

Numerical Simulation of a High-Pressure Reactive Furnace in Recovering Sulfur from Sour Gas

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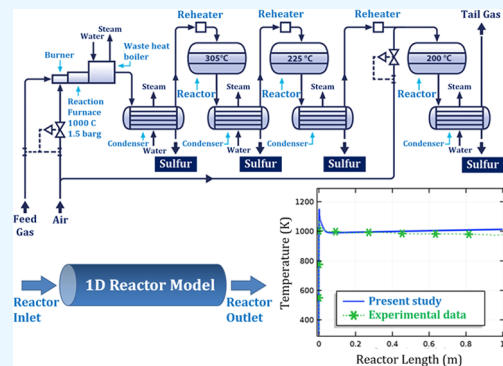
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ABSTRACT: Nowadays, the Claus process is one of the most efficient procedures to recover sulfur from acid gases. In the current study, the effect of working pressure and the role of initial species (sour gas, ammonia, carbon dioxide, hydrocarbon, nitrogen, and oxygen) are analyzed using COMSOL software. The reaction occurs between acid gases, which contain 88% H₂S, 10.5% CO₂, 0.49% N₂, and 1.01% CH₄ in terms of molar percentage, and pure air. A good agreement is obtained between the numerical simulation results and experimental data. According to the results, there is a direct correlation between the conversion rate of acid gases and the increase in pressure. However, this rise in reactor pressure also leads to an undesirable increase in the outlet temperature. It is also observed that reduction of hydrogen sulfide inflow decreases the sulfur monoxide production rate, which in turn significantly affects the reactor temperature and the sulfur recovery rate. The more the oxygen that enters the reactor, the more the hydrogen sulfides that change into sulfur.



1. INTRODUCTION

Sweetening of hydrogen sulfide and production of carbon dioxide are two of the most important factors in crude oil refineries and petrochemical industry processes.¹ Sulfur has a wide range of applications, including the production of vitriol, chemical organics and minerals, manures, explosives, rayon, reagents, color softeners, rubber, matches, and phosphate fertilizers. Therefore, recovery of sulfur from acid gases in a refinery is quite advantageous.² Most of the studies regarding sulfur recovery from sour gas have been devoted to the analysis of chemical kinetics, optimization of the recovery process, and assessment of different types of existing processes in this regard.³ One of the most progressive ways to recovery of sulfur is to utilize the Claus process or direct oxidation.⁴ This process consists of two steps, namely, thermal and catalytic processes. Reference⁴ highlights that the conversion of hydrogen sulfide is temperature-dependent, such that the thermal stage accounts for approximately 50% of the total reactions. The resulting sulfur from this segment can be recovered up to 99% in the catalytic section.⁵ More specifically, sulfur recovery processes based on the Claus method involve the following operating phases, as illustrated schematically in Figure 1.^{6,7}

- (1) The reactive furnace, where hydrocarbons and other combustible gases produce SO₂ in the Claus process.
- (2) A waste heat boiler to cool down combustion products to the typical range of 315–870 °C.
- (3) Catalysts, which improve H₂S and SO₂ reactions by 2–4 catalytic reactors.

- (4) Reheating is performed after condensation and separation of sulfur in order to maintain considerable gas flow at a temperature higher than the sulfur dew point temperature.
- (5) Some condensers are utilized to cool down the outlet gas flow from the catalytic converters to about 125 °C.

The Claus process is one of the most widely used methods in petrochemical refineries to recover sulfur from hydrogen sulfide.^{16,17} It has been significantly developed in recent years. The modified Claus method is one of the best approaches to enhance the sulfur recovery process. The literature shows that optimization of the modified Claus process to achieve enhanced sulfur recovery and reduced environmental impact requires sufficient knowledge about kinetics of various reactions occurring in the reaction furnace and the temperature recovery furnace.^{8–12} Different types of models have been proposed for the chemical kinetics of the Claus process.^{13–15} It was observed that the Claus process has been successful in improvement of sulfur recovery with a reduced cost.^{18,19} These studies have introduced new models for chemical kinetics and reaction among H₂S, SO₂, and CO₂ and side reactions, such as the

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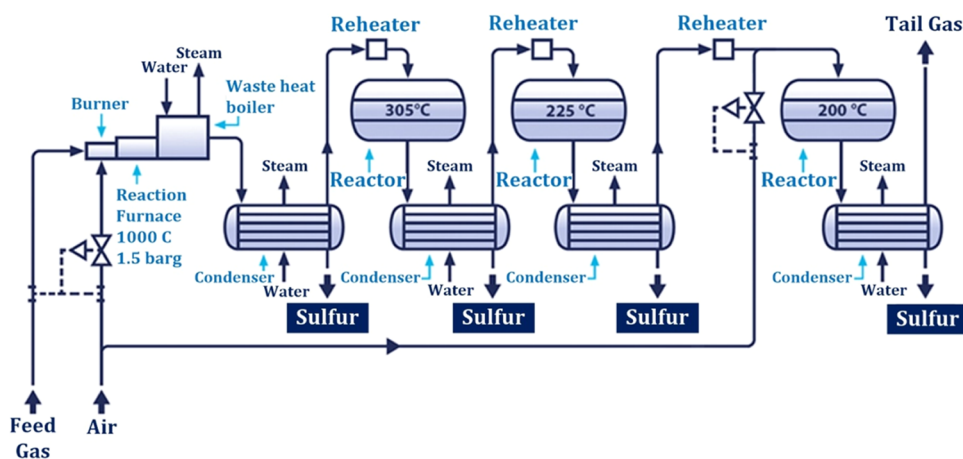


Figure 1. Schematic representation of the Claus process for sulfur recovery.

hydrolysis of COS and CS₂. However, there are numerous challenges in the Claus process such as the reaction mechanism in sulfur recovery units and the development of chemical kinetics. Additionally, such models are still not able to accurately calculate concentrations of CO, H₂, COS, and CS₂ due to restrictions in chemical kinetics. The present study attempts to correctly model such quantities. Another contribution of the current study is to examine the impact of pressure and inlet feed as two effective factors in the precision of chemical kinetics in sulfur recovery modeling.

By implementing computational fluid dynamics (CFD) in the COMSOL 5.5 software, this study investigates the challenges in the sulfur production rate, outlet temperature, and carbon dioxide production. In the next section, the setup of the computational model will be introduced. The results are presented in Section 3, with a discussion about the observed trends and physical impacts of the findings.

2. COMPUTATIONAL MODELING

A 1D plug-flow reactor is considered the computational model. It is used to describe chemical reactions within a cylindrical reactor operating under steady-state and adiabatic flow conditions. The length and diameter of the reactor are 1 and 0.35 m, respectively. Because of the high length (one-dimensional) assumption in such reactors, the concentration of gases is fixed. Due to the generation of hot spots inside the reactor induced by an exothermal reaction, internal temperature control is difficult. However, these reactions have the highest amount of H₂S conversion. Figure 2 schematically describes this kind of a reactor.

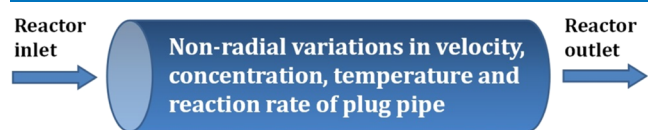


Figure 2. Schematic representation of the plug reactor in the current research.

2.1. Governing Equations. For thermosynthetic modeling of the problem, conservation of mass and the one-dimensional energy equation along the plug pipe are the main governing equations, as follows.

2.1.1. Conservation of Mass. In COMSOL as a finite element solver, the conservation of mass for the *j*th element and the *i*th species in the reaction can be expressed as follows¹¹

$$\frac{d(\alpha A_c C_{i,j})}{dt} = (F C_i)_{j-1} - (F C_i)_j + r_{i,j} \alpha A_c \text{ for } i = 1 \text{ to } NC$$

$$, j = 1 \text{ to } N \quad (1)$$

where $NC = 13$ is the number of existing species in the reaction of acid gases, air, and water steam. N is the number of participating elements in the discretization of equation in the finite element method. F_i (m³/s) and C_i (kmol/s) are the flow rate and the concentration of the *i*th species in the reaction, respectively. $r_{i,j}$ (kmol/m³s) represents the production rate of the *i*th species for the *j*th element. $\alpha = 1$ m is the reactor length, and A_c (m²) is the cross-sectional area of the plug pipe.

2.1.2. Conservation of Energy. For the *j*th element, the energy conservation equation is as follows

$$\frac{d(\rho C_v \alpha A_c C_v T_j)}{dt} = (F_M H)_{j-1} - (F_M H)_j \text{ for } j = 1 \text{ to } N \quad (2)$$

where F_{Mj} (kmol/s) is the molar rate of existing gases in the reaction, H (kJ/mol) is the molar enthalpy, C_v (J/kmol K) is the thermal capacity, and T (K) is the reaction temperature. The enthalpy of reaction can be calculated as follows

$$H = \sum_i Y_i \left[\Delta_f H_i^0 + \int_{T_{ref}}^T C_p^T dT \right] \quad (3)$$

where Y_i and $\Delta_f H_i^0$ (J/kmol) are the mass fraction and enthalpy of formation of the *i*th species at the standard condition, respectively, and C_p^T (J/kmol K) represents the thermal capacity. ANSYS Reaction Workbench 2021 software is used to calculate the thermodynamic properties of reactions.

2.2. Reaction Kinetics Modeling. Among numerous existing reactions in the reactive furnace during the Claus process as discussed in refs 12,14,15, a kinetic model consisting of 12 important reactions is considered for the present study. Previous studies indicate that the equilibrium assumption in modeling of reactions in the Claus process leads to incorrect results. In the current research, this is resolved by considering the finite rate model for chemical reactions. Table 1 summarizes 12 employed reactions in this research and the Arrhenius coefficients corresponding to each reaction.

Table 1. List of Employed Reactions in the Claus Process in the Present Research

reaction no.	reaction	reaction no.	reaction
R1	$\text{H}_2\text{S} + 1.5\text{O}_2 \rightarrow \text{SO}_2 + \text{H}_2\text{O}$ $r = A \exp\left(\frac{-E}{RT}\right) P_{\text{H}_2\text{S}}^{1.5} P_{\text{O}_2}$ $A = 1.4 \times 10^9, E = 1 \quad (\text{R1})$	R7	$\text{CH}_4 + \text{CO}_2 \rightarrow 2\text{CO} + \text{H}_2$ $r = A \exp\left(\frac{-E}{RT}\right) C_{\text{CH}_4} C_{\text{CO}_2}$ $A = 8.06 \times 10^9, E = 498 \quad (\text{R7})$
R2	$\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$ $r = A \exp\left(\frac{-E}{RT}\right) C_{\text{CH}_4}^{0.62} C_{\text{O}_2}^{0.51}$ $A = 348, E = 3.77 \quad (\text{R2})$	R8	$\text{CO} + 0.5\text{S}_2 \rightarrow \text{COS}$ $r = A_1 \exp\left(\frac{-6700}{T}\right) C_{\text{CO}} C_{\text{S}_2} - A_2 \exp\left(\frac{-21630}{T}\right) C_{\text{COS}}$ $A_1 = 3.18 \times 10^5, A_2 = 4.36 \times 10^9 \quad (\text{R8})$
R3	$\text{H}_2 + 0.5\text{O}_2 \rightarrow \text{H}_2\text{O}$ $r = A \exp\left(\frac{-E}{RT}\right) C_{\text{H}_2}^{0.229} C_{\text{O}_2}^{0.771}$ $A = 7.63 \times 10^{10}, E = 48.2 \quad (\text{R3})$	R9	$\text{CO} + \text{H}_2\text{S} \rightarrow \text{COS} + \text{H}_2$ $r = A \exp\left(\frac{-E}{RT}\right) C_{\text{CO}} C_{\text{H}_2\text{S}}^{0.5} - \exp\left(3.12 + \frac{334.47}{T}\right) C_{\text{COS}} C_{\text{S}_2} / C_{\text{H}_2\text{S}}^{0.5}$ $A = 1.59 \times 10^5, E = 26.5 \quad (\text{R9})$
R4	$\text{CO}_2 + \text{H}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$ $r = A \exp\left(\frac{-E}{RT}\right) (C_{\text{CO}_2} C_{\text{H}_2}^{0.5})^{0.229} C_{\text{O}_2}^{0.771} - \exp(-4.72 + 4800/T) (C_{\text{CO}} C_{\text{CO}} / C_{\text{H}_2}^{0.5})$ $A = 3.95 \times 10^{10}, E = 62.03 \quad (\text{R4})$	R10	$\text{CH}_4 + 2\text{S}_2 \rightarrow \text{CS}_2 + 2\text{H}_2\text{S}$ $r = A \exp\left(\frac{-19320}{T}\right) C_{\text{CH}_4} C_{\text{S}_2}$ $A = 5.53 \times 10^{10} \quad (\text{R10})$
R5	$\text{H}_2\text{S} \rightarrow 0.5\text{S}_2 + \text{H}_2$ $r = A_1 \exp\left(\frac{-E_1}{RT}\right) P_{\text{H}_2\text{S}}^{0.5} P_{\text{S}_2} - A_2 \exp\left(\frac{-E_2}{RT}\right) P_{\text{H}_2} P_{\text{S}_2}$ $A_1 = (5.263 \pm 0.26) \times 10^6, E_1 = (13.6 \pm 1) \times 10^6, E_2 = 45 \pm 0.3, E_2 = 23.4 \pm 0.2 \quad (\text{R5})$	R11	$\text{H}_2\text{S} + \text{SO}_2 + \text{H}_2 \rightarrow \text{S}_2 + 2\text{H}_2\text{O}$ $r = A \exp\left(\frac{-E}{RT}\right) (P_{\text{H}_2\text{S}} P_{\text{SO}_2} P_{\text{H}_2}) - 1/K_{\text{eq}} P_{\text{H}_2\text{O}}^2 P_{\text{S}_2}$ $A = 3.583 \times 10^7, E = 26 \quad (\text{R11})$
R6	$\text{CH}_4 + \text{S}_2 + \text{H}_2\text{O} \rightarrow \text{COS} + \text{H}_2\text{S} + 2\text{H}_2$ $r = A \exp\left(\frac{-E}{RT}\right) C_{\text{CH}_4} C_{\text{S}_2}$ $A = 5.53 \times 10^6, E = 38.7 \quad (\text{R6})$	R12	$\text{NH}_3 + 0.75\text{S}_2 \rightarrow 1.5\text{H}_2\text{O} + 0.5\text{N}_2$ $r = A \exp\left(\frac{-E}{RT}\right) P_{\text{NH}_3}^{0.75} P_{\text{S}_2}$ $A = 4.43 \times 10^6, E = 40 \quad (\text{R12})$

Table 2. Initial Conditions Considered for Case Studies 1, 2, and 3

parameters	value	unit	parameters	value	unit
reactor pressure	160 (1,2,3)	kPa	initial molar rate of N ₂	(1) 79.3306 (2) 80.4444 (3) 47.7306	mol/s
inlet gas temperature	350 (1,2,3)	K	initial concentration of H ₂ S	(1) 25.8384 (2) 22.0885 (3) 14.8032	mol/m ³
initial molar rate of H ₂ S	(1) 32.416 (2) 27.841 (3) 16.6028	mol/s	initial concentration of O ₂	(1) 12.5673 (2) 11.0203 (3) 6.05213	mol/m ³
initial molar rate of O ₂	(1) 49.6528 (2) 52.6028 (3) 31.1278	mol/s	initial concentration of H ₂ O	0.0000 (1,2,3)	mol/m ³
initial molar rate of H ₂ O	0.0000 (1,2,3)	mol/s	initial concentration of SO ₂	0.0000 (1,2,3)	mol/m ³
initial molar rate of SO ₂	0.0000 (1,2,3)	mol/s	initial concentration of CH ₄	(1) 0.0776 (2) 0.0676 (3) 0.0199	mol/m ³
initial molar rate of CH ₄	(1) 32.4167 (2) 27.8417 (3) 16.6028	mol/s	initial concentration of CO ₂	(1) 2.6167 (2) 2.2191 (3) 1.6870	mol/m ³
initial molar rate of CO ₂	(1) 32.4167 (2) 27.8417 (3) 16.6028	mol/s	initial Concentration of H ₂	0.0000 (1,2,3)	mol/m ³
initial molar rate of H ₂	0.0000 (1,2,3)	mol/s	initial concentration of CO	0.0000 (1,2,3)	mol/m ³
initial molar rate of CO	0.0000 (1,2,3)	mol/s	initial concentration of S ₂	0.0000 (1,2,3)	mol/m ³
initial molar rate of S ₂	0.0000 (1,2,3)	mol/s	initial concentration of COS	0.0000 (1,2,3)	mol/m ³
initial molar rate of COS	0.0000 (1,2,3)	mol/s	initial concentration of CS ₂	0.0000 (1,2,3)	mol/m ³
initial molar rate of CS ₂	0.0000 (1,2,3)	mol/s	initial concentration of NH ₃	(1) 3.7187 (2) 3.3242 (3) 0.000	mol/m ³
initial molar rate of NH ₃	(1) 9.7944 (2) 8.7556 (3) 0.0000	mol/s	initial concentration of N ₂	(1) 37.2507 (2) 41.7248 (3) 24.6092	mol/m ³

In the equations presented in Table 1, r (kmol/m³ s) is the reaction rate, E (J/kmol) is the activation energy, R (J/kmol K) is the universal gas constant, and A is a constant coefficient. C_i (kmol/m³) and P_i (Pa) represent the concentration and partial pressure of the i th species in the reaction, respectively.

2.3. Initial Conditions and Simulation. Considering $NC = 13$ as the number of species in the reaction and N as the number of computational elements, $N \cdot (NC + 1)$ ordinary differential equations should be solved simultaneously. The process is simulated in COMSOL 5.5 software based on the finite element method. The initial temperature is set to 298 K. Three case studies are considered, and their corresponding initial molar rates and initial concentrations are presented in Table 2. In all three case studies, the inlet temperature and reactor working pressure are set to 350 K and 160 kPa, respectively. The input configurations and working pressure are considered to be similar to references^{13,17} to validate the model accuracy. For the first two case studies, the rate of input reactants, inlet temperature, and working pressure are considered in the suitable range for industrial sulfur recovery furnaces, while the configuration considered in the third case study is to evaluate the model accuracy in a more extended scope.

3. RESULTS AND DISCUSSION

3.1. Validation of the Proposed Reactor Model. An adiabatic reactor is considered under steady-state conditions,

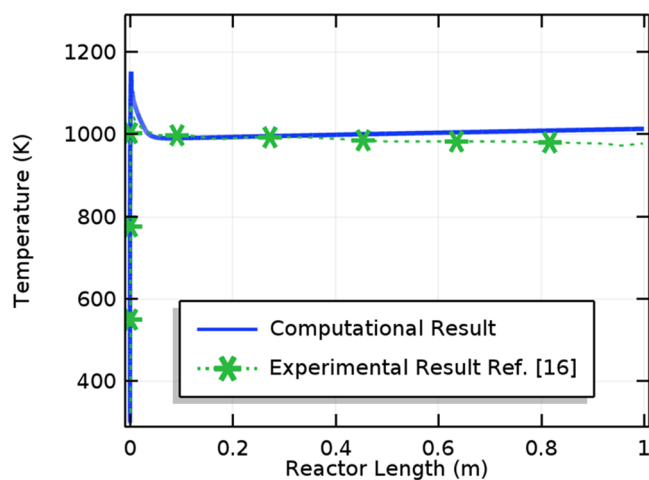
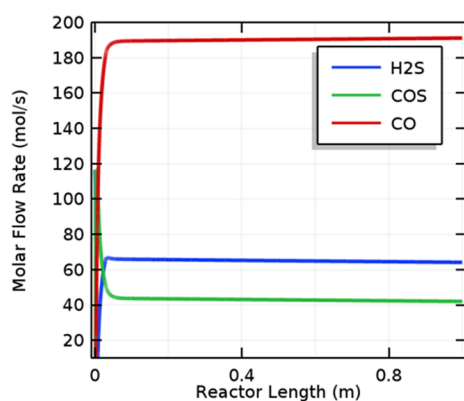


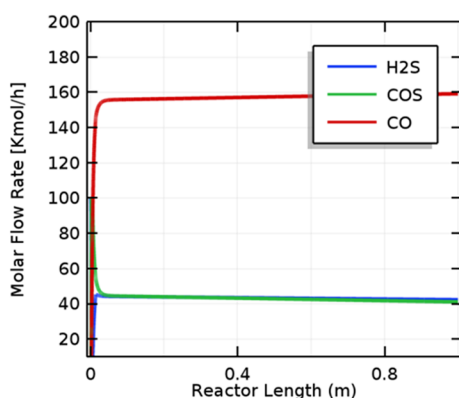
Figure 3. Comparison of simulation results for temperature along the pipe length with the experimental results of ref. [16].

where acid gases and air are regarded as ideal gases with high temperature and low pressure. In the simulated reactor, acid gases composed of 88% H₂S, 10.5% CO₂, 0.49% N₂ gas, and 1.01% CH₄ react with air (79% N₂ and 21% O₂) in a reactive furnace. The reactor working pressure is considered to be 160 kPa, and the inlet feed temperature for validation is 350 K.

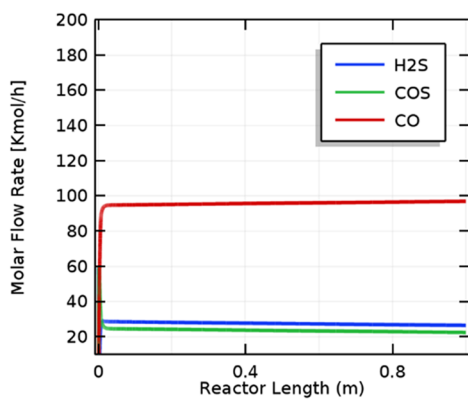
Figure 3 illustrates the longitudinal variation of temperature in the pipe for case study 1 and compares the simulation results



(a) First case study



(b) Second case study



(c) Third case study

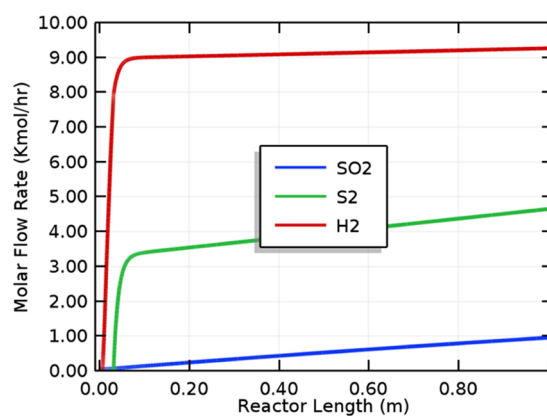
Figure 4. Molar fraction amounts of H₂S, COS, and CO in different concentrations.

Table 3. H₂S Conversion Amounts for the Three Case Studies

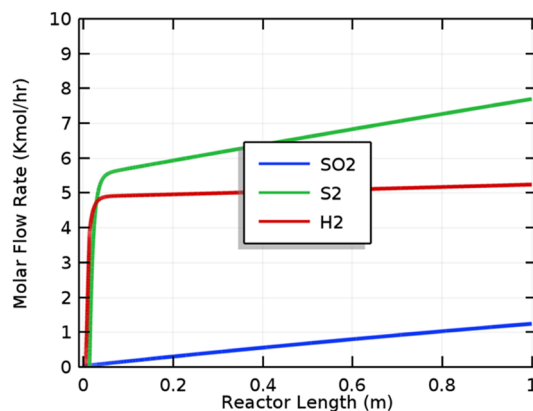
	case 1	case 2	case 3
H ₂ S conversion	45%	60%	55%

with the experimental data of.¹⁶ The experimental setup includes a three-dimensional reactor in which acid with salt gases and air are discharged.

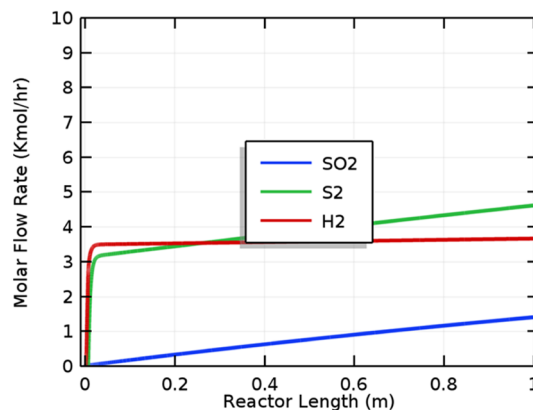
As is evident from Figure 3, there is a good agreement between the simulated temperature in the present study and the experimental data of reference.¹⁶ This figure exhibits the predicted kinetics for sulfur recovery analysis in the Claus reactive furnace precisely. It can be seen that the reactions happen in the frontal zone of the reactor where the temperature



(a) First case study



(b) Second case study



(c) Third case study

Figure 5. Molar fraction amounts of SO₂, S₂, and H₂ in various concentrations.

reaches 1150 K. It is worth mentioning that the highest temperature in industrial reactors in sulfur recovery furnaces is between 920 and 1080 K. The deviation between simulation results and experimental data is at most 6%, which is due to assumptions made in plug-flow modeling.

Since the major part of the chemical reaction occurs at the beginning of the reactor, a considerably lower reaction rate is expected downstream of the reactor. Thus, the temperature, which is a function of chemical reaction, slightly changes at this zone. However, according to Figure 3, there is a small discrepancy between simulation results and experimental data that can be explained as follows. In the current numerical simulations, a complete reaction for all components is assumed,

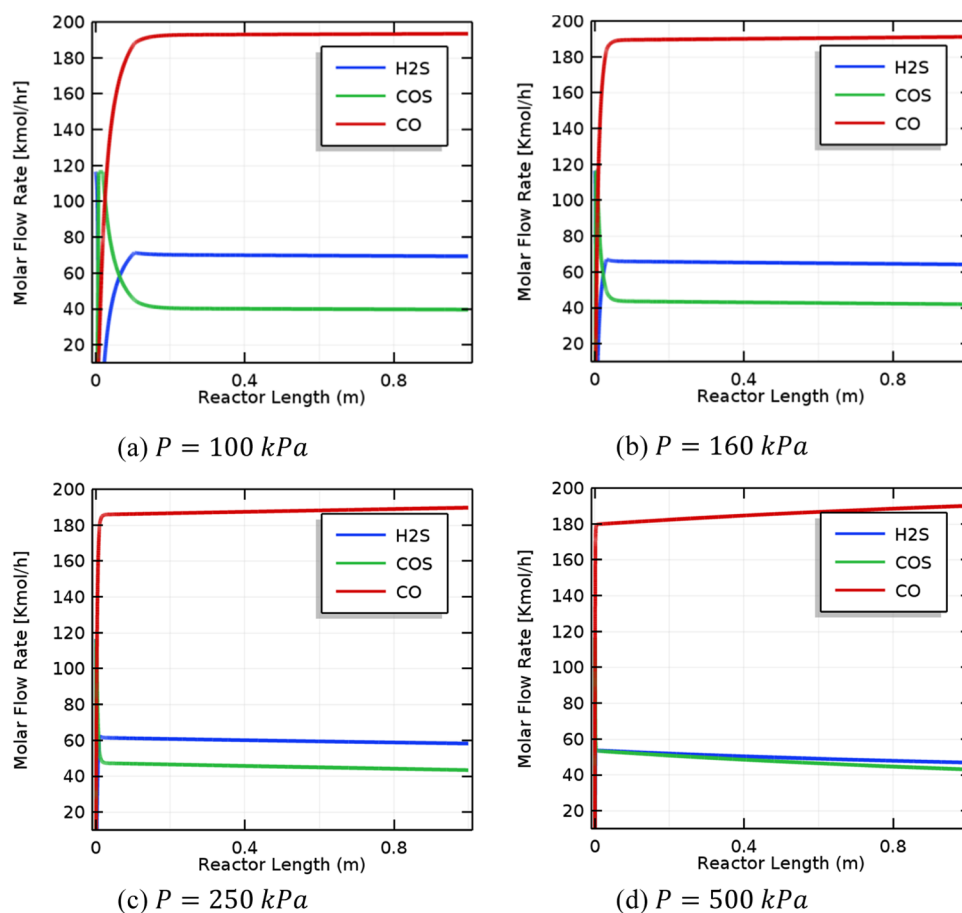


Figure 6. Molar flow rates of H₂S, COS, and CO along the reactor for different pressures.

as specified in the outlet boundary condition. However, in the real experimental scenario, some substances exit the reactor without reacting completely. The complete reaction of these components could lead to a gradual temperature increase similar to what occurs in the simulation.

3.2. Effect of Inlet Feed Concentration. Figure 4 illustrates the effect of the initial concentration of feed gas on the sulfur recovery rate for case studies 1, 2, and 3 based on Table 2. By reducing the inlet flow rate of hydrogen sulfide gas from case 1 to case 3, production of COS can also be decreased. This significantly affects the reactor temperature, as is seen later. According to the literature, the reaction between sulfur and carbon monoxide ($\text{CO} + 0.5\text{S}_2 \rightarrow \text{COS}$) significantly influences both the output temperature and the amount of sulfur recovery.^{16–18} To evaluate the amount of H₂S acidic gas conversion, the following equation can be used:

$$\text{H}_2\text{S conversion}(\%) = \frac{Y_{\text{H}_2\text{S}}^0 - Y_{\text{H}_2\text{S}}}{Y_{\text{H}_2\text{S}}^0} \times 100 \quad (4)$$

where $Y_{\text{H}_2\text{S}}^0$ is the mass fraction of H₂S acidic gas in the inlet feed gas. Table 3 presents the amounts of acidic gas conversion for the three case studies.

Because of the reduction of the hydrogen sulfide flow rate (from case 1 to case 3), it may be first expected that H₂S conversion should be reduced. However, Table 3 shows that in case 2, H₂S conversion is higher compared to that in the other two cases. This is because of the greater initial molar rate of O₂ in case 2 in comparison with those in cases 1 and 3.

Figure 5 compares the longitudinal variation of the flow rate of sulfur dioxide gas, hydrogen, and sulfur along the reactor for various concentrations (case studies). As can be seen, in the second case study in which the inlet airflow rate into the reactor is the highest (Table 2), the recovered sulfur amount is enhanced, as well. It can also be seen that increasing the concentration of hydrogen sulfide gas is more effective on sulfur recovery than reducing the amount of injected air.

3.3. Effect of the Reactor Working Pressure on Sulfur Recovery. It has been shown in the literature that when a chemical reaction occurs at temperatures lower than 1500 K, pressure is an effective factor.¹⁴ Figure 6 compares molar flow rates of H₂S, CO, and COS at pressures 100, 160, 250, and 500 kPa when the temperature is 350 K. As can be seen, the higher the pressure, the greater the H₂S concentration. Thus, production of COS as an influential component in chemical kinetics also increases. According to Figure 6, pressure does not have a significant effect on CO production. In other words, when the pressure increases, H₂S and other reactive components will be consumed more quickly along the reactor, causing acceleration of chemical reaction in the reactor.

Figure 7 demonstrates the variation of the conversion of hydrogen sulfide acid gas along the reactor for different pressures. It is evident that the higher the pressure, the greater the H₂S conversion. More specifically, H₂S conversion is 40, 45, 50, and 60% for the pressures 100, 160, 250, and 500 kPa, respectively. Thus, the pressure should be increased by a factor of 5 to reach a conversion higher than 50%, which is not practical and recommended. Thus, the selection of 160 kPa as the

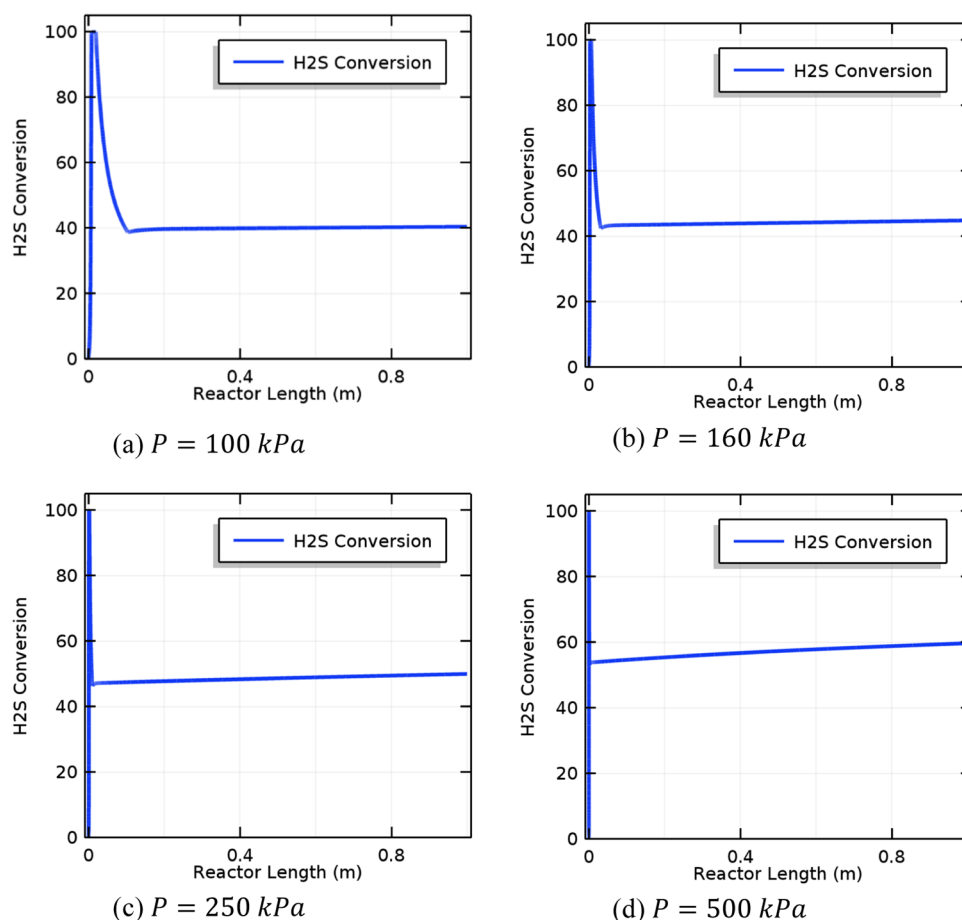


Figure 7. Longitudinal variation of H_2S conversion at different pressures.

pressure in the Claus process is reasonable as it aligns with values considered in previous studies on industrial sulfur recovery units.⁶ In our simulations, some mismatches were found between H_2S conversion at the pressure 160 kPa for the present study and that of the literature, which is due to assumptions made in the computational model of the current study. More specifically, mass concentration rate, thermal gradients, and flow effects are not considered in the numerical modeling, which can cause some deviations for H_2S conversion.

Figure 8 illustrates variation of the furnace temperature along the reactor length for different working pressures. It is evident that there is a peak of temperature immediately at the beginning of the reactor, which confirms the presence of a reaction and conversion at this zone. Although increase of pressure enhances sulfur recovery, it also causes the unfavorable effect of temperature rise in the reactor. This is one of the most important reasons for considering the reactor working pressure in the industry as 160 kPa, which confirms the results obtained in Figure 7.

4. CONCLUSIONS

In this research, 12 thermokinetic reactions with 13 species were modeled numerically for sulfur recovery in an adiabatic plug-flow reactor. The mass conservation and one-dimensional energy equations were solved simultaneously in the longitudinal direction of the plug pipe using COMSOL 5.5 software. To avoid modeling complexity, full mechanical-chemical kinetics was excluded. Based on the literature, implementation of balancing reaction hypothesis for prediction of sulfur amount

leads to some diversions and errors. The study presented here considered finite rate reactions to resolve this issue. The effect of kinetics, temperature, pressure, and inlet concentration on sulfur recovery was analyzed for three different case studies. Thermodynamic properties were extracted by using ANSYS Reaction Workbench 2021 software.

The results confirmed that utilizing the suggested kinetics and the plug-flow model is highly precise for the Claus process. It was observed that chemical reactions occur in the reactor frontal zone when the pressure is considerably high. Accordingly, one of the best ways to shorten the reactor length is to sufficiently increase the feed pressure in the reactor. Additionally, it was demonstrated that sulfur monoxide formation has a significant effect on the sulfur recovery process, similar to the findings of previous studies. In contrast, the temperature did not considerably affect production or consumption of different components in the reactor. When the inlet flow rate of hydrogen sulfide gas was reduced, the production of COS also decreased and, subsequently, the reactor temperature increased. The more the concentrated acidic gas entered the reactor, the more the H_2S conversion and the better the sulfur recovery achieved. The increase of the inlet airflow rate into the reactor also enhanced sulfur recovery. In the sulfur recovery process, the rise of the inlet airflow rate dominated the increase of the hydrogen sulfide gas concentration.

The results obtained in this research for the working pressure of 160 kPa had about a 25% deviation from sulfur recovery data on the industrial scale. Since fluid flow has a considerable influence on chemical reactions, it is recommended to model

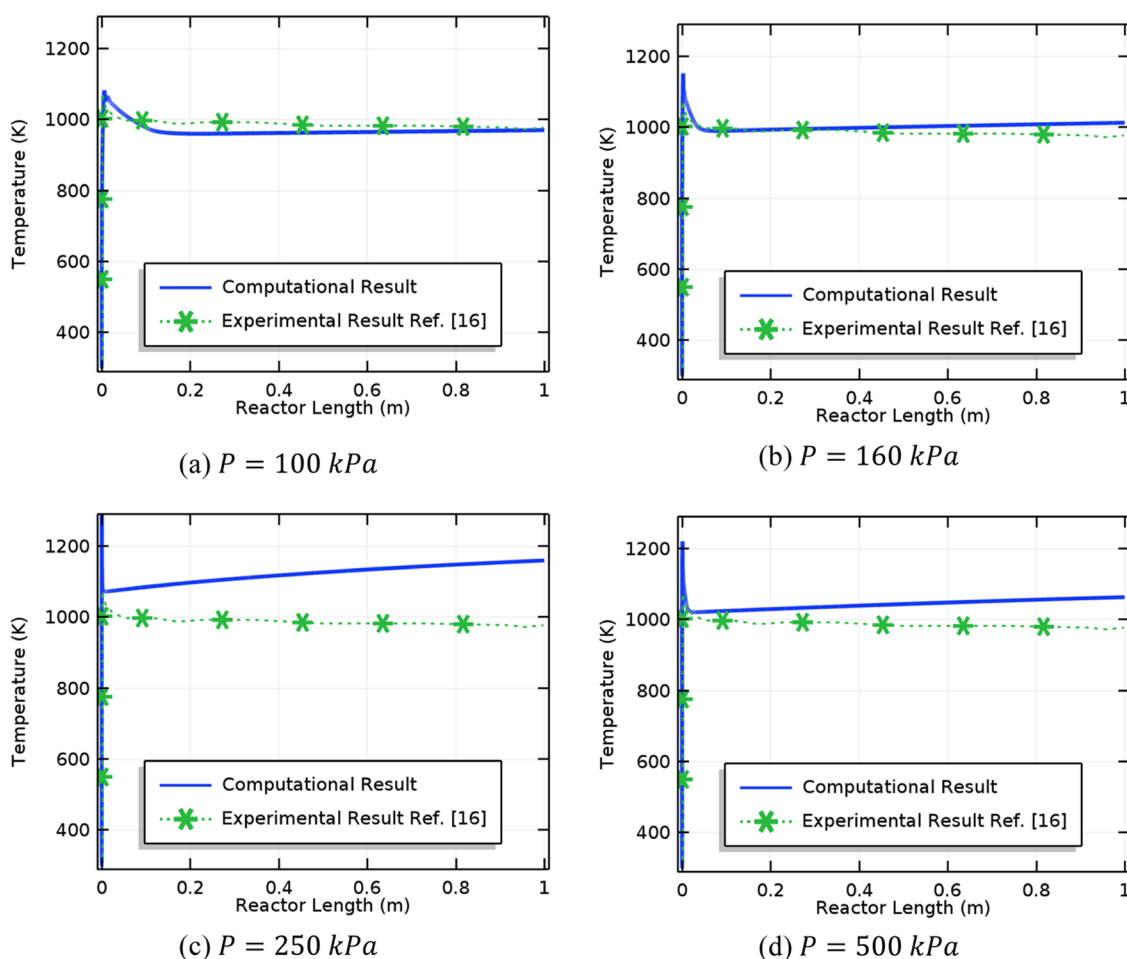


Figure 8. Variation of the furnace temperature along the reactive pipe length for different pressures.

turbulence flow characteristics in the CFD simulations in future studies. Additionally, since utilization of catalysts is one of the most effective ways for the enhancement of chemical reactions, it is suitable to analyze the effect of catalysts on the sulfur recovery process in future research.

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Notes

The authors declare no competing financial interest.

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