

An Automatic Approach to the Stabilization Condition in a HIx Distillation Simulation

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1. Introduction

In the Sulfur-Iodine(SI) thermochemical process to produce nuclear hydrogen, an H₂O-HI-I₂ ternary mixture solution discharged from the Bunsen reaction is primarily concentrated by electro-electrodialysis. The concentrated solution is distilled in the HIx distillation column to generate a high purity HI vapor. The pure HI vapor is obtained at the top of the HIx distillation column and the diluted HIx solution is discharged at the bottom of the column.

In order to simulate the steady-state HIx distillation column, a vapor-liquid equilibrium (VLE) model of the H₂O-HI-I₂ ternary system is required and the subprogram to calculate VLE concentrations has been already introduced by KAERI research group in 2006 [1]. The steady state simulation code for the HIx distillation process was also developed in 2007[2]. However, the intrinsic phenomena of the VLE data such as the steep slope of a T-x-y diagram caused the instability of the simulation calculation.

In this paper, a computer program to automatically find a stabilization condition in the steady state simulation of the HIx distillation column is introduced. A graphic user interface (GUI) function to monitor an approach to the stabilization condition was added in this program.

2. Method and Results

In order to stably run the existing code, the setting of the stabilization conditions is an important process because the stabilization conditions are closely related to convergence of steady state simulation for the HIx distillation process. Also, the setting procedure of the stabilization conditions is a gradual process from the existing converged values to new setting values. In the setting process of stabilization conditions, setting intervals were obtained by a trial-and-error method. Over the two sections, the stabilization conditions for the existing code running and an algorithm for automation setting of the stabilization conditions were introduced.

2.1 Stabilization conditions

The list of stabilization conditions for the code running is represented in Table 1. As shown in Table 1, the stabilization conditions consist of three parts: operation conditions, equipment specifications and initial guessing values. The operation conditions and equipment specifications are inputted into the code in the form of constant. The initial guessing values are inputted into the code in the form of a text file.

Table 1. List of the stabilization conditions

Stabilization condition	Unit	Reference
Column operation pressure	bar	Operation condition (constant)
Feed temperature	°C	
Total feed mole flow rate	mole/s	
Feed mole fraction (H ₂ O : HI : I ₂)	mole fraction	
Outlet HI mole flow rate	mole/s	
Outlet HI mole fraction	mole fraction	Equipment spec. (constant)
Total number of stage*	-	
Feed stage number from condenser	-	Initial guessing value (text file)
Liquid flowrate at each stage	mole/s	
Vapor flowrate at each stage	mole/s	
Temperature at each stage	°C	

*: Including condenser and reboiler.

2.2 Algorithm for automation setting of stabilization conditions

The sequence for automation setting of stabilization conditions are in the following steps:

- ① A new setting value which is the total liquid flow rate at the feed tray should be determined from the existing converged value.
- ② As a starting point, the existing converged value which is the column operation pressure should be approached to a new setting value by increasing or decreasing the 1 bar per each step.
- ③ As a starting point, the existing converged value which is feed temperature should be approached to a new setting value by increasing or decreasing the 0.1 degree C per each step.
- ④ As starting points, the existing converged values which are mole fraction of the H₂O-HI-I₂ chemical system should be approached to new setting values by increasing or decreasing the 10⁻⁵ per each step.
- ⑤ As a starting point, the existing converged value which is the HI outlet mole flow rate at the top should be approached to a new setting value by increasing or decreasing the 1.0 mole/s per each step.
- ⑥ As a starting point, the existing converged value which is the HI outlet mole fraction at the top should be approached to a new setting value by increasing or decreasing the 10⁻⁵ per each step.
- ⑦ As starting points, the existing converged values which are total number of stage and feed stage number should be approached to new setting values by increasing or decreasing the 1 per each step.

Figure 2 shows a flow chart for automation setting of stabilization conditions. As shown in Figure 2, after a setting of stabilization conditions, the convergence for steady state simulation is checked per each step.

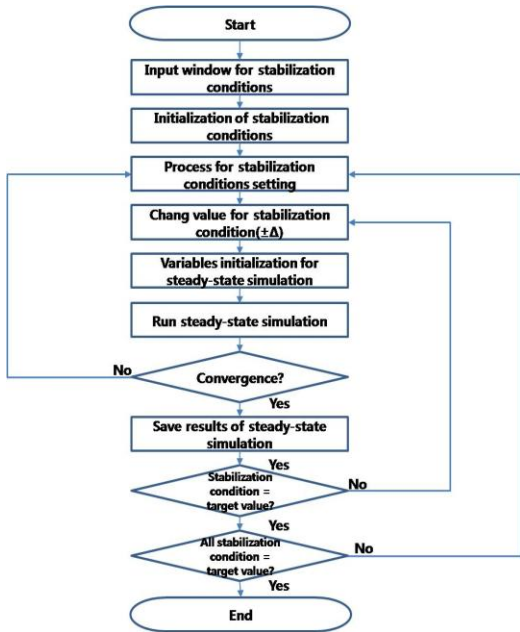


Fig. 2. Flow chart for automation setting of the stabilization conditions.

2.3 GUI Environment

Figure 3 shows input and main window for automation program of stabilization conditions. In figure 3, the stick graphs in main window are represented as matching degree between the target values and the setting values currently in progress.

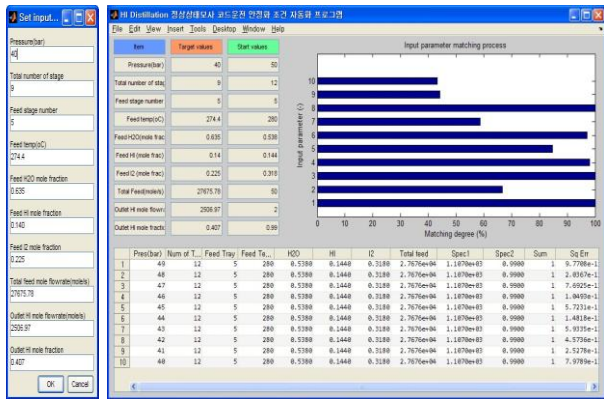


Fig. 3. Input and main window for automation program of stabilization conditions.

2.4 Testing for the developed program

Testing for the developed program has been performed by two cases of operation conditions. Table 3 shows the test cases for testing of the developed program. Based on the two operation conditions, Fig. 4 and Fig. 5 show results of steady state simulation for the HIX distillation process by using the developed program.

Table 3. Test cases for the automation program of stabilization condition

Stabilization condition	Test case 1	Test case 2
Column operation pressure (bar)	40	22
Total number of stage (-)	9	10

Feed stage number from condenser (-)	3	8
Feed temperature (°C)	274.00	249.00
Total feed mole flow rate (mole/s)	27675.78	37800.00
Feed mole fraction (-)	H ₂ O : 0.635 HI : 0.140 I ₂ : 0.225	H ₂ O : 0.516 HI : 0.116 I ₂ : 0.368
Outlet HI mole flow rate (mole/s)	2506.97	3877.30
Outlet HI mole fraction (-)	0.407	0.274

==== Converged after Iteration # = 45 =====

No.	Liquid composition			Vapor composition			Temp. oC	L	V
	Mole fraction, %			Mole fraction, %					
	H ₂ O	HI	I ₂	H ₂ O	HI	I ₂			
1	68.342	13.269	18.389	54.978	40.700	4.322	277.85	165.03	2506.97
2	65.400	12.863	21.737	55.803	39.006	5.191	280.26	163.53	2672.00
3	64.806	12.640	22.554	58.639	35.773	5.587	282.48	27871.74	1978.76
4	65.518	12.159	22.323	69.228	24.599	6.173	287.55	28320.60	2702.93
5	65.868	11.863	22.269	74.994	18.575	6.431	289.26	28437.98	3151.79
6	66.023	11.708	22.269	77.702	15.767	6.531	289.72	28446.60	3269.17
7	66.094	11.627	22.279	79.016	14.411	6.574	289.84	28436.20	3277.79
8	66.072	11.577	22.351	79.673	13.715	6.612	289.91	28418.14	3267.39
9	64.331	11.356	24.313	79.552	13.292	7.155	290.76	25168.81	3249.33

D B Reflux Boilup RR
2506.97 25168.81 165.03 3249.33 0.0658

Feed Bubble temperature (C) = 257.38
Heat in each exchanger, kcal/s
Q1 = 30001.52, Q2 = 13883.80, Q3 = -1121.08, Q4 = 20113.43, Q5 = -2332.01, Q6 = -71920.86
Enthalpy(kcal/s) of Feed = -1064452.33, Distillate = -66678.71, Bottom = -934895.95
Entropy(kcal/s/K) of Feed = -474525.40, Distillate = 7179.07, Bottom = -201668.92

Fig. 4. Results of steady state simulation for the HIX distillation process (pressure: 40 bar).

==== Converged after Iteration # = 205 =====

No.	Liquid composition			Vapor composition			Temp. oC	L	V
	Mole fraction, %			Mole fraction, %					
	H ₂ O	HI	I ₂	H ₂ O	HI	I ₂			
1	85.439	14.560	0.002	72.600	27.400	0.000	244.09	130854.17	3877.30
2	86.300	13.693	0.007	85.069	14.929	0.002	246.73	130788.25	134731.47
3	86.350	13.626	0.024	85.906	14.088	0.006	246.76	130694.47	134665.55
4	86.296	13.617	0.087	85.953	14.023	0.023	246.79	130655.18	134571.77
5	86.086	13.599	0.315	85.901	14.014	0.085	246.87	130537.95	134532.48
6	85.340	13.538	1.122	85.697	13.997	0.306	247.19	130130.54	134415.25
7	82.817	13.316	3.866	84.972	13.939	1.089	248.26	128772.48	134007.84
8	74.776	12.587	12.636	82.519	13.728	3.753	251.77	166964.61	132649.78
9	69.837	12.110	18.053	81.298	13.300	5.403	253.92	163459.61	133041.91
10	49.200	9.794	41.006	75.242	12.717	12.042	263.34	33922.70	129536.91

D B Reflux Boilup RR
3877.30 33922.70 130854.17 129536.91 33.7488

Feed Bubble temperature (C) = 250.64
Heat in each exchanger, kcal/s Q1 = -27544.88, Q2 = -1350.82, Q3 = -864725.03,
Q4 = 896816.07, Q5 = 2611.06, Q6 = 70203.19
Enthalpy(kcal/s) of Feed = -1072334.36, Distillate = -149299.17, Bottom = -919839.85
Entropy(kcal/s/K) of Feed = -414861.49, Distillate = -1120.01, Bottom = -76894.94

Fig. 5. Results of steady state simulation for the HIX distillation process (pressure: 22 bar).

3. Conclusion

The automation program as an approach to find the stabilization condition in the steady-state simulation of the HIX distillation column has been developed. This computer program effectively finds the setting of stabilization conditions and provides the conservation of the running time.

Acknowledgments

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REFERENCES

- [1] Jooho Lee, Youngjoon Shin, Kiyoung Lee, Vapor-Liquid Equilibrium of the HI-H₂O-I₂ chemical system, Calculation Note(NHDD-KA06-HP-004), 2006.
- [2] Youngjoon Shin, Kiyoung Lee, Jonghwa Chang, Thermal Efficiency of EED-embedded Sulfur Iodine Cycle, Calculation Note (NHDD-KA07-HP-001-00), 2007.