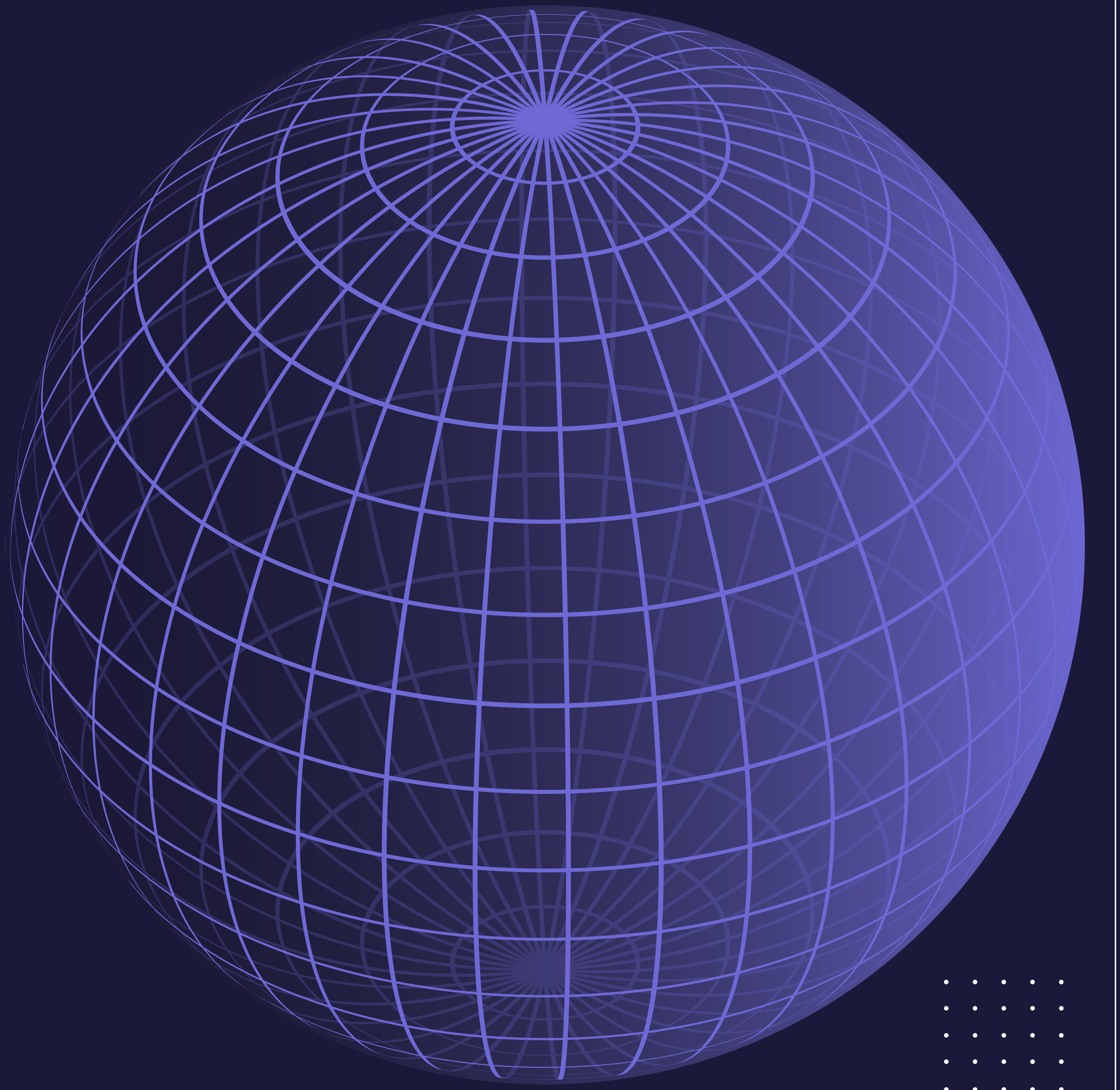
CHE 251 GROUP TERM PROJECT



GROUP 9

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TOPIC

Optimized Production of High Purity Sulphuric Acid via Contact Process

Sulphuric acid is a vital chemical in modern industry, crucial for agriculture, petroleum refining, pharmaceuticals, and metal processing. The contact process, optimized through Aspen Plus modeling, has improved efficiency and ensured high-purity production. Controlling factors like water flow rate maximizes output, ensuring a steady supply. Additionally, exploring alternatives like elemental sulphur enhances sustainability. This optimized production meets industrial demand, highlighting sulphuric acid's essential role in economic and technological progress.

CONTACT PROCCESS

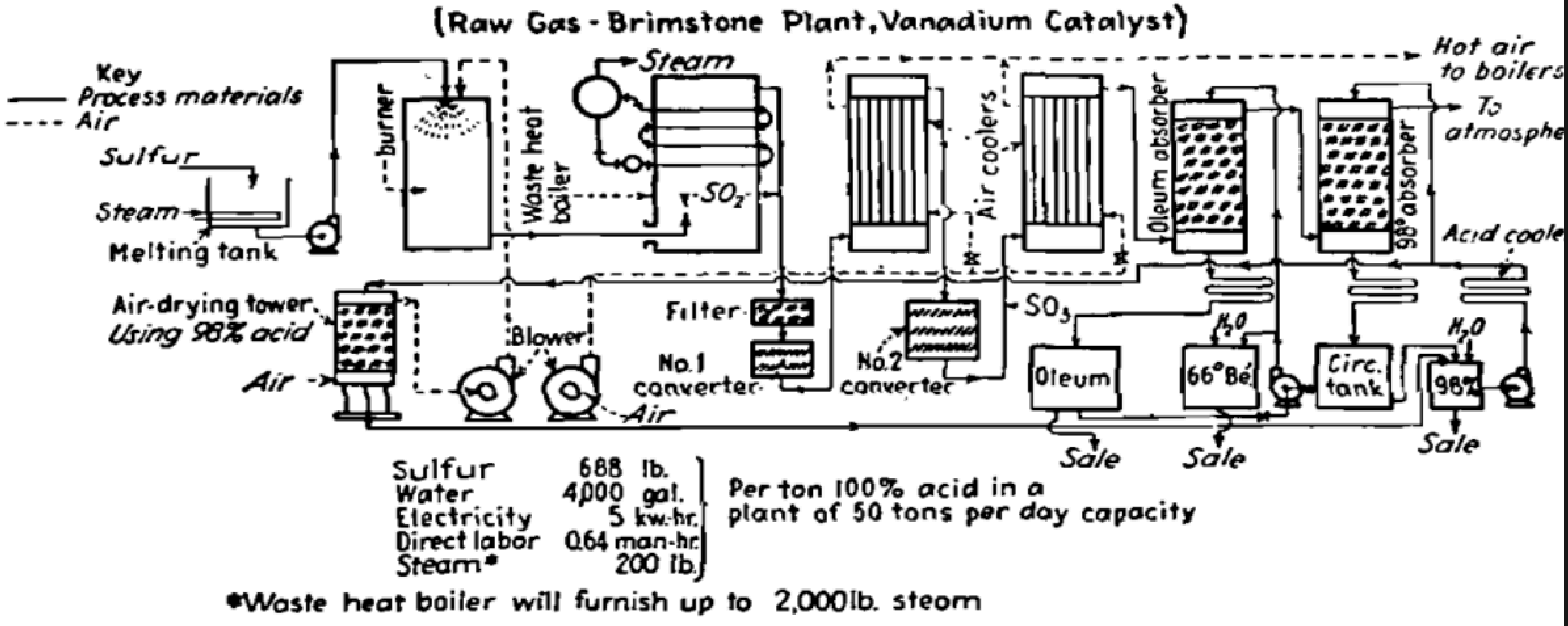


FIG. 8. Sulfuric acid manufacture by the contact process.

Book: The Chemical Process Industries, second edition Author: R. NORRIS SHREVE
Chapter 19: Sulphur and Sulphuric Acid, Page 384

OBJECTIVES

- To design a sulfuric acid (H_2SO_4) production plant using the contact process with a capacity of approximately 8 tonnes per hour
- The study aims to model, simulate, and optimize this process using Aspen Plus, identifying key parameters that maximize efficiency, reduce byproducts, conserve energy, and extend catalyst life.

METHODOLOGY

MODELING WITH ASPEN PLUS

Aspen Plus v14 was used to simulate H_2SO_4 production from elemental sulfur.

COMPONENT & FLUID PACKAGE

Chemical components include O_2, N_2, H_2O, S, H_2SO_4, SO_2, and SO_3. Common ideal model was used.

PROCESS SELECTION:

The double contact process was selected for its efficiency, high yield, and scalability for sulfuric acid recovery.

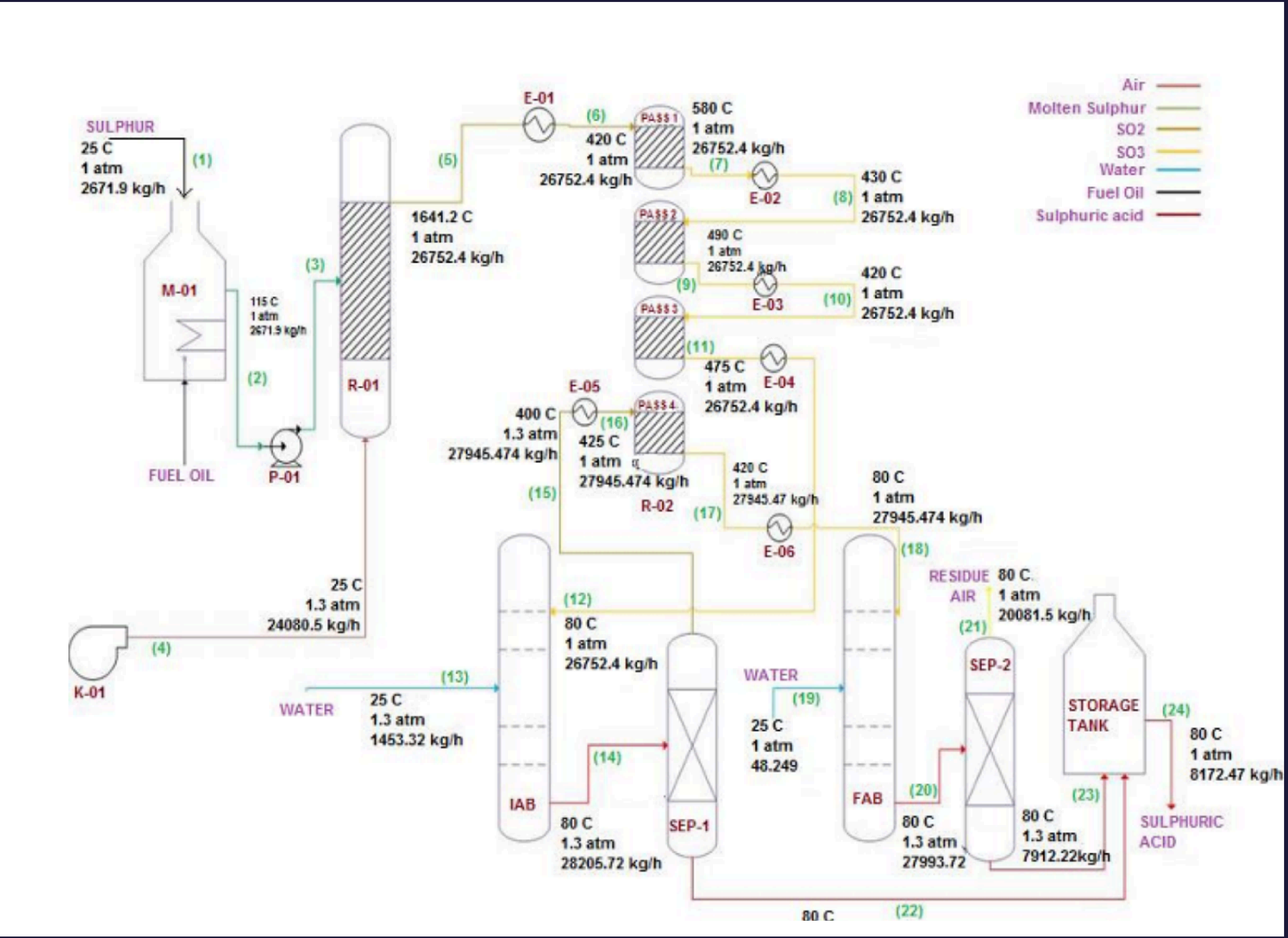
PROCESS FLOW

The flow includes SO_2 preparation, oxidation, SO_3, and dilution. Equipment includes pumps, reactors, heat exchangers, converters, and absorbers.

OPTIMIZATION

Sensitivity analysis on parameters like water flow and temperature was conducted to optimize process efficiency using Aspen Plus analytical tools.

As dive deeper into the process, we found a research paper (referenced below) along with a flow diagram. This resource provided a clearer and more efficient understanding of the process, which we then used to develop the Aspen model.



SOURCE: RSF Press Journal

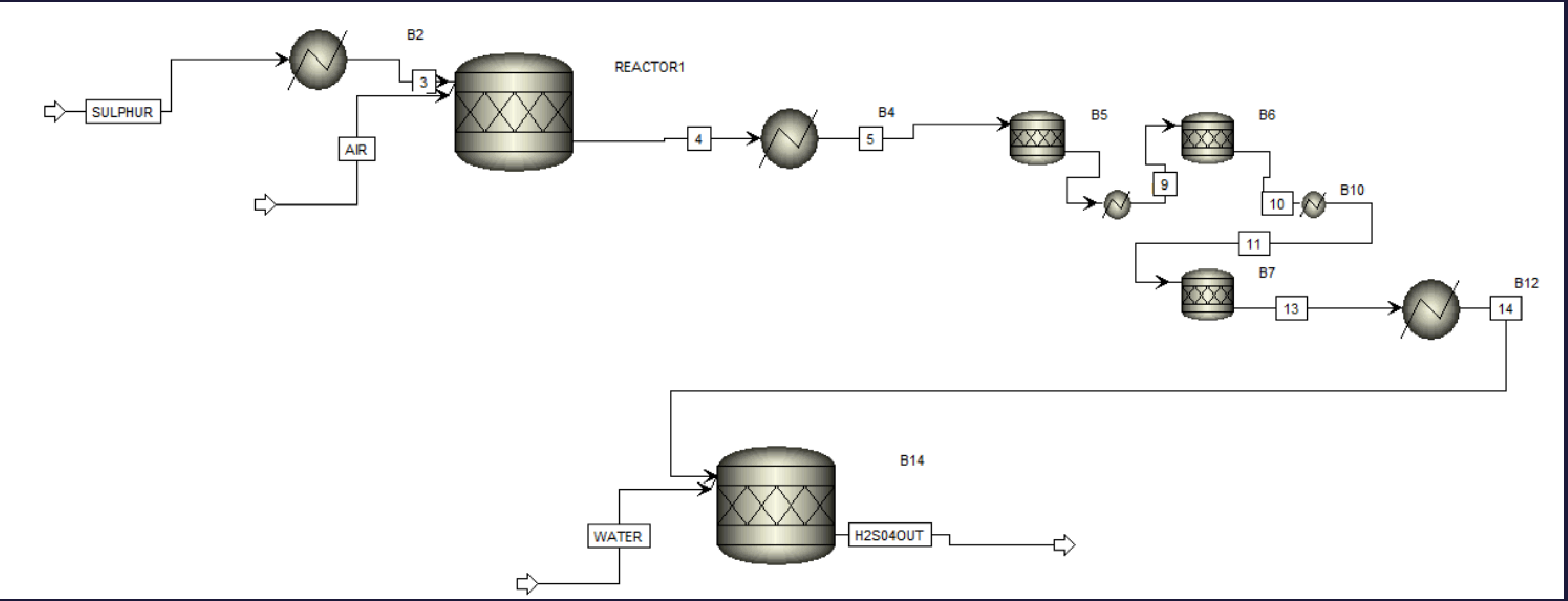
DISCUSSION

At first, we attempted to simulate a model without a separator to remove H2SO4, allowing SO3 to react with water again. Using this approach, the final output was 7,903.52 kg/hr.

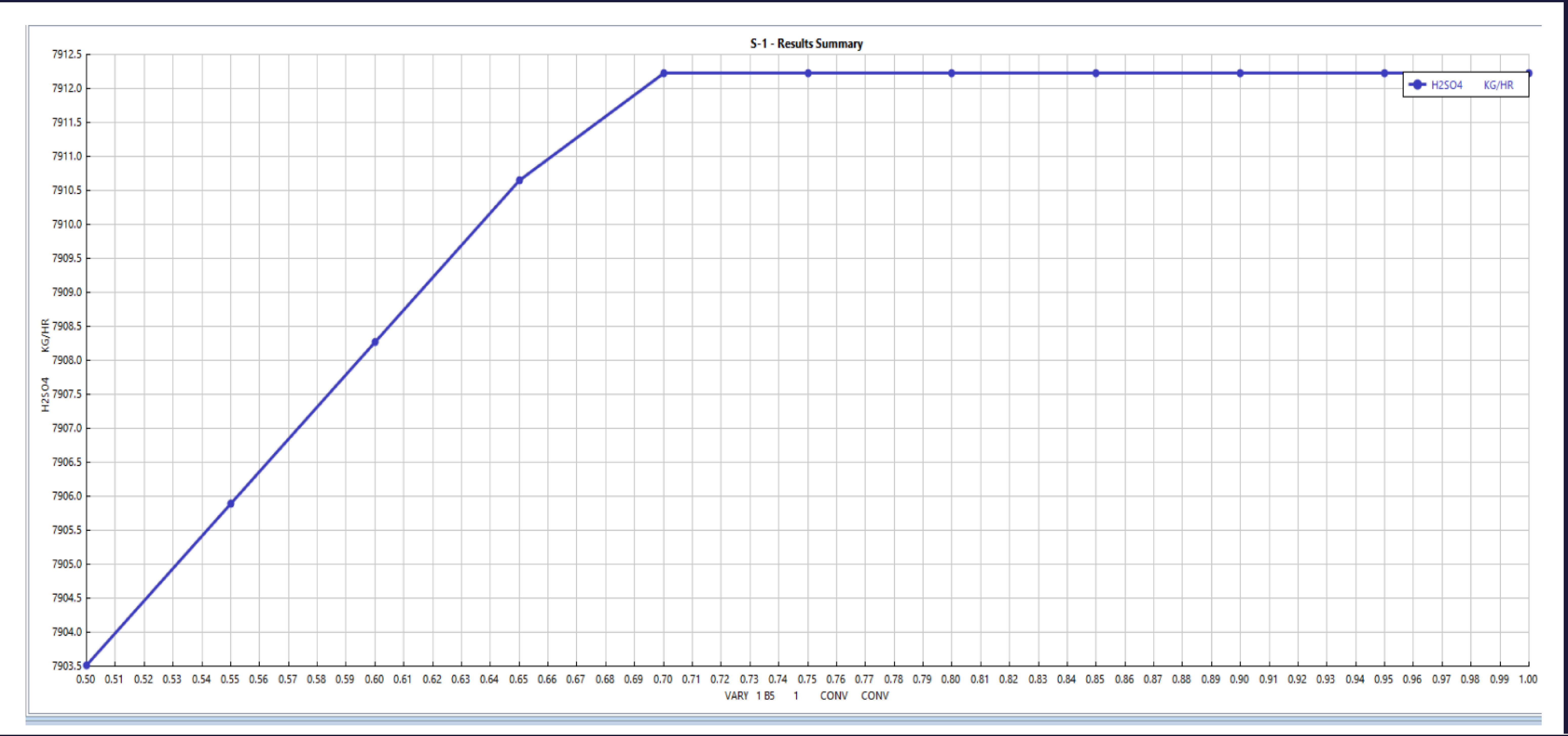
We conducted a sensitivity analysis on this model, focusing on H2SO4 production as the output. The analysis involved adjusting temperature, pressure, and the conversion rates of B5, B6, and B7 as key variables.

While, for temperature and pressure the output remained constant, we observed a span of linear increase before it became constant at 7912.22 Kg/hr.

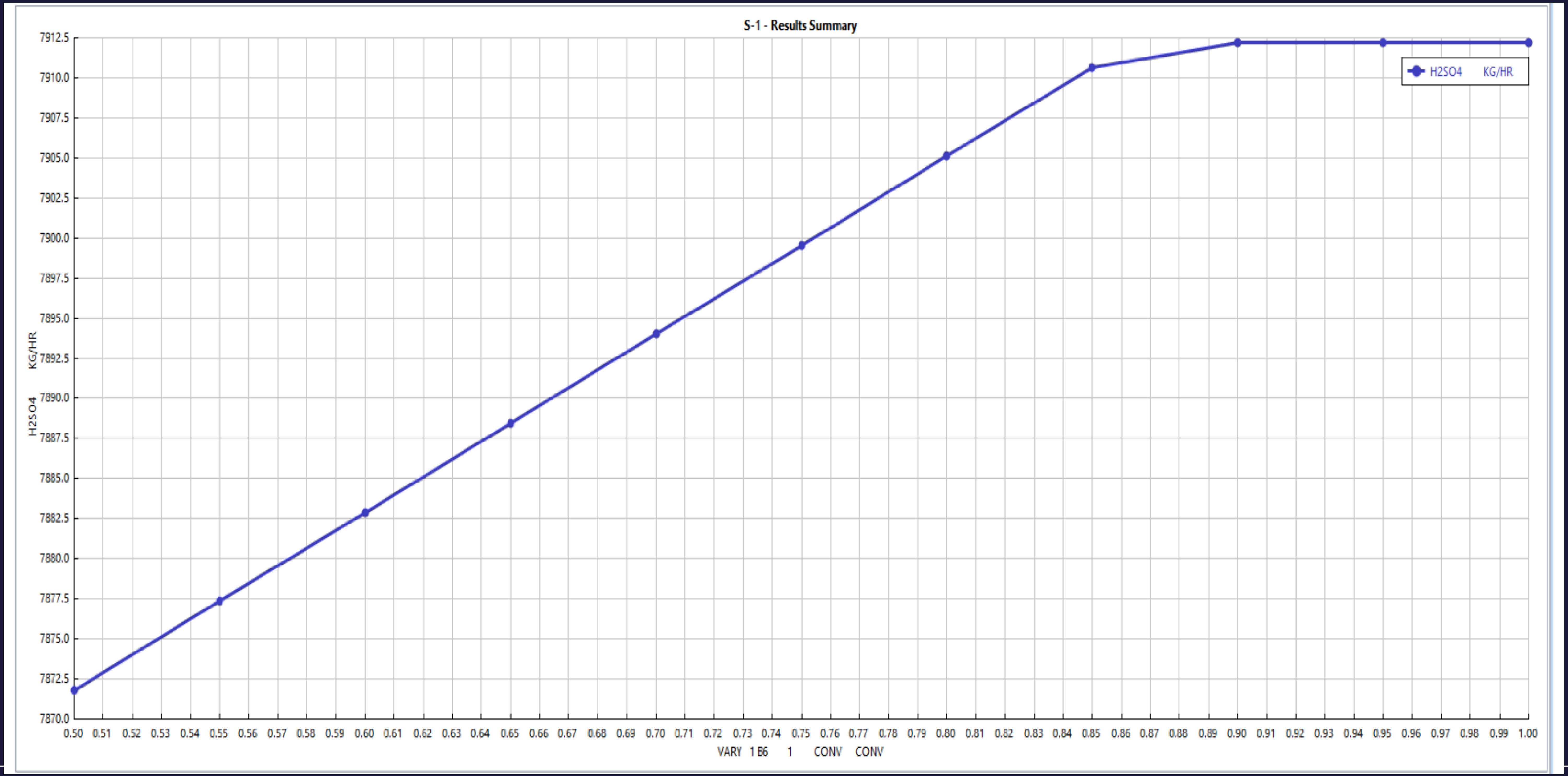
SIMULATION


B2
REACTOR1
3
SULPHUR
AIR
4
B4
5
B5
B6
9
10
B10
11
B7
B12
13
14
B14
WATER
H2S04OUT

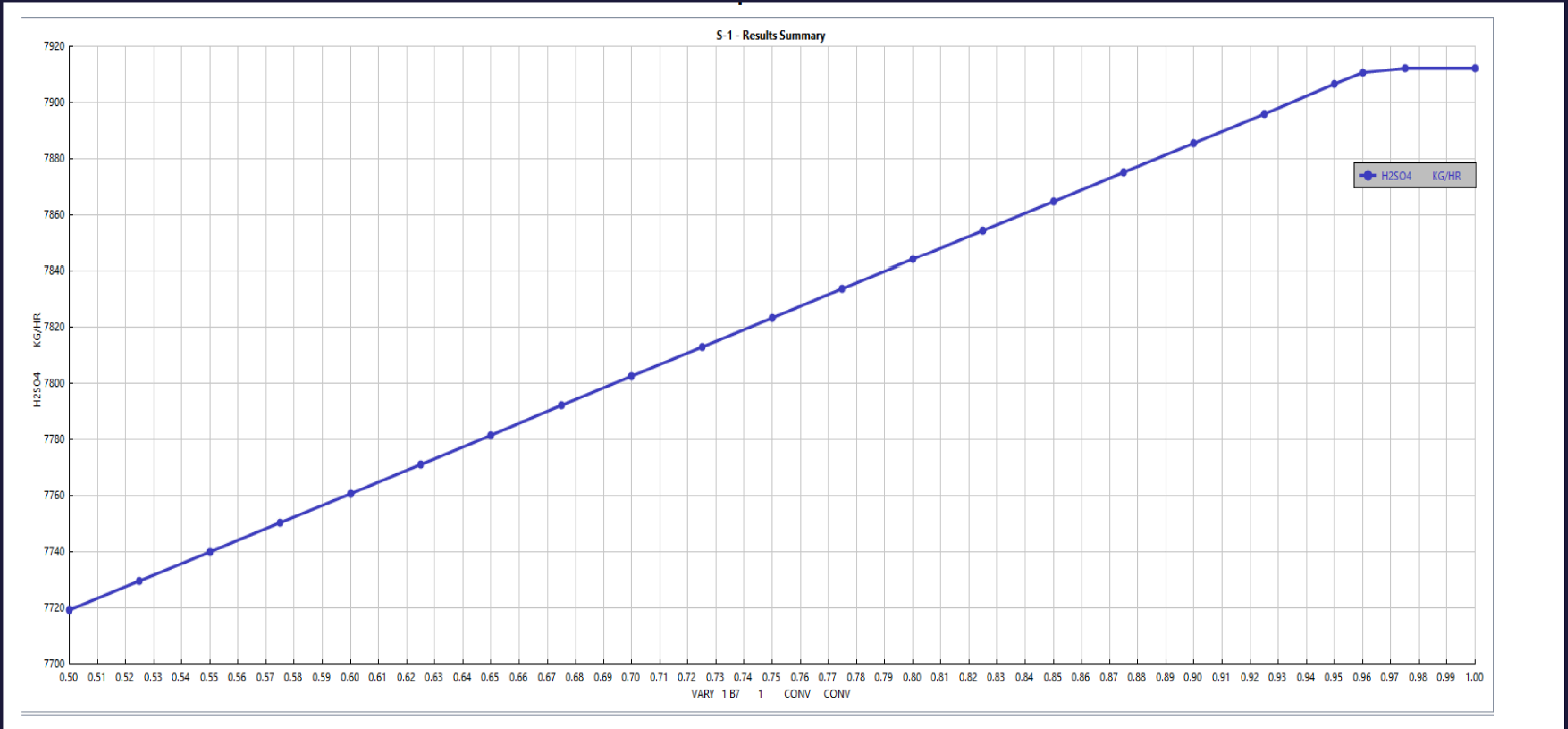
B5 CONVERSION RATE VS H2SO4 OUTPUT



B6 CONVERSION RATE VS H2SO4 OUTPUT



B7 CONVERSION RATE VS H2SO4 OUTPUT



RESULTS

Name	B3	B5	B6	B7	B8	REACTOR1
Property method	Ideal	Ideal	Ideal	Ideal	Ideal	Ideal
Use true species approach for electrolytes	Yes	Yes	Yes	Yes	Yes	Yes
Free water phase properties method	STEAM-TA	STEAM-TA	STEAM-TA	STEAM-TA	STEAM-TA	STEAM-TA
Water solubility method	3	3	3	3	3	3
Specified pressure[atm]	1.3	1	1	1	1.3	1
Specified Temperature[C]	80	580	490	475	80	1641.2
Outlet temperature[C]	80	580	490	475	80	1641.2
Outlet pressure[bar]	1.31723	1.01325	1.01325	1.01325	1.31723	1.01325
Calculated heat duty[cal/sec]	-581555	-55235.1	-50722.1	74765	-23195.3	17949.4
Net heat duty[cal/sec]	-581555	-55235.1	-50722.1	74765	-23195.3	17949.4
Calculated vapor fraction	0.897709	1	1	1	0.89518	1
First liquid / total liquid	1				1	
Total feed stream CO2e flow[kg/hr]	0	0	0	0	0	0
Total product stream CO2e flow [kg/hr]	0	0	0	0	0	0
Net stream CO2e production[kg/hr]	0	0	0	0	0	0
Utility CO2e production[kg/hr]	0	0	0	0	0	0

Name	B2	B4	B9	B10	B12
Property method	Ideal	Ideal	Ideal	Ideal	Ideal
Use true species approach for electrolytes	Yes	Yes	Yes	Yes	Yes
Free water phase properties method	STEAM-TA	STEAM-TA	STEAM-TA	STEAM-TA	STEAM-TA
Water solubility method	3	3	3	3	3
Specified pressure[atm]	1	1	1	1	1
Calculated pressure[bar]	1.01325	1.01325	1.01325	1.01325	1.01325
Calculated temperature[C]	115	420	420	420	420
Calculated vapor fraction	0	1	1	1	1
Calculated heat duty[cal/sec]	25060.4	-2.45018E+06	-281015	-129969	699849
Temperature change[C]	90	-1221.2	-150	-70	-395
Net duty[cal/sec]	25060.4	-2.45018E+06	-281015	-129969	699849

Conversion Rates by Pass: (Labeling according to the ASPEN Flowsheet)

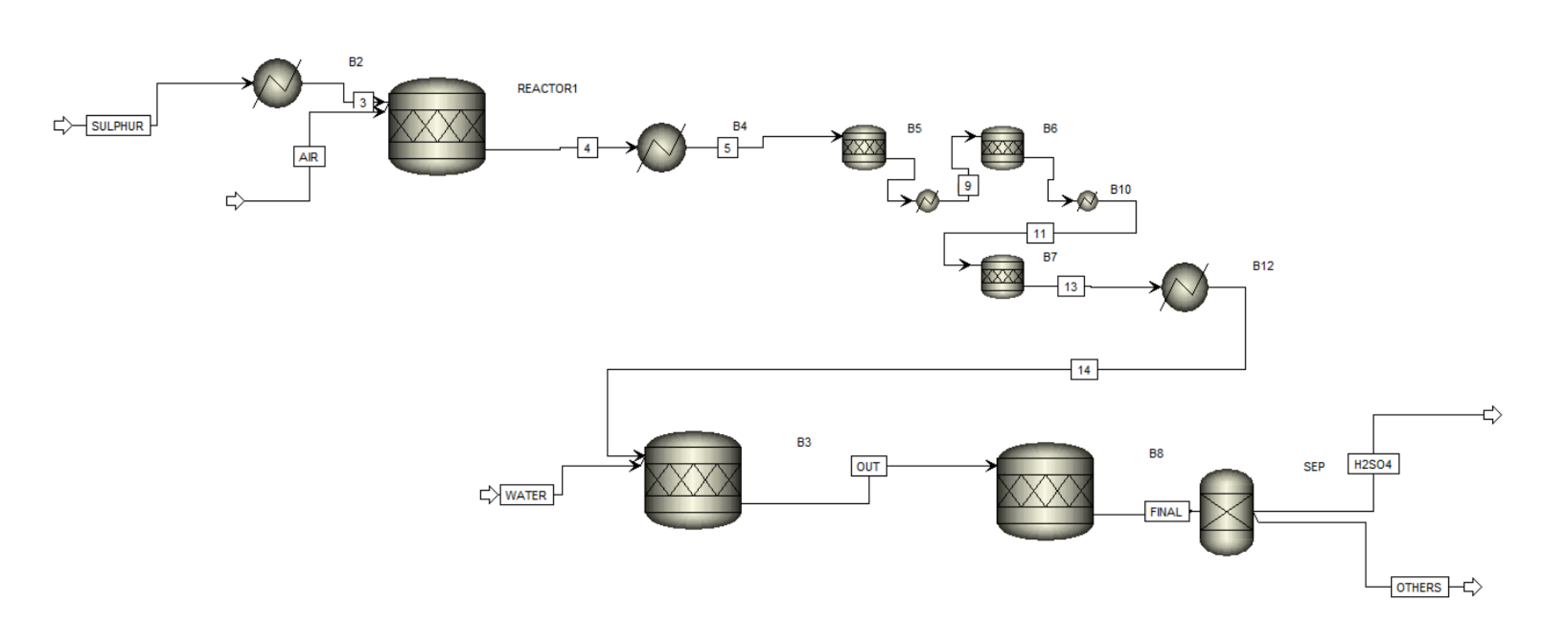
- First Pass (B5): ~60-65%
- Second Pass (B6): Increases overall conversion to around 80-85%
- Third Pass (B7): Increases conversion to around 90-95%

UPDTATED SIMULATION

- We modified the model by adding an additional reactor to the simulation, allowing the remaining SO_3 to react with water, which increased H_2SO_4 production. After separating the H_2SO_4, the final output was 8,134.07 kg/hr.

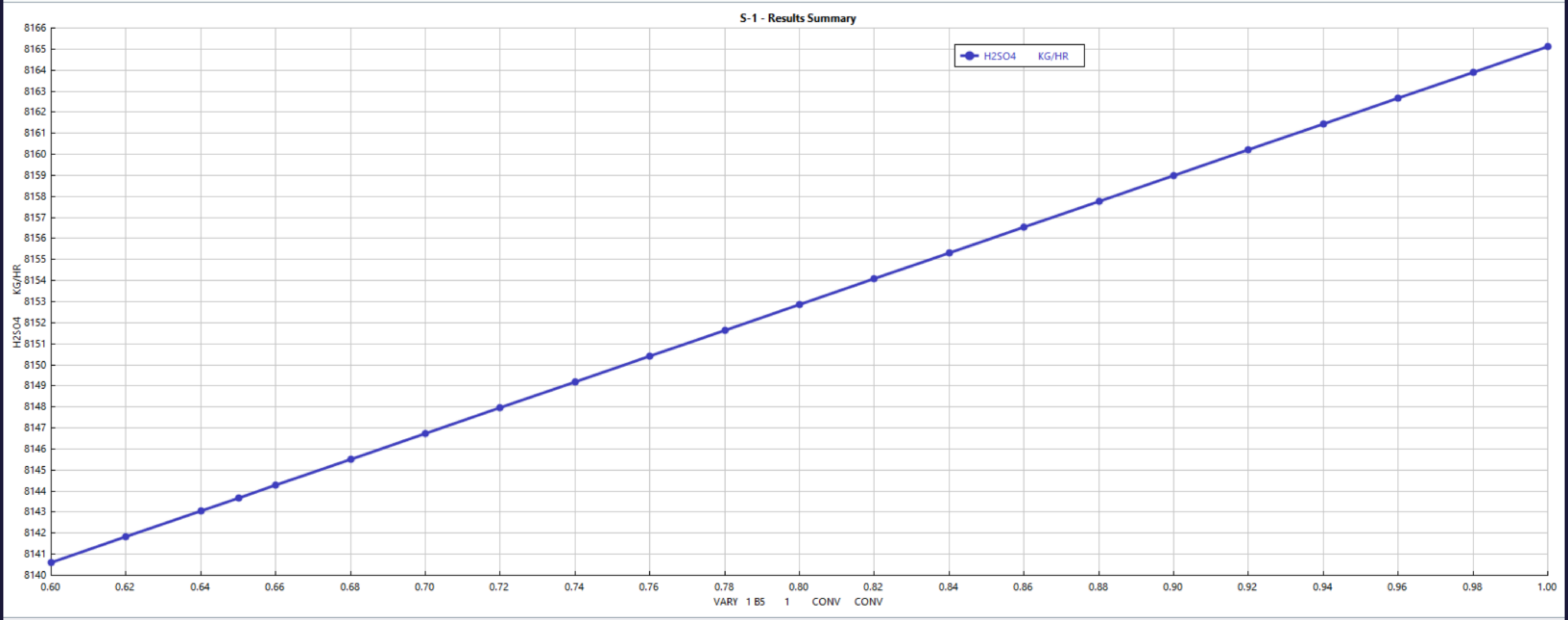
- We performed a sensitivity analysis on this model by adjusting the conversion rates of B3 and B5, as well as the temperature, pressure, and water flow rate. Like before, the output showed no sensitivity to pressure or temperature. However, unlike the previous run, the conversion rate continued to grow steadily without leveling off. As expected, increasing the water flow rate led to a rise in the final output, which eventually stabilized at 8,165.12 kg/hr.

SIMULATION

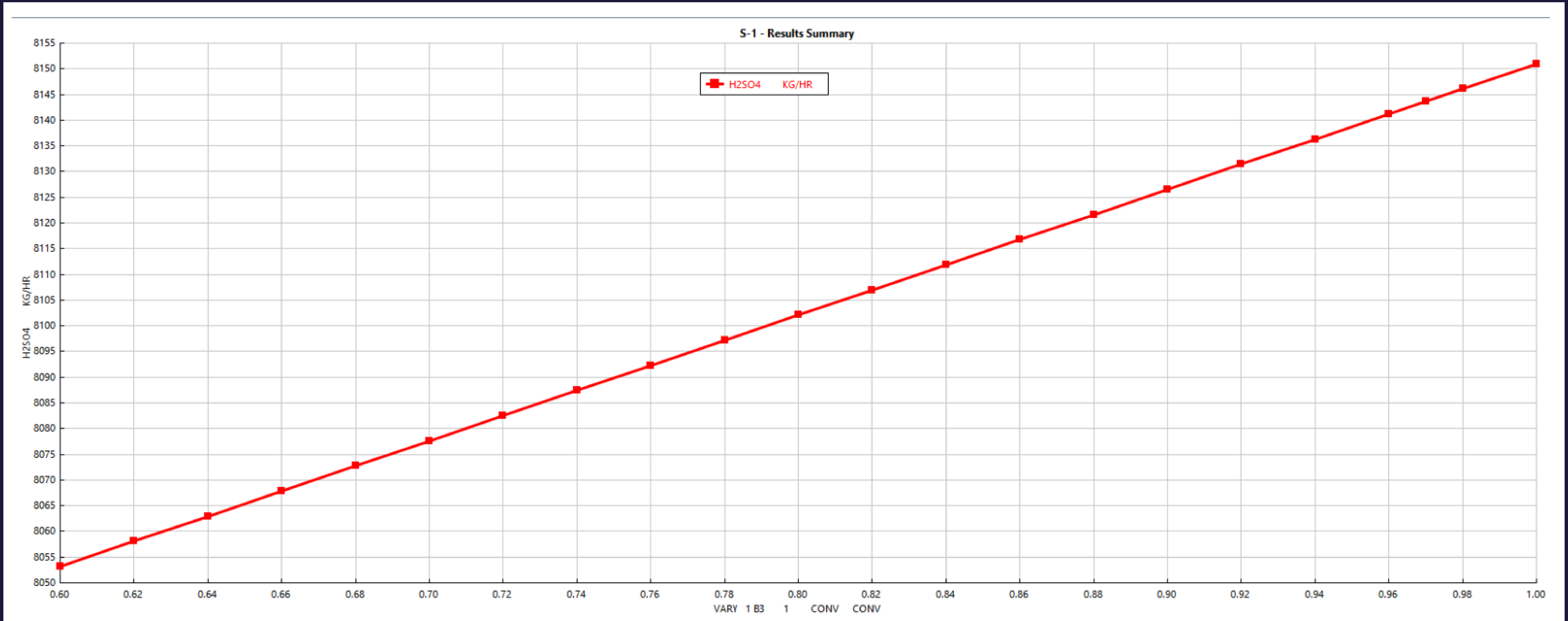


B2
REACTOR1
SULPHUR
3
AIR
4
B4
5
B5
B6
9
B10
11
B7
13
B12
14
B3
OUT
B8
SEP
H2SO4
WATER
FINAL
OTHERS

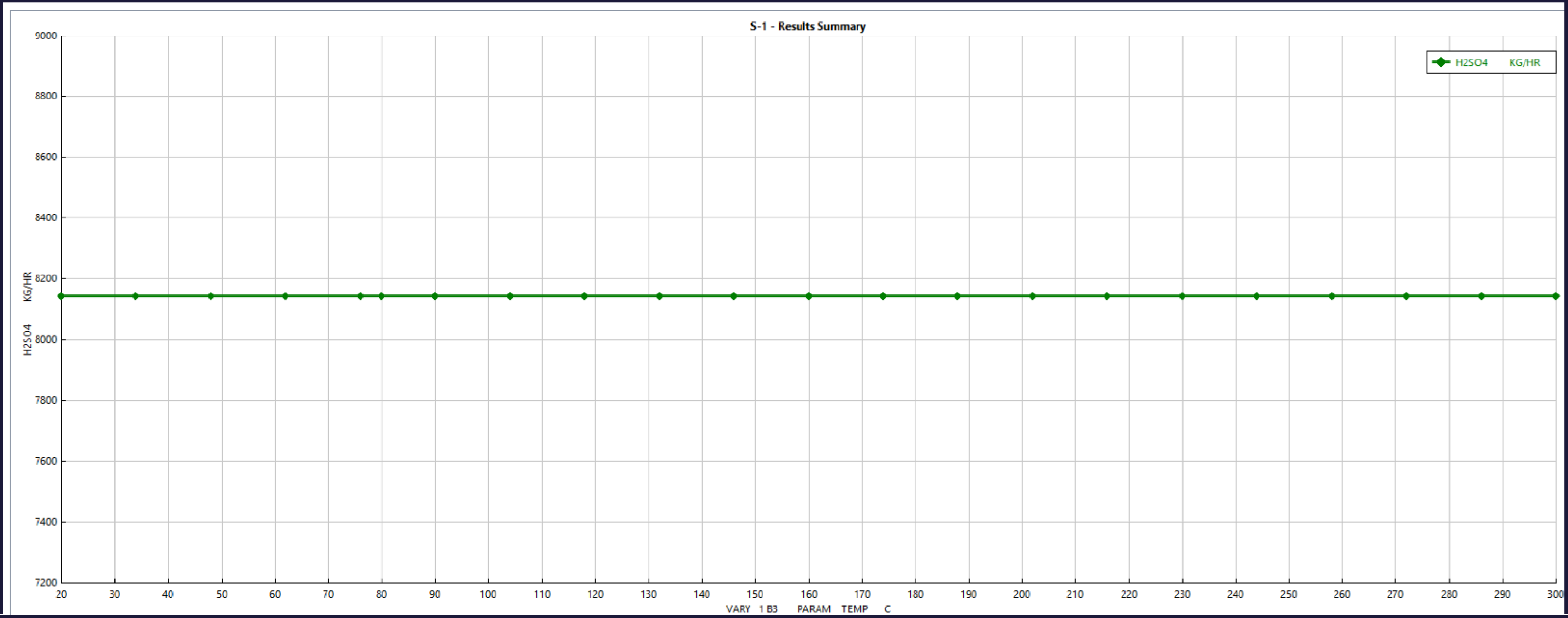
B5 CONVERSION RATE VS H2SO4 OUTPUT



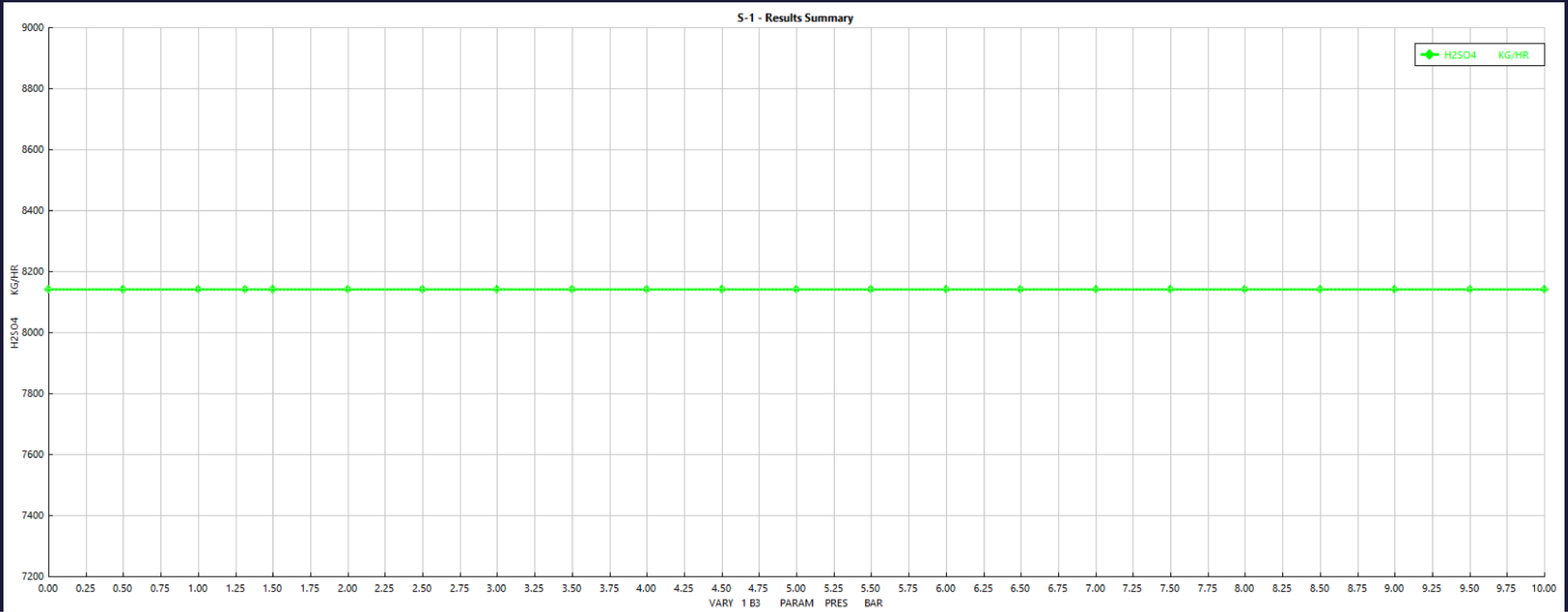
B3 CONVERSION RATE VS H2SO4 OUTPUT



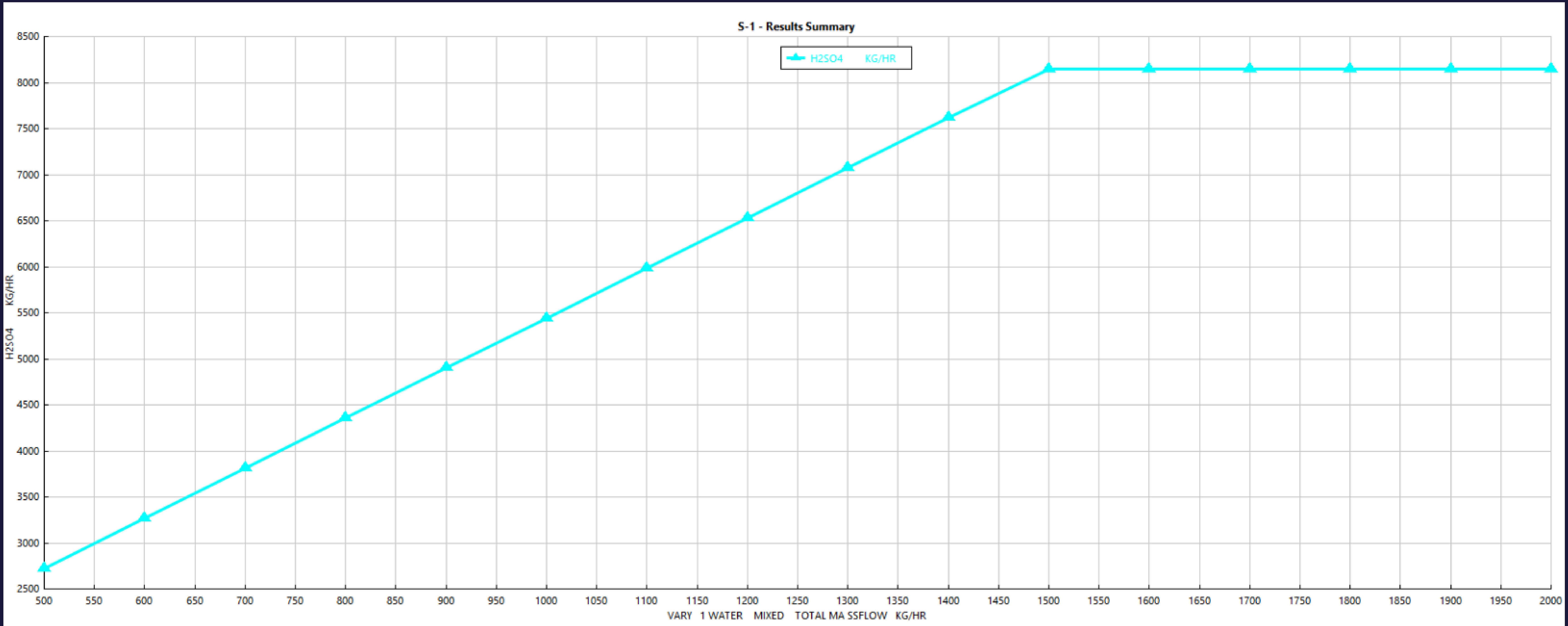
B3 TEMPERATURE VS H2SO4 OUTPUT



B3 PRESSURE VS H2SO4 OUTPUT



WATER MASS FLOW RATE VS H2SO4 OUTPUT.



STREAM FLOW RATES

Streams (Kg/hr)	3	4	5	8	9	10	11	13	Air	Final	H2SO4 Out	Sulphur	Water
Mass flow	2671.9	26752.4	26752.4	26752.4	26752.4	26752.4	26752.4	26752.4	24080.5	28252.4	28252.4	2671.9	1453.32
Sulphur	2671.9	0	0	0	0	0	0	0	0	0	0	2671.9	0
Air	0	0	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	18471.7	18471.7	18471.7	18471.7	18471.7	18471.7	18471.7	18471.7	18471.7	18471.7	0	0
Oxygen	0	2942.46	2942.46	2075.91	2075.91	1679.3	1679.3	1612.81	5608.76	0	1612.81	0	0
H2S2O7	0	0	0	0	0	0	0	0	0	0	0	0	0
SO2	0	5338.2	5338.2	1868.37	1868.37	280.256	280.256	14.0128	0	14.0128	14.0128	0	0
SO3	0	0	0	4336.38	4336.38	6321.1	6321.1	6653.84	0	5.98845	199.615	0	0
H2SO4	0	0	0	0	0	0	0	0	0	8143.69	7906.49	0	0
Water	0	0	0	0	0	0	0	0	0	4.1644	47.7324	0	1453.32

CONCLUSION

- This study highlights the effectiveness of refining our H_2SO_4 production model. Initially, without a separator to recycle SO_3, the output reached 7,903.52 kg/hr. Sensitivity analysis showed that only the conversion rates impacted the output, which stabilized at 7,912.22 kg/hr. To improve the model, we added a reactor and separator to allow the unused SO_3 to react further with water, increasing the output to 8,134.07 kg/hr.

- In the updated model, adjusting conversion rates and water flow rate continued to boost output, with water flow peaking at 8165.12 kg/hr. This refined model highlights the benefits of optimizing SO_3 recycling and water flow, achieving higher efficiency and production stability.

REFERENCES

- SOURCE: RSF Press Journal
- Book: The Chemical Process Industries, second edition Author: R. NORRIS SHREVE Chapter 19: Sulphur and Sulphuric Acid, Page 384

DATABANKS

- APV140 PURE40
- APV140 INORGANIC
- APV140 AQUEOUS
- APV140 SOLIDS
- APESV140 AP-EOS
- NISTV140 NIST-TRC

THANK YOU