_2S + 5O_2 \rightarrow SO_2 + 7S + 8H_2O$$

- The Claus process is the largest volume gas desulfurizing process and is used to recover elemental sulfur from hydrogen sulfide.
- H_2S is burned and then reduced to form elemental sulfur. Often ammonia is present in the feed and needs to be converted to N_2.
- Originally developed as a term project for an Advanced Chemical Reactor Design course.

Claus Process Reactor



Checkerwall

Vectorwall

- 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.

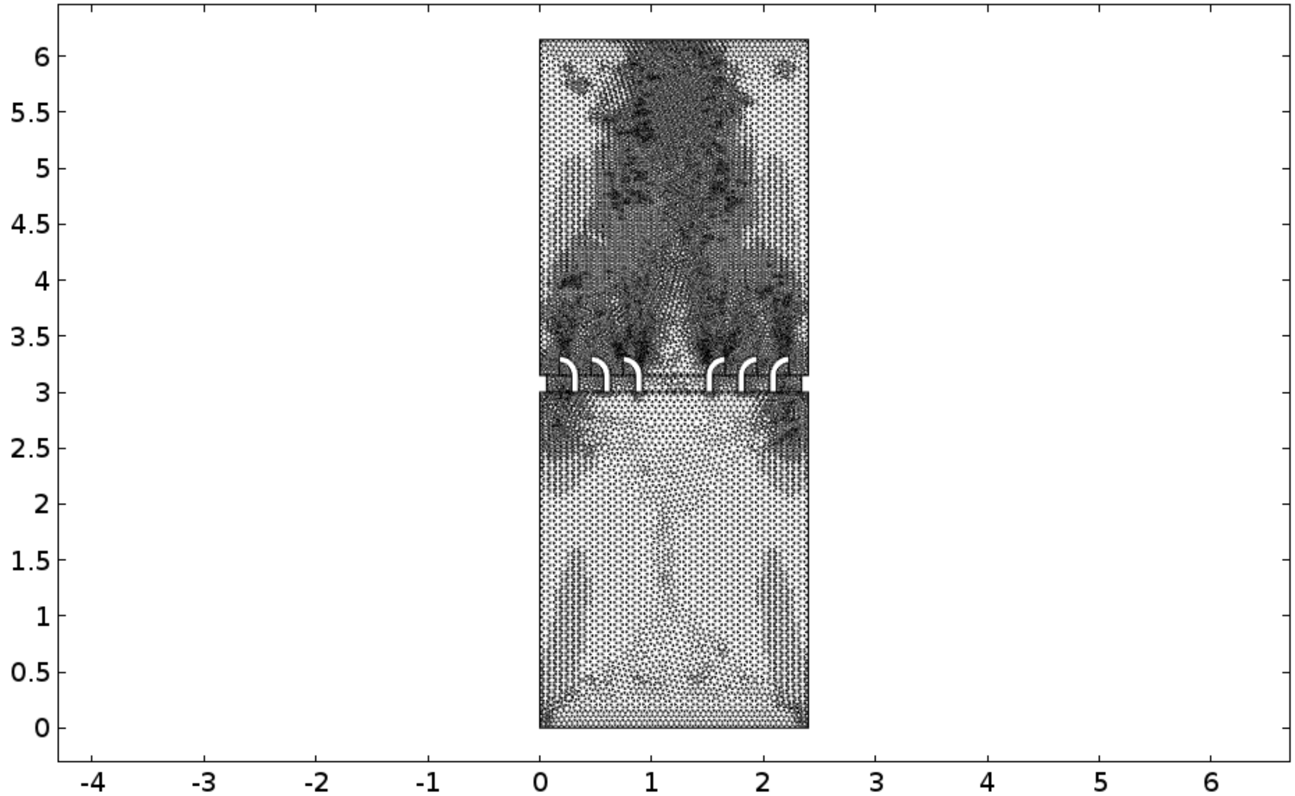
Claus Process Reactions

Reactions and Rate Laws	
$H_2S + \frac{3}{2}O_2 \xrightarrow{k_1} SO_2 + H_2O$ $r_1 = k_1 P_{H_2S} P_{O_2}^{1.5}$	$NH_3 + \frac{3}{4}SO_2 \xrightarrow{k_5} \frac{3}{8}S_2 + \frac{3}{2}H_2O + \frac{1}{2}N_2$ $r_5 = k_5 C_{NH_3}^{0.25} C_{SO_2}^{0.5}$
$NH_3 + \frac{3}{4}O_2 \xrightarrow{k_2} \frac{3}{2}H_2O + \frac{1}{2}N_2$ $r_2 = k_2 P_{NH_3} P_{O_2}^{0.75}$	$CH_4 + 2O_2 \xrightarrow{k_5} CO_2 + 2H_2O$ $r_6 = k_6 C_{CH_4}^{0.2} C_{O_2}^{1.3}$
$H_2 + \frac{1}{2}O_2 \xrightarrow{k_3} H_2O$ $r_3 = k_3 C_{H_2} C_{O_2}$	$H_2 + \frac{1}{2}S_2 \underset{k_{7r}}{\overset{k_{7f}}{\rightleftharpoons}} H_2S$ $r_7 = k_{7f} P_{H_2} P_{S_2} - k_{7r} P_{H_2S} P_{S_2}^{0.5}$
$CO + \frac{1}{2}O_2 \xrightarrow{k_4} CO_2$ $r_4 = k_4 C_{O_2}^{0.25} C_{CO} C_{H_2O}^{0.5}$	

- 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.

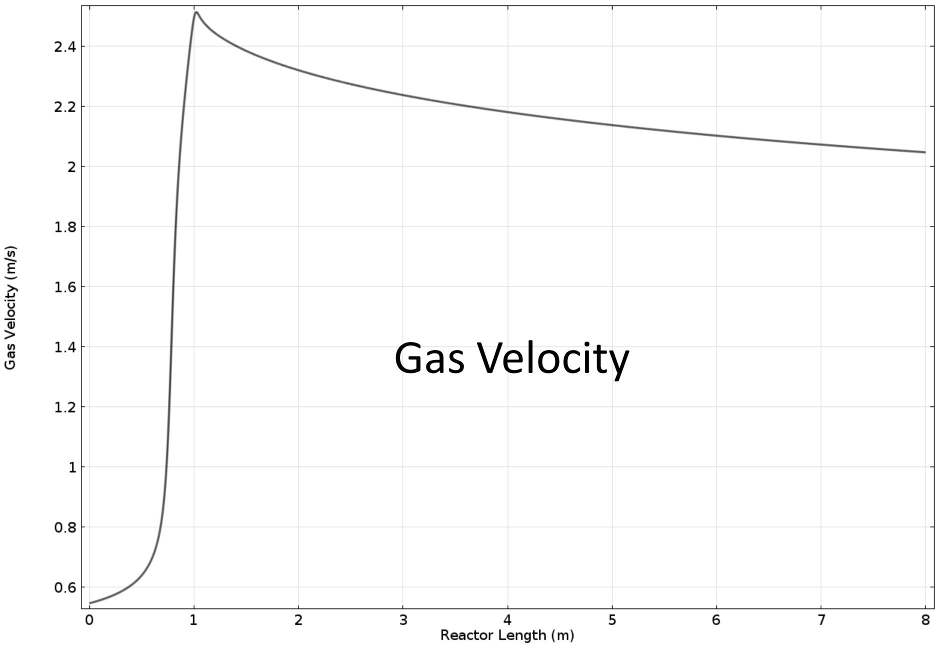
Claus Process Reactor
Comsol Implementation

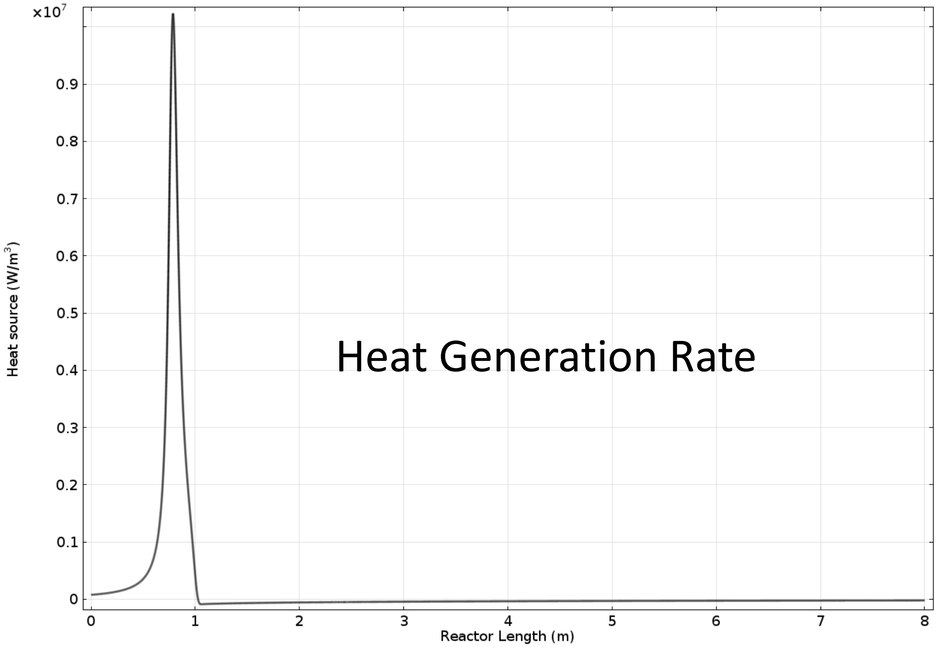
- The model coupled the Chemical Engineering, CFD, and Heat Transfer modules together and assumed compressible flow.
- Used simplified 1-D and eventually 2-D geometries. Adaptive meshing was required (~700,000 – 1,000,000 degrees of freedom).
- Class project solved the kinetics in ideal continuous stirred tank and plug flow reactors.



Claus Process Reactor
Comsol Implementation

- 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.

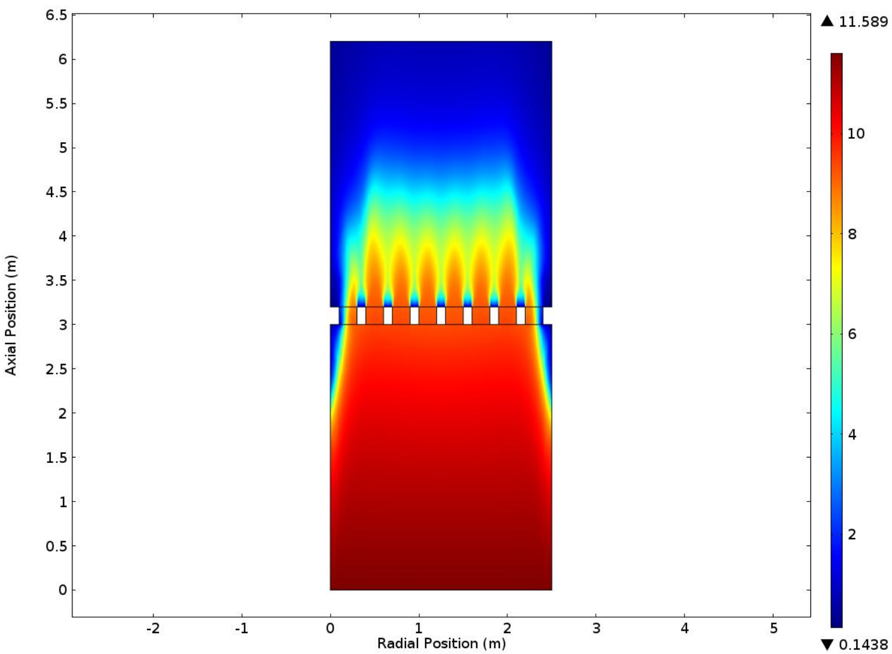




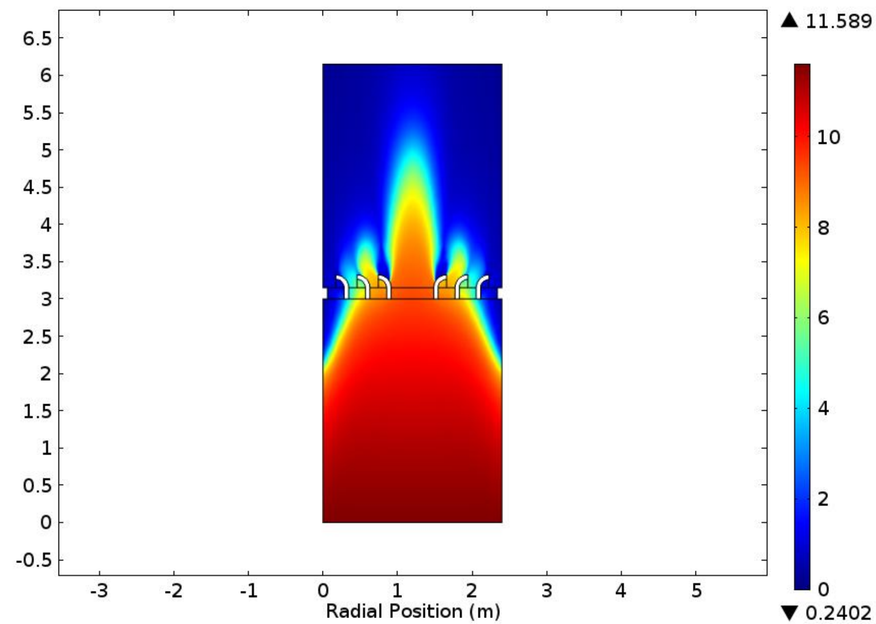
Claus Process Reactor Comsol Implementation

- 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.

Checkerwall



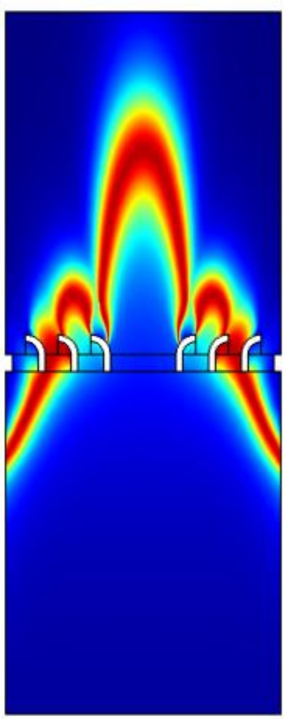
Vectorwall™



Hydrogen Sulfide Concentration Profiles

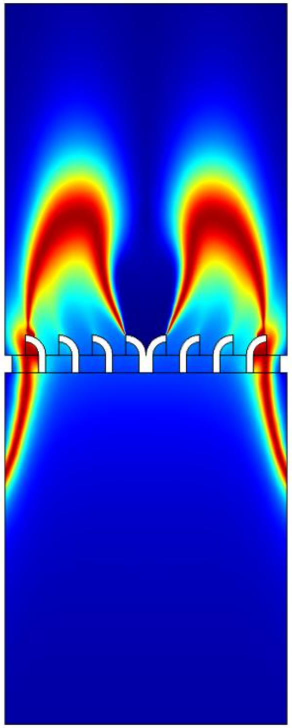
Claus Process Reactor
Comsol Implementation

- 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^{TM}, 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.

- Funding for this project was provided by:

New York State Pollution Prevention Institute