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A Cost Optimization Study of Simulation of Nitric Acid Production Using Hysys Software

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Abstract
Nitric acid production is an important chemical process. In our pa- per, we have generated data based on the simulation performed in HYSYS. This data can help us understand the process in differ- ent situation in industrial practice. From this project material and energy flows, sized unit operations blocks can be used to conduct economic assessment of each process and optimize each of them for profit maximization.
Key word: *economic developed fertilizers*
Our developed simulation model can also be used as a guide for understanding the process and the economics, and also a starting point for more sophisticated models for plant designing and process equipment specifying.
Keywords: *Oswald, simulation, passivation, ammonia*

I. INTRODUCTION

The common perception of ‘acid’ suggests stringency, corrosiveness and something capable of dissolution of another substance. How- ever, not all acids are, or can be seen to be thus, except that nitric acid[1–3]might be considered to be an extremely destructive com- pound in that it was the basis of explosives and also fertilizers – the almost diametric opposite of an explosive as it helps plants to grow.

However, this versatile acid (there’s many nitric acid uses) has found to capable of use in many industrial and chemical processes. As an integral part of explosives manufacture that, although known for a long time, derived from the lack of natural nitrates to fuel the Ger- man war effort prior to the First World War. Nitric acid can be used to manufacture components of trinitrotoluene (TNT).

As an agricultural fertilizer where it promotes vigorous growth in plants, there is, however, an unfortunate side effect in that nitrates are very soluble in water and when applied to well-drainingsoil,they leach into the watercourse and eventually reach streams and rivers.

Once in the water it stimulates the growth of algae that, in turn, deoxygenates the water to stifle growth in other plant forms and animal life.It can be used as an oxidizing agent in theproductiono fsomesolidfuelsforrocketpropulsion;componentofrocket fuel acting as an oxidizer.

As an ageing agent in woodworking where itcanbeusedinverydilute- forms (typically below 10%) to change the appearance of some woods and to produce a color similar to that of oiled or waxed sur- faces old.

In the jewelry trade, nitric acid can be used to identify low-grade alloys and assess purity of gold content.It can be used in a solution with alcohol and water to etch metals by removing some surfaces.

Nitric acid is commonly used in the food processing and dairy sec- tors to remove calcium and magnesium deposited during the manu- facturing or conversion processes or which may result from contin- ued exposure to hardwater. Most production of nitric acid is caused by the Ostwald process.

The Ostwald process is a chemical process for making nitricacid (HNO_3). Wilhelm Ostwald developed the process, and he patented it in 1902.

The Ostwald process was discovered just in time for the First World War, and it contributed greatly to the extended length of that war. This is because previously Germany had no nitrate deposits of its own from which to make the nitric acid that was essential for the production of the explosives used in artillery shells, such as TNT and nitroglycerine.

The Ostwald process is amainstay of the modern chemical indus- try[8], and it provides the main raw material for the most common type of fertilizer production. Historically and practically, the Ost- wald process is closely associated with the Haber process, which provides the requisite raw material, ammonia (NH_3).

In this work a detailed study is performed of the process by means of simulation in Aspen HYSYS v7.1. We will not get real life value through this simulation, but if the process is known and related data are available, it surely is the best way by which we will get ideas of an industrial process without conducting any experiment.

II. METHODOLOGY

The process of synthesis of ethanol by hydration of ethylene is sim- ulated in simulation software Aspen HYSYS 7.1. Aspen HYSYS is a widely used process simulator which provides quite accurate results compared to the real life result.

It provides comprehensive thermodynamics basis for accurate de- termination of physical properties, transport properties, and phase behavior. For our simulation we have chosen Peng Robinson fluid package.

Components for this simulation areAmmonia(NH3), Nitrogen(N2), Oxygen(O2), Water(H2O),Nitric-oxide(NO),Nitrogen di- oxide(NO2),Nitric acid (HNO3).

Process Description

Onceammoniahasbeenproducedbythe Haber process, it can be con- verted into nitric acid through a multi-step procedure known as the Ostwald process.

In the first step in this reaction, ammonia andoxygengas catalytically react to form nitrogen monoxide.The reaction is quite exothermic. In the commercial reaction, the catalyst used in aplatinum-rhodium metal gauze, that is heated to about 900 $^{\circ}$C. However, even a hot copper wire can catalyze the reaction in the laboratory.

Once the reaction hasstarted, the energy it produces is enough to keep the catalyst hot enough to sustain the reaction.In the next step, the NO[9] reacts with oxygen to produce NO_2.

No catalyst is required for this reaction, as it will occur in air at room temperature[10].The NO_2 can be compressed and cooled which will make it dim raze into N_2O_4, which can then be used as an oxidizer for rocket fuel.

$2NO_2\ (g) \qquad N_2O_4\ (g)\ + 58\ KJ$

FromleChâtelier’sprinciplewecan predict that at high pressures the equilibrium will be shifted to the right, since there are less mol- ecules of gas in the products.

Similarly, at lower temperatures the reaction will shift to the right. Instead of storing the NO_2, we can use it to producenitricacid.

TheNO_2(g)reacts with water to produce nitric acid (HNO_3) and NO.The nitric acid is separated by distillationandthe NO canbe re- cycled through reaction.

$4NO_2\ (g)\ + 2H_2O(l) + O_2\ (g) \rightarrow 4HNO_3\ (aq)$

Figure 1 shows the simplified block diagram of Ostwald process for nitric acid production.

Reactions Involved

There are three main reactions:

(a) Oxidization of ammonia to form nitric oxide

$4NH_3\ (g) + 5O_2\ (g) \rightarrow 4NO\ (g) + 6H_2 0\ (g)$; nH = Δ906 kJ

(b) Oxidization of nitric oxide to form nitrogen di-oxide

$4NO\ (g) + O_2\ (g)\ \rightarrow 4NO_2\ (g)$

(c) Conversion of nitrogen di-oxide into nitric acid

$4NO_2\ (g) + 2H_2O(l) + O2\ (g) \rightarrow 4HNO_3\ (aq)$

Figure 2 shows the HYSYS flow diagram of this process.

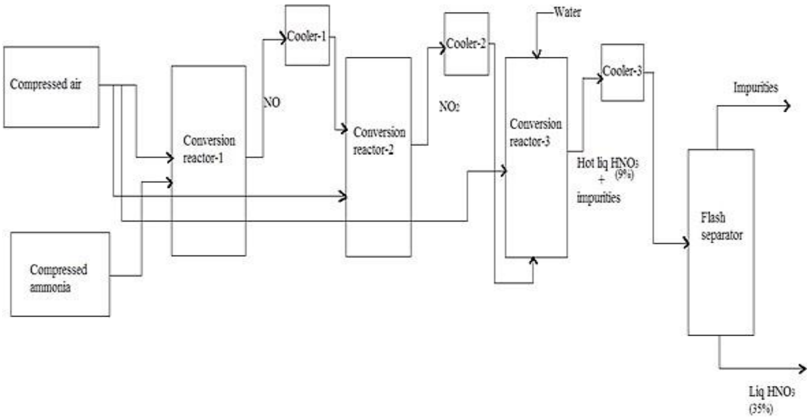

Fig.1: *Simplified Block Diagram of Ostwald Process for Nitric Acid Production.*

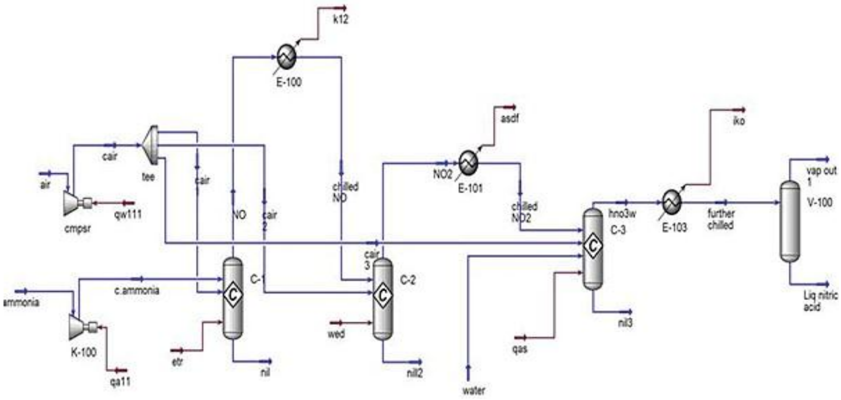

Fig. 2: *HYSYS Flow Diagram of Ostwald Process for Nitric Acid Production.*

III. CONCLUSIONS

Nitric acid has been known and esteemed for a long time. Most ni- tric acid is used in making ammonium nitrate. Its direct applications include photoengraving, metal pickling and passivation and the parting of gold and silver. Here the Oswald process is used to pro- duce nitric acid. This process is simulated using HYSYS simulation software. The purpose of this simulation was to observe the thermo- dynamic properties of the process. We also observed the changes which will occur if the properties of different unit were changed. By performing simulation 35.3% aqueous HNO3 is obtained for 11020 lbm/hr air and 500 lbm/hr ammonia input flow.

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