

Analysis of a Sulfuric Acid Concentration for a Nuclear Hydrogen Production Process by using ChemCAD

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1. Introduction

The thermo-chemical cycles are processes where water is decomposed into hydrogen and oxygen via chemical reactions using intermediate elements which are recycled. The sum of all the reactions is equivalent to the dissociation of a water molecule. Because they only use heat without having to convert it to electricity, these cycles have the potential of a better efficiency than an electrolysis and hence have the potential to significantly reduce the cost for a hydrogen production from water [1].

The concentration of the sulfuric acid solution and its decomposition are essential parts in this cycle. Sulfuric acid concentration is important because if a high purity of sulfuric acid can be obtained before the stream enters the acid decomposition unit operation, the decomposition can be carried out with high efficiency.

In this paper, we employed the ChemCAD to simulate a sulfuric acid concentration process at a steady state to obtain a prospective model.

2. Methods and Results

1. VLE Curves for H_2SO_4 - H_2O Binary System

To simulate the sulfuric acid concentration process, VLE models for concentrated acid are investigated. Fig. 1 shows the default VLE models in a commercial code.

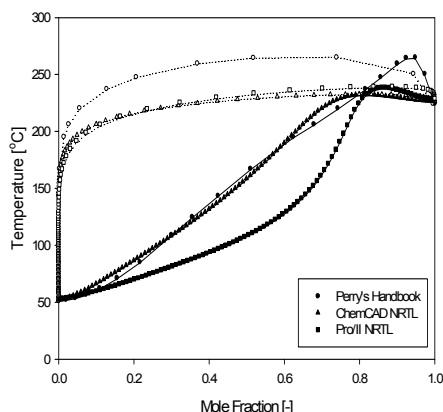


Fig. 1. Default VLE curves in commercial code(0.1bar).

From composition vs. partial-total pressure data [2], we can obtain a reference VLE curve of a H_2SO_4 - H_2O binary system. Default NRTL in ChemCAD is only well matched with a bubble point of a 0-0.7 mole fraction. Then, a new VLE model is needed to solve the problem.

By using the polynomial method in ChemCAD, a applicable model for a 0-0.9 mole fraction range is obtained. Fig. 2 represents this result and its problem does not reflect azeotropic points.

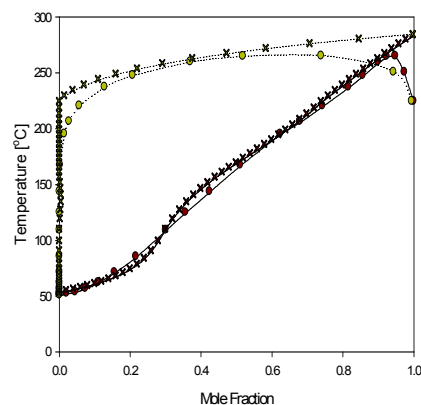


Fig. 2. Polynomial VLE curve(0.1bar).

Azeotropic point is very important because this point indicates a purity limitation. VLE model must have an azeotrope at a 0.9 mole fraction. Then, the VLE model for a 0.6-1.0 mole fraction is obtained from a BIP regression and a BIP modification. This result is shown in Fig. 3.

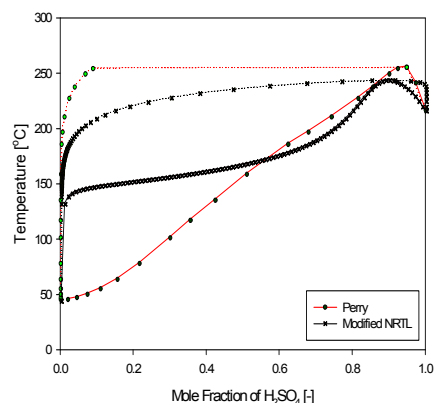


Fig. 3. VLE curve of modified NRTL(0.1bar).

Then, a polynomial equation for the K values can be applied to the 0-0.9 range and a modified NRTL can be applied to the azeotropic range.

2. Simulation Results



Fig. 4. Process diagram of the 2 step multiple effects flash evaporator.



Fig. 5. Process diagram of the 2 step multistage distillation column.

Fig. 4 and 5 show the process types for the sulfuric acid concentration. Both step 1 and step 2 consist of 3 flash evaporators or a 5 stage distillation column. Input and step output conditions based on a reference VLE curve are represented in Table 1.

Table 1. Input and step output conditions for H₂SO₄ concentration.

Stream		Input	Step 1	Step 2
Temp [°C]		77	170	240
Pressure [bar]		1.85	0.1	0.07
Total [kmol/s]		2.0407	2.0407	2.0407
Flowrates [kmol/s]	Sulfuric Acid	0.4862	-	-
	Water	1.5545	-	-
Mole Fraction [-]	Sulfuric Acid	0.2383	0.5231	0.9016
	Water	0.7617	0.4769	0.0984

Thermodynamic models are a polynomial equation for the K values for step 1 and a modified NRTL for step 2. 2nd step output must be azeotropic point and it affects the evaporation and decomposition process.

Table 2 shows the calculation results of the multiple effects for the flash evaporation process. Step 1 results agree with the reference data but step 2 results have a

high temperature of the bottom products compared with the reference data.

Results of 2 step 5 stage distillation columns are matched well with the reference data and it is shown in Table 3.

Table 2. Calculation results of the multiple effects for the flash evaporation process.

Concentration Step		Step 1		Step 2	
Stream No.		7	4	13	10
Temp [°C]		80.59	171.60	141.42	246.00
Heat Duty [kJ/s]		56828.63		20564.63	
Total [kmol/s]		1.1115	0.9292	0.3931	0.5360
Flowrates [kmol/s]	Sulfuric Acid	0	0.4862	0.0036	0.4826
	Water	1.1115	0.443	0.3896	0.0534
Mole Fraction [-]	Sulfuric Acid	0	0.5232	0.0092	0.9004
	Water	1	0.4768	0.9908	0.0996

Table 3. Calculation results of the 2 step multistage distillation column.

Concentration Step		Step 1		Step 2	
Stream No.		2	3	4	5
Temp [°C]		172.63	38	38	237.74
Heat Duty [kJ/s]		64189.918		25500.039	
Total [kmol/s]		0.9292	1.1115	0.4917	0.4375
Flowrates [kmol/s]	Sulfuric Acid	0.4862	0	0.0938	0.3924
	Water	0.443	1.1115	0.3979	0.0451
Mole Fraction [-]	Sulfuric Acid	0.5232	0	0.1908	0.8969
	Water	0.4768	1	0.8092	0.1031

3. Conclusion

The sulfuric acid concentration has been analyzed and an output forecast model for a steady state has been successfully established.

Acknowledgments

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