

Analysis for CFD of the Claus Reaction Furnace with Operating Conditions: Temperature and Excess Air for Sulfur Recovery

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ABSTRACT

In this work, a Claus reaction furnace was analyzed in a sulfur recovery unit (SRU) of the Abadan Oil Refinery where the combustion operating temperature is important since it ensures optimal performance in the reactor, this study focused on temperature of control of 1400, 1500 and 1600 K and excess air of 10, 20 and 30% to improve the reaction yield and H₂S conversion. The CFD simulation was carried out in Ansys Fluent in transitory state and in 3 dimensions, considering turbulence model $\kappa - \epsilon$ standard, energy model with transport by convection and mass transport with chemical reaction using the Arrhenius Finite – rate/Eddy dissipation model for a Kinetic model of destruction of acid gases H₂S and CO₂, obtaining a good approximation with experimental results of industrial process of the Abadan Oil Refinery, Iran. The percentage difference between experimental and simulated results varies between 0.5 to 5 % depending on species. The temperature of 1600 K and with excess air of 30% was the best, with one fraction mol of 0.054 of S₂ at the outlet and with conversion of the acid gas (H₂S) of 97.64%, which is quite good compared to the experimental one.

Keywords: CFD, SRU, Claus Reaction, Furnace, Sulfur.

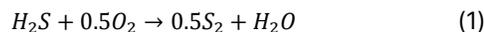
INTRODUCTION

High concentrations of sulfur and nitrogen are produced in crude oil processing, increasing the formation of hydrogen sulfide (H₂S) and ammonia (NH₃). Most of the H₂S is absorbed by the circulation of an amine solution (DEA process), and much of the ammonia is absorbed, along with proportional amounts of H₂S, in the wash with water (stripper of sour waters).

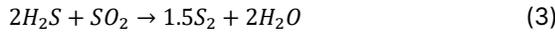
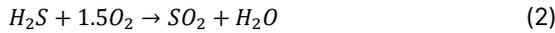
Applying a Claus process, the Sulfur Recovery Unit (SRU) converts H₂S present in sour amine gas and sour NH₃ gas to elemental (pure) sulfur. Environmental regulations have become stricter on sulfur dioxide emissions. One of the main strategies to reduce sulfur emissions is to increase the performance of sulfur recovery units (SRU) [1]. The modified Claus process is one of the main processes that convert toxic hydrogen sulfide into elemental sulfur from acid gas during natural gas processing and upgrading the refinery [2]. The main reactions of a

sulfur recovery unit occur in two stages:

A highly exothermic reaction occurs in which a large amount of heat is released, and a partially exothermic reaction occurs in which sulfur dioxide (SO₂) is produced in the reactor, and unreacted H₂S are burned together to produce sulfur elements [3]. The modified Claus process in which hydrogen sulfide is converted to sulfur can be represented by;



The sulfur recovery in the modified Claus process is obtained through thermal and catalytic reactions. The first step is thermal, where one-third of the hydrogen sulfide (H₂S) is partially oxidized, and Sulfur dioxide (SO₂) is produced at very high temperatures. The second step involves the reaction between unreacted hydrogen sulfide and sulfur dioxide over a catalytic bed at lower temperatures:



The conversion of H₂S to SO₂ in the modified Claus process is carried out in the reaction furnace, which is a cylindrical vessel with a refractory lining. The acid gas stream at a pressure typically ranging from 130 to 180 kPa is fed to the reaction furnace burner along with an appropriate amount of air to oxidize the feed contaminants and results in a 2:1 ratio of H₂S:SO₂ in the reactor effluent. The combustion of acid gases in the RF is carried out in temperature ranges of 975-1300 °C, and residence times of the gas are 0.5-2.0 s [4]. Another experimental investigation was on the effect of O₂ enrichment on the yield of the Claus process. It was observed that the rate of COS formation increased with O₂ enrichment due to the availability of higher amounts of CO, while that of CS₂ (carbon disulfide) decreased.

A tool that has been used lately is CFD (Computational Fluid Dynamics), where you can work with the kinetics of chemistry and the transport of mass, momentum, and heat, which helps us predict the temperature of combustion, recovery of sulfur and molar fractions of the products. The Abadan Oil Refining Company in Iran has introduced CFD to analyze the effect of O₂ enrichment on dry air, combustion temperature, sulfur recovery, and pollutant production [5].

A current study develops a new reduced kinetic model for simulating the destruction of acid gases in the industrial sector in a sulfur recovery unit reaction furnace. The proposed CFD model includes the reactions of the new kinetic mechanism and stationary laminar flamelet model. The relative error of the H₂S conversion calculated by CFD, using the new kinetic model, is 9.48% compared to industrial data [6].

The present work has focused on the effects of the operating temperature of the Claus reactor and excess air on the combustion and SRU emission characteristics, using a kinetic model of acid gas destruction (H₂S and CO₂) with Fluent to improve the reaction yield. The experimental data of a reaction furnace of Abadan Oil Refining Company in Iran was taken as a reference. [7] The kinetic studies Kinetic Modeling and Optimization of the Claus Reaction Furnace by Samane Zarei [8] and the evaluation of kinetic models to simulate Claus reaction furnaces in sulfur recovery units under different feeding conditions. This work has the following objective:

1. Simulate with Fluent the kinetic model of the destruction of acid gases H₂S and CO₂ and mass transfer in the furnace of the Claus reactor of SRU of the Abadan Oil Refinery. The novelty of this work is the study of different control temperatures 1400, 1500 and 1600 K, with excess air of 10, 20 and 30% to increase and ensure that more reactions occur in the

reaction oven, since in other works only modified operating conditions.

2. Use CFD to improve the reaction performance by modifying the operating temperature of the Claus reactor and removing excess air from the combustion.

METHODOLOGY

The following equations are involved in solving the problem posed by the physical phenomenon to be modelled: Navier-Stokes Reynolds average equation (RANS), turbulence model ($k - \epsilon$) standard, equations of state and coupled methods; FLUENT 16TM uses the method of finite volumes as a numerical method to solve the governing equations and those mentioned above [9]. The partial differential equations that describe the phenomenon of mass transport are the following:

The equation of conservation of mass or continuity.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m \quad (4)$$

The conservation equation of momentum or the momentum theorem in inertial reference frame is;

$$\frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\vec{\tau}) + \rho \vec{g} + \vec{F} \quad (5)$$

Where p is the static pressure, τ is the stress tensor, ρg is the gravitational force and F is the external force.

The stress tensor is given by:

$$\vec{\tau} = \mu \left[(\nabla \vec{v} + \nabla \vec{v}^T) - \frac{2}{3} \nabla \cdot \vec{v} I \right] \quad (6)$$

Where μ is the molecular viscosity, I is the unit tensor and the second term on the right side is the effect of volume expansion.

Standard turbulence model ($k - \epsilon$)

$$\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \epsilon - Y_M \quad (7)$$

$$\frac{\partial}{\partial t} (\rho \epsilon) + \frac{\partial}{\partial x_i} (\rho \epsilon u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] + C_1 \frac{\epsilon}{k} (G_k + C_3 G_b) - C_2 \rho \frac{\epsilon^2}{k} \quad (8)$$

κ is the turbulence kinetic energy, ϵ is the dissipation rate, G_k represents the generation of turbulence kinetic energy due to the mean velocity gradient, G_b is the generation of turbulence kinetic energy due to buoyancy.

The above equations are considered in Cartesian coordinates, C_1 , C_2 , C_3 , σ_k , and σ_ϵ are closure coefficients and the values of these coefficients are: 1.44, 1.92, 0.09, 1.0 and 1.3, respectively for the standard turbulence model ($\kappa - \epsilon$) equations 7 and 8 (Launder and Spalding 1972).

The energy conservation equation is given by the

following expression:

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\vec{v}(\rho E + p)) = \nabla \cdot \left(k_{eff} \nabla T - \sum_j h_j \bar{J}_j - (\bar{\tau}_{eff} \cdot \vec{v}) \right) + S_h \quad (9)$$

where k_{eff} is the effective conductivity ($k + k_t$, where k_t is the turbulent thermal conductivity, defined according to the turbulence model being used), and \bar{J}_j is the diffusion flux of species j . The combustion process in the Claus reaction furnace was modeled and simulated using Ansys Fluent to study the influence of furnace temperature and keep it under control and from excess intake air for sulfur recovery and pollutant production, The temperatures used were 1400 K, 1500 K and 1600 K, varying various excesses of air 10, 20 and 30 %.

The dimensions of the reaction furnace in SRU of the Abadan Oil Refinery were taken from Abdoli et al. (2018) and a representation is shown in Figure 1. The inner surface of the reaction furnace is covered by refractory to protect its wall.

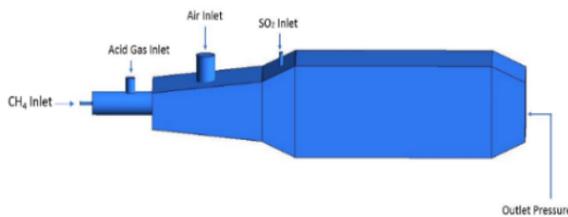


Figure 1. Reaction furnace in SRU of the Abadan Oil Refinery.

The reaction furnace consists of 4 inputs: CH₄ input, acid gas (H₂S) input, air input are located in the burner and SO₂ input is in the reaction furnace, there is a product output.

For the simulation the walls were assumed to be adiabatic, the mixture was treated as an incompressible, ideal gas, and there is no slip on the walls.

The furnace produces sulfur, but also oxidizes H₂S to SO₂. After the furnace there are catalytic reactors that produce sulfur from SO₂, but at lower temperatures than the reaction furnace. Also at the exit of the furnace there is a heat exchanger that cools the gases before the catalytic stage.

The study of hydrodynamics and mass transfer was carried out with CFD tools in Fluent 16.0, which will give us the profile of products obtained. A computer with 16 GB RAM and an Intel (R) Core™ i 7 -2600 CPU was used.

The essential parameters to carry out a study of this

type were to obtain an adequate mesh that represents our study area, propose ANSYS models to represent our process, turbulent model, reaction equations.

Table 1. shows the input operating conditions of the reagents.

Mole Fraction	acid gas	air	SO ₂	CH ₄
Inlet temperature (k)	353.15	463.15	324.15	3113.15
Mass flow (kg/s)	1.338	0.09028	0.25167	3.1025
Species				
H ₂	0.00197	0	0	0
O ₂	0	0.19291	0	0
H ₂ S	0.68952	0	0	0
SO ₂	0	0	0.90728	0
H ₂ O	0.147	0.07948	0.09272	0
CH ₄	0.00725	0	0	1

Simulation in CFD Preprocessing

Reactor meshing was performed in ANSYS ICEM software and boundary conditions were also entered into the mesh. The mesh was made with a hexahedral structure with a size of 364456 cells (see Figure 2).

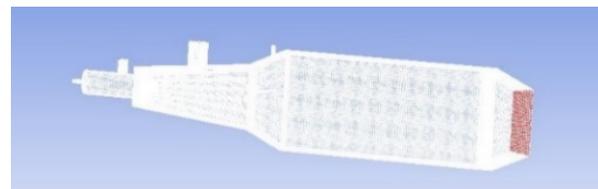
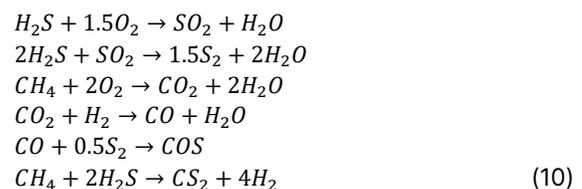


Figure 2. Mesh generated for the reactor.

Processing

The simulation in Fluent version 16.0 was performed in 3 dimensions, in transient state, using the viscous model of $k - \epsilon$ standard, the species transport model and for the reaction the Finite-rate/Eddy - Dissipation model. To simulate the combustion reaction in the Claus SRU furnace, the following reaction mechanism was followed [Amer Mehmood, 2020];



The transport equation was solved for each species.

Postprocessing

The profiles and temperature contours were obtained, the profiles of the products will be obtained, as well as those of the acid gas conversion profiles at various temperatures 1400, 1500 and 1600 K with excess air

10, 20 and 30 %, the mathematical model in Fluent will be validated with the experimental data.

RESULTS

The numerical results of the simulation are presented below, Figure 3 shows the behavior of the molar fraction of S_2 along the reactor at a temperature of 1400 K at 10, 20 and 30% excess air at 300 seconds of simulation. The air and acid gas inlets are the same in the reactor causing the concentration to increase in the first 2 meters by 0.032 which is where the chemical reaction takes place the most, the molar fraction of 0.043 at the exit for 10% excess air and a value of 0.045 for 20 and 30% excess air at 1400 K.

Figure 4 shows the profile of the S_2 molar fraction in the reactor at a temperature of 1500°K with 10, 20 and 30% excess air at 300 seconds of simulation. The concentration increases in the first 3 meters up to 0.032 because it is where the reaction gases come together and where the greatest reaction takes place and at the end it has a value of 0.042, for 10% excess air and 0.045 for 20% and 0.046 for 30% excess air at 1500°K.

Figure 5 shows the profile of the molar fraction of S_2 in the reactor at a temperature of 1600 ° K at 10, 20 and 30% excess air at 300 seconds of simulation. As in the other cases, the concentration increases in the first meters of the reactor length up to 0.042 and at the exit there is less reaction and a value of 0.046 is obtained for 10% excess air and 0.055 for 20% and 0.054 for 30% excess air at 1600 K. It is observed that there is a greater conversion of S_2 at 1600 ° K and at 30% excess air.

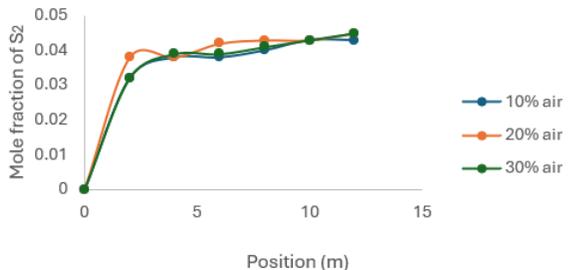


Figure 3. Mole fraction profiles of S_2 at 1400 K with 10, 20 and 30% excess air in the SRU reaction oven.

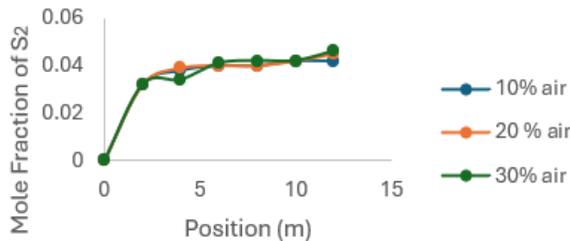


Figure 4. Mole fraction profiles of S_2 at 1500 K with 10, 20 and 30% excess air in the SRU reaction oven.

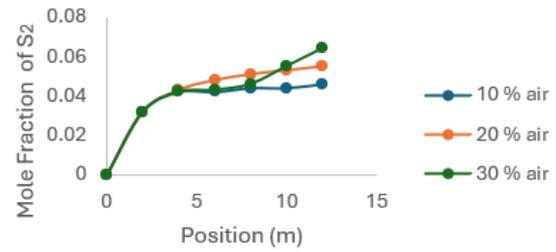


Figure 5. Mole fraction profiles of S_2 at 1600 K with 10, 20 and 30% excess air in the SRU reaction oven.

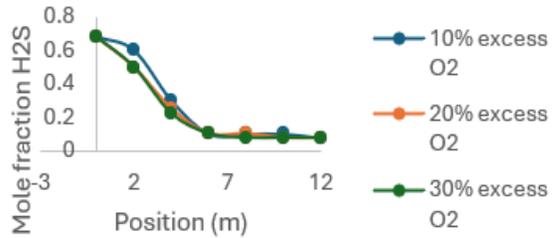


Figure 6. Mole fraction profiles of H_2S at 1400 K with 10, 20 and 30% excess air in the furnace at 300 seconds of simulation.

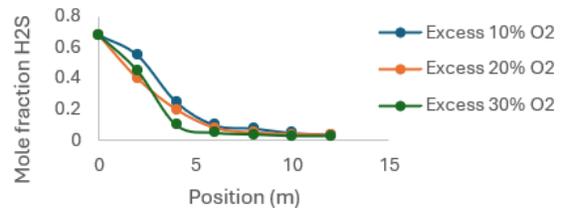


Figure 7. Mole fraction profiles of H_2S at 1600 K with 10, 20 and 30% excess air in the furnace at 300 seconds of simulation.

The following results show the acid gas (H_2S) conversion profile at the various temperatures 1400, 1500 and 1600 K and with the various excesses of air 10, 20 and 30% respectively. The fluctuations in figures 3, 4 and 5 depend on the reaction turbulence and the equipment design.

Figure 6 shows the H_2S conversion profiles in the reactor at 1400 K at different air excesses 10, 20 and 30%, it starts with a value of 0.68 molar fraction of acid gas, after 4 and 5 meters it consumes up to 0.1, and at the reactor exit it reaches a value of 0.075, with a conversion of 89.12%, due to the design of the equipment, it could be raised if there was more contact and turbulence of the reactants.

Figure 7 shows the H_2S conversion profiles in the reactor at 1600 K at different air excesses 10, 20 and 30%, it starts with a value of 0.68 molar fraction of acid gas at the inlet, after 4 and 5 meters it is consumed up to 0.05 is where the reaction takes place, at the reactor outlet it reaches a value of 0.03, a conversion of 97.64% is

obtained, this is similar to the experimental conversion with a value of 97.98%.

The results are presented only as a function of axial position (graph 1-D) to analyze the behavior profiles on action lines in the reactor. No experimental points were added in the figures to show how the model compares to reality, because I do not have all the experimental data from the company, only output results.

The temperature as a function of the molar fraction of CO₂, CO and COS, H₂O species with 30% excess air was the best result, compared with the industrial data of Abadan Oil Refining Company. S₂, SO₂ and H₂O species tend to increase at the exit of the Claus furnace, and CO₂, COS and CO tend to decrease.

The results of the simulation were compared with the experimental data of the Abadan Oil Refining company. The results of the simulation for 30% excess air and the experimental data for the species of S₂, SO₂, CO, CO₂, H₂O, COS and H₂S. The relative error with respect to the temperature of 1400, 1500 and 1600 K is 0.02, 0.01 and 0.02% respectively.

CONCLUSIONS

In this work, the SRU (sulfur recovery unit) process was analyzed to improve the performance of the reaction and sulfur recovery using the CFD tool, a standard k- ϵ turbulence model, an energy model with convective transport and mass transport were used. with chemical reaction using the Finite - rate/Eddy model. - Proposed model for the destruction of acid gases (H₂S and CO₂).

This work presents a CFD analysis controlling the temperature and excess air of 10, 20 and 30% to improve the reaction performance, outlet temperature, sulfur recovery. It was obtained a good approximation with the experimental results of the industrial process of the Abadan Oil refinery, Iran. Control temperatures of 1400, 1500 and 1600 K were analyzed, as well as excess air of 10, 20 and 30% respectively. It was found that at the highest temperature of 1600 K and at 30 of excess air there is a higher reaction yield, producing 0.0728 mole fraction of S₂, compared to the experimental one of 0.0709, which has an error of 2.6 %.

For the conversion of H₂S, a value of 0.03 mole fraction was obtained at the reactor outlet compared to the experimental one, with an error of 4%, a good approximation to the experimental results of the process. was obtained a conversion of the acid gas (H₂S) of 95.64%, which is quite good compared to the experimental one. The results of simulation or numerical predictions confirm that, at higher temperatures and higher excess air, the acid gas increases combustion and sulfur conversion. The results confirm that the excess air for combustion and more than 30% and with a temperature of 1600 K improve the recovery of sulfur and reduce the amount of

pollutants such as COS and CO₂ and CO. The experimental conversion of sulfur was 99.1% and the conversion for the temperature of 1600 K and 30% with excess air was 99.5% with a percentage deviation of 0.4%, for the other temperatures of 1400, 1500 with 30% with excess air conversion was lower with a value of 98%.

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REFERENCES

1. El-Bishtawi, Haimour No' man, Claus recycle with double combustion process. *Fuel Process Technol* 86:245–260 (2004)
<https://doi.org/10.1016/j.fuproc.2004.04.001>
2. Dowling, N.I., Hyrne, J.B., Moon, D.L., Clark, P.O., Un horno Claus de craqueo térmico de H₂S Modificación Para la Producción de Hidrógeno, Reunión Técnica Anual (1995)
3. Maddox RN, Gas Conditioning and Processing: gas and liquid sweetening. Campbell Petroleum Series, Norman, Oklahoma (1983)
4. Monnery, W.D., Svrcek, W.Y., Behie, L.A., Modelling the modified Claus process reaction furnace and the implications on plant design and recovery, *The Canadian Journal of Chemical Engineering*, 71, 711-724, (1993)
<https://doi.org/10.1002/cjce.5450710509>
5. Abdoli P, Hosseini SA, Abdul Mujeebu M, Influence of O₂ enrichment in dry air on combustion temperature, contaminant production and sulfur recovery, in SRU reaction furnace. *Forschung im Ingenieurwesen* 82:99–106, (2018).
<https://doi.org/10.1007/s10010-017-0260-y>
6. Bayazid Mahmoodi, A new acid gas destruction kinetic model for reaction furnace of an industrial sulfur recovery unit: A CFD study, *Chemical Engineering Science*, 256, 117692 (2022).
<https://doi.org/10.1016/j.ces.2022.117692>
7. Pedram Abdoli¹, Seyed Amin Hosseini, Muhammad Abdul Mujeebu, Effect of Preheating Inlet Air and Acid Gas on the Performance of Sulfur Recovery Unit—CFD Simulation and Validation, *Forsch Ingenieurwesen*, 83:81–89 (2019)
<https://doi.org/10.1007/s10010-019-00299-9>
8. Samane Zarei, Hamid Ganji, Maryam Sadi, Mehdi Rashidzadeh, Kinetic Modeling and Optimization of Claus Reaction Furnace, *Journal of Natural Gas*

Science and Engineering, 747 – 757, (2016)

<https://doi.org/10.1016/j.jngse.2016.03.086>

9. ANSYS, Inc., (2016), ANSYS Fluent User's Guide.

Canonsburg, PA, USA.

https://www.afs.enea.it/project/neptunius/docs/fluent/html/ug/main_pre.htm

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