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Steady state simulation of production of sulfuric acid by contact process using Aspen Hysys V8.8

Mohamed Nasser and Mahmoud Emad
Military Technical Collage, Cairo, Egypt

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Abstract
The aim of this study was to simulate the production of sulfuric acid by contact process using Aspen Hysys V8.8 with steady state mode making some assumptions and using hypothetical reactors. Antoine Model is used as fluid package in this simulation where the values of minimum and maximum temperature and the coefficients (A through F) are estimated for each component. The increase of boiler outlet temperature shows linearly decrease relation with waste energy heat flow. Inlet water temperature shows no effect on molar enthalpy of sulfuric acid product and value of molar enthalpy of sulfuric acid product remains constant and equal to -9.329e+005 kJ/kg mole. Air temperature also shows no effect on product sulfuric acid flow rate. Flu gas temperature shows linearly increase relation with absorber inlet water temperature for the range of 10 to 120 ^{0}C and sharply increase for the range of 120 to 130 ^{0}C and finally become roughly constant after 130 ^{0}C with the increase of absorber inlet water temperature.

Keywords: Sulfuric acid, aspen hysys, Antoine model, steady state

1. Introduction
Sulfuric acid is one kind of fundamental chemicals. It's generally utilized in fertilizer industry. Sulfuric acid is utilized to produce fertilizer including ammonia sulfate, magnesium sulfate, potassium sulfate and etc (Wagenfeld, Al-Ali, Almheiri, Slavens, & Calvet, 2019) [8]. It's also utilized in military chemical plant and metallurgy industry. Sulfuric acid is acting as main additives in a lot of the processes of pharmaceutical production. It's likewise used to dry chemicals in dozens chemical process (Sanders, 2015) [7]. Worldwide market of sulfuric corrosive in 2021 is assessed to be around 11.1 billion USD (Peng, 2000) [6].
Sulfur, Oxygen and water are used to produce sulfuric acid by the contact process. In the initial step, sulfur is burned to yield sulfur dioxide then sulfur dioxide is sulfur trioxide utilizing oxygen within the sight of a vanadium (V) oxide catalyst (Weil, Sandler, & Gernon, 2000) [9]. At last the sulfur trioxide is reacted with water to produce 98-99% sulfuric acid. The high support cost of sulfuric acids plants, rigid necessities on SO2 discharges, significance of energy proficiency, precise equipment sizing and rating has made the renewal of the plant testing. Due to overall strain to lessen SO2 discharges, most new plants currently use Double Contact Double Absorption and many existing plants have been changed to utilize it (Mousdale, 2010) [5].
Computer assisted modeling and simulation has increasingly become popular in all fields of engineering and in particular in chemical engineering, oil & gas and petrochemical industries (Klatt, Marquardt, & Engineering, 2009) [3]. Nowadays, a number of simulators are developed and/or updated in order for engineers to make fast and precise calculations. Among all of the simulators, chemical engineering simulators assist a chemical engineer to simulate design and operation of a chemical equipment and plant, which saves a lot of time and money. They also enable chemical engineers to design large plants by using defined thermodynamic or other equations of state, kinetic data, practical and mathematical models and equations, and other user input data. Without simulators modeling and design of such large plants would be expensive and time consuming (Dobre & Marcano, 2007) [2].
Today Aspen HYSYS software is the master process modeling solution that gives large economic benefits throughout the process engineering lifecycle (Al-Lagtah, Al-Habsi, Onaizi, & Engineering, 2015) [1]. Now-a-days chemical engineer used Aspen HYSYS to design new plants and also optimize production for greater margins.
The present work aims to simulate the production of sulfuric acid by contact process using Aspen Hysys V8.8 with steady state.

2. Methodology
2.1 Process description: Liquid sulfur is burnt with air in a burner of sulfur to produce sulfur dioxide. The main important steps in this process are to change sulfur dioxide to sulfur trioxide and at that time combining sulfur trioxide with water to produce a solution containing 98-99%. This is done by using four converter beds where sulfur dioxide is passing through them. Due to the constraint of Aspen HYSYS programming four individual converters were utilized as converter bed. The produced sulfur dioxide from a burner is gone through a waste heat boiler to lower the temperature of the produced sulfur dioxide before entering the 1st bed converter (Converter-1). The exit stream from a waste heat boiler is entering to Converter-1 where the conversion of sulfur dioxide to sulfur trioxide is done but it isn't complete conversion. The exit stream from Converter-1 is cooled and passed to Converter-2 to complete the convert of remaining of sulfur dioxide to sulfur trioxide. The exit stream from Converter-2 is cooled and passed to Converter-3. Then the exit stream from Converter-3 is cooled and passed to Converter-4 where complete conversion of sulfur dioxide to sulfur trioxide. The exit stream from Converter – 4 is gone through a cooler to keep up temperature as excessively high. The cooled sulfur trioxide is passed to an absorption tower where sulfur trioxide reacts with 98% sulfuric acid to form 98.5 % sulfuric acid. At the top of absorption tower, the vent of stack gas which contains mainly of Nitrogen. The produced sulfuric acid from absorption tower is cooled and split into two streams where one of them is the final product.

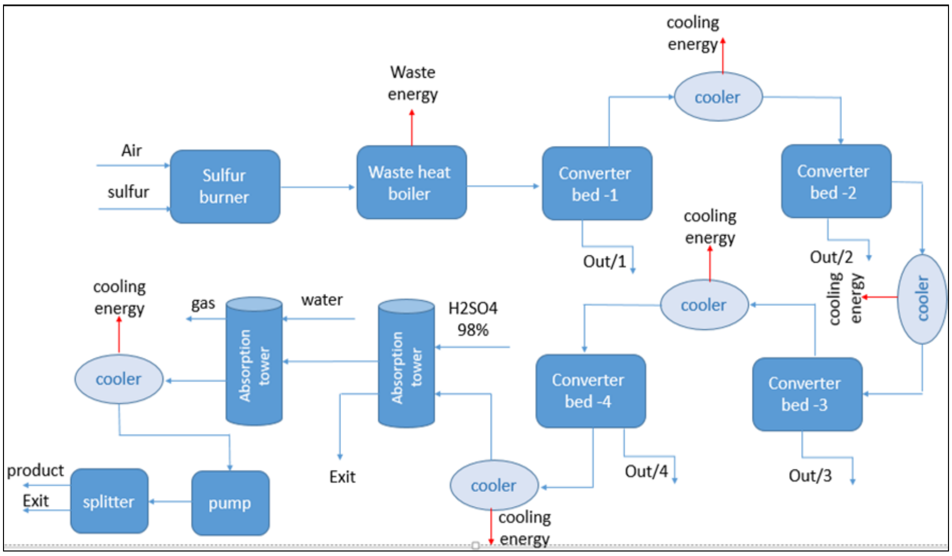

Fig 1: Block diagram of the process of production of sulfuric acid by contact

2.2 Simulation of the process by aspen hysys

Simulation of the process of production of sulfuric acid by contact process is done by using aspen hysys v8.8. Figure (2) shows the Hysys process flow diagram production of sulfuric acid by contact process. The procedure of this simulation is as the following:

2.2.1 List of component

The component used in this simulation are as the following:

a) Liquid sulfur
b) Sulfur dioxide
c) Sulfur trioxide
d) Sulfuric acid
e) Water
f) Oxygen
g) Nitrogen

2.2.2 Fluid package

In this simulation the used fluid package is Antoine Model where the values of minimum and maximum temperature and the coefficients (A through F) are estimated for each component.

2.2.3 Reaction involved

There are three reactions involved in this simulation. Reaction (1) occurs in the sulfur burner while reaction (2) occurs in the four converter reactor bed with different conversion percentage. Finally, reaction (3) occurs in the absorber tower (Leiva, Flores, & Aguilar, 2020) [4].

$$S + O2 \rightarrow SO2 \qquad (Sulfur\ burner)$$

$$SO2 + 0.5\ O2 \rightarrow SO3 \qquad (First\ bed\ reactor\ with\ conversion\ 67\ \%)$$

$$SO2 + 0.5\ O2 \rightarrow SO3 \qquad (second\ bed\ reactor\ with\ conversion\ 90\ \%)$$

$$SO2 + 0.5\ O2 \rightarrow SO3 \qquad (third\ bed\ reactor\ with\ conversion\ 95.7\ \%)$$

$$SO2 + 0.5\ O2 \rightarrow SO3 \qquad (Fourth\ bed\ reactor\ with\ conversion\ 99.5\ \%)$$

$$SO3 + H2O \rightarrow H2SO4 \qquad (Absorption\ tower)$$

2.2.3 Process condition

The process conditions of this simulation is described below

2.2.3.1 Streams

The streams condition used in this simulation are shown in table (1).

Table 1: Conditions of streams.

Condition	Liquid sulfur	Air	water	Sulfuric acid (product)
Temperature (^{0}C)	105	50	30	25
Pressure (KPa)	1500	1500	250	250
Flow rate (kgmole/hr)	24.95	251.3	90	15.65

2.2.3.2 Converters

The conditions of four converters used in this simulation are shown in table (2).

Table 2: Conditions of four converters

Converter bed number	Inlet Temperature (^{0}C)	Outlet Temperature (^{0}C)	Conversion (%)
First bed	422	612	67
Second bed	450	534	90
Third bed	420	429.1	95.7
Fourth bed	420	420.4	99.5

2.2.3.3 Absorption tower

The conditions of two absorption tower used in this simulation are shown in table (3).

Table 3: Conditions of two absorption tower

Condition	First absorption tower	Second absorption tower
Number of stages	15	15
Top Pressure (KPa)	250	200
Bottom Pressure (KPa)	300	250
Efficiency type	overall	overall

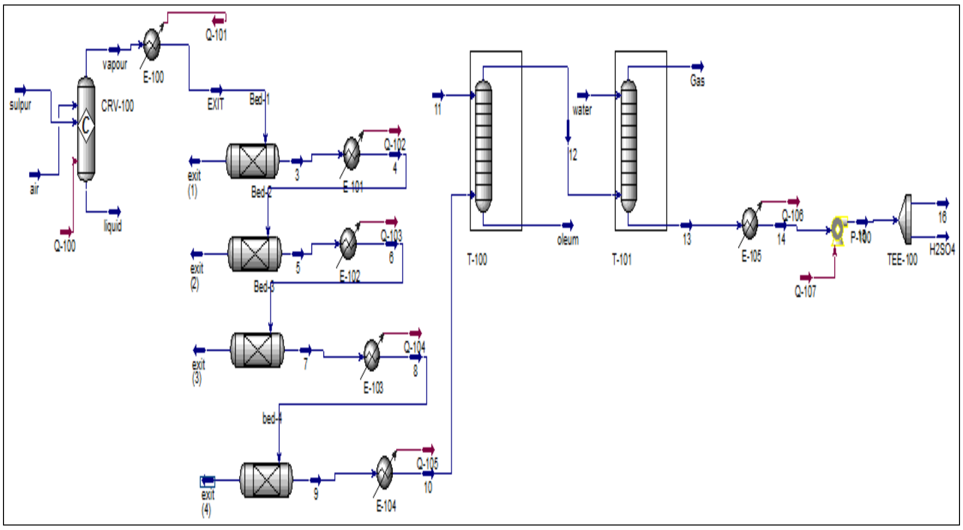

Fig 2: Hysys process flow diagram production of sulfuric acid by contact process

3. Result and Discussions

After performing the simulation, the influence of different processing parameters on the process are observed. From the simulation result, those effects are described in below.

3.1. Effect of boiler outlet temperature on waste energy heat flow

From figure 3, it is shown that the increase of boiler outlet temperature cause linearly decrease in waste energy heat flow. Waste energy heat flow comes to a value of practically 8.204 e+006 kJ/h. With extra increase in boiler outlet temperature at 300^{0}C of boiler outlet temperature, waste energy heat flow decreases in a linear way and arrives at a value of practically 2.1e+006 kJ/h at 1000^{0}C of boiler outlet temperature.

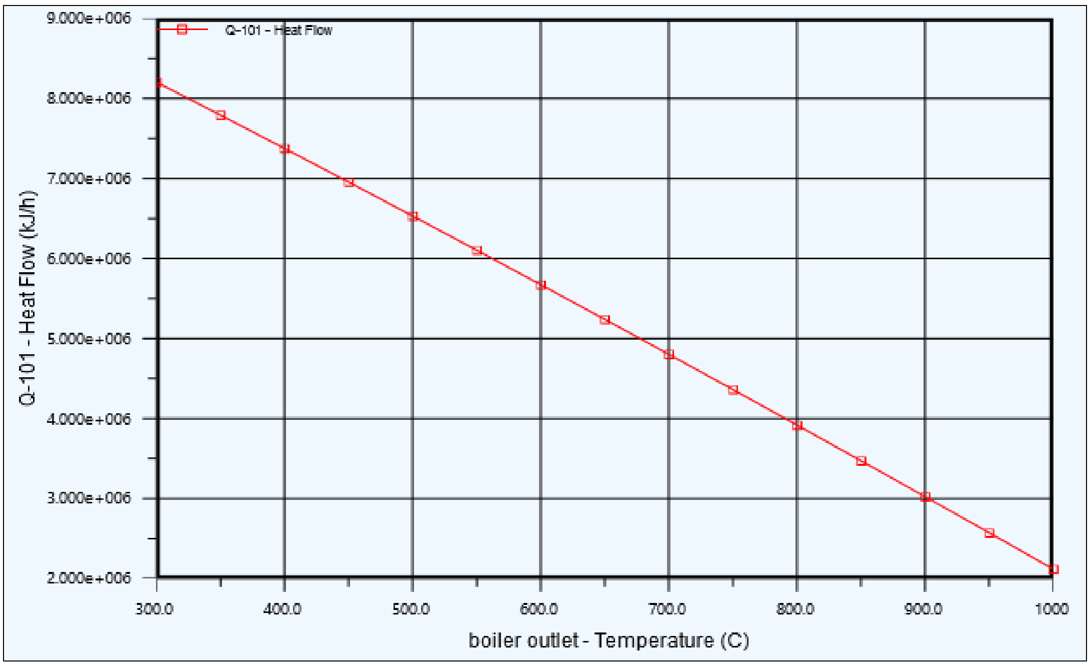

Fig 3: Effect of boiler outlet temperature (^{0}C) on waste energy heat flow (kJ/h).

3.2 Effect of inlet water temperature on molar enthalpy of sulfuric acid product.

From figure 4, it is noticed that molar enthalpy of sulfuric acid product is -9.329e+005 kJ/kg mole and remains constant throughout the change of inlet water temperature so, inlet water temperature has no effect on molar enthalpy of sulfuric acid product.

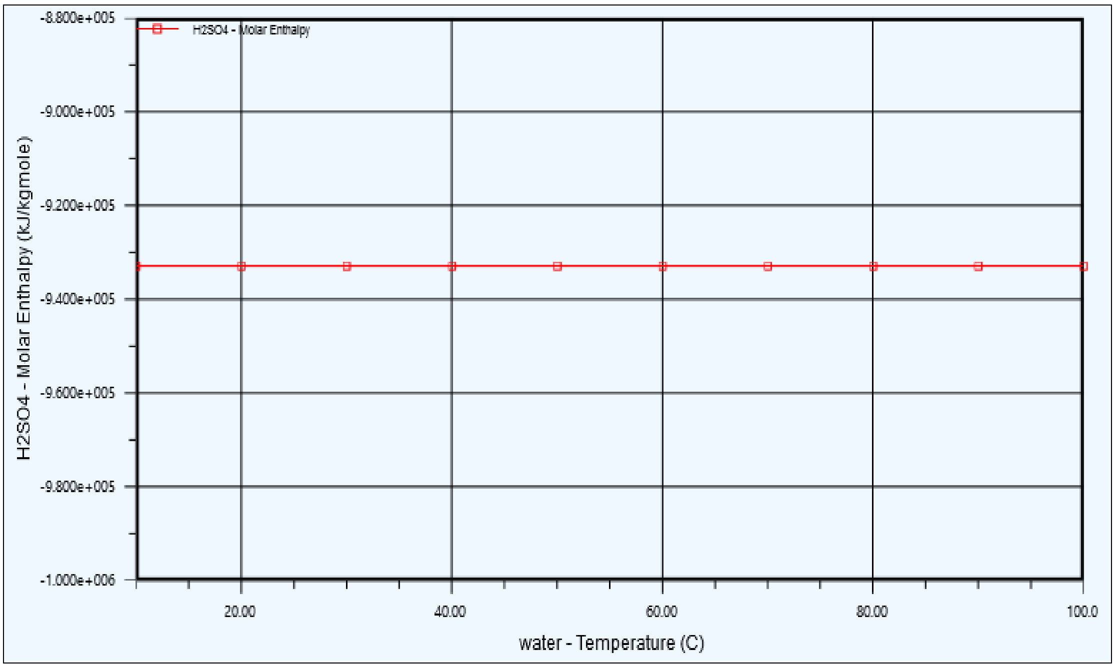

Fig 4: Effect of inlet water temperature (^{0}C) on molar enthalpy of sulfuric acid product (kJ/kg mole).

3.3 Effect of air temperature on product sulfuric acid flow rate

From figure 5, it is noticed that product sulfuric acid flowrate is 1520 kJ/hr and remains constant throughout the change of air temperature so, air temperature has no effect on product sulfuric acid flow rate.

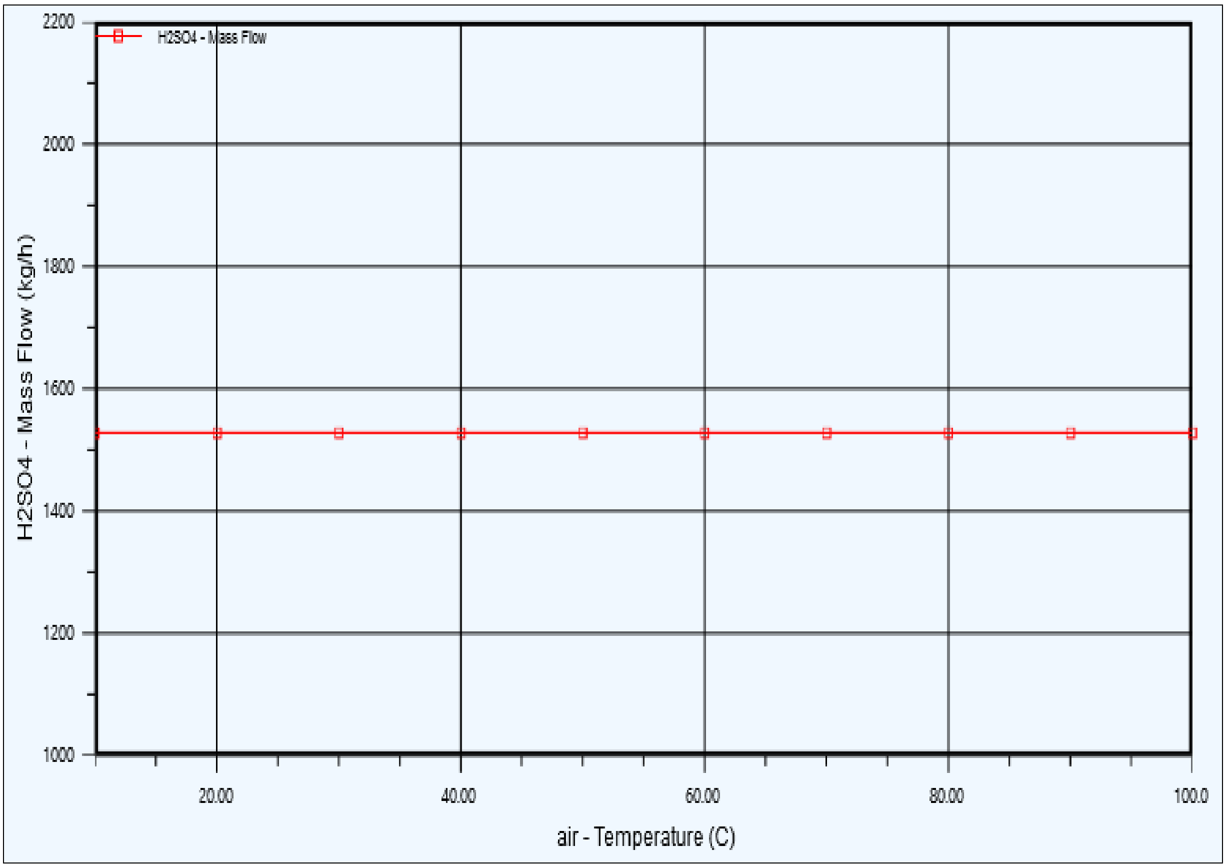

Fig 5: Effect of inlet water temperature (^{0}C) on product sulfuric acid flow rate (kJ/hr).

3.4 Effect of absorber inlet water temperature (^{0}C) on flu gas temperature (^{0}C)

From figure 6, it is observed that flu gas temperature increase linearly with the increase of absorber inlet water temperature for the range of 10 to 120 ^{0}C and increases sharply for the range of 120 to 130 ^{0}C then becomes roughly constant after 130 ^{0}C with the increase of absorber inlet water temperature.

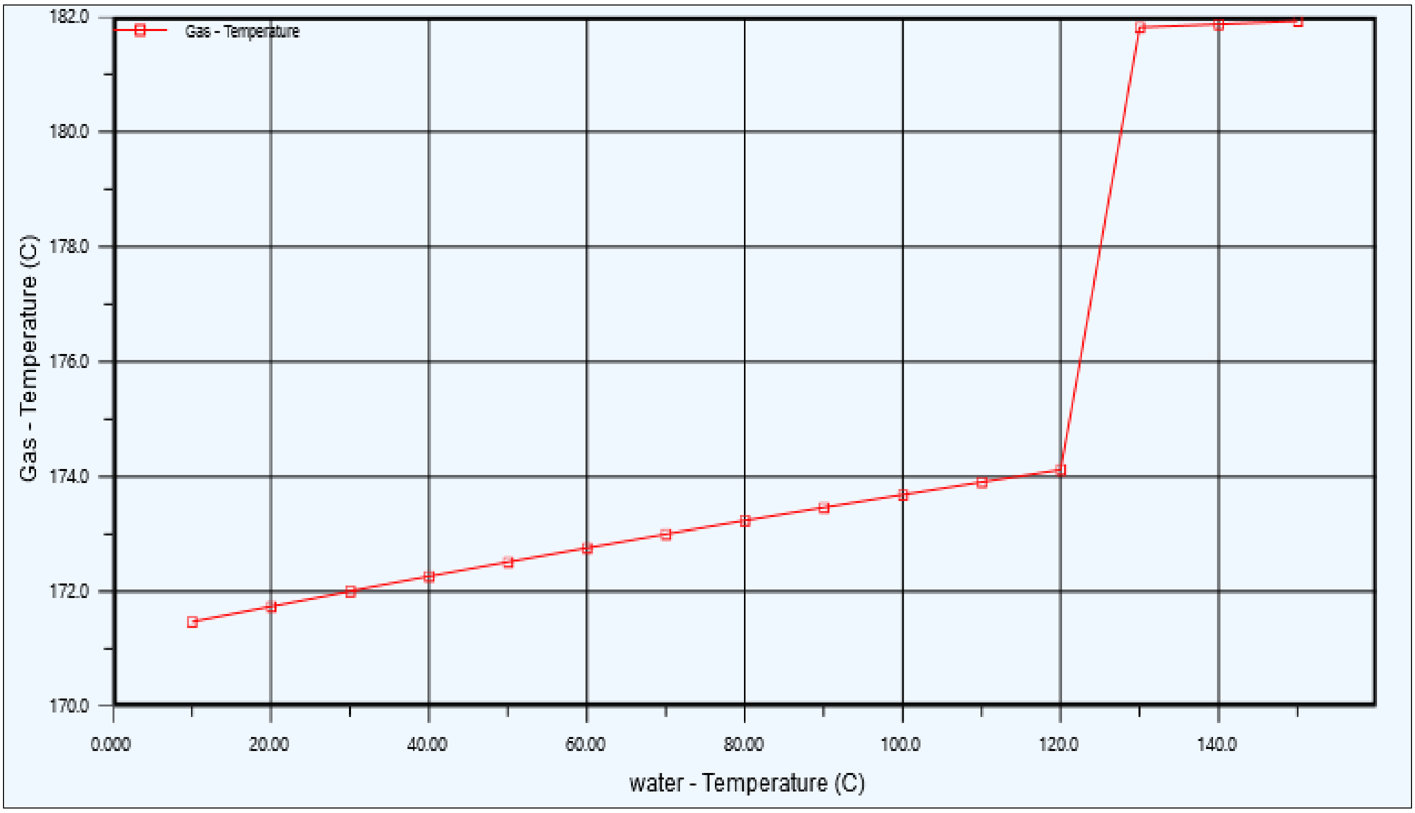

Fig 6: Effect of absorber inlet water temperature (^{0}C) on flu gas temperature (^{0}C)

3. Conclusion

In this work the simulation of Sulfuric acid process was done by using aspen hysys software. This simulation model was able to be used as guide for understanding the process of production Sulfuric acid. In addition to studying of the impact of different parameter on this process can be taken in consideration when commissing these simulation design where the increase of boiler outlet temperature shows linearly decrease relation with waste energy heat flow. Inlet water temperature shows no effect on molar enthalpy of sulfuric acid product and value of molar enthalpy of sulfuric acid product remains constant and equal to -9.329e+005 kJ/kg mole. Air temperature also shows no effect on product sulfuric acid flow rate. Flu gas temperature shows linearly increase relation with absorber inlet water temperature for the range of 10 to 120^{0}C and sharply increase for the range of 120 to 130^{0}C and finally become roughly constant after 130^{0}C with the increase of absorber inlet water temperature.

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