

Making soda ash manufacture more sustainable. A modeling study using ASPEN Plus

Ana-Maria Cormos, Calin-Cristian Cormos, Paul Ş. Agachi

*Babes – Bolyai University, Faculty of Chemistry and Chemical Engineering
11 Arany Janos Street, RO-400028, Cluj – Napoca, Romania
E-mail: cani@chem.ubbcluj.ro; cormos@chem.ubbcluj.ro; sagachi@chem.ubbcluj.ro*

Abstract

The quality of the products, operational costs and environmental impact are important factors in the actual context of world economy globalization. The models are used to describe closer the real physicochemical processes that take place in a real plant. In this paper, the modeling and simulation of soda ash manufacturing process were done using ASPEN PLUS. The evolutions of the processes parameters (flows, composition, temperatures, pressures etc.) were studied during the synthesis steps: ammonia absorption into brine, carbonation process of ammoniacal brine and recovery of ammonia from the process wastewater. The simulation results were compared with real plant operation data in order to validate the applications. From the comparison, one can observe a close similarity between simulation results and the real plant data. This fact validates the applications developed for process simulation and proves the utility of the model in analyzing and optimization of the real plant operation.

Keywords: Sustainable development, soda ash, ASPEN Plus, sensitivity studies

1. Introduction

Sodium carbonate is a common inorganic industrial chemical, also known as soda ash (Na_2CO_3). It is widely used in the manufacture of glass, chemicals,

such as sodium silicates and sodium phosphates, the pulp and paper industries, the manufacture of detergents and for the treatment of water.

The decrease of energy consumption and efficient use raw materials for the soda ash manufacture leads to important economic and environmental benefits (decreasing the operational costs; increasing the profit gross margin; making soda ash manufacture more sustainable, reduction of the process effluents etc.). Soda ash manufacture by Solvay technology is a very complex process [1]. The natural sodium chloride solution (brine) is extracted and purified (removal of solid impurities by filtration and removal of calcium and magnesium ions by precipitation). Then ammonia is absorbed into the purified sodium chloride solution. After ammonia absorption, the solution is carbonated with gaseous carbon dioxide coming from two main sources: thermal decomposition of the limestone (CaCO_3) and sodium bicarbonate calcination process. After carbonation of ammoniacal brine, a suspension of sodium bicarbonate is obtained. Sodium bicarbonate is filtered and the residual liquid phase is treated with calcium hydroxide solution (slaked lime) in order to recover the ammonia from ammonium salts (ammonium chloride, carbonate, bicarbonate etc.). The recovered ammonia is recycled back into the process at absorption stage into the sodium chloride solution (brine). Sodium bicarbonate resulted after filtration is washed, dried and calcined in order to obtain sodium carbonate (soda ash).

2. Modeling and simulation of the ammonia absorption process

The ammonia absorption process is done using an absorption columns sequence. Because the absorption process is an exothermic process, the columns are provided with cooling systems [1]. The purified brine is distributed in the ammonia recovering column I *B2* (see Fig. 1) and in ammonia recovering column III *B3*. The sodium chloride solution (brine) rich in ammonia passes in the ammonia recovering column II *B5*, and into the first absorber *B4*. In the absorbers *B4* and *B6*, the brine flows in counter-current with cold gas coming from ammonia distillation process.

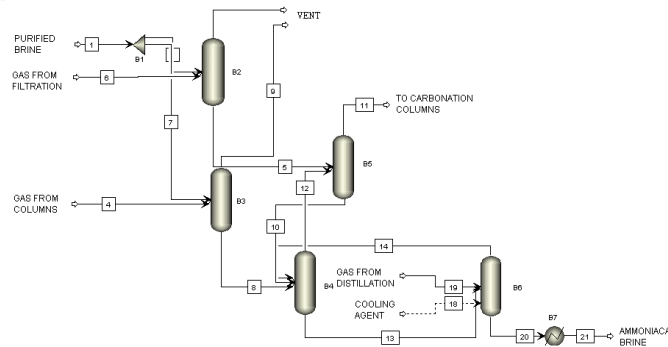


Figure 1. Simulation of the ammonia absorption process into brine solution using ASPEN Plus

The modeling and simulation of the ammonia absorption process were done using ASPEN Plus software package (see Fig. 1) [1-3]. The electrolyte package was used as thermodynamic option for simulation of the processes [2,3]. The calculated properties of output gaseous streams resulted from the simulation of the ammonia absorption process in sodium chloride solution (brine) are presented in the Table 1.

Table 1 . The properties of the gaseous streams leaving the ammonia recovering columns

Parameter	Measuring Unit	Gas from ammonia recovering column I	Gas from ammonia recovering column III	Gas from ammonia recovering column II	First absorber	Second absorber
Temperature	[°C]	20	20	54	59	59
CO ₂	[mole %]	2.2	0	49.45	0.21	0.07
CO	[mole %]	2.29	0	0	0.02	0.01
O ₂	[mole %]	19.17	2.07	1.83	0.32	0.12
N ₂	[mole %]	76.67	94.66	10.44	80.86	79.68
H ₂ O	[mole %]	1.88	1.87	10.9	14.37	13.96
NH ₃	[mole %]	0	0.02	75.65	4.21	6.16
Flow	[kg/h]	822	777	32	9.67	26.21

3. Modeling and simulation of the carbonation process

The carbonation process of ammoniacal sodium chloride solution is a complex process because of the following factors: presence of a three phase system (gas – liquid – solid), diversity of chemical species present in the liquid, chemical reactions that take place, the carbonation process is exothermic, precipitation of sodium bicarbonate that affects the heat transfer coefficients etc [1-4].

The main ASPEN Plus window of the application is presented in the Fig. 2.

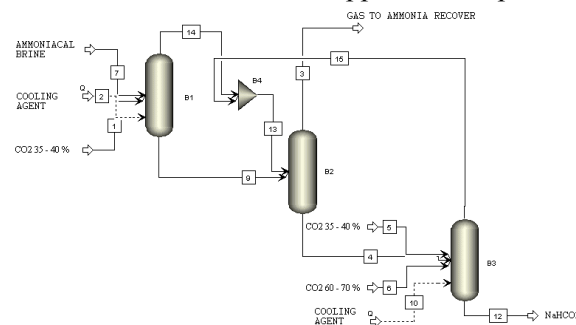


Figure 2. Simulation of the carbonation process of ammoniacal brine using ASPEN Plus

The properties of output gaseous streams resulted from the simulation of the distillation columns are presented in Table 3.

Table 3. The properties of the gaseous streams leaving the distillation columns

Parameter	Measuring Unit	Ammonia “large” distillation	Ammonia “small” distillation
Temperature	[°C]	86	31
NH ₃	[mole %]	64.5	32.7
CO ₂	[mole %]	10.5	14.3
H ₂ O	[mole %]	25	53
Debit	[kg/h]	17522	8210

The simulation results presented above were compared with data collected from real plant operation [1,3,4]. From the comparison, one can observe a close similarity between simulation results and experimental data.

In order to analyzing and optimization of the real plant operation, a large numbers of sensitivity studies were done. The sensitivity study regarding the influence of the principal inlet flows (brine and ammonia from recovery stage) to ammonia absorption process are presented in figure 4 and 5. Concluding to those studies the performance of the ammonia absorption process is increasing with gas flow from distillation and decreasing brine flow.

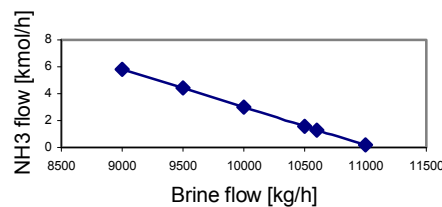


Figure 4. The influence of brine flow to ammonia absorption process

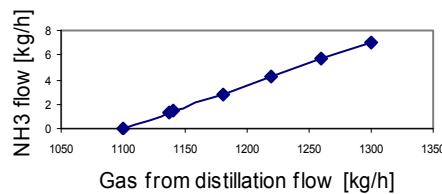


Figure 5. The influence of the distillation gas flow to ammonia absorption process

The sensitivity study regarding the influence of the principal inlet flows (hydrated lime flow and distillate without chlorine flow) to ammonia recovery

process are presented in figure 6 and 7. The figures showed the inlet flow are important for ammonia recovery process (increase of ammonia recovery).

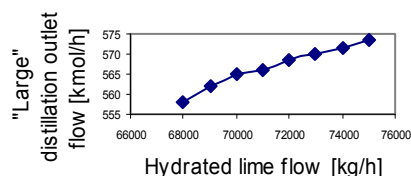


Figure 6. The influence of hydrated lime flow to ammonia recovery process

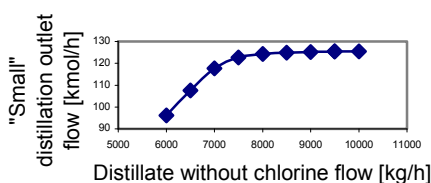


Figure 7. The influence of distillate without chlorine flow to ammonia recovery process

The close similarity between simulation results and experimental data and sensitivity studies validate the applications developed for simulation of the soda ash production process and proves the utility of the model in analyzing and optimization of the real plant operation

5. Conclusion

Modeling and simulation of the sodium carbonate (soda ash) manufacturing process by ammoniacal technology (Solvay) was done using ASPEN Plus software package.

The evolutions of the process parameters (liquid and gaseous flows, composition, temperatures and pressures) for different steps in soda ash manufacture were studied. The simulation results were compared with real plant operation data in order to validate the applications developed for the manufacturing process of soda ash. The mathematical model and the simulation results proved to be a reliable tool for analyzing and optimizing the real plant operation of the soda ash manufacturing process using Solvay technology.

References

1. L. Filipescu, Tehnologia produselor sodice si clorosodice, Ed.Tehnica, Bucuresti, 1983
2. C.C. Cormos, A.M. Cormos, S. Agachi, Rev. Chim., 56 (2005) 581
3. C.C. Cormos, A.M. Cormos, S. Agachi, Rev. Chim., 57 (2006) 130
4. L. Kucka, I. Muller, E. Kenig, A. Gorak, Chem. Eng. Sci. 58 (2003) 3571