Claus Process Reactor Simulation

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Abstract

A model was developed to simulate the reaction, concentration field, flow field, and temperature distribution inside a Claus reactor for converting hydrogen sulfide to sulfur. The model considered two ideal reactors, a continuous stirred tank reactor and a plug flow reactor. As expected, two ideal reactors showed much different behaviors in terms of reactant conversion and operating temperature. Operation in the plug flow reactor was much less severe. A full 1D model was developed for this system as well. This is a dispersed plug flow model able to mimic the performance of the two idea reactors discussed above. The model included the thermodynamics of the reactions, the actual transport properties of the gaseous species, the fluid flow, and the heat transfer that would occur in a more realistic version of the Claus system.

The problem was an especially challenging one due to the flow rates of material involved, the overall size of the reactor, and the highly exothermic nature of the reactions. Temperatures approaching 1800 K were predicted within the flame zone. A 2D simulation was also conducted at a reduced heat generation rate due to limitations in the capability of the hardware. A traditional checkerwall configuration and a simplified VectorWall™ configuration from Blasch Precision Ceramics, Inc. were used. The ability to alter the flow field using the VectorWall™ and thereby affect the reaction and heat generation rate are shown in Figures 1 and 2.

This is likely the first time that the details of the flow, temperature, concentration, and heat generation fields have been simulated for a reactor of this type. The simulation was run in COMSOL Multiphysics® using reaction engineering, transport of dilute species, laminar flow, and heat transfer in fluids physics. NASA polynomials were used to calculate the reaction and thermodynamic parameters for each of the seven reactions and eleven species in the model and the transport parameters were all evaluated within COMSOL using built in kinetic theory approximations and Lennard-Jones constants for each species. The 2D simulation was conducted using adaptive meshing and the final simulation required approximately 60,000 elements.

Figures used in the abstract

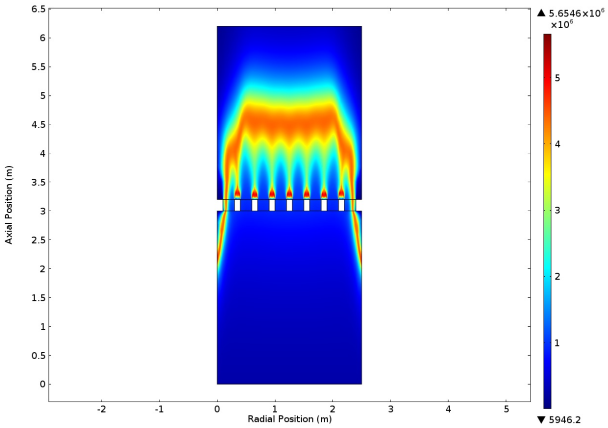

Figure 1: Heat generation rate in a Claus reactor using a checkerwall configuration.

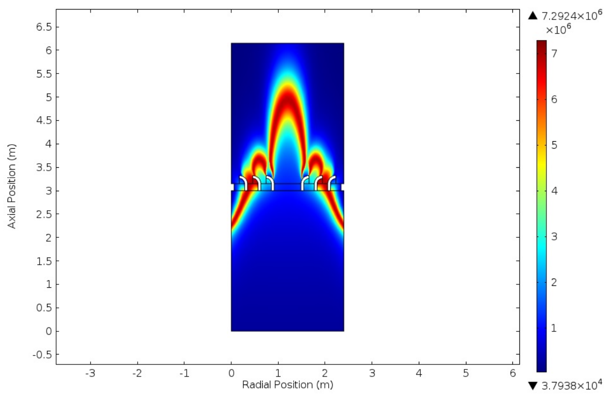

Figure 2: Heat generation rate in a Claus reactor using a Vectorwall configuration.