



Cairo University

# **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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**Title of Thesis:**

**Three-Dimensional CFD Simulation of Industrial Claus Reactors**

**Key Words:**

Claus Reactor; COMSOL; CFD Simulation; Reaction Kinetics

**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<sub>2</sub> and H<sub>2</sub>S 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 <sup>3</sup>
$C_{pL}$	Liquid heat capacity at constant pressure, J/(mol.K)
$D$	Diffusion coefficient,
$E$	Activation energy, J/mole
Eq.	Equilibrium
$\Delta H_{ri}$	Enthalpy of reaction i, J
$k$	Permeability of the porous medium, m <sup>2</sup>
$k_0$	Constant, h <sup>-1</sup>
$k_{eq}$	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 <sup>3</sup> .atm/mol.K
$R_i$	Rate of reaction j, mol/(m <sup>3</sup> .s)
$T$	Absolute temperature, K
$u$	Velocity vector, m/s

## **Greek Symbols**

$\mu$	Denotes the dynamic viscosity of the fluid, Pa.s
$\rho$	The density of the fluid, kg/m <sup>3</sup>
$\rho_L$	Liquid density, kg/m <sup>3</sup>
$\varepsilon_p$	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 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  $\text{SO}_2$  and  $\text{H}_2\text{S}$  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.