Computer simulation and optimization of the oxidation process in the production of nitric acid in the Aspen Plus environment

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Abstract. The article presents a method for determining the optimal technological and design parameters of the process, as well as the procedure for conducting technological analysis in the Aspen Plus environment. With the help of a wide range of thermodynamic models and process property databases, this modeling environment allows for an accurate representation of their behavior in the production of nitric acid. By using computer modeling in Aspen Plus, a 60.09% aqueous solution of HNO3 was obtained for 93465.8 kg/h of air and 5458.9 kg/h of ammonia. The objective of this modeling was to determine the optimal process parameters and its configuration, conduct a technological analysis, and determine the flows and properties of substances at various points. The main process parameters were analyzed, and their interrelation is shown in the graphs.

1 Introduction

Nitric acid is one of the most important acids and ranks second after sulfuric acid in terms of production volume. The consumption of nitric acid is not limited to the production of fertilizers. Modern methods for the production of nitric acid are based on the contact oxidation of ammonia. The raw materials for the production of nitric acid are ammonia, air, water.

The production of nitric acid can lead to the formation of nitric oxide II (N2O) as a by-product. The formation of N2O occurs in a two-stage process for the production of nitric acid:

1. The first stage is the oxidation of ammonia catalytically at high temperature to obtain nitric oxide (II);
2. The second stage is the oxidation of nitric oxide (II) to nitrogen dioxide (NO2), which then reacts with water to form nitric acid.

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N2O is a greenhouse gas that contributes to global warming. Therefore, reducing its emissions is very important for the environmental sustainability of nitric acid production.The production process of nitric acid includes several steps.

1) Synthesis gas: a gas mixture of natural gas and air passes through a catalyst where the gas mixture is converted into synthesis gas, consisting mainly of hydrogen and carbon monoxide.
2) Ammonia production: synthesis gas is mixed with steam water and passed through a catalyst, where a hydrogenation reaction takes place, resulting in the formation of ammonia.
3) Catalytic oxidation of ammonia: Ammonia and air are fed into the reactor where the catalytic oxidation of ammonia takes place in the presence of a catalyst. This reaction results in the formation of nitric oxide.
4) Formation of nitric acid: Nitric oxide is oxidized to form nitrogen dioxide, which then reacts with water to form nitric acid.
5) Purification and separation: nitric acid passes through a series of purification and separation plants, where it is purified and separated into the required concentrations.

The reaction is highly exothermic, and in many modern high pressure plants, the thermal energy of the tail gas is recovered as it passes through the turbine, increasing the power required to compress the process gas [2]. Although each individual step of the overall process is relatively simple, there are a number of variables within each that allow a wide range of combinations of operating conditions to be possible [3].

2 Materials and methods

One of the main processes in the production of nitric acid is the contact oxidation of ammonia in a combustion reactor. This process is simulated in the Aspen Plus14.0 computer simulation environment, which is used to simulate chemical processes and optimize technological processes in various industries. The environment uses a large database of physical properties such as thermodynamic properties, thermal conductivity, viscosity, density, etc., which can be set by the user or selected from standard libraries. For modeling, NRTL (Non-Random Two-Liquid) was chosen as the main method for calculation: this is a method for calculating activity coefficients for simulating phase equilibrium in liquid mixing systems, and the ESRK method (Equation of State, Rigorous Kubicka) was additionally used to calculate thermodynamic properties of phases using the equation of state [4].

Aspen Plus is the market leading chemical process optimization software used by various industries to design, operate and improve industrial plants. The product has the ability to solve problems and tasks of varying degrees of complexity directly during the technological process.

Aspen Plus provides a wide range of tools for developing and optimizing process models, including a best-in-class set of physico-chemical properties, the ability to handle solid, liquid, gas, and electrolyte processes.

Aspen Plus is constantly being updated to improve performance and add new modeling features. For example, this software has the ability to compare data obtained as a result of the program and production in real time. This allows you to reduce the resources of the enterprise and improve the quality of the product. The staff has the opportunity to use the product in supervisory mode [5].

To obtain nitric acid, the description of the technological process for the production of nitric acid is as follows. Ammonia-air mixture, at 221.2 °C and 4.07 barg (0.407 MPa) is fed into the catalytic combustion reactor of the reactor, in which it passes through a perforated gas distribution grid, which evenly distributes the gas over the platinum-rhodium alloy catalyst gauzes.

To start the ignition, a hydrogen ignition rod is ignited. The pilot rod flame is extinguished immediately when the reaction starts. Gas distribution, speed, contact time and oxidation temperature on platinum catalyst gauzes are optimized to achieve high ammonia conversion and minimize catalyst losses. The overall oxidation reaction (1) occurs at approximately 890°C with the efficient formation of NO:

$$NH_3 + \frac{5}{4}O_2 \rightarrow NO + \frac{3}{2}H_2O \qquad \Delta H = -226\ 241\frac{kj}{kmole}NH_3 \tag{1}$$

The high temperature of the catalytic gauzes (overheating) and the long contact time contribute to the decomposition of NO and the complete oxidation of ammonia (2):

$$NO \rightarrow \frac{1}{2}N_2 + \frac{1}{2}O_2 \tag{2}$$

The ratio controller is adjusted to maintain this temperature of the catalyst grid. The temperature control of the catalytic gauzes is important to achieve maximum NO yield and is done by adjusting the air to ammonia ratio (3), which is calculated as follows [1]:

$$R = \frac{(\frac{Nm_3}{h})_{NH_3}}{(\frac{Nm_3}{h})_{NH_3} + (\frac{Nm_3}{h})_{AIR} + 5H} * 100 \tag{3}$$

Process description. The liquid ammonia is vaporized and mixed with primary air before being oxidized in a reactor at low pressure (approximately 4.2 barg). The maximum utilization of energy is carried out by cooling the nitrous gas and obtaining steam and further cooling the tail gas by cross heat exchange [6-7].

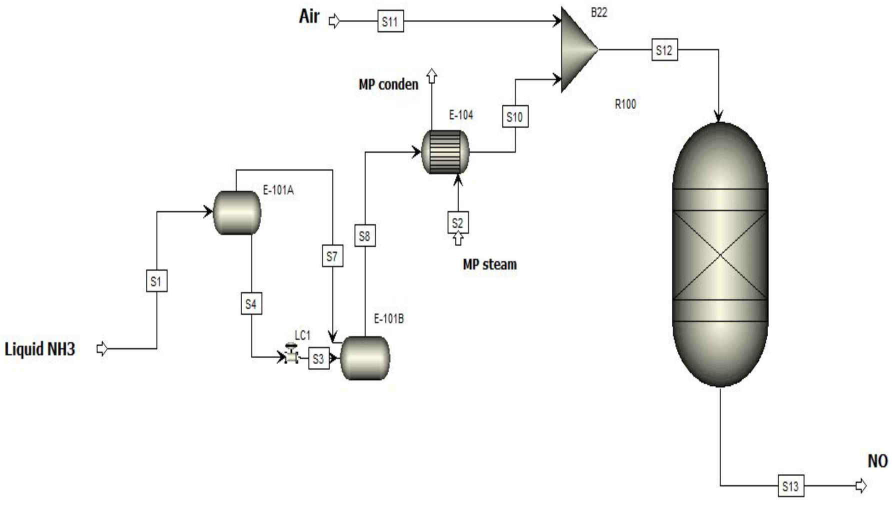


Fig. 1. Technological scheme of the ammonia oxidation process in the Aspen Plus program.

This two-stage cooling allows both the production of steam with parameters corresponding to the requirements of the steam turbine, and an increase in the temperature of the tail gas, thereby achieving an increase in the energy production of the turboexpander [1-2]. The final cooling of low-pressure nitrous gases with simultaneous condensation of a weak acid is carried out by cooling water. After the extraction of the weak acid, the nitrous gases are compressed to a low pressure in the NOx compressor to 10.5 barg. The high-pressure nitrous gases are then cooled by cross heat exchange with the tail gas and further condensation of the weak acid, after which they are fed to an absorber where they react with water to produce nitric acid. The resulting nitric acid is bleached with secondary air and cooled to a temperature below 45°C, and then fed to the border of the nitric acid plant, i.e. to the nitric acid storage tanks. From these reservoirs, nitric acid is removed further.

3 Results

The results obtained and their discussion. When modeling, 60.09% nitric acid HNO3 was found in the final product. We can change the amount of HNO3 by changing various parameters. Some charts are shown.

Influence of the ammonia inlet flow on the temperature of the combustion reactor at a constant air flow Figure 2

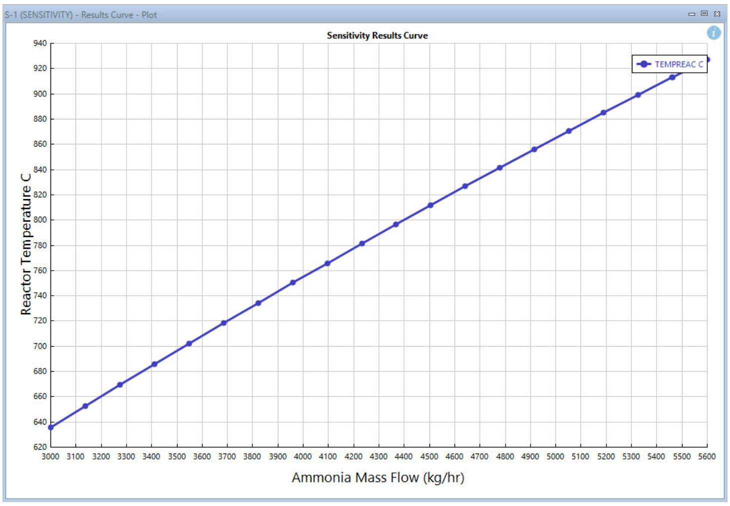


Fig. 2. Graph of the ratio of ammonia consumption and temperature of the contact oxidation reactor.

Figure 2 shows that the temperature in the reactor increases with increasing ammonia flow. Influence of the ammonia input flow on the consumption of the final product. 3 The figure shows that an increase in the consumption of ammonia leads to an increase in the consumption of nitric acid [8-11].

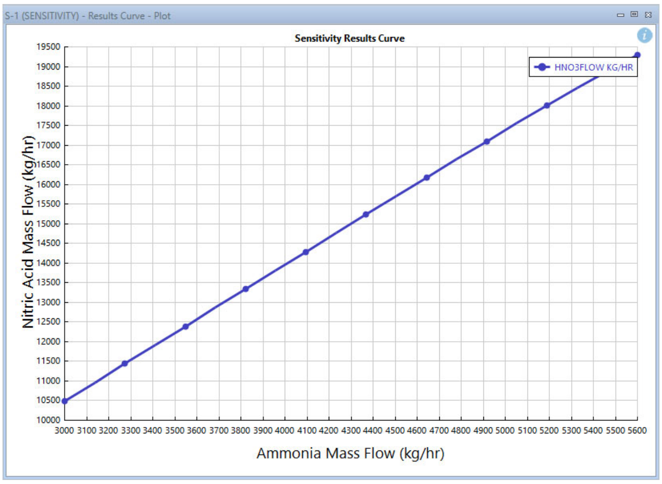
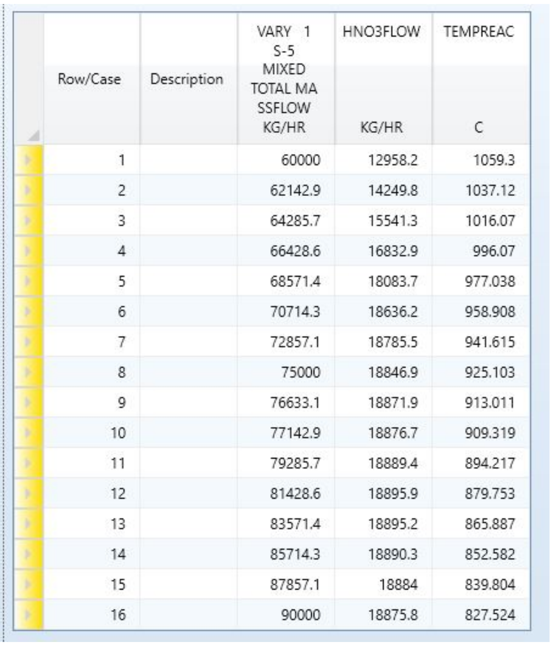


Fig. 3. Graph of the relationship between the consumption of ammonia and the final product HNO3.

Influence of air on the temperature in the reactor and the flow rate of the final product 4-5. It can be seen from the table and figure that an increase in air flow reduces the temperature of the reactor, and also increases the flow rate of the final product to a certain value [12-13].



Row/Case	Description	VARY 1 S-5 MIXED TOTAL MASSFLOW KG/HR	HNO3FLOW KG/HR	TEMPREAC C
1		60000	12958.2	1059.3
2		62142.9	14249.8	1037.12
3		64285.7	15541.3	1016.07
4		66428.6	16832.9	996.07
5		68571.4	18083.7	977.038
6		70714.3	18636.2	958.908
7		72857.1	18785.5	941.615
8		75000	18846.9	925.103
9		76633.1	18871.9	913.011
10		77142.9	18876.7	909.319
11		79285.7	18889.4	894.217
12		81428.6	18895.9	879.753
13		83571.4	18895.2	865.887
14		85714.3	18890.3	852.582
15		87857.1	18884	839.804
16		90000	18875.8	827.524

Fig. 4. Table of the results of the ratios of air flow, reactor temperature and final product.

Influence of air flow on temperature and flow of sodium chloride. The study of the real process and the simulation of the process in the Aspen Plus software shows the optimal solution for obtaining the finished product [14-16].

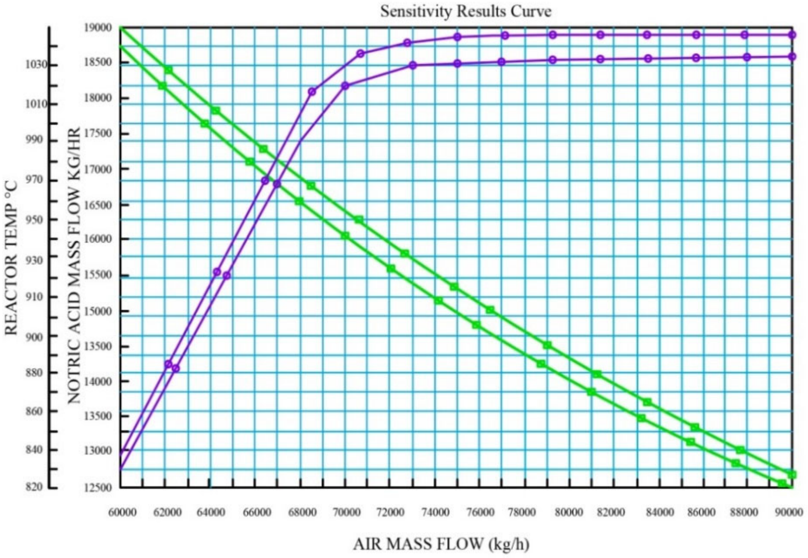


Fig. 5. Graph of the ratio of air flow, reactor temperature and final product.

Influence of water consumption on irrigation of the absorption column and consumption and consumption of the final product HNO3 Figure 6. The figure shows an increase in water consumption for irrigation increases the consumption of nitric acid [17-20].

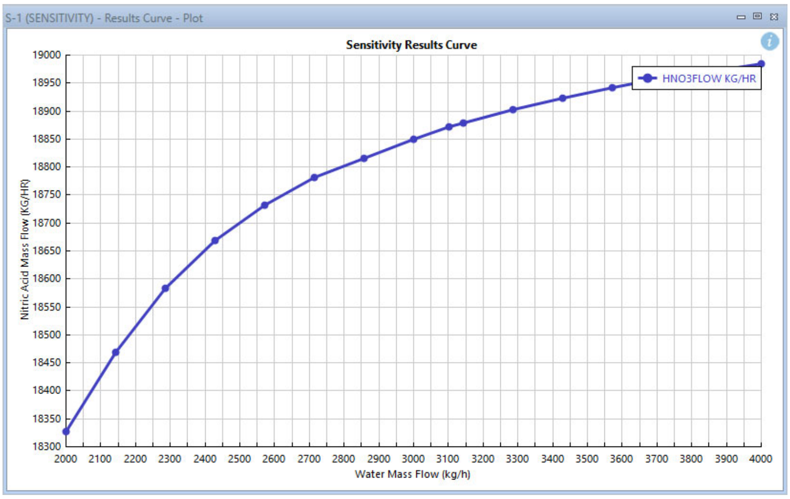


Fig. 6. Graph of the ratio of water consumption and the final product HNO3.

4 Conclusion

In the article, the data was obtained based on the simulation on Aspen Plus. With this data, you can understand the process in various situations in industrial practice. Computer simulation of processes in Aspen Plus provides several advantages. The integration of various process blocks combines several modules and blocks, which allows the integration of various processes and technologies, such as reactions, separation, etc. This allows you to speed up the development process and reduce the cost of research and development of new technologies. The environment also provides the possibility of real-time simulation, which allows you to optimize processes and improve their efficiency. The flexibility of Aspen Plus allows you to simulate processes under various conditions, taking into account various parameters such as temperature, pressure, concentration, etc.

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