THREE-DIMENSIONAL CFD SIMULATION OF INDUSTRIAL CLAUS REACTORS

By

Abdel Samea Abdel Fattah Abdel Samea

A Thesis Submitted to the
Faculty of Engineering at Cairo University
in Partial Fulfillment of the
Requirements for the Degree of
DOCTOR OF PHILOSOPHY
in
Chemical Engineering

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Three-Dimensional CFD Simulation of Industrial Claus Reactors

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Summary:

The Claus process is used extensively in the industry to recover elementary sulfur from hydrogen sulfide present in gases from refineries and natural gases. It involves thermal oxidation of hydrogen sulfide and its reaction with sulfur dioxide to form sulfur and water vapor. In this study, we used a computational fluid dynamics (CFD) tool to build a three-dimensional finite-element model that describes the detailed flow fields and chemical reactions for two different industrial cases. The first case consisted of three Claus industrial reactors in series (R1A,R1B and R1C) and the second case consists of two Claus industrial reactors in series (R2A and R2B), each having one inlet and one outlet with different operating temperatures and feed concentrations. The flow behavior and the outlet compositions of the partially-packed Claus reactors at temperature range of 458 K to 570 K, with varying SO_2 and H_2S feed concentrations are presented and discussed. We present two sets of empirical kinetic rate equations, both of which give good agreement with the available industrial data.

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Nomenclature

C_i	Concentration of the each species i, mol/m^3
C_{pL}	Liquid heat capacity at constant pressure, J/(mol.K)
D	Diffusion coefficient,
E	Activation energy, J/mole
Eq.	Equilibrium
ΔH_{ri}	Enthalpy of reaction i, J
k	Permeability of the porous medium, m^2
k_0	Constant, h^{-1}
k_{eq}	Equivalent thermal conductivity, W/(m.K)
k_L	Liquid conductivity, W/(m.K)
k_p	Solid conductivity, W/(m.K)
Op.	Operating
P	Total pressure, Pa
P_i	Partial pressure of component i, atm
Q	Mass source or mass sink.
Q_H	Heat source (or sink), J
R	Universal gas constant, m^3.atm/mol.K
R_i	Rate of reaction j, mol/(m^3.s)
T	Absolute temperature, K
u	Velocity vector, m/s

Greek Symbols

μ	Denotes the dynamic viscosity of the fluid, Pa.s
ρ	The density of the fluid,kg/m^3
ρ_L	Liquid density,kg/m^3
ε_p	Bed porosity

Subscripts

eq	Equivalent
f	Fluid Phase
L	Liquid Phase
p	Solid particles
ri	Reaction
s	Solid Phase

Abstract

The Claus process is used extensively in industry to recover elemental sulfur from hydrogen sulfide present in gases from refineries and natural gas. It involves thermal oxidation of hydrogen sulfide and its reaction with sulfur dioxide to form sulfur and water vapor. In this study, we used a computational fluid dynamics (CFD) tool is used to build a three-dimensional finite-element model that describes the detailed flow fields and chemical reactions for two different industrial cases. The first case consists of three Claus industrial reactors while the second case consists of two Claus industrial reactors, both cases in series, and each having one inlet and one outlet with different operating temperatures and feed concentrations. The flow behavior and outlet compositions of the partially-packed Claus reactors at temperature range of 458 K to 570 K, with varying SO_2 and H_2S feed concentrations are presented and discussed. Two sets of empirical kinetic rate equations, are presented, both of which give good agreement with the available industrial data.