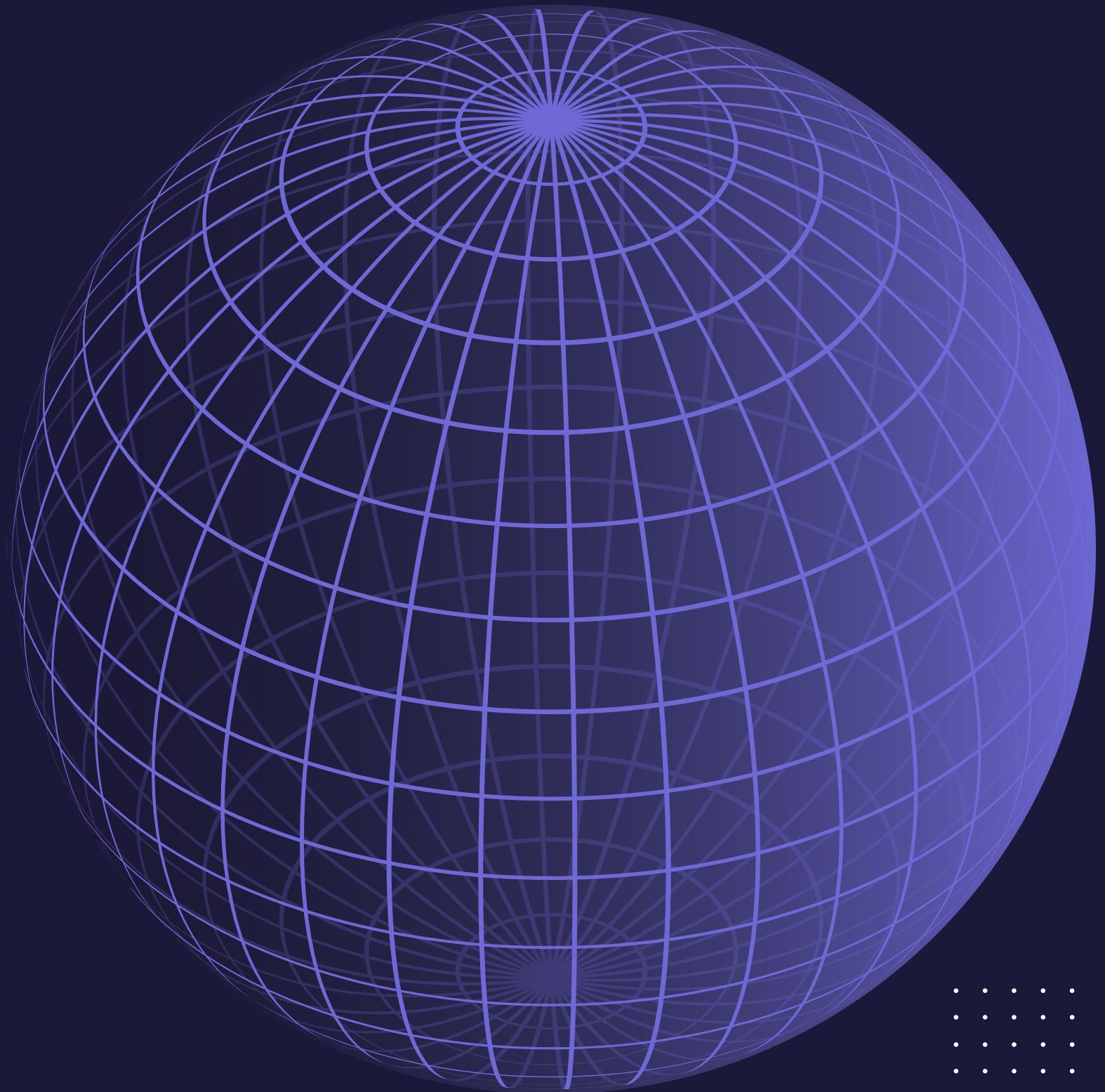




CHE 251 GROUP TERM PROJECT

GROUP 9



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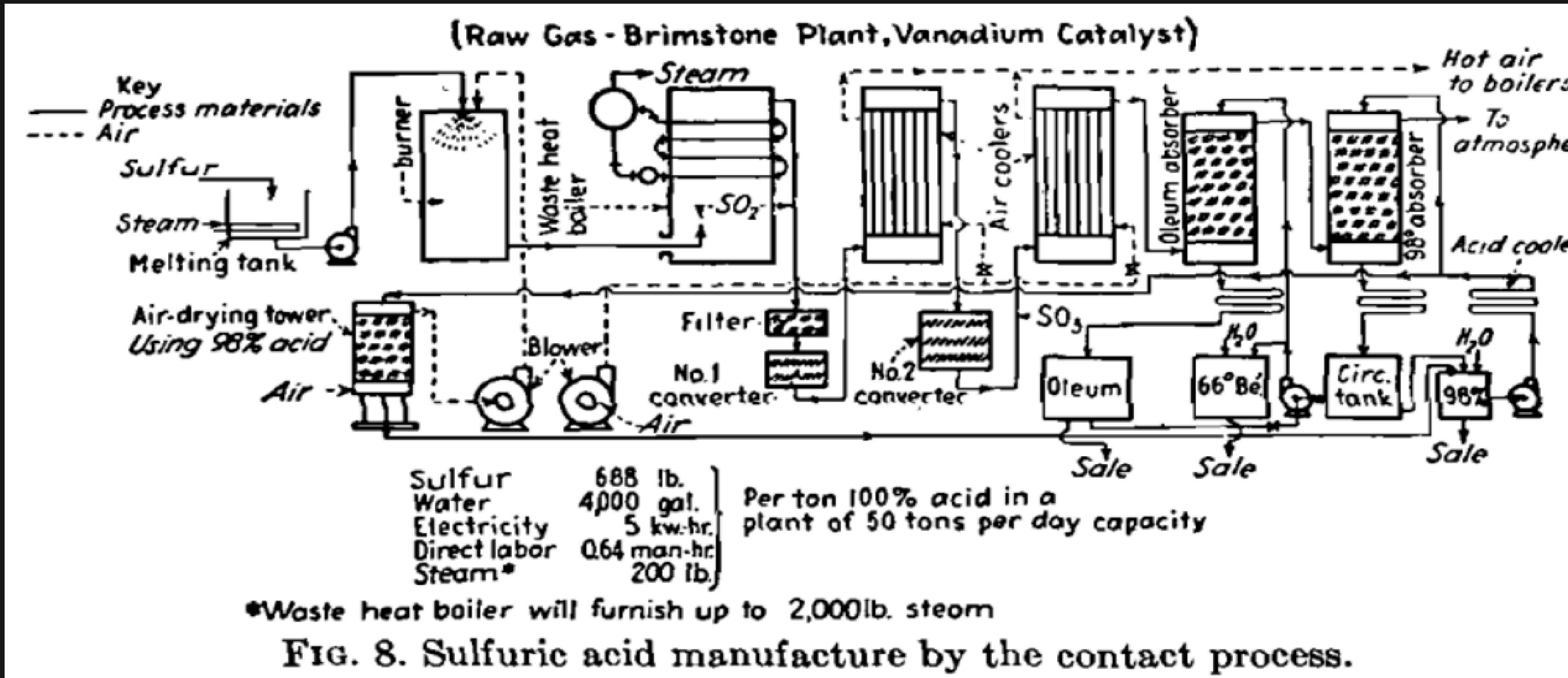
TOPIC

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 PROCESS





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.

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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

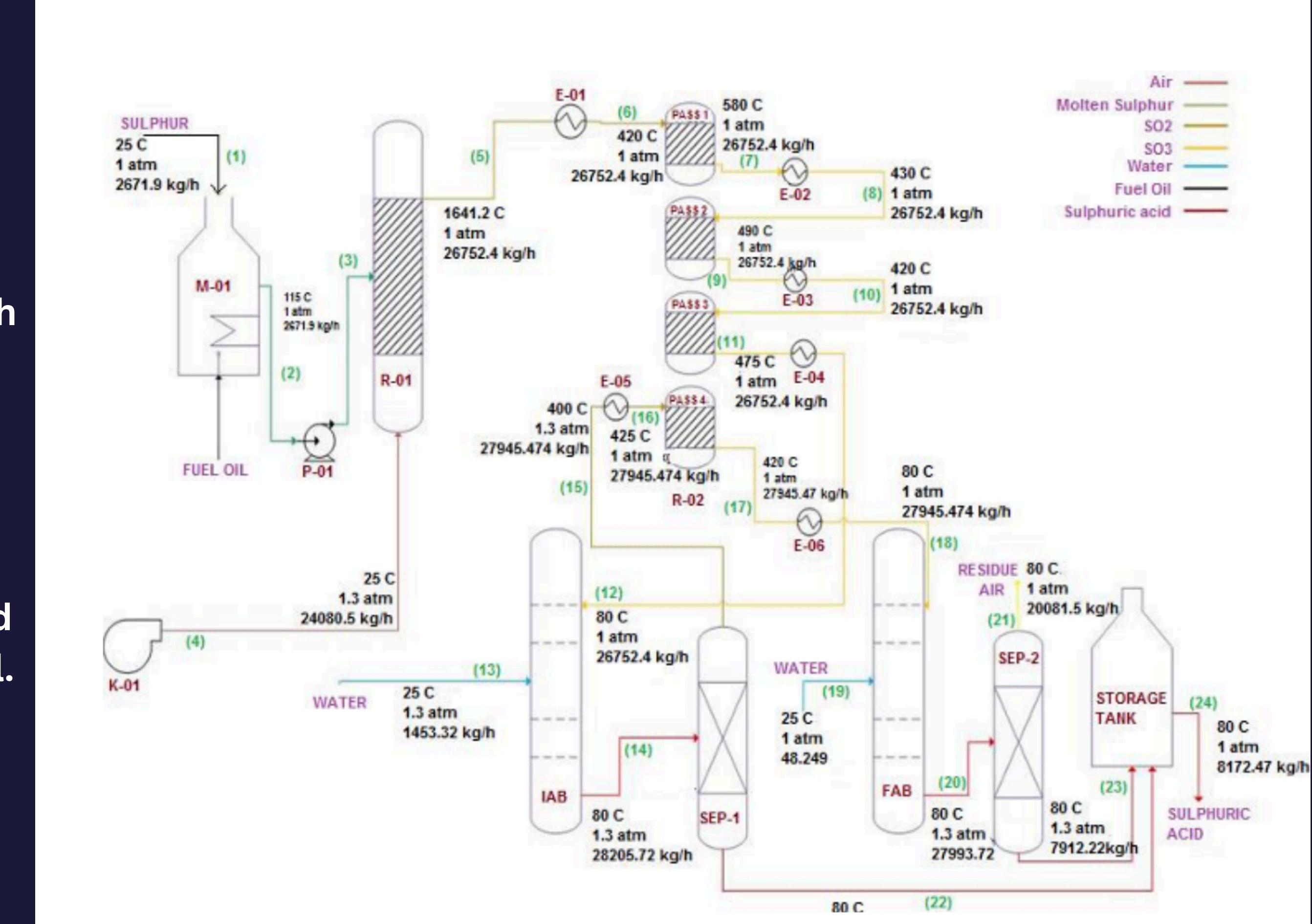
The flow includes SO_2 preparation, oxidation, SO_3 , and dilution.
Equipment includes pumps, reactors, heat exchangers, converters, and absorbers.

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





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.

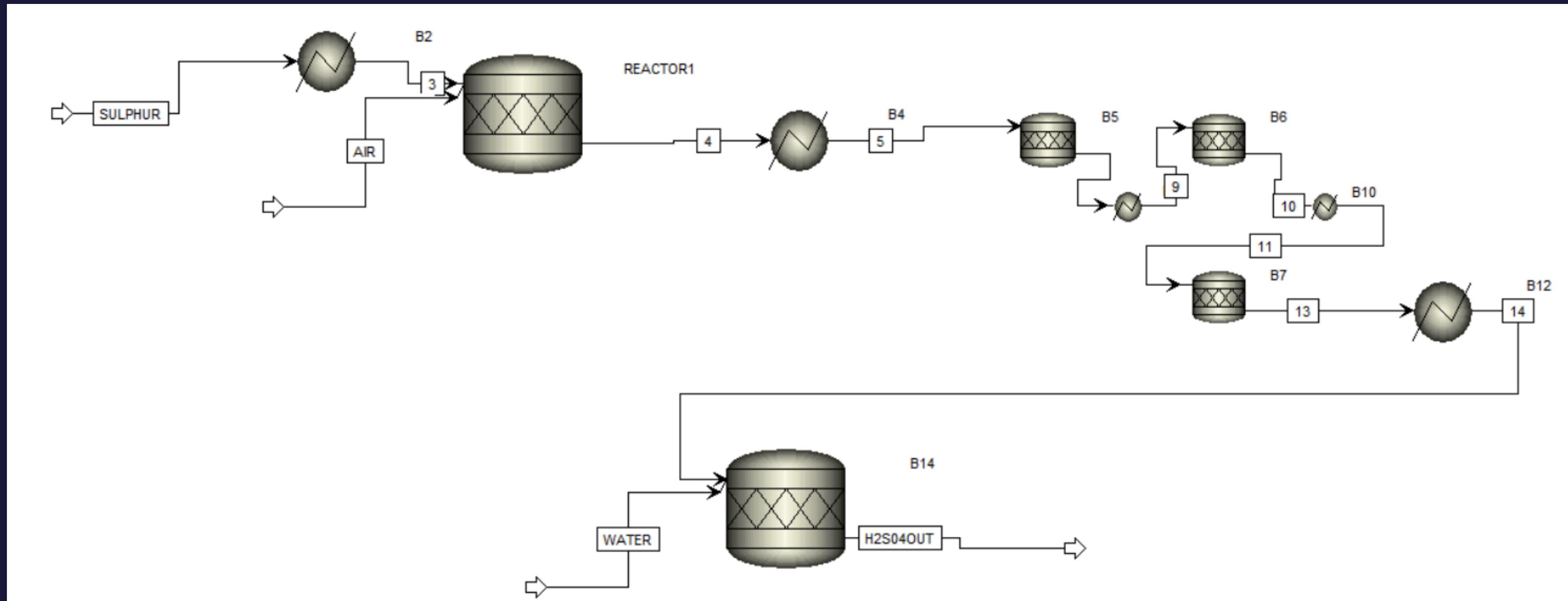
We conducted a sensitivity analysis on this model, focusing on H₂SO₄ production as the output. The analysis involved adjusting temperature, pressure, and the conversion rates of B5, B6, and B7 as key variables.

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.

DISCUSSION

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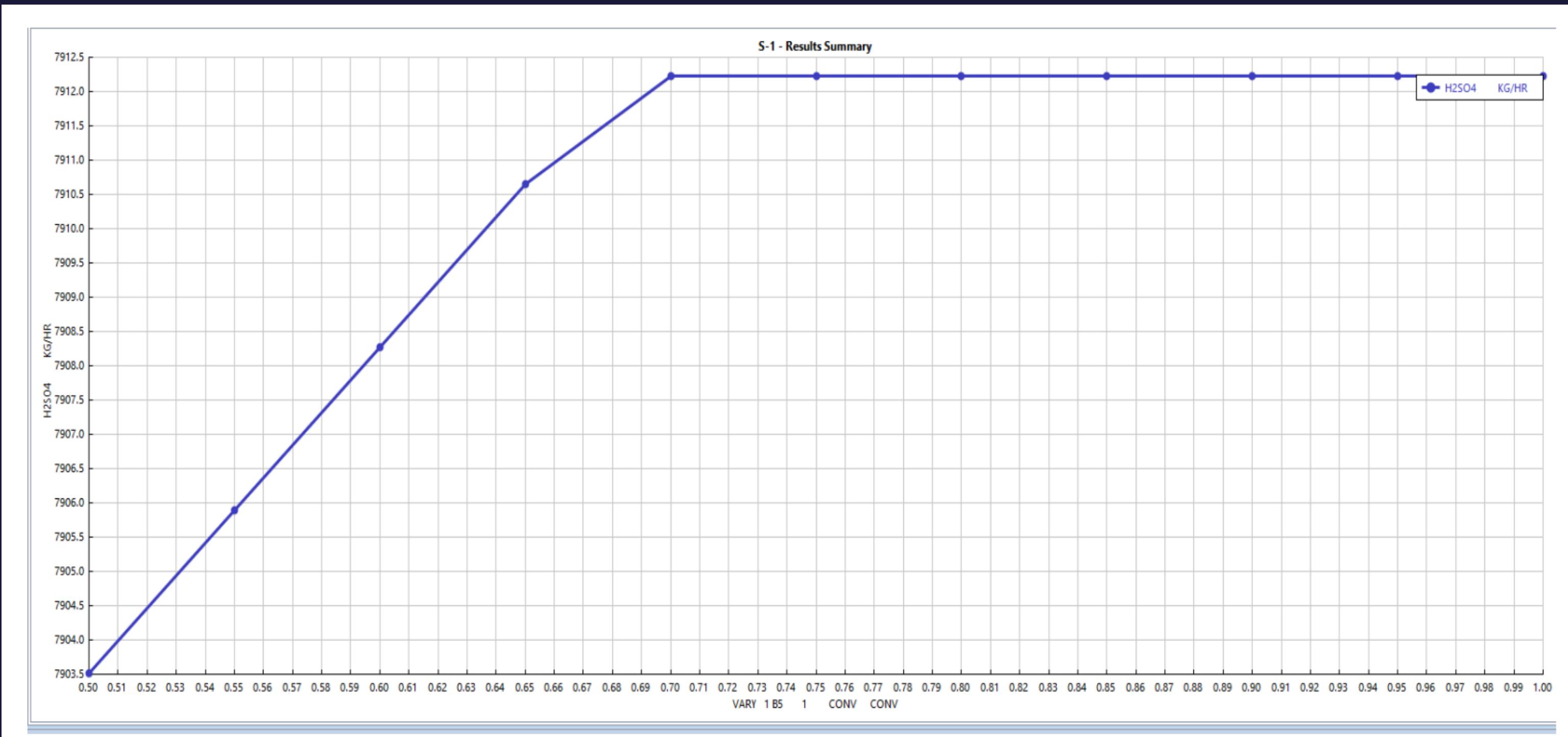
SIMULATION



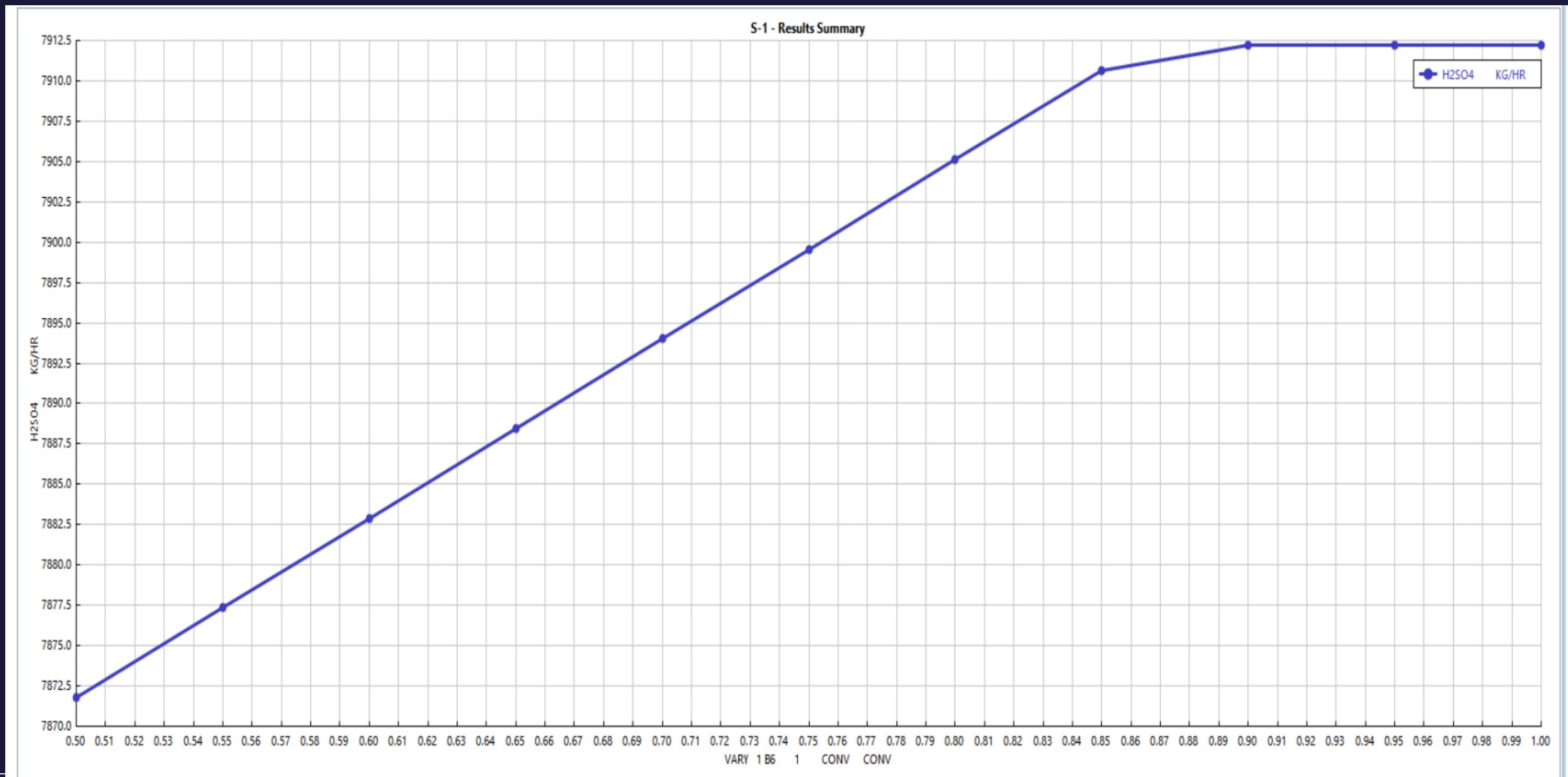
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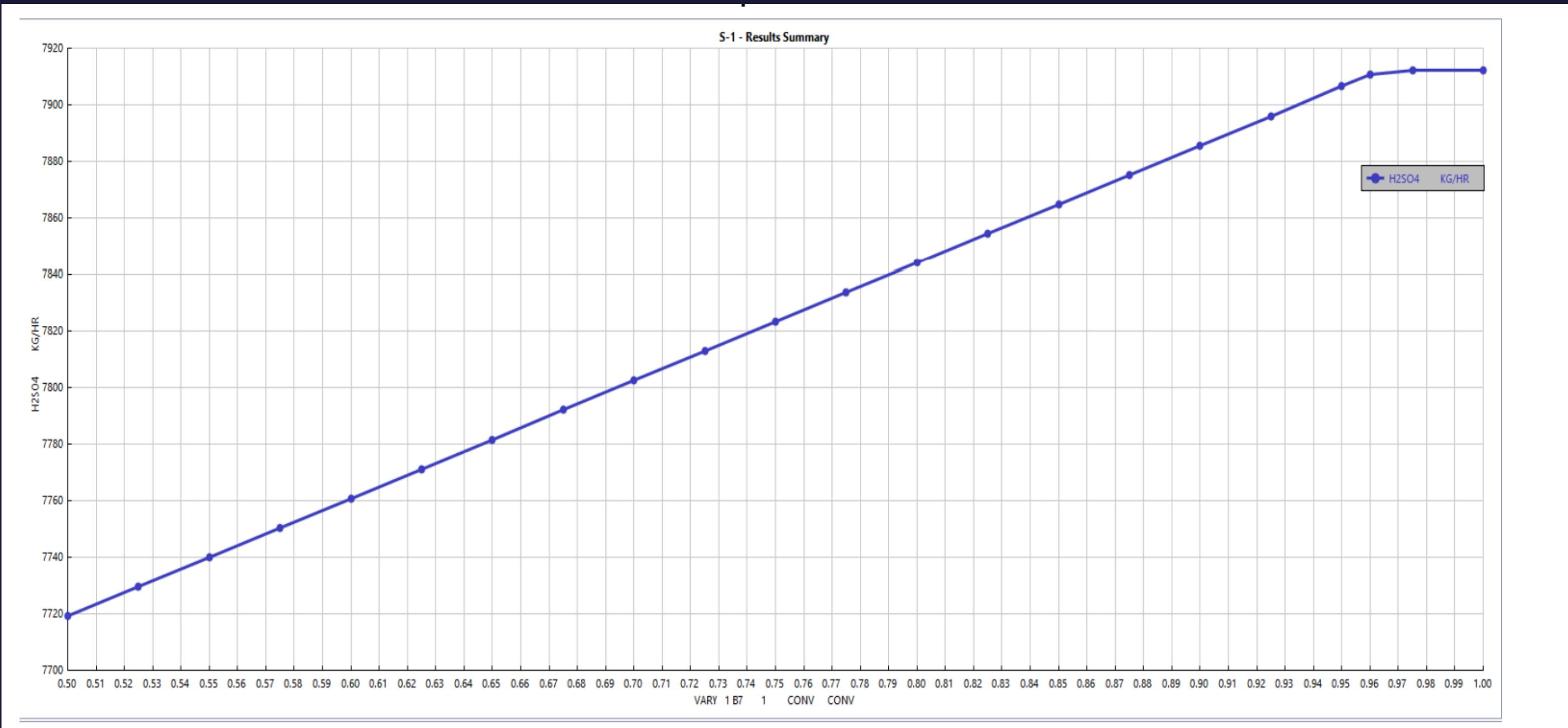
B5 CONVERSION RATE VS H₂S04 OUTPUT



B6 CONVERSION RATE VS H₂S₀4 OUTPUT



B7 CONVERSION RATE VS H₂S₀4 OUTPUT



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

RESULTS

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%**

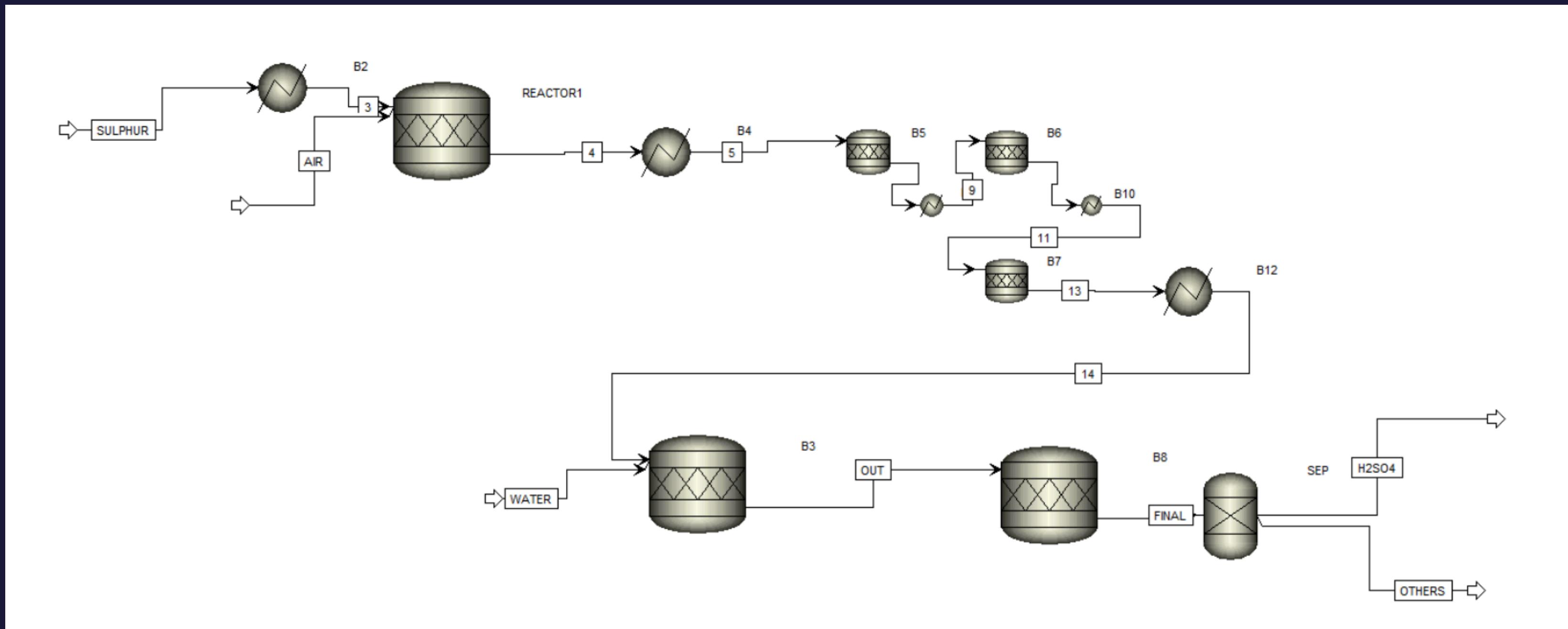


UPDATED SIMULATION

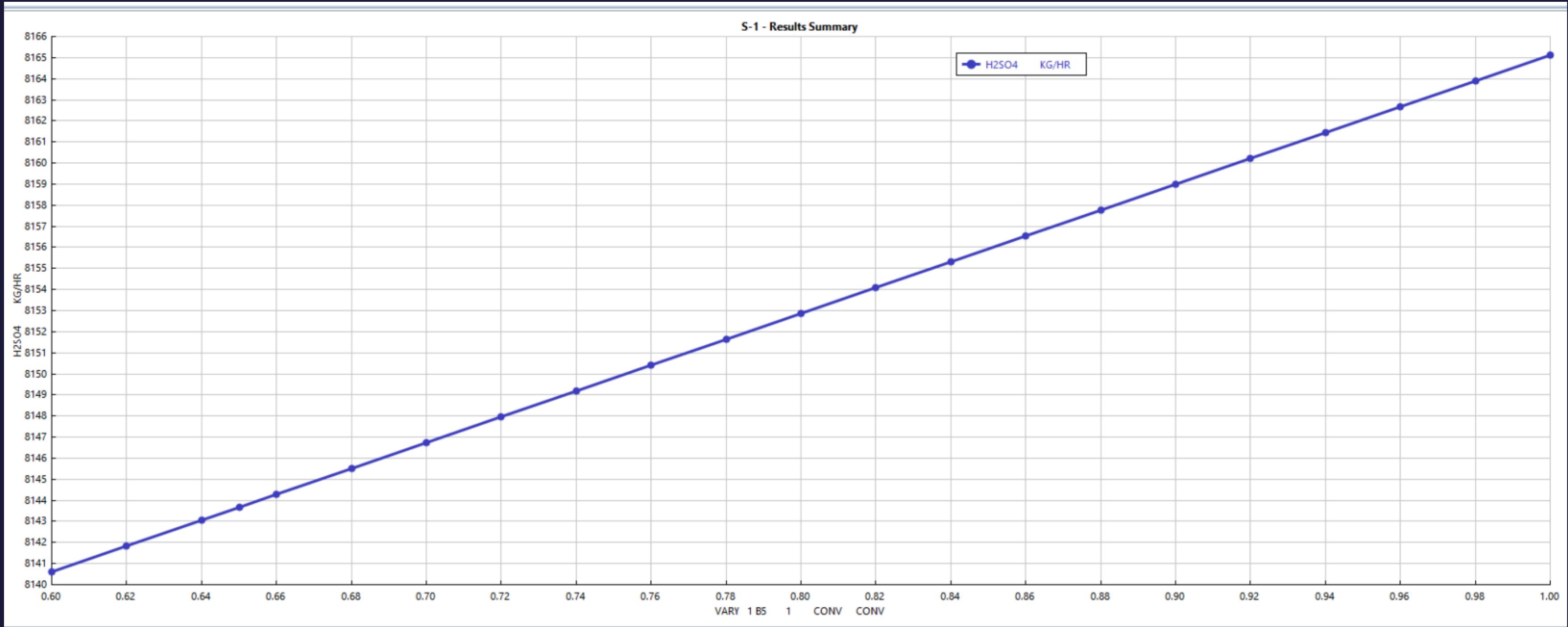
- We modified the model by adding an additional reactor to the simulation, allowing the remaining SO₃ to react with water, which increased H₂SO₄ production. After separating the H₂SO₄, the final output was 8,134.07 kg/hr.
- We performed a sensitivity analysis on this model by adjusting the conversion 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.



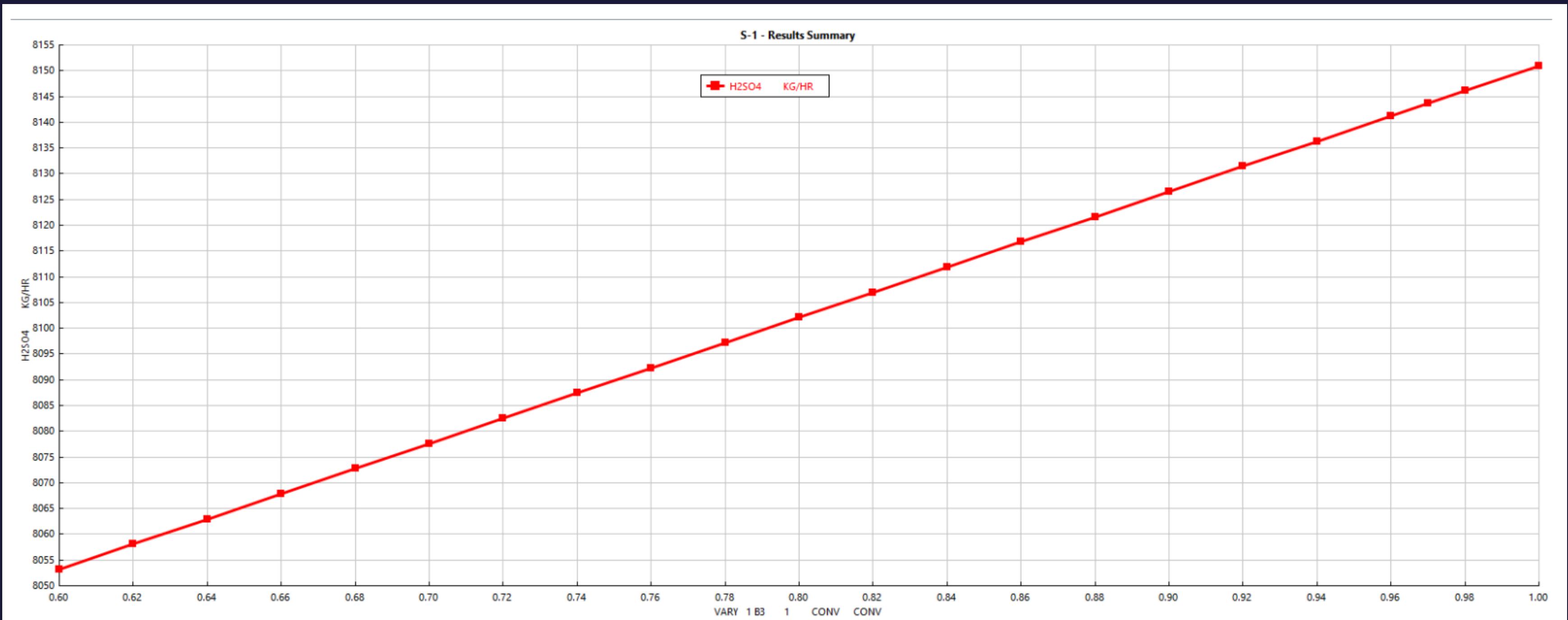
SIMULATION



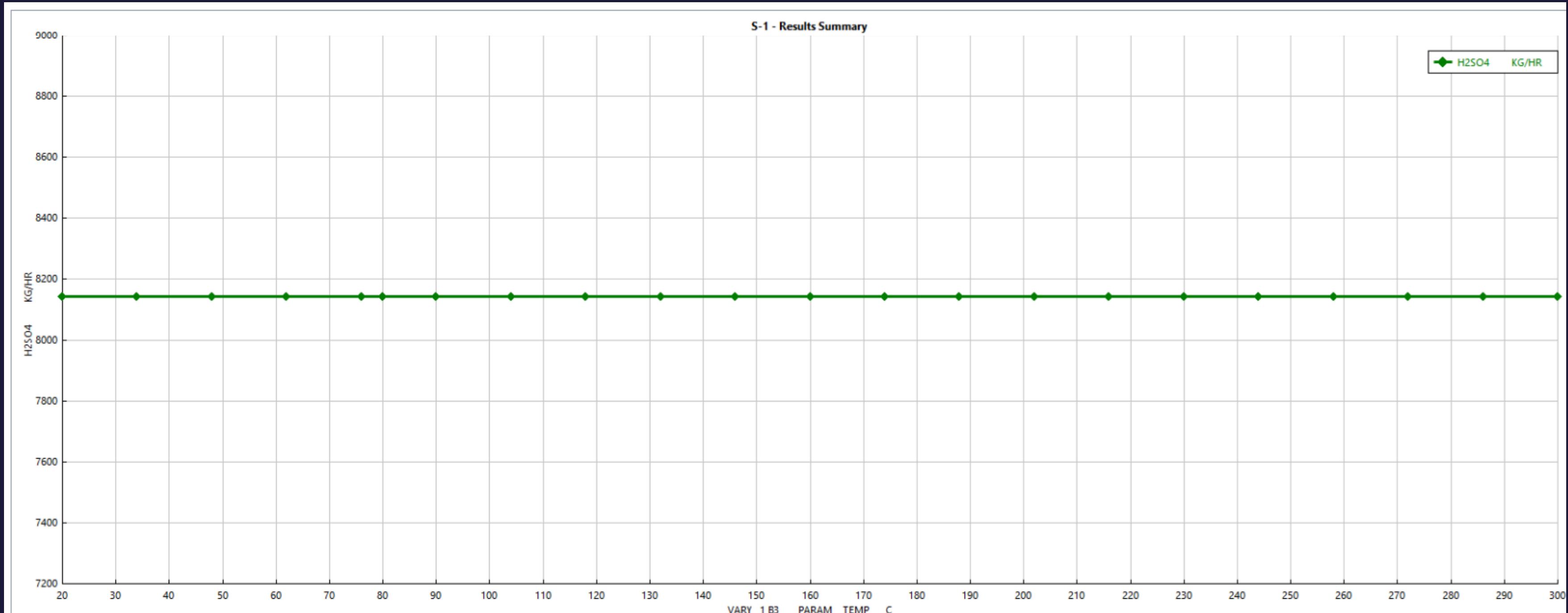
B5 CONVERSION RATE VS H₂S₀4 OUTPUT



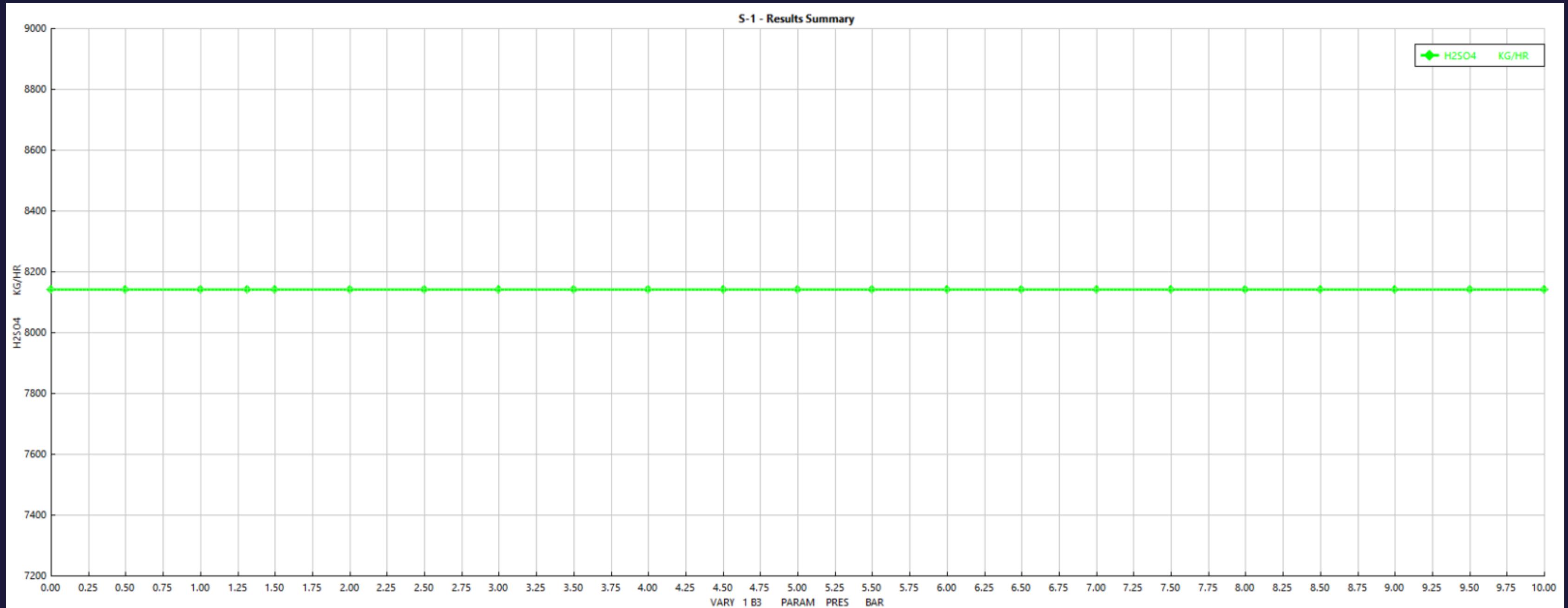
B3 CONVERSION RATE VS H₂S₀4 OUTPUT



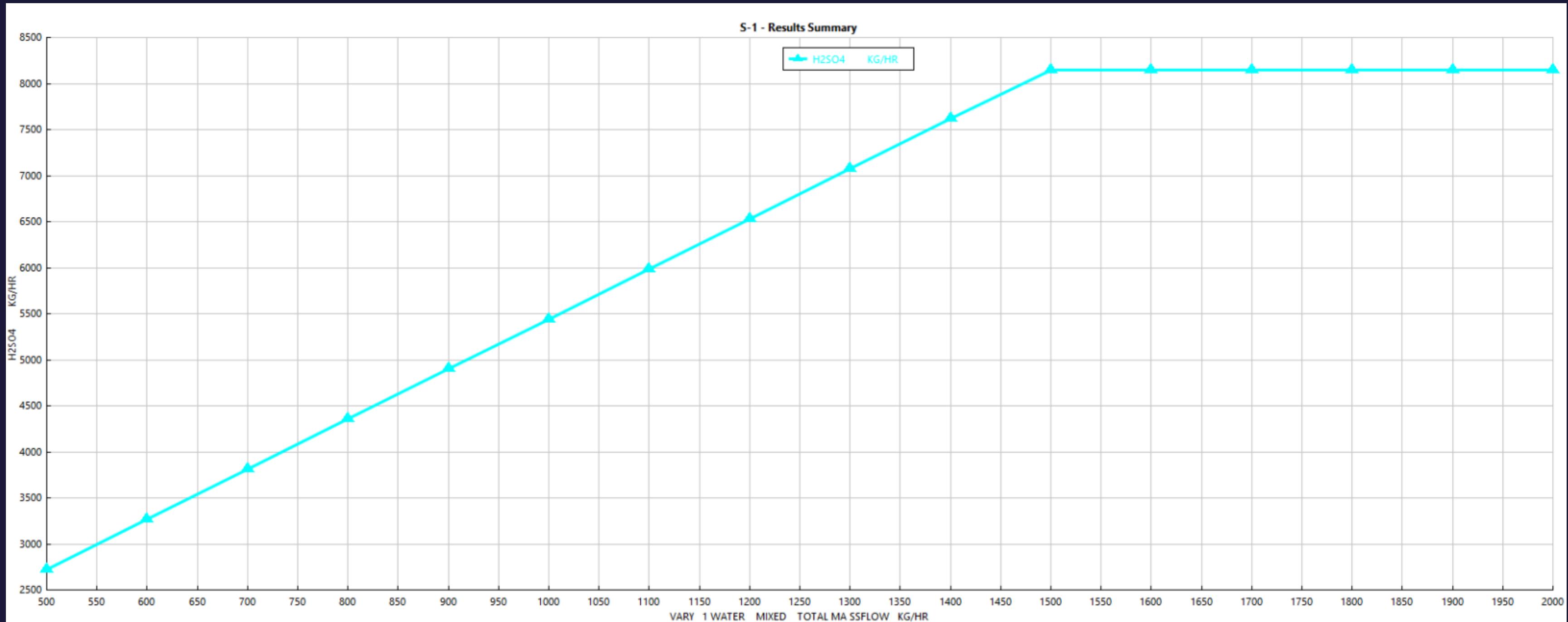
B3 TEMPERATURE VS H₂S₀₄ OUTPUT



B3 PRESSURE VS H₂S₀₄ OUTPUT



WATER MASS FLOW RATE VS H₂S₀4 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

