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Salahaddin University-
Erbil College of
Engineering
Chemical-Petrochemical Engineering Department



Production of nitric acid

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Abstract

The production of nitric acid (HNO_3) is a fundamental process in the chemical industry, supporting a wide array of applications across agriculture, explosives manufacturing, pharmaceuticals, and metallurgy. This abstract presents an overview of nitric acid production, emphasizing the significance of two primary methods: the single and dual processes.

The single process, exemplified by the Ostwald process, involves the catalytic oxidation of ammonia (NH_3) to nitric oxide (NO), followed by the subsequent oxidation of NO to nitrogen dioxide (NO_2), and ultimately the absorption of NO_2 in water to yield nitric acid. Conversely, the dual process, typified by the Birkeland–Eyde process, integrates the production of nitrogen oxides with the synthesis of nitric acid in a single operation, utilizing atmospheric nitrogen and oxygen as raw materials

Results from both processes indicate their efficacy in yielding high-purity nitric acid suitable for various industrial applications. However, environmental concerns persist due to the emission of nitrogen oxides (NO_x) during production, necessitating ongoing efforts to develop more sustainable and environmentally friendly synthesis methods.

the production of nitric acid via single and dual processes plays a critical role in modern industrial processes, with advancements geared towards enhancing efficiency, reducing environmental impact, and meeting the evolving demands of industry and society.

Acknowledgement

All the thanks, praises and glorifying is due to almighty ALLAH. To our parents who grew us up and guided us through life.

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Big thanks to our colleagues and all thanks for all doctors and teaching assistance of Chemical Engineering Department through these four years..

Supervisor's Certificate

I certify that the engineering project titled "**production of nitric acid**" was done under my supervision at the Chemical-Petrochemical Engineering Department, College of Engineering - Salahaddin University–Erbil. In the partial fulfillment of the requirement for the degree of Bachelor of Science in Chemical-Petrochemical Engineering

Supervisor

Signature:

Name:

Date: / /

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Nomenclature

Q	total energy of the system
$H(x_0)$	enthalpy
C_p	heat capacity
d_w	wire diameter
f_w	wire area per gauza cross sectional area
A_{wr}	surface area of screen / volume of one screen The density of catalyst
n_s	number of screen per gauza
ϵ	<i>Porcity</i>
G	<i>mass velocity</i>
V^*_{*w}	gas mass flow rate per unit cross – sectional area $kg/m^2.s$
σ_b	bending stress
σ_c	Elastic Stability

Chapter 1

Introduction

Chapter One

Introduction

1.1 Name and history of Nitric Acid

1.1.1 Name

IUPAC : Nitric acid

Other name : Hydrogen nitrate , Aqua fortis

Color : colorless (pure),yellow(old)

Properties : a) highly corrosive , can cause severe burns

b) miscible in water at all concentration

c) will decompose at high temperature to form nitrogen oxide

d) poisonous liquid

Nitric acid, a colorless, highly corrosive liquid, stands as one of the most potent oxidizing agents known in chemistry. Its remarkable reactivity

renders it indispensable across various industrial sectors. However, in its highly pure form, nitric acid is not entirely stable and necessitates careful preparation. Typically, it is obtained from its azeotrope through distillation with concentrated sulfuric acid, a process essential for ensuring its purity and stability.

Notably, nitric acid exhibits a gradual yellowing phenomenon attributed to its decomposition into nitrogen dioxide over time. This characteristic change underscores its dynamic nature and underscores the need for proper storage and handling protocols. Solutions comprising more than 80% nitric acid are termed fuming nitric acids, reflecting their heightened reactivity and tendency to release nitrogen dioxide fumes.

In its commonly encountered form, reagent-grade nitric acid exists as a water solution containing approximately 68% by weight nitric acid. This concentration corresponds to the constant-boiling mixture of nitric acid with water, which consists of 68.4% nitric acid by weight and boils at 121.9°C. Nitric acid exhibits complete miscibility with water, forming distinct hydrates, including a monohydrate ($\text{HNO}_3 \cdot \text{H}_2\text{O}$) with a melting point of -38°C and a dihydrate ($\text{HNO}_3 \cdot 2\text{H}_2\text{O}$) with a melting point of -18.5°C . These hydrates contribute to the diverse physical properties exhibited by nitric acid solutions.

The multifaceted nature of nitric acid, encompassing its reactivity, stability considerations, and various hydrate forms, underscores its significance in chemical synthesis, industrial processes, and laboratory applications. This introduction sets the stage for a comprehensive exploration of nitric acid's properties, applications, and broader implications across diverse fields.

1.1.2 History

Scholars have known nitric acid for many centuries. Probably the earliest description of its synthesis occurs in the writings of the Arabic alchemist Abu Musa Jabir Ibn Hayyan (c. 721–c. 815), better known by his Latinized name of Geber. The compound was widely used by the alchemists, although they knew nothing of its chemical composition. It was not until the middle of the seventeenth century that an improved method for making nitric acid was invented by German chemist Johann Rudolf Glauber (1604–1670). Glauber produced the acid by adding concentrated sulfuric acid (H_2SO_4) to saltpeter (potassium nitrate; KNO_3). A similar method is still used for the laboratory preparation of nitric acid, although it has little or no commercial or industrial value.

The chemical nature and composition of nitric acid were first determined in 1784 by the English chemist and physicist Henry Cavendish (1731–1810). Cavendish applied an electric spark to moist air and found that a new compound - nitric acid – was formed. Cavendish was later able to determine the acid's chemical and physical properties and its chemical composition. The method of preparation most commonly used for nitric acid today was one invented in 1901 by the Russian born German chemist Friedrich Wilhelm Ostwald (1853–1932). The Ostwald process involves the oxidation of ammonia over a catalyst of platinum or a platinum-rhodium mixture.

Today, nitric acid is one of the most important chemical compounds used in industry. It ranks number thirteen among all chemicals produced in the United States each year. In 2005, about 6.7 million metric tons (7.4 million short tons) of the compound were produced in the United States

1.2 Applications

Nitric acid is used in the production of ammonium nitrate for fertilizers, making plastics, and in the manufacture of dyes. It is also used for making explosives such as nitroglycerin and TNT. When it is combined with hydrochloric acid, an element called aqua regia is formed. This is a reagent that is capable of dissolving gold and platinum. Additionally, it is used in a colorimetric test to distinguish heroin and morphine.

Nitric acid is commonly used in science laboratories at schools for experimenting when specifically testing for chloride. This is accomplished by adding a sample with silver nitrate solution and nitric acid to test if a white precipitate, silver chloride is present. In the field of medicine, nitric acid is used in its pure state as a caustic to remove chancres and warts. Diluted solutions are used in the treatment of dyspepsia.

Nitric acid has been used in various forms as the oxidizer in liquid-fueled rockets. These forms include red fuming nitric acid, white fuming nitric acid, mixtures with sulfuric acid, and forms with HF inhibitor.

It is also typically used in the digestion process of turbid water samples, solid sludge samples, as well as other types of unique samples that require elemental analysis via ICP-MS, ICP-OES, ICP-AES, GFAA and flame atomic absorption spectroscopy.

In organic synthesis, nitric acid may be used to introduce the nitro group. When used with sulfuric acid, it generates the nitronium ion, which electrophilically reacts with aromatic compounds such as benzene.

In electrochemistry, nitric acid is used as a chemical doping agent for organic semiconductors, and in purification processes for raw carbon nanotubes.

In a low concentration, nitric acid is often used in woodworking to artificially age pine and maple. The color produced is a gray–gold, very much like very old wax or oil-finished wood.

Nitric acid can be used as a spot test for alkaloids like LSD, producing a variety of colors, depending on the alkaloid.

1.3 Physical properties

Table 1-1 physical properties

1. Molecular weight	63,012 g / mol
2. Physical appearance	Colorless or pale yellow liquid, which may turn reddish-brown
3. Smell	Sharp, distinctive smothering.
4. Boiling point	Degrees Fahrenheit to 760 mmHg (83 ° C).
5. Melting point	-41.6 ° C.
6. Water solubility	very soluble and not miscible with water.
7. Density	1513 g / cm ³ at 20 ° C.
8. The relative density	1.50 (with respect to water = 1).
9. The relative density of vapor	2 or 3 times the estimated (with respect to air = 1).
10. steam pressure	63.1 mm Hg at 25 ° C
11. Viscosity	1,092 MPa at 0 ° C, and 0.617 MPa at 40 ° C .
12. enthalpy evaporation	39.1 kJ / mol at 25 ° C .
13.. enthalpy Standard molar	-207 kJ / mol (298 degrees Fahrenheit) .
14. Molar entropy	146 kJ / mol (298 degrees Fahrenheit).
15. .Surface tension	-0.04356 N / m at 0 ° C .

Molecular Weight: Nitric acid has a molecular weight of 63.012 g/mol, which is crucial for understanding its chemical behavior and stoichiometry in reactions.

Physical Appearance: While primarily colorless or pale yellow, nitric acid can undergo color changes, turning reddish-brown due to exposure to light or impurities. These variations in color can indicate changes in purity or concentration.

Smell: Nitric acid emits a sharp and distinctive odor, often described as suffocating or pungent. This characteristic smell serves as a warning sign of its presence and potential hazards.

Boiling Point: Nitric acid boils at 83°C (degrees Fahrenheit to 760 mmHg), indicating its volatility and susceptibility to vaporization. Knowledge of its boiling point is essential for various applications involving distillation or evaporation.

Melting Point: With a melting point of -41.6°C, nitric acid exists in liquid form at typical ambient temperatures. Understanding its freezing point is crucial for storage and handling, especially in cold environments.

Water Solubility: Nitric acid exhibits high water solubility, being very soluble and non-miscible with water. This property facilitates its use in aqueous solutions and reactions involving water as a solvent.

Density: The density of nitric acid at 20°C is 1.513 g/cm³, indicating its relatively high mass per unit volume. Knowledge of its density is essential for calculating concentrations and for proper storage and handling practices.

Relative Density: With a relative density of 1.50 compared to water, nitric acid is denser than water. This property influences its behavior in aqueous solutions and its interactions with other substances.

Relative Density of Vapor: The relative density of nitric acid vapor is estimated to be 2 to 3 times that of air, indicating its tendency to form dense vapors that may accumulate in confined spaces or low-lying areas.

Vapor Pressure: Nitric acid has a vapor pressure of 63.1 mm Hg at 25°C, reflecting its tendency to evaporate and form vapors even at moderate temperatures. This property is important for understanding its volatility and potential for inhalation exposure.

Viscosity: Nitric acid exhibits variable viscosity, with values of 1.092 MPa at 0°C and 0.617 MPa at 40°C. Understanding its viscosity is crucial for processes involving fluid flow, such as pumping and mixing.

Enthalpy of Evaporation: The enthalpy of evaporation of nitric acid is 39.1 kJ/mol at 25°C, representing the energy required to convert liquid nitric acid into vapor at a constant temperature. This property is important for understanding its phase behavior and energy requirements for vaporization.

Standard Molar Enthalpy: With a standard molar enthalpy of -207 kJ/mol at 298°F, nitric acid exhibits exothermic behavior when undergoing standard state reactions. This property is significant for thermodynamic calculations and reaction kinetics.

Molar Entropy: Nitric acid has a molar entropy of 146 kJ/mol at 298°F, reflecting the degree of disorder or randomness associated with its molecular configuration at a given temperature. Knowledge of entropy is crucial for understanding its thermodynamic stability and spontaneity in reactions.

Surface Tension: Nitric acid displays a surface tension of -0.04356 N/m at 0°C, which influences its interactions with other substances at interfaces. Understanding surface tension is important for processes such as wetting, spreading, and emulsification.

These complete insights into the physical properties of nitric acid provide a foundation for expertise its behavior, reactivity, and capacity dangers in diverse applications, ranging from business processes to laboratory experiments. Proper understanding and control of these homes are critical for ensuring secure handling, storage, and use of nitric acid.

1.4 Chemical properties

Table 1-2 Chemical properties

1	Nitrogen acid is a strong monomeric acid that easily reacts with water to form mono (HNO ₃ H ₂ O) and triple (HNO ₃ 3H ₂ O) solid hydrates.
2	It is affected by heat or light, which causes it to decompose, as shown below $4\text{HNO}_3 \rightarrow 2\text{H}_2\text{O} + 4\text{NO}_2 + \text{O}_2$
3	Acid and strong oxidizing agent, when at high concentrations, it oxidizes nonmetallic elements such as carbon (C), iodine (I), phosphorous (P) and sulfur (S), and gives their oxides, or oxygen acids, and nitrogen dioxide (NO ₂), for example: $\text{S} + 6\text{HNO}_3 \rightarrow \text{H}_2\text{SO}_4 + 6\text{NO}_2 + 2\text{H}_2\text{O}$
4	Concentrated nitric acid oxidizes water chloric acid, forming chlorine and chlorine oxide, ClO ₂ .
5	Water-soluble nitrate salts result from the reaction of nitric acid with minerals, their oxides, hydroxides, or carbonates. All nitrates decompose when heated, and they may do so explosively.
6	The nitric acid reacts with minerals, and it is reduced (i.e., a decrease in the oxidation state of nitrogen), and causes its dissolution and forms metallic oxides with it, and the reaction products differ according to the concentration of nitric acid, the reaction metal, and temperature.
7	Relatively unreacted minerals such as copper (Cu), silver (Ag), and lead (Pb) reduce the concentrated nitric acid, mainly to NO ₂ , while the reactive minerals such as zinc (Zn) and iron (Fe) react with the dilute nitric acid to form N ₂ O or nitrous oxide. (laughing gas).
8	Nitric acid interacts with proteins, and is used to detect them, as in proteins in human skin, to produce a yellow substance called xanthoprotein

9	Highly corrosive and non-flammable toxic substance.
10	is very sensitive to water and causes painful and severe first- degree burns.
11	A solution containing more than 86% is called fumigated nitric acid.
12	It needs to be kept in a dry and cool place

1.5 Safety properties

Nitric acid's potency as a strong acid and oxidizing agent warrants a comprehensive understanding of its safety considerations. Beyond its capacity for chemical burns, which can cause significant harm upon contact with living tissues, nitric acid poses additional risks and demands stringent handling protocols.

The corrosive nature of nitric acid extends beyond its immediate contact with skin or flesh. Upon exposure, it initiates a cascade of chemical reactions known as acid hydrolysis, effectively breaking down proteins and fats present in biological tissues. This process not only leads to the destruction of cells but can also result in long-term damage if not promptly addressed. The severity of these burns is often exacerbated by the concentration and duration of exposure to the acid.

In addition to its corrosive effects on biological matter, nitric acid exhibits distinctive staining properties. The yellow discoloration observed on the skin following contact with concentrated nitric acid stems from its reaction with keratin, the protein responsible for the structural integrity of skin, hair, and nails. This visual indicator serves as a warning sign of exposure and underscores the need for immediate intervention.

While systemic effects from nitric acid exposure are relatively rare, its status as a non-carcinogenic and non-mutagenic substance provides some reassurance regarding its long-term health implications. Nonetheless, the importance of adhering to strict safety measures cannot be overstated,

particularly when dealing with concentrated solutions or prolonged exposures.

Effective first aid for nitric acid spills involves rapid and thorough irrigation with copious amounts of water. This not only helps to dilute the acid and mitigate its corrosive effects but also serves to cool the surrounding tissue and prevent further damage. Prompt removal of contaminated clothing and meticulous cleansing of exposed skin are essential steps in minimizing the extent of injury.

Beyond its direct corrosive effects, nitric acid presents additional hazards due to its potent oxidizing properties. Reactions with certain compounds, such as cyanides, carbides, and metallic powders, have the potential to yield explosive outcomes, highlighting the importance of careful handling and storage practices. Similarly, interactions with organic materials, including turpentine, can result in violent and spontaneous ignition, emphasizing the need for segregation from such substances.

To mitigate the risk of accidents or chemical reactions, nitric acid should be stored in dedicated areas away from bases and organic materials. Proper labeling, containment, and ventilation are essential considerations in ensuring the safe handling and storage of this hazardous substance. Additionally, thorough training and adherence to established safety protocols are indispensable for minimizing the likelihood of incidents and safeguarding both personnel and the surrounding environment.

Chapter 2

Methodology

Chapter Two

Methodology

2.1 The Nitric Acid Production Processes

All commercially produced nitric acid is now prepared by the oxidation of ammonia. The requirement for a nitric acid product of 60% (wt.) immediately restricts the choice of a recommended production process. Only two processes

are possible, both highly efficient, each offering distinct advantages under different market conditions .

2.1.1 The Single-Pressure Process

The Single -Pressure process was developed to take full advantage of operating pressure in enabling equipment sizes to be reduced throughout the process . A single compression step is used to raise the pressure through the entire process sufficiently to favor absorption. Operating pressures range from 800 kPa as used by the Sumitomo Chemical Company Ltd. to 1100 kPa

as used in the C&I Girdler single-pressure process. Increased ammonia oxidation and complete ammonia/air mixing, and uniform flow distribution can minimize increased consumption of ammonia due to the higher-pressure operation across the gauze "inside the reactor". The higher oxidation temperature results in an increased consumption of platinum and rhodium and the need to rework the gauze every five to seven weeks. The higher temperature and the favorable pressure effect make possible a greater recovery of energy from the process.

The process begins with the vaporization of ammonia at 1240 kPa and 35°C using process heat "as shown in the given flow sheet, Fig. (1). Steam is then used to superheat the ammonia to 180°C, filtered air is compressed by an axial compressor to an interstage level and then, following cooling, by a centrifugal compressor to a discharge pressure of 1090 kPa. A portion of the air is diverted for acid bleaching; the remainder is circulated through a jacket surrounding the tail-gas preheater and then used for ammonia oxidation.

In this process; the heated air and the ammonia vapor (10.3% ammonia by volume) are then mixed and passed through the platinum/ rhodium gauze reactor where the heat of reaction (producing nitric oxide) raises the temperature to be between 927°C and 937°C. The reaction gas flows through a series of heat exchangers in which energy is recovered either as high-pressure superheated steam or as shaft horsepower from the expansion of hot tail gas. Approximately 70% of the oxidation to nitrogen dioxide occurs as the gas passes through the energy recovery train and is cooled to 185°C. After further cooling to 63°C in the primary cooler/condenser, separation of approximately one third acid product as 42% strength nitric acid is achieved. The remaining gas reaches a 43% oxidation conversion to nitrogen dioxide, with approximately 20% dimerization. The gas is combined with bleached air containing additional nitrogen peroxide; it then passes through an empty

oxidation vessel and the secondary cooler. In cooling to 66°C, the gas provides heat to a recirculating hot water system used for vaporizing the ammonia.

The gas entering the absorber is 95% oxidized to nitrogen peroxide. In the absorber deionized water is added to the top tray, and weak acid from the low-pressure condenser is added to a tray corresponding to its strength.

Down-flowing acid and up-flowing acid alternately mix as the chemical steps of action formation and nitric oxide oxidation take place with the liberation of heat. There are three operational zones in the absorber, these are the lower zone cooled with plant cooling water, the middle zone cooled with chilled water, and the upper zone which is essentially adiabatic. High efficiency of heat removal in the middle and lower zones is particularly important due to its effect on the oxidation and dimerization reactions.

For this process, chilled water at 7°C is used and the tail-gas exit temperature is approximately 10°C. Acid from the bottom of the absorber is bleached at 1010 kPa with partially cooled compressed air. The bleach air, containing nitrogen peroxide stripped from the acid, is then added to the main gas stream before entering the oxidation vessel. The cold gas is warmed by heat exchange with the hot compressed bleached air, and then heated to the expander inlet temperature of 620°C by two exchangers in the recovery train. The expander recovers 80% of the required compressor power. Expanded tail gas at 300°C flows through an economizer, providing heat to high-pressure boiler feed water and to low pressure de ionized deaerator make-up water. Subsequently tail gas is exhausted to the atmosphere at 66°C and less than 1000 ppm of nitrogen oxides.

The chilled water (7°C) for absorption refrigeration unit, using heat, supplies the absorber recovered from the compressor and intercooler as the energy source. Heat for ammonia vaporization, as previously noted, is available at

35°C and is recovered from the secondary gas cooler. The system uses circulating condensate as the energy transfer medium.

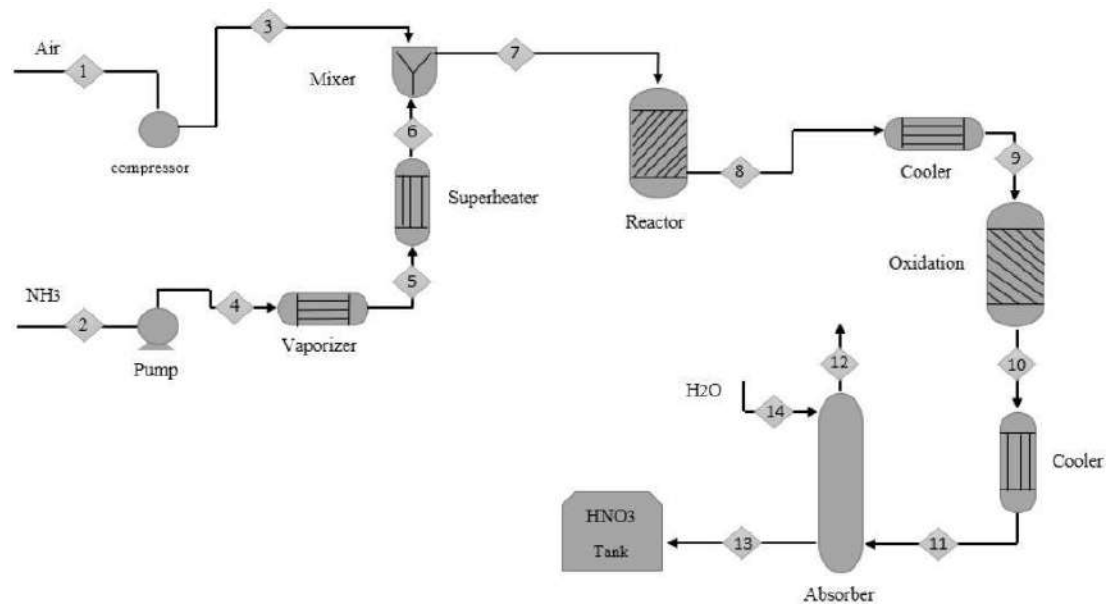


Figure 2-1 The Single-Pressure Process

2.1.2 The Dual-Pressure Process

The dual-pressure process was developed to take advantage of two factors:

- a) Low-pressure ammonia oxidation;
- b) High-pressure absorption for acid production

In addition to the higher conversion, the lower catalyst gauze temperature (associated with the low-pressure ammonia oxidation) results in a much lower rate of platinum deterioration. Both advantages are maximized at the lowest pressure. In contrast, however, absorption is best performed at the highest pressure.

The low-pressure ammonia oxidation is usually performed in the pressure range of 101.3 kPa to 344 kPa. High-pressure absorption is usually performed in the operating range of 800 kPa up to 1010 kPa. This process begins with the vaporization of ammonia at 550 kPa and 7°C "as shown in its flow sheet of Fig. (2)" followed by superheating to 76°C using heat from

the compressed bleached air. Filtered air is 12 compressed in an axial compressor to 350 kPa and is mixed

with the superheated ammonia vapor (1 O-1 1% ammonia by volume) prior to entering the converter/reactor. In the converter, the gases react over the platinum/rhodium gauze catalyst.

The gases leaving the reactor at 330 kPa and 865°C flow through a series of heat exchangers for recovery of energy, either as high-pressure superheated steam or shaft horsepower from expansion of hot tail gas. Approximately 40% of the oxidation to nitrogen dioxide occurs in the gas as it passes through the energy recovery train and is cooled to 135°C (exit from the tail-gas preheater). After further cooling to 45°C in the medium-pressure condenser, and separation of 20% of the acid product as 30% strength nitric acid, the gas reaches 50% oxidation to nitrogen peroxide with approximately 20% dimerization.

The gas is combined with bleach air containing additional nitrogen peroxide and is compressed in a centrifugal nitrous-gas compressor to 1025 kPa. The exit temperature of 224°C is achieved due to the combined heat effects of the compression, the further oxidation to 80% nitrogen peroxide, and the virtual disappearance of the dimer. The compressed gas flows through an empty oxidation chamber, a high-pressure boiler feed water economizer, and a low-pressure deionized water economizer, and thus is cooled to 95°C. Residence time in the system and the effect of increased pressure result in at least 95% oxidation to nitrogen peroxide, but the dimerization is low due to the temperature level.

The gas is then cooled to the dew point (50°C) for entry into the absorber. The dimerization increases to 48%, adding significantly to the heat removed prior to the absorber.

The system uses circulating condensate as the energy transfer medium. The absorber is essentially the same as that previously described for the single pressure process. Chilled water at 15°C is used in the absorber and the outlet gas temperature is 18°C. Refrigeration for the chilled water is provided by the ammonia vaporizer which operates at 7°C. Weak acid from the bottom of the absorber is let down to 330 kPa for bleaching with air from the axial compressor. This air, with nitrogen peroxide stripped from the acid, flows to the suction of the nitrous-gas compressor together with the main nitrous gas stream from the condenser

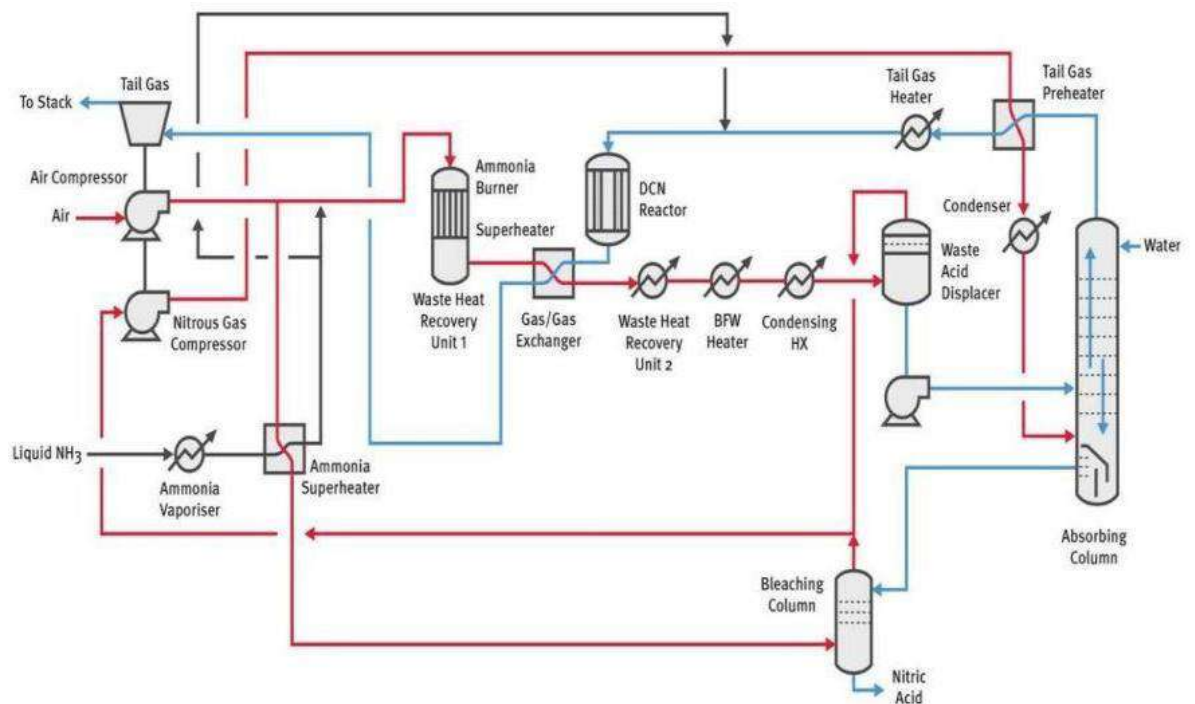


Figure 2-2 The Dual-Pressure Process

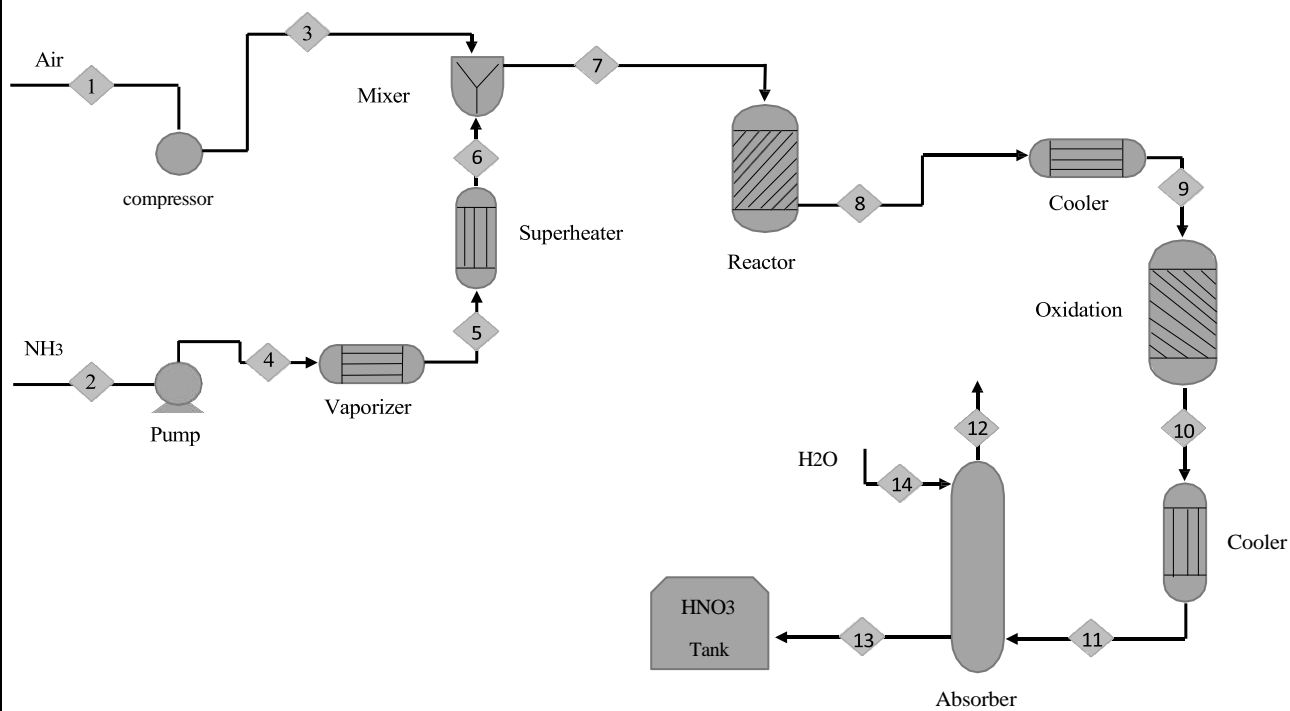
Chapter 3

Material Balance

2.1 Process Description

The process begins with the vaporization of ammonia at 1240 kPa and 35°C using process heat. Steam is then used to superheat the ammonia about 170°C, filtered air is compressed by a centrifugal compressor, discharge pressure of 1200 kPa. In our process; the air and the ammonia vapor are mixed and passed through the platinum/ rhodium gauze reactor where the heat of reaction raises the temperature to be between 650°C and 630°C. The reaction gas flows of heat exchangers to cooled down to 70 oC. Approximately 95% of the oxidation to nitrogen dioxide occurs as the gas passes in the Oxidation unit, after that cooled to 60°C, then sent to absorber to produce nitric acid (60%) purity.

2.2 Flow sheet of process :

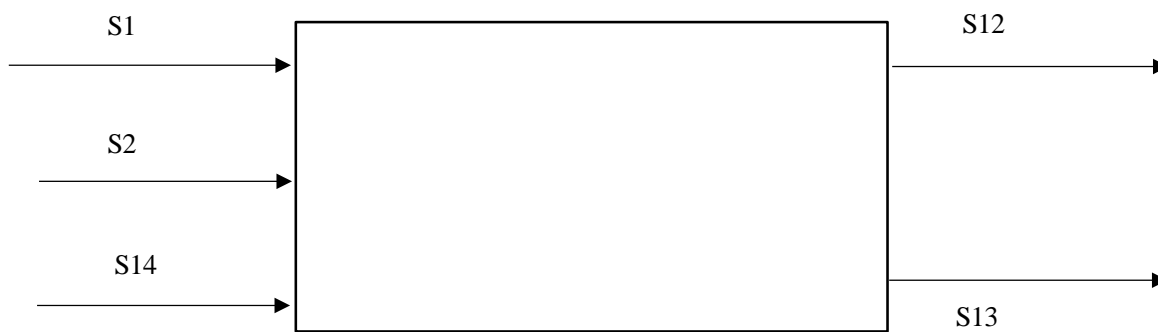


2.3 Over all material balance

Production = $150000 \frac{\text{ton}}{\text{year}}$ of 60% nitric acid

$$150000 \frac{\text{ton}}{\text{year}} = 20833 \frac{\text{kg}}{\text{hr}}$$

$$\text{HNO}_3 = 0.6 \times 20833 = 12499.8 \text{ kg/hr} = 198.4 \text{ kmol/hr}$$



Conversion of ammonia 95%

HNO₃ :

$$= 198.4 \frac{\text{kmole}}{\text{hr}}$$

NH₃ :

$$= 231.40 \frac{\text{kmole}}{\text{hr}}$$

O₂ :

$$= 198.4 \times 2 = 396.8 \frac{\text{mole}}{\text{hr}} \text{ (reacted)}$$

Excess 20%

$$= 496 \frac{\text{kmole}}{\text{hr}}$$

N₂:

$$= \frac{496 \times 32 \times 0.79}{28 \times 0.21} = 2132.46 \frac{\text{kmol}}{\text{hr}}$$

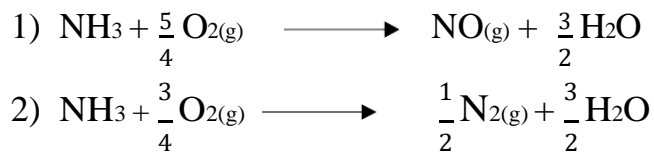
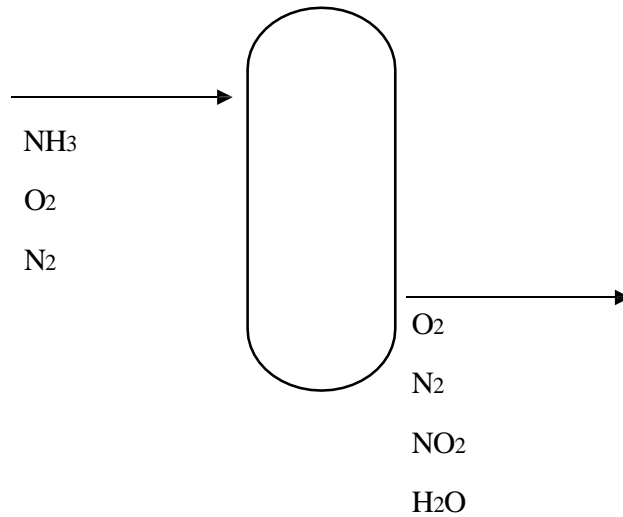
Make up H₂O :

$$= 462.95 - 198.4 = 264.55 \frac{\text{kmole}}{\text{hr}}$$

Tail gases

$$= 231.40 + 496 + 2132.46 - 198.4 - 264.55 = 2396.91 \text{ kmole/hr}$$

2.4 Reactor material balance :



Reaction one:

Conversion of ammonia = 95%

$$\text{NH}_3 \text{ (reacted)} = 231.40 \times 0.95 = 219.83 \frac{\text{kmole}}{\text{hr}}$$

$$\text{O}_2 \text{ (reacted)} = \frac{5}{4} \times 219.83 = 274.78 \frac{\text{kmole}}{\text{hr}}$$

$$\text{NO (produced)} = 219.83 \frac{\text{kmole}}{\text{hr}}$$

$$\text{H}_2\text{O (produced)} = \frac{3}{2} \times 219.83 = 329.74 \frac{\text{kmole}}{\text{hr}}$$

Reaction two :

Conversion of ammonia =5%

$$\text{NH}_3 \text{ (reacted)} = 0.05 \times 231.40 = 11.57 \frac{\text{kmole}}{\text{hr}}$$

$$\text{O}_2 \text{ (reacted)} = \frac{3}{4} \times 11.57 = 8.677 \frac{\text{kmole}}{\text{hr}}$$

$$\text{N}_2 \text{ (produced)} = \frac{1}{2} \times 11.57 = 5.785 \frac{\text{kmole}}{\text{hr}}$$

$$\text{H}_2\text{O} \text{ (produced)} = \frac{3}{2} \times 11.57 = 17.355 \frac{\text{kmole}}{\text{hr}}$$

Output products:

$$\text{O}_2 = \text{inlet} - \text{reacted} = 496 - 274.78 - 8.677 = 212.543 \frac{\text{kmole}}{\text{hr}}$$

$$\text{N}_2 = \text{inlet} + \text{produced} = 2132.46 + 5.785 = 2138.245 \frac{\text{kmole}}{\text{hr}}$$

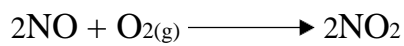
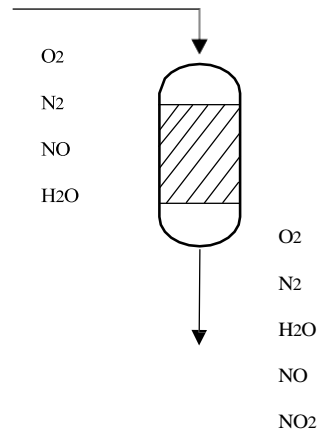
$$\text{NO} = \text{inlet} + \text{produced} = 0 + 219.83 = 219.83 \frac{\text{kmole}}{\text{hr}}$$

$$\text{H}_2\text{O} = \text{inlet} + \text{produced} = 0 + 329.74 + 17.355 = 347.095 \frac{\text{kmole}}{\text{hr}}$$

Table 1 Summary of reactor mass balance

compound	Input				Output			
	Mole/hr	Kg/hr	Wt%	Mole %	Mole/hr	Kg/hr	Wt%	Mole %
NH3	231.40	3933.8	4.94	8.09	-----	-----	-----	-----
O2	496	15872	19.96	17.343	212.543	6801.376	8.55	7.284
N2	2132.46	59708.88	75.09	74.565	2138.245	59870.86	75.29	73.284
NO	-----	-----	-----	-----	219.83	6594.9	8.29	7.534
H2O	-----	-----	-----	-----	347.095	6247.71	7.86	11.896
TOTAL	2859.86	79514.8			2917.713	79514.8		

2.5 Oxidation material balance :



Conversion of NO = 95%

$$\text{NO (inlet)} = 219.83 \frac{\text{kmole}}{\text{hr}}$$

$$\text{NO (reacted)} = 219.83 \times 0.95 = 208.838 \frac{\text{kmole}}{\text{hr}}$$

$$\text{NO (outlet)} = 219.83 - 208.838 = 10.992 \frac{\text{kmole}}{\text{hr}}$$

$$\text{N}_2 \text{ (outlet)} = 2138.245 \frac{\text{kmole}}{\text{hr}}$$

$$\text{H}_2\text{O (outlet)} = 347.095 \frac{\text{kmole}}{\text{hr}}$$

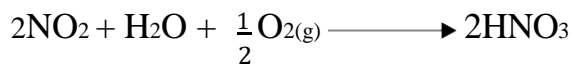
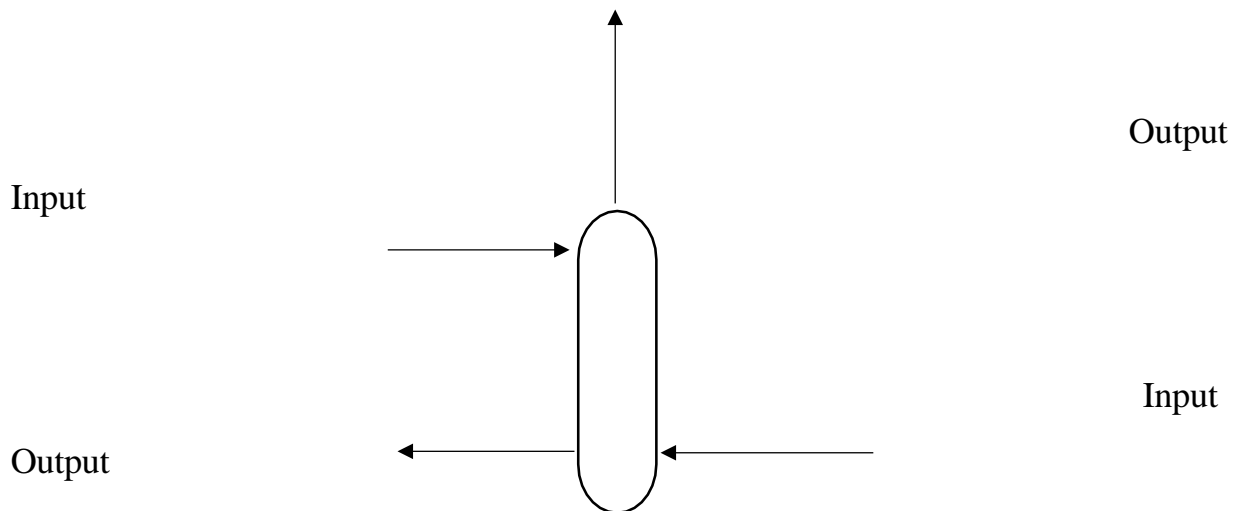
$$\text{O}_2 \text{ (outlet)} = 212.543 - \frac{1}{2}(208.838) = 108.124 \frac{\text{kmole}}{\text{hr}}$$

$$\text{NO}_2 \text{ (outlet)} = 0 + 208.838 \frac{\text{kmole}}{\text{hr}} = 208.838 \frac{\text{kmole}}{\text{hr}}$$

Table(2) : Summery of oxidation mass balance

component	Input				Output			
	Mole/hr	Kg/hr	Wt%	Mole fraction	Mole/hr	Kg/hr	Wt%	Mole fraction
NO	219.83	6594.9	8.29	7.53	10.992	329.76	0.41	0.3907
O ₂	212.543	6801.376	8.55	7.28	108.124	3459.968	4.35	3.843
N ₂	2138.245	59870.86	75.3	73.28	2138.245	59870.86	75.3	76.005
H ₂ O	347.095	6247.71	7.85	11.896	347.095	6247.71	7.85	12.337
NO ₂	-----	-----	-----	-----	208.838	9606.548	12.08	7.42
TOTAL	2917.713	79514.8			2813.29	79514.8		

2.6 Absorber material balance :



Conversion of $\text{NO}_2 = 95\%$

$$\text{NO}_2 (\text{inlet}) = 208.838 \frac{\text{kmole}}{\text{hr}}$$

$$\text{NO}_2 (\text{reacted}) = 208.838 \times 0.95 = 198.396 \frac{\text{kmole}}{\text{hr}}$$

$$\text{NO}_2 (\text{outlet}) = 208.838 - 198.396 = 10.442 \frac{\text{kmole}}{\text{hr}}$$

$$\text{HNO}_3 (\text{outlet}) = 0 + (198.396) = 198.396 \frac{\text{kmole}}{\text{hr}}$$

$$\text{O}_2 (\text{outlet}) = 108.124 - \frac{0.5}{2}(198.396) = 58.525 \frac{\text{kmole}}{\text{hr}}$$

$$\text{N}_2 (\text{outlet}) = 2138.245 \frac{\text{kmole}}{\text{hr}}$$

$$\text{H}_2\text{O} (\text{outlet}) = 347.095 - \frac{1}{2}(198.396) = 247.897 \frac{\text{kmole}}{\text{hr}}$$

$$\text{NO} = 10.992$$

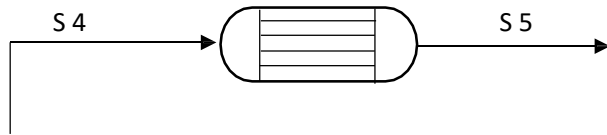
Table(3) Summary of absorber mass balance

component	Input				Output			
	Mole/hr	Kg/hr	Wt%	Mole %	Mole/hr	Kg/hr	Wt%	Mole %
NO ₂	208.838	9606.548	12.08	7.42	10.442	480.332	0.6	0.391
O ₂	108.124	3459.968	4.35	3.84	58.525	1872.8	2.36	2.196
N ₂	2138.24	59870.72	75.3	76.00	2138.245	59870.86	75.3	80.24
HNO ₃	-----	-----	-----	-----	198.396	12498.948	15.7	7.44
NO	10.992	329.76	0.41	0.390	10.992	329.76	0.41	0.412
H ₂ O	347.095	6247.71	7.85	12.33	247.897	4462.146	5.61	9.303
Total	2813.29	79514.8			2664.49	79514.8		

Chapter 4

Energy Balance

4.1 Vaporizer Energy Balance :



For S4: NH₃ at -15 C ° and S5: NH₃ at 35 C °

T_{ref} = -15 C °

$$Q = \sum n_{out}H_{out} - \sum n_{in}H_{in}$$

$$\sum H_{in} = \int_{-15}^{-15} CP dT$$

$$Q = \sum n_{out}H_{out} - 0$$

$$H_{out} = n \left[\int_{T_{ref}}^{T_{boil}} Cp dT + H_{vap} + \int_{T_{boil}}^{T_{out}} Cp dT \right]$$

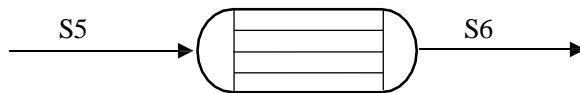
$$H = \int_{35}^{-15} Cp dT = 35.15 \times 10^{-3}(35 + 15) + 2.954 \times \frac{10^{-5}}{2} (35^2 + 15^2) +$$

$$0.4421 \times \frac{10^{-8}}{3} (35^3 + 15^3) - 6.686 \times \frac{10^{-12}}{4} (35^4 + 15^4)$$

$$\sum H_{out} = 1000 \times 231.40 \left[1.78 + \left(\frac{1133.642}{1000} \times 17 + 0.07232 \right) \right]$$

$$\sum H_{out} = Q = 4888147.748 \frac{kJ}{h}$$

4.2 Superheater Energy Balance :



For S5: NH₃ at 35 C ° and S6: NH₃ at 177 C °

$$Q = \sum n H_{out} - \sum n H_{in}$$

$$T_{ref} = 35 \text{ C } ^\circ$$

$H_{in} = \text{Zero}$

$$H_{(out)} = \int_{T_1}^{T_2} Cp \, dT$$

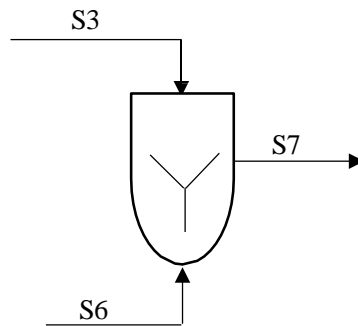
For NH₃ :

$$H = \int_{35}^{177} Cp \, dT = 35.15 \times 10^{-3}(177 - 35) + 2.954 \times \frac{10^{-5}}{2}(177^2 - 35^2) + 0.4421 \times \frac{10^{-8}}{3}(177^3 - 35^3) - 6.686 \times \frac{10^{-12}}{4}(177^4 - 35^4)$$

$$H_{out} = 1000 \times 231.40 \times 5.442 = 1259278.8 \text{ KJ/h}$$

$$Q = H_{out} = 1259278.8 \text{ KJ/h}$$

4.3 Mixer Energy Balance :



For S3: NH_3 at 177 C° , S6: Air at 262 C° and S7: $\text{NH}_3 + \text{Air}$ at ?

$$Q = 0 \text{ (Adiabatic)}$$

Energy required to heat ammonia = Energy lost by air

$$mC_p(T_{out} - T_{in}) = mC_p(T_{out} - T_{in})$$

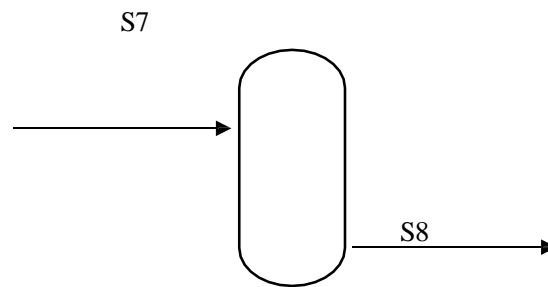
$$C_p(\text{NH}_3) = 2.38 \frac{\text{KJ}}{\text{Kg} \cdot \text{C}^\circ}$$

$$C_p(\text{Air}) = 1.05 \frac{\text{KJ}}{\text{Kg} \cdot \text{C}^\circ}$$

$$2335.88 \times 2.38 \times (T_{out} - 177) = 43537.52 \times 1.05 \times (262 - T_{out})$$

$$T_{out} = 250\text{ C}^\circ$$

4.4 Reactor Energy Balance :

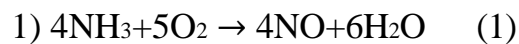


For S7: NH₃ + Air at 250 C ° and S8: Air + NO + H₂O at 645 C °

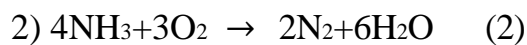
Table 4: Summary of enthalpy components in reactor

Component	Input S7 (kJ/mol)	Output S8 (kJ/mol)
H (Air)	6.654	19
H (NH ₃)	8.84	
H (NO)		19.744
H (H ₂ O)		23

$$Q = \sum n_{out} H_{out} - \sum n_{in} H_{in} + n_{product 1} \Delta H_{r1} + n_{product 2} \Delta H_{r2}$$



Conversion=95%



Conversion=5%

$$\Delta H_r = \sum (F \Delta H_f)_{Product} - \sum (F \Delta H_f)_{Reactant}$$

$$\Delta H_{r1} = -1311.04 \frac{\text{kJ}}{\text{mol}}$$

Based on NO

$$\Delta H_{r1} = -\frac{1311.04}{4} = -327.76 \text{ KJ/mol}$$

$$\Delta H_{r2} = -1446.24 \text{ KJ/mol}$$

Based on H₂O

$$\Delta H_{r2} = -\frac{1446.24}{6} = -241.04 \text{ KJ/mol}$$

$$H = \int_{T_1}^{T_2} C_p dT = a(T_2 - T_1) + \frac{b}{2} (T_2^2 - T_1^2) + \frac{c}{3} (T_2^3 - T_1^3) + \frac{d}{4} (T_2^4 - T_1^4)$$

For NH₃ :

$$H = \int_{25}^{250} C_p dT = 35.15 \times 10^{-3}(250 - 25) + 2.954 \times \frac{10^{-5}}{2} (250^2 - 25^2) + 0.4421 \times \frac{10^{-8}}{3} (250^3 - 25^3) - 6.686 \times \frac{10^{-12}}{4} (250^4 - 25^4) = 8.84 \text{ KJ/mol}$$

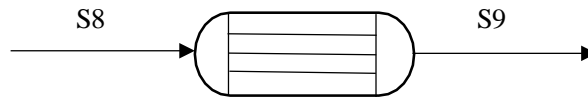
T_{ref} = 25 C °

Component	Input S7 (kJ/mol)	Output S8 (kJ/mol)
H (Air)	6.654	19
H (NH ₃)	8.84	—
H (NO)	—	19.744
H (H ₂ O)	—	23

$$Q = 39294150 + F_{out}(NO) \cdot \Delta H_{r1} + F_{out}(H_2O) \cdot \Delta H_{r2}$$

$$Q = -11641109 \text{ KJ/h}$$

4.5 Heat Exchanger Energy Balance (1st Cooler) :



For S8 : Air + NO + H₂O at 645 C°

For S9 : Air + NO + H₂O at 70 C °

$$Q = \sum(FH)_{out} - \sum(FH)_{in}$$

$$T_{ref} = 70 \text{ C } ^\circ$$

$$H_{(out)} = \text{Zero}$$

Input :

$$H = \int_{T_1}^{T_2} Cp dT = a(T_2 - T_1) + \frac{b}{2}(T_2^2 - T_1^2) + \frac{c}{3}(T_2^3 - T_1^3) + \frac{d}{4}(T_2^4 - T_1^4)$$

For Air :

$$H = \int_{70}^{645} Cp dT = 28.94 \times 10^{-3}(645 - 70) + 0.4147 \times \frac{10^{-5}}{2}(645^2 - 70^2) + 0.3191 \times \frac{10^{-8}}{3}(645^3 - 70^3) - 1.965 \times \frac{10^{-12}}{4}(645^4 - 70^4) = 17.693 \text{ KJ/mol}$$

For NO :

$$H = \int_{70}^{645} Cp dT = 18.400 \text{ KJ/mol}$$

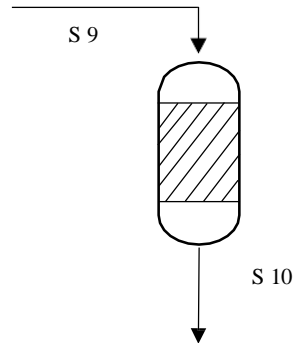
For H₂O :

$$H = \int_{70}^{645} Cp dT = 21.173 \text{ KJ/mol}$$

$$Q = -[(2350.788 \times 17.693) + (219.83 \times 18.400) + (347.095 \times 21.173)]$$

$$Q = - 52986.40652 \text{ KJ/h}$$

4.6 Oxidation Energy Balance :



For S9 : Air + NO + H₂O at 70 C °

For S10 : Air + NO + H₂O + NO₂ at 140 C °

Conversion = 95%

$$\Delta Hr = \sum(F\Delta H_f)_{Product} - \sum(F\Delta H_f)_{Reactant}$$

$$\Delta Hr = -139957.8592 \text{ KJ/mol}$$

Based on (NO₂) :

$$\Delta Hr = -139957.8592 / 2 = -69978.92958 \text{ KJ/mol}$$

$$Q = \sum(FH)_{out} - \sum(FH)_{in} + n_{proud} \Delta Hr$$

$$H = \int_{T_1}^{T_2} Cp dT = a(T_2 - T_1) + \frac{b}{2}(T_2^2 - T_1^2) + \frac{c}{3}(T_2^3 - T_1^3) + \frac{d}{4}(T_2^4 - T_1^4)$$

$$T_{ref} = 25 \text{ C } ^\circ$$

$$H = \int_{25}^{70} Cp dT \quad \text{For input}$$

For (H₂O)_g

$$H = \int_{25}^{70} Cp dT = 33.46 \times 10^{-3}(70 - 25) + 0.6880 \times \frac{10^{-5}}{2}(70^2 - 25^2) +$$

$$0.7604 \times \frac{10^{-8}}{3}(70^3 - 25^3) - 3.593 \times \frac{10^{-12}}{4}(70^4 - 25^4) = 1.521 \text{ KJ/mol}$$

$$H = \int_{25}^{140} Cp \, dT \quad \text{For output}$$

For (H₂O)_g

$$H = \int_{25}^{140} Cp \, dT = 33.46 \times 10^{-3}(140 - 25) + 0.6880 \times \frac{10^{-5}}{2} (140^2 - 25^2) + 0.7604 \times \frac{10^{-8}}{3} (140^3 - 25^3) - 3.593 \times \frac{10^{-12}}{4} (140^4 - 25^4) = 3.919 \text{ KJ/mol}$$

Table (4)

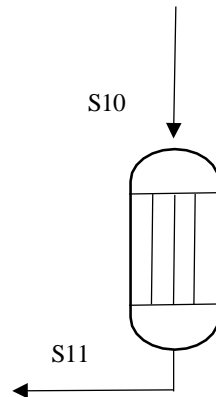
Component	Input S9 (KJ/mol)	Output S10 (KJ/mol)
H (H ₂ O) _g	1.521	3.919
H (Air)	1.312	3.37
H (NO)	1.345	3.47
H (NO ₂)	—	4.5

$$\sum(FH)_{in} = 3907.84 \text{ KJ/h}$$

$$\sum(FH)_{out} = 9908.44 \text{ KJ/h}$$

$$Q = - 63978.32958 \text{ KJ/h}$$

4.7 Heat Exchanger Energy Balance (2nd Cooler) :



For S10 : Air + NO + H₂O + NO₂ at 140 C °and

S11 : Air + NO + H₂O + NO₂ at 60 C °

$T_{ref} = 60\text{ C }^\circ$

$$Q = \sum(FH)_{out} - \sum(FH)_{in}$$

$$H = \int_{T_1}^{T_2} Cp dT = a(T_2 - T_1) + \frac{b}{2}(T_2^2 - T_1^2) + \frac{c}{3}(T_2^3 - T_1^3) + \frac{d}{4}(T_2^4 - T_1^4)$$

$H_{out} = \text{Zero}$

Input :

For H₂O

$$H = \int_{60}^{140} Cp dT = 33.46 \times 10^{-3}(140 - 60) + 0.6880 \times \frac{10^{-5}}{2}(140^2 - 60^2) + 0.7604 \times \frac{10^{-8}}{3}(140^3 - 60^3) - 3.593 \times \frac{10^{-12}}{4}(140^4 - 60^4) = 2.737 \text{ KJ/mo}$$

For Air

$$H = \int_{60}^{140} Cp dT = 2.350 \text{ KJ/mol}$$

For NO

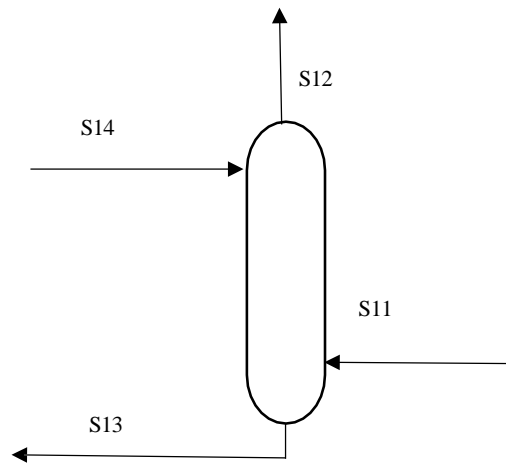
$$H = \int_{60}^{140} Cp dT = 2.4230 \text{ KJ/mol}$$

For NO₂

$$H = \int_{60}^{140} Cp dT = 3.1796 \text{ KJ/mol}$$

$$Q = - 33526.579 \text{ KJ/mol}$$

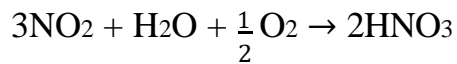
4.8 Absorber Energy Balance :



Basis : $T_{ref} = 25 \text{ C } ^\circ$

For S11 : Air + NO + H₂O + NO₂ at 60 C ° , S11 : H₂O at 20 C °

For S12 : Air + NO + H₂O at 30 C ° and S13 : HNO₃ + H₂O at 30 C °



Conversion = 95 %

$$\Delta Hr = \sum(F\Delta Hf)_{Product} - \sum(F\Delta Hf)_{Reactant}$$

$$\Delta Hr = -300258.6481 \text{ KJ/mol}$$

Based on (HNO₃) :

$$\Delta Hr = -300258.6481 / 2 = -150129.3241 \text{ KJ/mol}$$

$$Q = \sum(FH)_{out} - \sum(FH)_{in} + n_{proud} \Delta Hr$$

$$H = \int_{T_1}^{T_2} Cp dT = a(T_2 - T_1) + \frac{b}{2}(T_2^2 - T_1^2) + \frac{c}{3}(T_2^3 - T_1^3) + \frac{d}{4}(T_2^4 - T_1^4)$$

For (H₂O)_g in S12

$$H = \int_{25}^{30} C_p dT = 33.46 \times 10^{-3}(30 - 25) + 0.6880 \times \frac{10^{-5}}{2}(30^2 - 25^2) + 0.7604 \times \frac{10^{-8}}{3}(30^3 - 25^3) - 3.593 \times \frac{10^{-12}}{4}(30^4 - 25^4) = 0.166 \text{ KJ/mol}$$

$$T_{ref} = 25 \text{ C}^\circ$$

Component	Input S11 (KJ/mol)	Input S14 (KJ/mol)	Output S12 (KJ/mol)	Output S13 (KJ/mol)
H (H ₂ O) _g	1.18	—	0.166	—
H (H ₂ O) _L	—	-0.375	—	0.375
H (Air)	1.02	—	0.145	—
H (NO)	1.044	—	0.149	—
H (NO ₂)	1.32	—	—	—
H (HNO ₃)	—	—	—	0.55

$$\Sigma(FH)_{in} = 2857.845 \text{ KJ/mol}$$

$$\Sigma(FH)_{out} = 563.399 \text{ KJ/mol}$$

$$Q = -152423.7701 \text{ KJ/mol}$$

Chapter 5

Chemical and Mechanical Design

5.1 Design of Reactor:

Introduction:

CHOICE OF REACTOR TYPE

The choice of reactor is dictated by the process conditions, the type of reaction and the mode of catalyst exposition. The oxidation of ammonia is a gas-solid reaction of catalytic type. Since the catalyst is in the form of wire gauze, so a fixed bed reactor is best suited. The reaction is exothermic and the heat of reaction is to be conserved as it will be used to supply power required for compression, to generate steam and to preheat air, hence the mode of operation will be adiabatic.

The reactor is classified as a heterogeneous, catalytic, shallow fixed bed, adiabatic, down flow reactor. Most of the reactors employed in nitric acid industry are tapered along with 700 angles.

CHOICE OF CATALYST

Catalysts which increase the rate of oxidation of ammonia to nitrogen oxide (NO) include platinum, its alloys with metals of platinum group, oxides of iron, manganese, cobalt etc. The activity of platinum and platinum alloy catalysts is higher than that of others. Non platinum catalysts are cheaper but they are less active and unstable. For these reasons at most of plants where HNO₃ is made from ammonia, platinum catalysts are used. 90% Pt with 10% Rh is selected as catalyst for this reaction because it can operate at high temperatures, maximum yield is obtained and the contact time can be accurately controlled.

Kinetic of reaction

The catalyst of ammonia oxidation is so rapid that the amount of catalyst required is very small and heat transfer is not feasible. Typically configuration of this system is the woven – wire gauze. This reaction completely by mass transfer, and the design of screen packs has been based on pilot –plant studies and plant experience.

Assumption:

1. The reactions are mainly controlled by diffusion.
2. The partial pressure of ammonia on the catalyst surface is negligible.
3. The design model is developed as plug flow.
4. Typical reported data are used.
5. Ratio of mass of ammonia /hr.: mass of catalyst =85.
6. Cross sectional area = $0.256 \times 10^{-3} \text{ m}^2/\text{ton HNO}_3$, daily.

Let:

$N_w = 80$ inch mesh size

$A_w = \text{area /ton HNO}_3 = 0.256 \text{ m}^2/\text{ton HNO}_3$

$d_w = \text{wire diameter} = 0.003 \text{ inch} = 76 \times 10^{-4} \text{ cm}$

$f_w = \text{wire area per gauza cross sectional area}$

$A_{wr} = \text{surface area of screen / volume of one screen}$

The density of catalyst = 0.0214 kg / cm^3

$n_s = \text{number of screen per gauza}$

$X = 0.95$

$V_g = \text{volume of one screen} = 110 \text{ cm}^3$

$Y_{\text{NH}_3} = 0.09$

$$a_{wr} = \pi N_w^2 \left[\left(\frac{1}{N_w} \right)^2 + d_w^2 \right]^{0.2} = 122.6 \text{ cm}^{-1} = 294.39 \text{ inch}^{-1}$$

$$f_w = a_{wr} \times 2d_w = 294.39 \times 2 \times 0.003 = 1.77$$

$$\epsilon = \text{Porcity} = 1 - \frac{a_w d_w}{4} = 1 - \frac{122.6 \times 76 \times 10^{-4}}{4} = 0.8$$

$$G = \text{mass velocity} = \frac{\frac{M_A}{M_w}}{Y_A \times X_A \times a_w \times 2000}$$

$$= \frac{30}{24 \times 3600 \times 0.96 \times 0.09 \times 0.027547}$$

$$G = 4.63 \frac{\text{lbm}}{\text{ft}^2 \cdot \text{s}} = 2.1 \frac{\text{g}}{\text{cm}^2 \cdot \text{s}}$$

→ Superficial velocity

$$u_s = 2.1 \times \frac{1}{\rho} = 2.1 \times \frac{82.06 \times 1209}{7.8 \times 30} = 890 \frac{\text{cm}}{\text{s}} = 28.3 \frac{\text{ft}}{\text{s}}$$

$$u_s = \frac{1 - X_A \times \epsilon^{0.352} \times d_w^{0.648} \times G^{0.648} \times u^{0.0190}}{-\ln 5.81761 \times 10^{-5}) \times f_w \times T^{0.333} \times (28.85 + 11.82 \times y_{A_o})^{0.667}}$$

$n_s = 19 \text{ gauza}$

$$\text{ratio} = \frac{\text{mass ammonia}}{\text{mass catalyst}} = 85$$

The mass of ammonia /85=mass of catalyst

$$m_{\text{cat}} = \frac{17 \times 231.40}{85} = 46.28 \text{ kg}$$

$$\text{Area required} = A = 0.256 \times 300 = 76.8 \text{ m}^2$$

Volume of catalyst = the mass of catalyst/ density of catalyst

$$\text{Volume of catalyst} = \frac{27.5}{0.0214} = 1284 \text{ cm}^3$$

$$N_c = \text{number of screen} = \frac{V_c}{V_g - (1 - \epsilon)} = 12 \text{ screen}$$

$$\text{height} = 0.5 \times 50 + 1 \text{ TOP} + 1 \text{ bottom} = 8 \text{ m}$$

$$\text{Area} = \pi \times D \times L$$

$$D = \frac{76.8}{\pi \times 8} = 3.05 \text{ m}$$

Mechanical design :

Shell

$$e = \frac{p_i D_i}{2F - p} + c$$

C= thickness of shell mm

Pi=design pressure N/mm²

Di=inside shell diameter

F=design stress N/mm.

c= corrosion constant.

Di = 3.055m=3055mm.

Operating pressure =8 bar.

Design pressure $P_i = 1.1 \times 8 = 8.8 \text{ bar} = 0.88 \text{ N/mm}^2$

$C=1 \text{ mm}$

At $T=645 \text{ }^\circ\text{C}$ design stress of stainless steel

$$F = 55 \frac{\text{N}}{\text{mm}^2} \text{ table 13.2}$$

$$e = \frac{0.88 \times 3055}{2 \times 55 - 0.88} + 1 = 25 \text{ mm}$$

Ellipsoidal head:

$$e = \frac{P_i}{2Jf - 0.2P_i} + c$$

Where :

C =thickness of ellipsoidal head mm

J = joint factor = 0.8

$$e = \frac{0.88 \times 3055}{2 \times 0.8 \times 55 - 0.2 \times 0.88} + 1 = 31 \text{ mm}$$

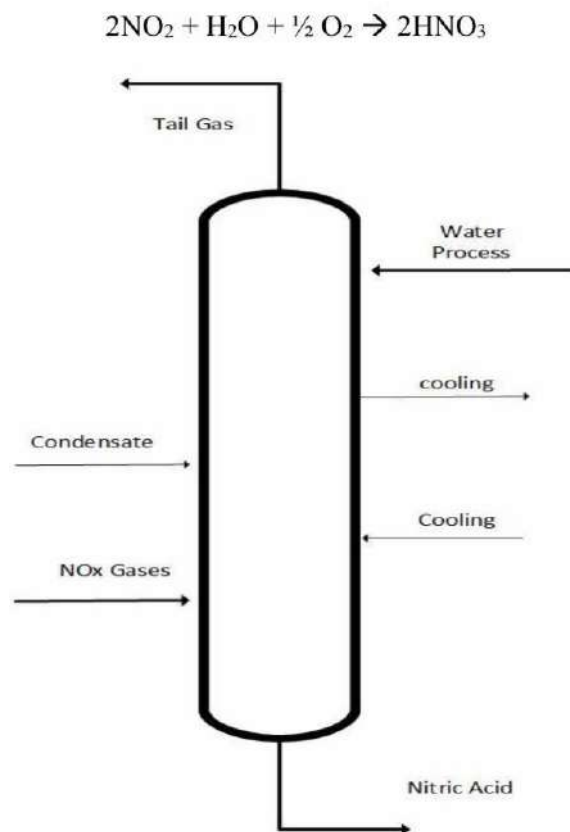
Type	Fixed bed
Volume m^3	1.284
Height m	8
Dimeter m	3
Material of const	St.st

5.2 Design of Absorber ;

Introduction

The most important step of manufacturing nitric acid is Absorption of NO_x. When it is compared to other absorptions operation. Absorption of NO_x is the most complex. This is for several reasons:

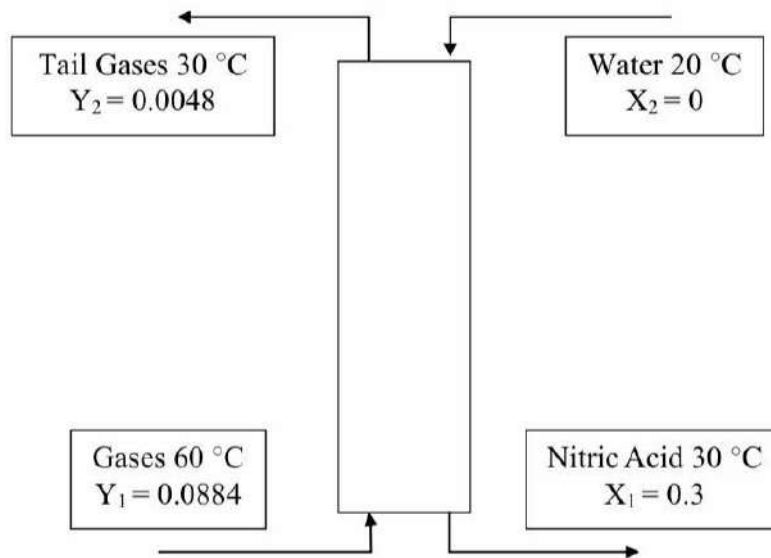
1. NO_x is a mixture of several components of NO,NO₂,N₂O₃ and N₂O₄.
2. In absorption tower many reversible and irreversible reactions.
3. Simultaneous absorption of many gases occurs followed by chemical reaction.
4. Heat Generated from the reactions, which affect the absorption.



The objective ;

To design an absorption tower to absorb NO₂ from the mixer gas stream using water to form nitric acid with 60% weight.

Absorber design calculation



Stream temperature and NO₂ molar composition

Number of Gases moles entered the absorber= Gm= 1417.09 Kmol/hr

Number of water moles entered the absorber=Lm=373.19 Kmol/hr

Compositions of income gases

Component	Mole fraction	Mole fraction
NO ₂	0.0884	46
NO	0.0037	30
O ₂	0.0386	32
N ₂	0.869	28

Average Molecular Weight (Mwt)

$$\begin{aligned} &= (46 \times 0.0884) + (30 \times 0.0037) + (32 \times 0.0386) + (0.869 \times 28) \\ &= 29.74 \text{ Kg/ Kmole} \end{aligned}$$

$$\begin{aligned} \text{Density of Gases (assuming ideal Gas)} = \rho_v &= \frac{P \times \text{mwt}}{R \times T} = \frac{120000 \times 29.74}{8314.34 \times 333} \\ &= 12.89 \text{ Kg/m}^3 \end{aligned}$$

P= 1200000 Pa T=60 °C = 333 K R= 8314.34 m³ × Pa/Kmole × K
Density of water at 20 °C , 1200 kPa = ρ_l= 998.23 Kg/m³

Diameter Calculation

$$U_v = (-0.171 L t^2 + 0.21 L t - 0.047) \left(\frac{\rho_l - \rho_v}{\rho_v} \right)^{0.5}$$

L_t=plat spacing=0.9 m

$$U_v = (-0.171 \times (0.9)^2 + 0.21 \times 0.9 - 0.047) \left(\frac{998.23 - 12.89}{12.89} \right)^{0.5} = 0.51 \text{ m/sec}$$

Taking 60% U_v = 0.3 m/s

$$D = \sqrt{\frac{4V_m}{\pi \rho_m U_v}}$$

$$D = \sqrt{\frac{4 \times 11.71}{3.14 \times 12.98 \times 0.3}} = 1.96 \approx 2 \text{ m}$$

Design

Assumptions

1. N_2O_4 ($2NO_2$) is the only species, which dissolved in the Liquid.
2. Neglect the reactions occurs in the column.
3. Isothermal Operation and the temperature is $45^\circ C$.
4. The design of the column is trays absorption column.

Height of Absorber

Equilibrium line can be specified:

$$Y = mX$$

From Raoult's law

$$m = \frac{p^{sat}}{P_{total}}$$

P^{sat} for NO_2 at $45^\circ C$

From Antoine Equation:

$$\ln P^{sat} = A - \frac{B}{T - C}$$

$$A = 20.5324$$

$$B = 4141.29$$

$$C = 3.65$$

$$T = 45^\circ C = 318 \text{ K}$$

$$\ln P^{sat} = 20.5324 - \frac{4141.29}{318 + 3.65} = 7.6572$$

$$P^{sat} = 2115.944 \text{ mmHg} = 282.01 \text{ kPa}$$

So, the slope of the equilibrium line

$$m = \frac{282.01}{1200} = 0.234$$

$$\text{Number of stage } N = \frac{\ln\left[\left(1 - \frac{m G_m}{L_m}\right) \left(\frac{Y_1 - m X_2}{Y_2 - m X_2}\right) + \frac{m G_m}{L_m}\right]}{\ln\left(\frac{L_m}{L_m G_m}\right)}$$

$$m = 0.235$$

$$G_M = 1417.09 \text{ kmol/hr}$$

$$L_m = 373.191 \text{ kmol/hr}$$

$$Y_1 = 0.0048$$

$$Y_2 = 0.0884$$

$$X_2 = 0$$

$$N = \frac{\ln\left[\left(1 - 0.893\right) \left(\frac{0.0884 - 0}{0.0048 - 0}\right) + 0.893\right]}{\ln\left(\frac{1}{0.893}\right)} = 9.3 \approx 10 \text{ stages}$$

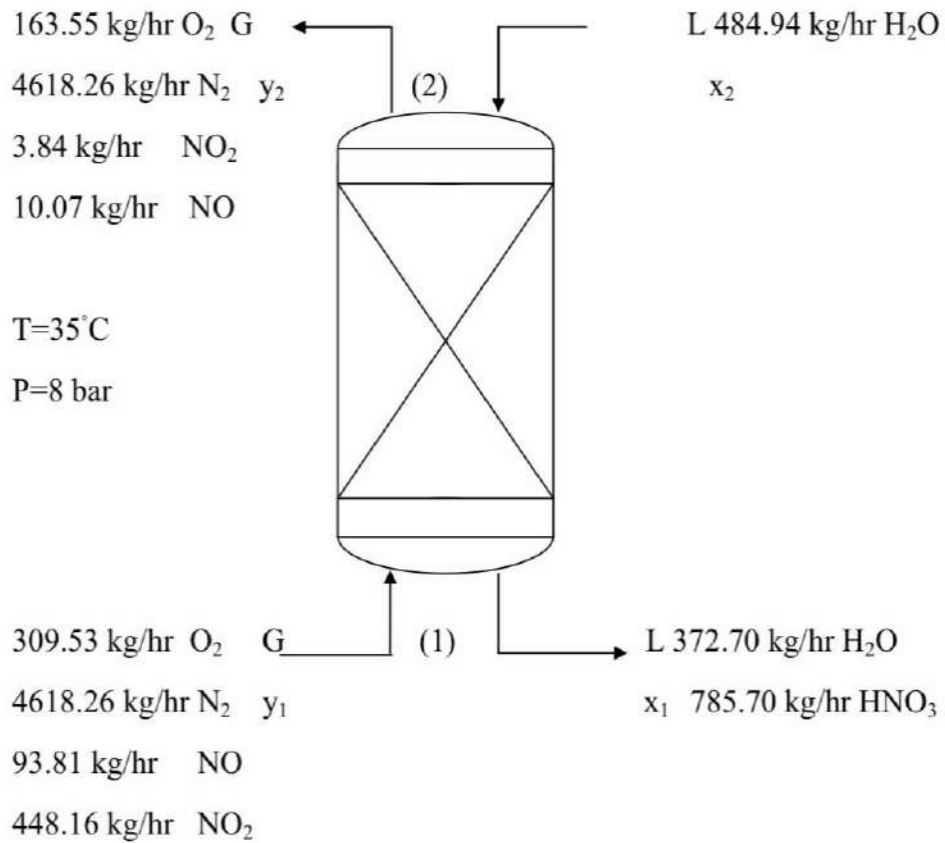
$$\text{Height of Absorber} = \text{Number of stages} \times \text{Plate spacing}$$

$$= N \times Lt$$

$$= 10 \times 0.9$$

$$= 9m$$

Mechanical Design of Absorber



Inlet gas

Component	Kg/hr	M .wt	K mol /hr	Mol% y
O ₂	309.53	32	9.673	5.16
N ₂	4618.26	28	164.938	87.98
NO	93.81	30	3.127	1.66
NO ₂	448.81	46	9.743	5.20
Total	5469.76		187.481	

Liquid density

Density of H₂O at 35 °C

$$\rho_l = 994 \text{ kg/m}^3$$

$$L = 484.94 \text{ kg/hr}$$

$$L = 0.135 \text{ kg/s}$$

$$G = 5469.76 \text{ kg/hr}$$

$$G = 1.519 \text{ kg/s}$$

$$F_{L.V} \left(\frac{0.135}{1.519} \right) \left(\frac{9.12}{994} \right)^{0.5} = 0.01$$

$$V_W^* = \left[\frac{K_4 \rho V (\rho_L - \rho V)}{13.1 F_p (\mu_L)^{0.1}} \right]^{0.5}$$

Where:

V_W^* = gas mass flow rate per unit cross – sectional area $\text{kg/m}^2 \cdot \text{s}$

K_4 = constant

μ_L = liquid viscosity $\text{kg/m} \cdot \text{s}$

F_p = packing factor .

Design pressure drop for absorber from from 15 to 50 mmH₂O /m packing

Select $\Delta p = 42 \text{ mmH}_2\text{O /Packing}$

For $F_{L.V} = 0.01$ and $\Delta P = 42 \text{ mmH}_2\text{O /m packing}$

$$K_4 = 3$$

$$F_p = 170 \text{ m}^{-1} \text{ table 11.2}$$

Viscosity of H₂O at 35°C

$$\mu_L = 0.722 \text{ } \mu_L = 0.722 * 10^{-3} \text{ kg/m} \cdot \text{s}$$

$$V_W^* = \left(\frac{3 \times 9.12(998 - 9.12)}{13.1 \times 170 \left(\frac{0.772 \times 10^{-3}}{994} \right)^{0.1}} \right)^{0.5}$$

$$= 7.052 \text{ Kg/m}^2 \cdot \text{s}$$

$$A = \frac{G}{V_W^*}$$

A = cross-sectional area of column m².

$$A = \frac{1.519}{7.052} = 0.215 \text{ m}^2$$

$$A = \frac{\pi D^2}{4}$$

$$0.215 = \frac{\pi D^2}{4}$$

$$D = 0.52 \text{ m}$$

Height of column

$$Z = \text{HOG} \cdot \text{NOG}$$

Where :

Z = height of packing m.

HOG = over all height of gas phase transfer unit m.

NOG = number of transfer unit .

HOG was obtained from table (15.4) "separation process engineering" For ceramic packing with size 2 in → HOG = 0.65 m

Absorption with chemical reaction , vapour pressure of NO₂ over the solution can be negligible .

$$P_A^* = 0$$

$$P_A^* = P_A^\circ X_A$$

$$\frac{P_A^*}{P_T} = \frac{P_A^\circ}{P_T} X_A$$

$$y^*_A = m x_A$$

$$m = \left(\frac{P_A^*}{P_T} \right) = 0 \rightarrow y^*_A = 0$$

$$\text{NOG} = \int_{y_2}^{y_1} \frac{dy}{y}$$

For absorption with chemical reaction $y^*=0$

$$\text{NOG} = \int_{y_2}^{y_1} \frac{dy}{y} = \ln \frac{y_1}{y_2}$$

$$y_1 = 0.052$$

$$y_2 = \frac{\frac{3.85}{46}}{\frac{163.55}{32} + \frac{4618.26}{28} + \frac{10.07}{30} + \frac{3.84}{46}} = 0.0005$$

$$\text{NOG} = \ln \frac{0.052}{0.0005} = 4.64$$

$$Z = (0.65) (4.64)$$

$$= 3.02 \text{ m}$$

Pipe sizing

$$d = 293 G^{0.53} \rho^{-0.37}$$

where:

d = optimum pipe diameter mm .

G = fluid mass flow rate kg/s .

ρ = fluid density kg/m³ .

inlet gases

$$G = 5469.76 \text{ kg/hr} = 1.519 \text{ kg/s}$$

$$\rho = 9.12 \text{ kg/m}^3$$

$$d = 293 (1.519)^{0.53} (9.12)^{-0.37} = 162 \text{ mm}$$

outlet gases

$$G = 4795.72 \text{ kg/hr} = 1.332 \text{ kg/s}$$

$$\rho = 8.79 \text{ kg/m}^3$$

$$d = 293 (1.332)^{0.53} (8.79)^{-0.37} = 153 \text{ mm}$$

inlet liquid

$$G = 484.94 \text{ kg/hr} = 0.135 \text{ kg/s}$$

$$\rho = 994 \text{ kg/m}^3$$

$$d = 293 (0.135)^{0.53} (994)^{-0.37} = 8 \text{ mm}$$

outlet liquid

$$G = 1158.4 \text{ kg/hr} = 0.322 \text{ kg/s}$$

$$\rho = 1390 \text{ kg/m}^3$$

$$d = 293 (0.322)^{0.53} (1390)^{-0.37} = 11 \text{ mm}$$

Mechanical design

Shell

$$e = \frac{P_i \cdot D_i}{2f - p_i} + c$$

where

e = thickness of shell mm.

P_i = Design pressure N/ mm² .

D_i = shell inside diameter mm .

f = design stress N/ mm² .

C = corrosion constant mm.

$$d = 0.52 \text{ m} = 520 \text{ mm}$$

operating pressure = 8 bar

design pressure $p_i = 1.1 * (8-1) = 7.7 \text{ atm} = 0.77 \text{ N/mm}^2$

$C = 2 \text{ mm}$

At $T = 35 \text{ }^\circ\text{C}$ design stress of high silicon iron

$f = 135 \text{ N/mm}^2$ Table 13.2

$$e = \frac{0.77 \times 520}{2 \times 135 - 0.77} + 2 = 3.48 \text{ mm}$$

Ellipsoidal head

$$e = \frac{p_i \times D_i}{2Jf - 0.2p_i}$$

where

e = thickness of ellipsoidal head mm .

J = joint factor = 0.8

$$e = \frac{0.77 \times 520}{2 \times 0.8 \times 135 - 0.2 \times 0.77} + 2 = 3.85 \text{ mm}$$

weight loads

weight of vessel (shell)

$$W_v = C_v \pi \rho_m D_m g (H_v + 0.8D_m) t \times 10^{-3}$$

W_v = total weight of shell excluding internal fitting N .

C_v = constant.

ρ_m = density of vessel material kg/m^3 .

H_v = height (length) of shell m .

D_m = mean diameter of shell m.

t = wall thickness mm

$$t = e = 3\text{mm}$$

$$C_V = 1.15$$

$$\rho_m = 7100 \text{ kg/m}^3$$

$$D_m = (D_i + t \cdot 10^{-3})$$

$$D_m = (0.52 + 3 \cdot 10^{-3}) = 0.523\text{m}$$

$$H_v = 3.02 \text{ m}$$

$$W_v = 1.15\pi \cdot 7100 \cdot 0.523 \cdot 9.81 (3.02 + 0.8 \cdot 0.523)(3 \cdot 10^{-3})$$

$$W_v = 1358 \text{ N}$$

Weight of fluid

$$W_f = v \rho g$$

Where

W_f = Weight of fluid N .

V = volume of fluid m^3 .

ρ = density of fluid kg / m^3 .

$$W_f = \frac{\pi}{4} (0.52)^2 (3.02) (7100) (9.81) = 8746 \text{ kg/m}^3$$

$W = w_v + w_f$ total weight

$$W = 1358 + 8746 = 10104 \text{ N}$$

Added 10% above total weight

$$W = 1.1 (10104) = 11114 \text{ N}$$

design of bracket support

$$F_{bs} = 60 L_c t_c$$

Where

F_{bs} = design load per bracket N.

L_c = depth of bracket mm.

t_c = thickness of plate mm.

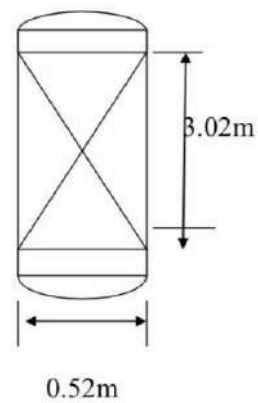
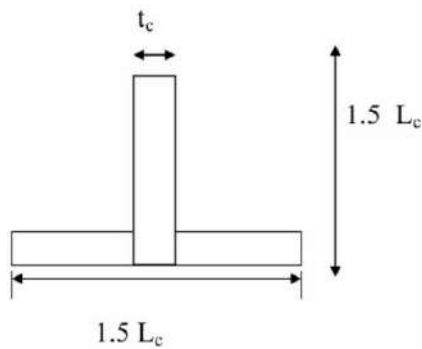
use four brackets

$$F_{bs} = \frac{11114}{4} = 2779 \text{ N}$$

Take $t_c = 3 \text{ mm}$

$$2779 = 60 * 3 L_c$$

$$L_c = 16 \text{ mm}$$



Analysis Stress (σ):

Longitudinal Stress σ_L :

$$\begin{aligned} \sigma_l &= \frac{P \times d}{4 \times 0.0338} \\ &= \frac{7.7 \times 0.52}{4 \times 0.0338} = 26 \frac{N}{m^2} \end{aligned}$$

Dean weight stress σ_w :

$$\begin{aligned} \sigma_w &= \frac{w_{total}}{\pi(D_i + e)e} \\ &= \frac{11.114}{3.14(0.52 + 0.0385)0.0385} = \frac{1.64N}{m^2} \end{aligned}$$

Bending stress σ_b :

$$\sigma_b = \pm \frac{M}{L_v} \left(\frac{d_i}{2} + e \right)$$

$$L_v = \frac{\pi}{64} \times (d_o^4 - d_i^4)$$

Where; $d_o = d_i + (2 * e) = 0.52 + (2 * 0.0385) = 0.59 \text{ m}$

$$L_v = \frac{\pi}{64} (0.59^4 - 0.52^4) = 0.118 \text{ m}$$

$$M = \frac{f_w}{2} (H_v)^2 = \frac{14378.43}{2} (7)^2 = 35227 \text{ N.m}$$

$$\sigma_b = \pm \frac{35227}{0.118} \left(\frac{0.52}{2} + 0.0385 \right) = \pm 89.1123 \text{ N/m}^2$$

$$\sigma_z(\text{downwind}) = \sigma_l - \sigma_w - \sigma_b = 26.45 \text{ N/m}^2$$

$$\sigma_z(\text{upwind}) = \sigma_l - \sigma_w - \sigma_b = 62 \text{ N/m}^2$$

Elastic Stability σ_c :

$$\sigma_c = 2 \times 10^4 \left(\frac{e}{d_o} \right) = 2 \times 10^4 \left(\frac{0.0385}{0.52} \right) = 148.07 \frac{\text{N}}{\text{m}^2}$$

Type	Packed
Length packing	3.02m
Dimeter	0.52m
Volum $= \frac{\pi D^2 L}{4}$	0.614
Temp. °C	35°C
Pressure bar	8 bar
Material of count	High silicon iron
Shell thickness	3.48mm

thickness of ellipsoidal head	3.85mm
total weight	11114N
Longitudinal Stress σ_L	26N/m ²
Dean weight stress σ_w :	1.64N/m ²
σ_z (downwind)	26.45N/m ²
σ_z (upwind)	62N/m ²
Elastic Stability σ_c ;	148.07 N/m ²
Bending stress σ_b ;	89.1123 N/m ²

Chapter 6

Conclusion

Conclusion

our exploration of nitric acid production has traversed through the fundamental principles, methodological intricacies, and design considerations essential for understanding and optimizing this vital industrial process.

Commencing with an introduction to nitric acid and its significance in various industries, we underscored the importance of efficient and sustainable production methods to meet growing demands. This laid the foundation for our comprehensive analysis of production methodologies and their associated material and energy balances.

Through meticulous material and energy balance calculations, we quantified the inputs, outputs, and energy requirements of nitric acid production, providing valuable insights into process efficiency and resource utilization. This quantitative assessment informed our subsequent design considerations and optimization efforts.

Our focus on reactor and absorber design exemplifies the intersection of theory and practice in nitric acid production. By applying engineering principles to develop efficient and reliable systems, we aimed to enhance product quality, minimize waste generation, and improve overall process performance.

In conclusion, our report encapsulates the multidimensional nature of nitric acid production, integrating theoretical insights with practical applications to address key challenges and opportunities in the field. By leveraging advances in process optimization, equipment design, and sustainability practices, we pave the way for continued innovation and improvement in nitric acid production technologies.

As we conclude this project, we recognize the ongoing imperative for research, collaboration, and knowledge exchange in advancing nitric acid production methods. By embracing interdisciplinary approaches and fostering industry partnerships, we can collectively propel the field towards greater efficiency, sustainability, and economic viability.

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Appendix

(Physical Properties Data)

Table B.1 Selected Physical Property Data^a

Compound	Formula	Mol. Wt.	SG (20°/4°)	$T_m(^{\circ}\text{C})^b$	$\Delta\hat{H}_m(T_m)^{c,d}$ kJ/mol	$T_b(^{\circ}\text{C})^e$	$\Delta\hat{H}_v(T_b)^{c,d}$ kJ/mol	$T_c(\text{K})^f$	$P_c(\text{atm})^g$	$(\Delta\hat{H}_f^{\circ})^{h,i}$ kJ/mol	$(\Delta\hat{H}_c^{\circ})^{h,i}$ kJ/mol
Acetaldehyde	CH ₃ CHO	44.05	0.783 ¹⁸	-123.7	—	20.2	25.1	461.0	—	-166.2(g)	-1192.4(g)
Acetic acid	CH ₃ COOH	60.05	1.049	16.6	12.09	118.2	24.39	594.8	57.1	-486.18(l)	-871.69(l)
Acetone	C ₃ H ₆ O	58.08	0.791	-95.0	5.69	56.0	30.2	508.0	47.0	-438.15(g)	-919.73(g)
Acetylene	C ₂ H ₂	26.04	—	—	—	-81.5	17.6	309.5	61.6	-248.2(l)	-1785.7(l)
Ammonia	NH ₃	17.03	—	-77.8	5.653	-33.43	23.351	405.5	111.3	-216.7(g)	-1821.4(g)
Ammonium hydroxide	NH ₄ OH	35.03	—	—	—	—	—	—	—	+226.75(g)	-1299.6(g)
Ammonium nitrate	NH ₄ NO ₃	80.05	1.725 ²⁵	169.6	5.4	—	—	—	—	-67.20(l)	-382.58(g)
Ammonium sulfate	(NH ₄) ₂ SO ₄	132.14	1.769	513	—	—	—	—	—	-46.19(g)	—
Aniline	C ₆ H ₅ N	93.12	1.022	-6.3	—	184.2	—	699	52.4	-365.14(c)	—
Benzaldehyde	C ₆ H ₅ CHO	106.12	1.046	-26.0	—	179.0	38.40	—	—	-399.36(aq)	—
Benzene	C ₆ H ₆	78.11	0.879	5.53	9.837	80.10	30.765	562.6	48.6	-1179.3(c)	-1173.1(aq)
Benzoic acid	C ₇ H ₆ O ₂	122.12	1.266 ¹⁵	122.2	—	249.8	—	—	—	—	—
Benzyl alcohol	C ₇ H ₈ O	108.13	1.045	-15.4	—	205.2	—	—	—	-88.83(l)	-3520.0(l)
Bromine	Br ₂	159.83	3.119	-7.4	10.8	58.6	31.0	584	102	-40.04(g)	—
1,2-Butadiene	C ₄ H ₆	54.09	—	-136.5	—	10.1	—	446	—	+48.66(l)	-3267.6(l)
1,3-Butadiene	C ₄ H ₆	54.09	—	-109.1	—	-4.6	—	425	42.7	+82.93(g)	-3301.5(g)
n-Butane	C ₄ H ₁₀	58.12	—	-138.3	4.661	-0.6	22.305	425.17	37.47	—	-3226.7(g)
Isobutane	C ₄ H ₁₀	58.12	—	-159.6	4.540	-11.73	21.292	408.1	36.0	—	-3741.8(l)
1-Butene	C ₄ H ₈	56.10	—	-185.3	3.8480	-6.25	21.916	419.6	39.7	-124.7(g)	-2878.5(g)
Calcium carbide	CaC ₂	64.10	2.22 ¹⁸	2300	—	—	—	—	—	-158.4(l)	-2849.0(l)
Calcium carbonate	CaCO ₃	100.09	2.93	—	—	—	—	—	—	-134.5(g)	-2868.8(g)
Calcium chloride	CaCl ₂	110.99	2.152 ¹⁵	782	28.37	>1600	—	—	—	+1.17(g)	-2718.6(g)
Calcium hydroxide	Ca(OH) ₂	74.10	2.24	—	—	—	—	—	—	-62.76(c)	—
Calcium oxide	CaO	56.08	3.32	2570	50	2850	—	—	—	Decomposes at 825°C	-1206.9(c)
Calcium phosphate	Ca ₃ (PO ₄) ₂	310.19	3.14	1670	—	—	—	—	—	—	—
Calcium silicate	CaSiO ₃	116.17	2.915	1530	48.62	—	—	—	—	—	—
Calcium sulfate	CaSO ₄	136.15	2.96	—	—	—	—	—	—	-1432.7(c)	—
Calcium sulfate (gypsum)	CaSO ₄ ·2H ₂ O	172.18	2.32	—	—	—	—	—	—	-1450.4(aq)	—
Carbon (graphite)	C	12.010	2.26	3600	46.0	4200	—	—	—	(-1.5 H ₂ O at 128°C)	-2021(c)
Carbon dioxide	CO ₂	44.01	—	-56.6 at 5.2 atm	8.33	(Sublimes at -78°C)	304.2	72.9	—	0(c)	-393.51(c)
Carbon disulfide	CS ₂	76.14	1.261 ^{22/20}	-112.1	4.39	46.25	26.8	552.0	78.0	-412.9(l)	—
Carbon monoxide	CO	28.01	—	-205.1	0.837	-191.5	6.042	133.0	34.5	-393.5(g)	—
Carbon tetrachloride	CCl ₄	153.84	1.595	-22.9	2.51	76.7	30.0	556.4	45.0	+87.9(l)	-1075.2(l)
Chlorine	Cl ₂	70.91	—	-101.00	6.406	-34.06	20.4	417.0	76.1	+115.3(g)	1102.6(g)
Chlorobenzene	C ₆ H ₅ Cl	112.56	1.107	-45	—	132.10	36.5	632.4	44.6	-110.52(g)	-282.99(g)
Chloroethane	C ₂ H ₅ Cl	See ethyl chloride	—	—	—	—	—	—	—	-139.5(l)	-352.2(l)

^aAdapted in part from D. M. Himmelblau, *Basic Principles and Calculations in Chemical Engineering*, 3rd Edition, ©1974, Tables D1 and F1. Adapted by permission of Prentice-Hall, Inc., Englewood Cliffs, NJ.

^bMelting point at 1 atm.

^cHeat of fusion at T_m and 1 atm.

^dBoiling point at 1 atm.

^eHeat of vaporization at T_b and 1 atm.

^fCritical temperature.

^gCritical pressure.

^hHeat of formation at 25°C and 1 atm.

ⁱHeat of combustion at 25°C and 1 atm. Standard states of products are CO₂(g), H₂O(l), SO₂(g), HCl(aq), and N₂(g). To calculate $\Delta\hat{H}_c^{\circ}$ with H₂O(g) as a product, add 44.01*n_w* to the tabulated value, where *n_w* = moles H₂O formed/mole fuel burned.

^jTo convert $\Delta\hat{H}$ to kcal/mol, divide given value by 4.184; to convert to Btu/lb-mole, multiply by 430.28.

(continued)

Table B.1 (Continued)

Compound	Formula	Mol. Wt.	SG (20°/4°)	T_m (°C) ^b	$\Delta\hat{H}_m(T_m)^{c,d}$ kJ/mol	T_b (°C) ^e	$\Delta\hat{H}_v(T_b)^{c,f}$ kJ/mol	T_c (K) ^g	P_c (atm) ^h	$(\Delta\hat{H}_v)^{g,i}$ kJ/mol	$(\Delta\hat{H}_c)^{g,j}$ kJ/mol
Chloroform	CHCl ₃	119.39	1.489	-63.7	—	61.0	—	536.0	54.0	-131.8(l)	-373(l)
Copper	Cu	63.54	8.92	1083	13.01	2595	304.6	—	—	0(c)	—
Cupric sulfate	CuSO ₄	159.61	3.606 ^{18*}	—	—	Decomposes > 600°C		—	—	-769.9(c)	—
Cyclohexane	C ₆ H ₁₂	84.16	0.779	6.7	2.677	80.7	30.1	553.7	40.4	-843.1(aq)	-3919.9(l)
Cyclopentane	C ₅ H ₁₀	70.13	0.745	-93.4	0.609	49.3	27.30	511.8	44.55	-123.1(g)	-3953.0(g)
<i>n</i> -Decane	C ₁₀ H ₂₂	142.28	0.730	-29.9	—	173.8	—	619.0	20.8	-105.9(l)	-3290.9(l)
Diethyl ether	(C ₂ H ₅) ₂ O	74.12	0.708 ^{28*}	-116.3	7.30	34.6	26.05	467	35.6	-77.2(g)	-3319.5(g)
Ethane	C ₂ H ₆	30.07	—	-183.3	2.859	-88.6	14.72	305.4	48.2	-249.7(l)	-6778.3(l)
Ethyl acetate	C ₄ H ₈ O ₂	88.10	0.901	-83.8	—	77.0	—	523.1	37.8	-6829.7(g)	-2726.7(l)
Ethyl alcohol (Ethanol)	C ₂ H ₅ OH	46.07	0.789	-114.6	5.021	78.5	38.58	516.3	63.0	-463.2(l)	-2246.4(l)
Ethyl benzene	C ₈ H ₁₀	106.16	0.867	-94.67	9.163	136.2	35.98	619.7	37.0	-426.8(g)	-1366.91(l)
Ethyl bromide	C ₂ H ₅ Br	108.98	1.460	-119.1	—	38.2	—	504	61.5	-277.63(l)	-2726.7(l)
Ethyl chloride	C ₂ H ₅ Cl	64.52	0.903 ^{15*}	-138.3	4.452	13.1	24.7	460.4	52.0	-235.31(g)	-1409.25(g)
3-Ethylhexane	C ₈ H ₁₈	114.22	0.717	—	—	118.5	34.27	567.0	26.4	-12.46(l)	-4564.9(l)
Ethylene	C ₂ H ₄	28.05	—	-169.2	3.350	-103.7	13.54	283.1	50.5	+29.79(g)	-4607.1(g)
Ethylene glycol	C ₂ H ₄ O ₂	62.07	1.113 ^{19*}	-13	11.23	197.2	56.9	—	—	-54.4(g)	—
Ferrie oxide	Fe ₂ O ₃	159.70	5.12	—	—	Decomposes at 1560°C		—	—	-822.2(c)	—
Ferrous oxide	FeO	71.85	5.7	—	—	—	—	—	—	-1409.25(g)	—
Ferrous sulfide	FeS	87.92	4.84	1193	—	—	—	—	—	-266.5(c)	—
Formaldehyde	H ₂ CO	30.03	0.815 ^{20*}	-92	—	-19.3	24.48	—	—	-95.1(c)	—
Formic acid	CH ₂ O ₂	46.03	1.220	8.30	12.68	100.5	22.25	—	—	-115.90(g)	-563.46(g)
Glycerol	C ₃ H ₈ O ₃	92.09	1.260 ^{20*}	18.20	18.30	290.0	—	—	—	-409.2(l)	-262.8(l)
Helium	He	4.00	—	-269.7	0.02	-268.9	0.084	5.26	2.26	-362.6(g)	-1661.1(l)
<i>n</i> -Heptane	C ₇ H ₁₆	100.20	0.684	-90.59	14.03	98.43	31.69	540.2	27.0	-115.90(g)	-563.46(g)
<i>n</i> -Hexane	C ₆ H ₁₄	86.17	0.659	-95.32	13.03	68.74	28.85	507.9	29.9	-4816.9(l)	-4853.5(g)
Hydrogen	H ₂	2.016	—	-259.19	0.12	-252.76	0.904	33.3	12.8	-198.8(l)	-4163.1(l)
Hydrogen bromide	HBr	80.92	—	-86	—	-67	—	—	—	-167.2(g)	-4194.8(g)
Hydrogen chloride	HCl	36.47	—	-114.2	1.99	-85.0	16.1	324.6	81.5	0(g)	-285.84(g)
Hydrogen cyanide	HCN	27.03	—	-14	—	26	—	—	—	+130.54(g)	—
Hydrogen fluoride	HF	20.0	—	-83	—	20	—	503.2	—	-268.6(g)	—
Hydrogen sulfide	H ₂ S	34.08	—	-85.5	2.38	-60.3	18.67	373.6	88.9	-316.9(aq, 200)	—
Iodine	I ₂	253.8	4.93	113.3	—	184.2	—	826.0	—	-19.96(g)	-562.59(g)
Iron	Fe	55.85	7.7	1535	15.1	2800	354.0	—	—	0(c)	—
Lead	Pb	207.21	11.337 ^{20*} / ^{20*}	327.4	5.10	1750	179.9	—	—	0(c)	—
Lead oxide	PbO	223.21	9.5	886	11.7	1472	213	—	—	-219.2(c)	—
Magnesium	Mg	24.32	1.74	650	9.2	1120	131.8	—	—	0(c)	—
Magnesium chloride	MgCl ₂	95.23	2.325 ^{25*}	714	43.1	1418	136.8	—	—	-641.8(c)	—
Magnesium hydroxide	Mg(OH) ₂	58.34	2.4	—	—	Decomposes at 350°C		—	—	—	—
Magnesium oxide	MgO	40.32	3.65	2900	77.4	3600	—	—	—	-601.8(c)	—
Mercury	Hg	200.61	13.546	-38.87	—	-356.9	—	—	—	0(c)	—
Methane	CH ₄	16.04	—	-182.5	0.94	-161.5	8.179	190.70	45.8	-74.85(g)	-890.36(g)
Methyl acetate	C ₃ H ₆ O ₂	74.08	0.933	-98.9	—	57.1	—	506.7	46.30	-409.4(l)	-1595(l)
Methyl alcohol (Methanol)	CH ₃ OH	32.04	0.792	-97.9	3.167	64.7	35.27	513.20	78.50	-238.6(l)	726.6(l)
Methyl amine	CH ₃ N	31.06	0.699 ^{11*}	-92.7	—	-6.9	—	429.9	73.60	-201.2(g)	-764.0(g)
Methyl chloride	CH ₃ Cl	50.49	—	-97.9	—	-24	—	416.1	65.80	-28.0(g)	-1071.5(l)

(continued)

Table B.1 (Continued)

Compound	Formula	Mol. Wt.	SG (20/4°)	$T_m(^{\circ}\text{C})^a$	$\Delta\hat{H}_m(T_m)^{b,d}$ kJ/mol	$T_b(^{\circ}\text{C})^c$	$\Delta\hat{H}_v(T_b)^{e,f}$ kJ/mol	$T_c(\text{K})^g$	$P_c(\text{atm})^h$	$(\Delta\hat{H}_f^{\circ})^{i,j}$ kJ/mol	$(\Delta\hat{H}_f^{\circ})^{k,l}$ kJ/mol
Methyl ethyl ketone	$\text{C}_4\text{H}_8\text{O}$	72.10	0.805	-87.1	—	78.2	32.0	—	—	—	-2436(l)
Naphthalene	C_{10}H_8	128.16	1.145	80.0	—	217.8	—	—	—	—	-5157(g)
Nickel	Ni	58.69	8.90	1452	—	2900	—	—	—	0(c)	—
Nitric acid	HNO_3	63.02	1.502	-41.6	10.47	86	30.30	—	—	-173.23(l)	—
										-206.57(aq)	—
Nitrobenzene	$\text{C}_6\text{H}_5\text{O}_2\text{N}$	123.11	1.203	5.5	—	210.7	—	—	—	—	-3092.8(l)
Nitrogen	N_2	28.02	—	-210.0	0.720	-195.8	5.577	126.20	33.5	0(g)	—
Nitrogen dioxide	NO_2	46.01	—	-9.3	7.335	21.3	14.73	431.0	100.0	+33.8(g)	—
Nitric oxide	NO	30.01	—	-163.6	2.301	-151.8	13.78	179.20	65.0	+90.37(g)	—
Nitrogen pentoxide	N_2O_5	108.02	1.63 ^{18f}	30	—	47	—	—	—	—	—
Nitrogen tetraoxide	N_2O_4	92.0	1.448	-9.5	—	21.1	—	431.0	99.0	+9.3(g)	—
Nitrous oxide	N_2O	44.02	1.226 ^{-89f}	-91.1	—	-88.8	—	309.5	71.70	+81.5(g)	—
<i>n</i> -Nonane	C_9H_{20}	128.25	0.718	-53.8	—	150.6	—	595	23.0	-229.0(l)	-6124.5(l)
										—	-6171.0(g)
<i>n</i> -Octane	C_8H_{18}	114.22	0.703	-57.0	—	125.5	—	568.8	24.5	-249.9(l)	-5470.7(l)
										-208.4(g)	-5512.2(g)
										-826.8(c)	-251.9(s)
Oxalic acid	$\text{C}_2\text{H}_2\text{O}_4$	90.04	1.90	—	Decomposes at 186°C			—	—	—	—
Oxygen	O_2	32.00	—	-218.75	0.444	-182.97	6.82	154.4	49.7	0(g)	—
<i>n</i> -Pentane	C_5H_{12}	72.15	0.63 ^{18f}	-129.6	8.393	36.07	25.77	469.80	33.3	-173.0(l)	-3509.5(l)
										-146.4(g)	-3536.1(g)
Isopentane	C_5H_{12}	72.15	0.62 ^{19f}	-160.1	—	27.7	—	461.00	32.9	-179.3(l)	-3507.5(l)
										-152.0(g)	-3529.2(g)
1-Pentene	C_5H_{10}	70.13	0.641	-165.2	4.94	29.97	—	474	39.9	-20.9(g)	-3375.8(g)
Phenol	$\text{C}_6\text{H}_5\text{OH}$	94.11	1.071 ^{23f}	42.5	11.43	181.4	—	692.1	60.5	-158.1(l)	-3063.5(s)
										—	-90.8(g)
Phosphoric acid	H_3PO_4	98.00	1.834 ^{18f}	42.3	10.54	(-½H ₂ O at 213°C)	—	—	—	-1281.1(c)	—
										-1278.6(aq, 1H ₂ O)	—
Phosphorus (red)	P ₄	123.90	2.20	590 ^{43 atm}	81.17	Ignites in air, 725°C	—	—	—	-17.6(c)	—
										0(c)	—
Phosphorus (white)	P ₄	123.90	1.82	44.2	2.51	280	49.71	—	—	—	—
Phosphorus pentoxide	P ₂ O ₅	141.95	2.387	—	Sublimes at 250°C			—	—	-1506.2(c)	—
Propane	C_3H_8	44.09	—	-187.69	3.52	-42.07	18.77	369.9	42.0	-119.8(l)	-2334.0(l)
										-103.8(g)	-2720.0(g)
Propylene	C_3H_6	42.08	—	-185.2	3.00	-47.70	18.42	365.1	45.4	+20.41(g)	-2058.4(g)
<i>n</i> -Propyl alcohol	$\text{C}_3\text{H}_7\text{OH}$	60.09	0.804	-127	—	97.04	—	536.7	49.95	-300.70(l)	-2010.4(l)
										-255.2(g)	-2068.6(g)
Isopropyl alcohol	$\text{C}_3\text{H}_7\text{OH}$	60.09	0.785	-89.7	—	82.24	—	508.8	53.0	-310.9(l)	-1986.6(l)
<i>n</i> -Propyl benzene	C_9H_{12}	120.19	0.862	-99.50	8.54	159.2	38.24	638.7	31.3	-38.40(l)	-5218.2(l)
										+7.82(g)	-5264.48(g)
Silicon dioxide	SiO ₂	60.09	2.25	1710	14.2	2230	—	—	—	-851.0(c)	—
Sodium bicarbonate	NaHCO ₃	84.01	2.20	—	Decomposes at 270°C			—	—	-945.6(c)	—
Sodium bisulfate	NaHSO ₄	120.07	2.742	—	—	—	—	—	—	-1126.3(c)	—
Sodium carbonate	Na ₂ CO ₃	105.99	2.533	—	Decomposes at 854°C			—	—	-1130.9(c)	—
Sodium chloride	NaCl	58.45	2.163	808	28.5	1465	170.7	—	—	-411.0(c)	—
Sodium cyanide	NaCN	49.01	—	562	16.7	1497	155	—	—	-89.79(c)	—
Sodium hydroxide	NaOH	40.00	2.130	319	8.34	1390	—	—	—	-426.6(c)	—
										-469.4(aq)	—
Sodium nitrate	NaNO ₃	85.00	2.257	310	15.9	Decomposes at 381°C	—	—	—	-466.7(c)	—
Sodium nitrite	NaNO ₂	69.00	2.168 ^{6f}	271	—	Decomposes at 321°C	—	—	—	-359.4(c)	—
Sodium sulfate	Na ₂ SO ₄	142.05	2.698	880	24.3	—	—	—	—	-1384.5(c)	—
Sodium sulfide	Na ₂ S	78.05	1.856	950	6.7	—	—	—	—	-373.2(c)	—
Sodium sulfite	Na ₂ SO ₃	126.05	2.633 ^{18f}	—	Decomposes			—	—	-1090.3(c)	—

(continued)

Table B.1 (Continued)

Compound	Formula	Mol. Wt.	SG (20°/4°)	$T_m(^{\circ}\text{C})^b$	$\Delta\hat{H}_m(T_m)^{c,j}$ kJ/mol	$T_b(^{\circ}\text{C})^d$	$\Delta\hat{H}_v(T_b)^{c,j}$ kJ/mol	$T_c(\text{K})^f$	$P_c(\text{atm})^g$	$(\Delta\hat{H}_f^{\circ})^{h,j}$ kJ/mol	$(\Delta\hat{H}_f^{\circ})^{i,j}$ kJ/mol
Sodium thiosulfate	$\text{Na}_2\text{S}_2\text{O}_3$	158.11	1.667	—	—	—	—	—	—	-1117.1(c)	—
Sulfur (rhombic)	S_8	256.53	2.07	113	10.04	444.6	83.7	—	—	0(c)	—
Sulfur (monoclinic)	S_8	256.53	1.96	119	14.17	444.6	83.7	—	—	+0.30(c)	—
Sulfur dioxide	SO_2	64.07	—	-75.48	7.402	-10.02	24.91	430.7	77.8	-296.90(g)	—
Sulfur trioxide	SO_3	80.07	—	16.84	25.48	43.3	41.80	491.4	83.8	-395.18(g)	—
Sulfuric acid	H_2SO_4	98.08	1.834 ^{8f}	10.35	9.87	Decomposes at 340°C		—	—	-811.32(l) -907.51(aq)	—
Toluene	C_7H_8	92.13	0.866	-94.99	6.619	110.62	33.47	593.9	40.3	+12.00(l) +30.00(g)	-3909.9(l) -3947.9(g)
Water	H_2O	18.016	1.00 ^{8f}	0.00	6.0095	100.00	40.656	647.4	218.3	-285.84(l) -241.83(g)	—
<i>m</i> -Xylene	C_8H_{10}	106.16	0.864	-47.87	11.569	139.10	36.40	619	34.6	-25.42(l) +17.24(g)	-4551.9(l) -4594.5(g)
<i>o</i> -Xylene	C_8H_{10}	106.16	0.880	-25.18	13.598	144.42	36.82	631.5	35.7	-24.44(l) +18.99(g)	-4552.9(l) -4596.3(g)
<i>p</i> -Xylene	C_8H_{10}	106.16	0.861	13.26	17.11	138.35	36.07	618	33.9	-24.43(l) 17.95(g)	-4552.91(l) -4595.2(g)
Zinc	Zn	65.38	7.140	419.5	6.674	907	114.77	—	—	0(c)	—



Table B.2 Heat Capacities*

Form 1: C_p [kJ/(mol·°C)] or [kJ/(mol·K)] = $a + bT + cT^2 + dT^3$
 Form 2: C_p [kJ/(mol·°C)] or [kJ/(mol·K)] = $a + bT + cT^{-2}$

Example: $(C_p)_{\text{acetone(g)}} = 0.07196 + (20.10 \times 10^{-5})T - (12.78 \times 10^{-8})T^2 + (34.76 \times 10^{-12})T^3$, where T is in °C.

Note: The formulas for gases are strictly applicable at pressures low enough for the ideal gas equation of state to apply.

Compound	Formula	Mol. Wt.	State	Form	Temp. Unit	$a \times 10^3$	$b \times 10^5$	$c \times 10^8$	$d \times 10^{12}$	Range (Units of T)
Acetone	CH ₃ COCH ₃	58.08	l	1	°C	123.0	18.6			-30-60
					K	71.96	20.10	-12.78	34.76	0-1200
Acetylene	C ₂ H ₂	26.04	g	1	°C	42.43	6.053	-5.033	18.20	0-1200
					K	28.94	0.4147	0.3191	-1.965	0-1500
Air		29.0	g	1	°C	28.09	0.1965	0.4799	-1.965	273-1800
					K	35.15	2.954	0.4421	-6.686	0-1200
Ammonia	NH ₃	17.03	g	1	°C	215.9				273-328
Ammonium sulfate	(NH ₄) ₂ SO ₄	132.15	c	1	K	126.5	23.4			6-67
Benzene	C ₆ H ₆	78.11	l	1	°C	74.06	32.95	-25.20	77.57	0-1200
					K	89.46	30.13	-18.91	49.87	0-1200
Isobutane	C ₄ H ₁₀	58.12	g	1	°C	92.30	27.88	-15.47	34.98	0-1200
n-Butane	C ₄ H ₁₀	58.12	g	1	°C	82.88	25.64	-17.27	50.50	0-1200
Isobutene	C ₄ H ₈	56.10	g	1	°C	68.62	1.19	-8.66 × 10 ¹⁰		298-720
Carbon carbide	CaC ₂	64.10	c	2	K	82.34	4.975	-12.87 × 10 ¹⁰		273-1033
Calcium carbonate	CaCO ₃	100.09	c	2	K	89.5				276-373
Calcium hydroxide	Ca(OH) ₂	74.10	c	1	K	41.84	2.03	-4.52 × 10 ¹⁰		273-1173
Calcium oxide	CaO	56.08	c	2	K	11.18	1.095	-4.891 × 10 ¹⁰		273-1373
Carbon	C	12.01	c	2	K	36.11	4.233	-2.887	7.464	0-1500
Carbon dioxide	CO ₂	44.01	g	1	°C	28.95	0.4110	0.3548	-2.220	0-1500
Carbon monoxide	CO	28.01	g	1	°C	93.39	12.98			273-343
Carbon tetrachloride	CCl ₄	153.84	l	1	K	33.60	1.367	-1.607	6.473	0-1200
Chlorine	Cl ₂	70.91	g	1	°C	22.76	0.6117			273-1357
Copper	Cu	63.54	c	1	K					

*Adapted in part from D. M. Himmelblau, *Basic Principles and Calculations in Chemical Engineering*, 3rd Edition, © 1974, Table E.1. Adapted by permission of Prentice-Hall, Inc., Englewood Cliffs, NJ.

(continued)

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Table B.2 (Continued)

Compound	Formula	Mol. Wt.	State	Form	Temp. Unit	$a \times 10^3$	$b \times 10^5$	$c \times 10^8$	$d \times 10^{12}$	Range (Units of T)
Cumene (Isopropyl benzene)	C ₉ H ₁₂	120.19	g	1	°C	139.2	53.76	-39.79	120.5	0-1200
					K					
Cyclohexane	C ₆ H ₁₂	84.16	g	1	°C	94.140	49.62	-31.90	80.63	0-1200
Cyclopentane	C ₅ H ₁₀	70.13	g	1	°C	73.39	39.28	-25.54	68.66	0-1200
Ethane	C ₂ H ₆	30.07	g	1	°C	49.37	13.92	-5.816	7.280	0-1200
Ethyl alcohol (Ethanol)	C ₂ H ₅ OH	46.07	l	1	°C	103.1				0
					K	158.8				100
Ethylene	C ₂ H ₄	28.05	g	1	°C	61.34	15.72	-8.749	19.83	0-1200
					K	+40.75	11.47	-6.891	17.66	0-1200
Ferric oxide	Fe ₂ O ₃	159.70	c	2	K	103.4	6.711	-17.72 × 10 ¹⁰		273-1097
Formaldehyde	CH ₂ O	30.03	g	1	°C	34.28	4.268	0.0000	-8.694	0-1200
Helium	He	4.00	g	1	°C	20.8				0-1200
n-Hexane	C ₆ H ₁₄	86.17	l	1	°C	216.3				20-100
					K	137.44	40.85	-23.92	57.66	0-1200
Hydrogen	H ₂	2.016	g	1	°C	28.84	0.00765	0.3288	-0.8698	0-1500
Hydrogen bromide	HBr	80.92	g	1	°C	29.10	-0.0227	0.9887	-4.858	0-1200
Hydrogen chloride	HCl	36.47	g	1	°C	29.13	-0.1341	0.9715	-4.335	0-1200
Hydrogen cyanide	HCN	27.03	g	1	°C	35.3	2.908	1.092		0-1200
Hydrogen sulfide	H ₂ S	34.08	g	1	°C	33.51	1.547	0.3012	-3.292	0-1500
Magnesium chloride	MgCl ₂	95.23	c	1	K	72.4	1.58			273-991
Magnesium oxide	MgO	40.32	c	2	K	45.44	0.5008	-8.732 × 10 ¹⁰		273-2073
Methane	CH ₄	16.04	g	1	°C	34.31	5.469	0.3661	-11.00	0-1200
					K	19.87	5.021	1.268	-11.00	273-1500
Methyl alcohol (Methanol)	CH ₃ OH	32.04	l	1	°C	75.86	16.83			0-65
					K	42.93	8.301	-1.87	-8.03	0-700
Methyl cyclohexane	C ₇ H ₁₄	98.18	g	1	°C	121.3	56.53	-37.72	100.8	0-1200
Methyl cyclopentane	C ₆ H ₁₂	84.16	g	1	°C	98.83	45.857	-30.44	83.81	0-1200
Nitric acid	HNO ₃	63.02	l	1	°C	110.0				25
Nitric oxide	NO	30.01	g	1	°C	29.50	0.8188	-0.2925	0.3652	0-3500

Table B.2 (Continued)

Compound	Formula	Mol. Wt.	State	Form	Temp. Unit	$a \times 10^3$	$b \times 10^5$	$c \times 10^8$	$d \times 10^{12}$	Range (Units of T)
Cumene (Isopropyl benzene)	C ₉ H ₁₂	120.19	g	1	°C	139.2	53.76	-39.79	120.5	0-1200
Cyclohexane	C ₆ H ₁₂	84.16	g	1	°C	94.140	49.62	-31.90	80.63	0-1200
Cyclopentane	C ₅ H ₁₀	70.13	g	1	°C	73.39	39.28	-25.54	68.66	0-1200
Ethane	C ₂ H ₆	30.07	g	1	°C	49.37	13.92	-5.816	7.280	0-1200
Ethyl alcohol (Ethanol)	C ₂ H ₅ OH	46.07	l	1	°C	103.1				0
			l	1	°C	158.8				100
			g	1	°C	61.34	15.72	-8.749	19.83	0-1200
Ethylene	C ₂ H ₄	28.05	g	1	°C	+40.75	11.47	-6.891	17.66	0-1200
Ferric oxide	Fe ₂ O ₃	159.70	c	2	K	103.4	6.711	-17.72 × 10 ¹⁰	—	273-1097
Formaldehyde	CH ₂ O	30.03	g	1	°C	34.28	4.268	0.0000	-8.694	0-1200
Helium	He	4.00	g	1	°C	20.8				0-1200
<i>n</i> -Hexane	C ₆ H ₁₄	86.17	l	1	°C	216.3				20-100
			g	1	°C	137.44	40.85	-23.92	57.66	0-1200
Hydrogen	H ₂	2.016	g	1	°C	28.84	0.00765	0.3288	-0.8698	0-1500
Hydrogen bromide	HBr	80.92	g	1	°C	29.10	-0.0227	0.9887	-4.858	0-1200
Hydrogen chloride	HCl	36.47	g	1	°C	29.13	-0.1341	0.9715	-4.335	0-1200
Hydrogen cyanide	HCN	27.03	g	1	°C	35.3	2.908	1.092		0-1200
Hydrogen sulfide	H ₂ S	34.08	g	1	°C	33.51	1.547	0.3012	-3.292	0-1500
Magnesium chloride	MgCl ₂	95.23	c	1	K	72.4	1.58			273-991
Magnesium oxide	MgO	40.32	c	2	K	45.44	0.5008	-8.732 × 10 ¹⁰		273-2073
Methane	CH ₄	16.04	g	1	°C	34.31	5.469	0.3661	-11.00	0-1200
			g	1	K	19.87	5.021	1.268	-11.00	273-1500
Methyl alcohol (Methanol)	CH ₃ OH	32.04	l	1	°C	75.86	16.83			0-65
			g	1	°C	42.93	8.301	-1.87	-8.03	0-700
Methyl cyclohexane	C ₇ H ₁₄	98.18	g	1	°C	121.3	56.53	-37.72	100.8	0-1200
Methyl cyclopentane	C ₆ H ₁₂	84.16	g	1	°C	98.83	45.857	-30.44	83.81	0-1200
Nitric acid	HNO ₃	63.02	l	1	°C	110.0				25
Nitric oxide	NO	30.01	g	1	°C	29.50	0.8188	-0.2925	0.3652	0-3500
Nitrogen	N ₂	28.02	g	1	°C	29.00	0.2199	0.5723	-2.871	0-1500
Nitrogen dioxide	NO ₂	46.01	g	1	°C	36.07	3.97	-2.88	7.87	0-1200
Nitrogen tetraoxide	N ₂ O ₄	92.02	g	1	°C	75.7	12.5	-11.3		0-300
Nitrous oxide	N ₂ O	44.02	g	1	°C	37.66	4.151	-2.694	10.57	0-1200
Oxygen	O ₂	32.00	g	1	°C	29.10	1.158	-0.6076	1.311	0-1500
<i>n</i> -Pentane	C ₅ H ₁₂	72.15	l	1	°C	155.4	43.68			0-36
			g	1	°C	114.8	34.09	-18.99	42.26	0-1200
Propane	C ₃ H ₈	44.09	g	1	°C	68.032	22.59	-13.11	31.71	0-1200
Propylene	C ₃ H ₆	42.08	g	1	°C	59.580	17.71	-10.17	24.60	0-1200
Sodium carbonate	Na ₂ CO ₃	105.99	c	1	K	121				288-371
Sodium carbonate decahydrate	Na ₂ CO ₃ · 10H ₂ O	286.15	c	1	K	535.6				298
Sulfur	S	32.07	c	1	K	15.2	2.68			273-368
			(Rhombic)							
			c	1	K	18.3	1.84			368-392
			(Monoclinic)							
Sulfuric acid	H ₂ SO ₄	98.08	l	1	°C	139.1	15.59			10-45
Sulfur dioxide	SO ₂	64.07	g	1	°C	38.91	3.904	-3.104	8.606	0-1500
Sulfur trioxide	SO ₃	80.07	g	1	°C	48.50	9.188	-8.540	32.40	0-1000
Toluene	C ₇ H ₈	92.13	l	1	°C	148.8	32.4			0-110
			g	1	°C	94.18	38.00	-27.86	80.33	0-1200
Water	H ₂ O	18.016	l	1	°C	75.4				0-100
			g	1	°C	33.46	0.6880	0.7604	-3.593	0-1500

Table B.4 Antoine Equation Constants^a

$$\log_{10} p^* = A - \frac{B}{T + C} \quad p^* \text{ in mm Hg, } T \text{ in } ^\circ\text{C}$$

Example: The vapor pressure of acetaldehyde at 25°C is determined as follows:

$$\log_{10} p_{\text{C}_2\text{H}_4\text{O}}^*(25^\circ\text{C}) = 8.00552 - \frac{1600.017}{25 + 291.809} = 2.9551$$

$$\Rightarrow p_{\text{C}_2\text{H}_4\text{O}}^*(25^\circ\text{C}) = 10^{2.9551} = 902 \text{ mm Hg}$$

Compound	Formula	Range (°C)	A	B	C
Acetaldehyde	C ₂ H ₄ O	-0.2 to 34.4	8.00552	1600.017	291.809
Acetic acid	C ₂ H ₄ O ₂	29.8 to 126.5	7.38782	1533.313	222.309
Acetic acid*	C ₂ H ₄ O ₂	0 to 36	7.18807	1416.7	225
Acetic anhydride	C ₄ H ₆ O ₃	62.8 to 139.4	7.14948	1444.718	199.817
Acetone	C ₃ H ₆ O	-12.9 to 55.3	7.11714	1210.595	229.664
Acrylic acid	C ₃ H ₄ O ₂	20.0 to 70.0	5.65204	648.629	154.683
Ammonia*	NH ₃	-83 to 60	7.55466	1002.711	247.885
Aniline	C ₆ H ₇ N	102.6 to 185.2	7.32010	1731.515	206.049
Benzene	C ₆ H ₆	14.5 to 80.9	6.89272	1203.531	219.888
n-Butane	n-C ₄ H ₁₀	-78.0 to -0.3	6.82485	943.453	239.711
i-Butane	i-C ₄ H ₁₀	-85.1 to -11.6	6.78866	899.617	241.942
1-Butanol	C ₄ H ₁₀ O	89.2 to 125.7	7.36366	1305.198	173.427
2-Butanol	C ₄ H ₁₀ O	72.4 to 107.1	7.20131	1157.000	168.279
1-Butene	C ₄ H ₈	-77.5 to -3.7	6.53101	810.261	228.066
Butyric acid	C ₄ H ₈ O ₂	20.0 to 150.0	8.71019	2433.014	255.189
Carbon disulfide	CS ₂	3.6 to 79.9	6.94279	1169.110	241.593
Carbon tetrachloride	CCl ₄	14.1 to 76.0	6.87926	1212.021	226.409
Chlorobenzene	C ₆ H ₅ Cl	62.0 to 131.7	6.97808	1431.053	217.550
Chlorobenzene*	C ₆ H ₅ Cl	0 to 42	7.10690	1500.0	224.0
Chlorobenzene*	C ₆ H ₅ Cl	42 to 230	6.94504	1413.12	216.0
Chloroform	CHCl ₃	-10.4 to 60.3	6.95465	1170.966	226.232
Chloroform*	CHCl ₃	-30 to 150	6.90328	1163.03	227.4
Cyclohexane	C ₆ H ₁₂	19.9 to 81.6	6.84941	1206.001	223.148
Cyclohexanol	C ₆ H ₁₂ O	93.7 to 160.7	6.25530	912.866	109.126
n-Decane	n-C ₁₀ H ₂₂	94.5 to 175.1	6.95707	1503.568	194.738
1-Decene	C ₁₀ H ₂₀	86.8 to 171.6	6.95433	1497.527	197.056
1,1-Dichloroethane	C ₂ H ₄ Cl ₂	-38.8 to 17.6	6.97702	1174.022	229.060
1,2-Dichloroethane	C ₂ H ₄ Cl ₂	-30.8 to 99.4	7.02530	1271.254	222.927
Dichloromethane	CH ₂ Cl ₂	-40.0 to 40	7.40916	1325.938	252.616
Diethyl ether	C ₄ H ₁₀ O	-60.8 to 19.9	6.92032	1064.066	228.799
Diethyl ketone	C ₅ H ₁₀ O	56.5 to 111.3	7.02529	1310.281	214.192
Diethylene glycol	C ₄ H ₁₀ O ₂	130.0 to 243.0	7.63666	1939.359	162.714
Dimethyl ether	C ₂ H ₆ O	-78.2 to -24.9	6.97603	889.264	241.957
Dimethylamine	C ₂ H ₇ N	-71.8 to 6.9	7.08212	960.242	221.667
N,N-Dimethylformamide	C ₃ H ₇ NO	30.0 to 90.0	6.92796	1400.869	196.434
1,4-Dioxane	C ₆ H ₈ O ₂	20.0 to 105.0	7.43155	1554.679	240.337
Ethanol	C ₂ H ₅ O	19.6 to 93.4	8.11220	1592.864	226.184
Ethanolamine	C ₂ H ₇ NO	65.4 to 170.9	7.45680	1577.670	173.368
Ethyl acetate	C ₄ H ₈ O ₂	15.6 to 75.8	7.10179	1244.951	217.881
Ethyl acetate*	C ₄ H ₈ O ₂	-20 to 150	7.09808	1238.710	217.0
Ethyl chloride	C ₂ H ₅ Cl	-55.9 to 12.5	6.98647	1030.007	238.612
Ethylbenzene	C ₈ H ₁₀	56.5 to 137.1	6.95650	1423.543	213.091

^aAdapted from T. Boublik, V. Fried, and E. Hala, *The Vapour Pressures of Pure Substances*, Elsevier, Amsterdam, 1973. If marked with an asterisk (*), constants are from *Lange's Handbook of Chemistry*, 9th Edition, Handbook Publishers, Inc., Sandusky, OH, 1956.

(continued)

Table B.4 (Continued)

Compound	Formula	Range (°C)	A	B	C
Ethylene glycol	C ₂ H ₆ O ₂	50.0 to 200.0	8.09083	2088.936	203.454
Ethylene oxide	C ₂ H ₄ O	0.3 to 31.8	8.69016	2005.779	334.765
1,2-Ethylenediamine	C ₂ H ₈ N ₂	26.5 to 117.4	7.16871	1336.235	194.366
Formaldehyde	HCHO	-109.4 to -22.3	7.19578	970.595	244.124
Formic acid	CH ₂ O ₂	37.4 to 100.7	7.58178	1699.173	260.714
Glycerol	C ₃ H ₈ O ₃	183.3 to 260.4	6.16501	1036.056	28.097
<i>n</i> -Heptane	<i>n</i> -C ₇ H ₁₆	25.9 to 99.3	6.90253	1267.828	216.823
<i>i</i> -Heptane	<i>i</i> -C ₇ H ₁₆	18.5 to 90.9	6.87689	1238.122	219.783
1-Heptene	C ₇ H ₁₄	21.6 to 94.5	6.91381	1265.120	220.051
<i>n</i> -Hexane	<i>n</i> -C ₆ H ₁₄	13.0 to 69.5	6.88555	1175.817	224.867
<i>i</i> -Hexane	<i>i</i> -C ₆ H ₁₄	12.8 to 61.1	6.86839	1151.401	228.477
1-Hexene	C ₆ H ₁₂	15.9 to 64.3	6.86880	1154.646	226.046
Hydrogen Cyanide	HCN	-16.4 to 46.2	7.52823	1329.49	260.418
Methanol	CH ₃ OH	14.9 to 83.7	8.08097	1582.271	239.726
Methanol*	CH ₃ OH	-20 to 140	7.87863	1473.11	230.0
Methyl acetate	C ₃ H ₆ O ₂	1.8 to 55.8	7.06524	1157.630	219.726
Methyl bromide	CH ₃ Br	-70.0 to 3.6	7.09084	1046.066	244.914
Methyl chloride	CH ₃ Cl	-75.0 to 5.0	7.09349	948.582	249.336
Methyl ethyl ketone	C ₄ H ₈ O	42.8 to 88.4	7.06356	1261.339	221.969
Methyl isobutyl ketone	C ₆ H ₁₂ O	21.7 to 116.2	6.67272	1168.408	191.944
Methyl methacrylate	C ₅ H ₈ O ₂	39.2 to 89.2	8.40919	2050.467	274.369
Methylamine	CH ₃ N	-83.1 to -6.2	7.33690	1011.532	233.286
Methylcyclohexane	C ₇ H ₁₄	25.6 to 101.8	6.82827	1273.673	221.723
Naphthalene	C ₁₀ H ₈	80.3 to 179.5	7.03358	1756.328	204.842
Nitrobenzene	C ₆ H ₅ NO ₂	134.1 to 210.6	7.11562	1746.586	201.783
Nitromethane	CH ₃ NO ₂	55.7 to 136.4	7.28166	1446.937	227.600
<i>n</i> -Nonane	<i>n</i> -C ₉ H ₂₀	70.3 to 151.8	6.93764	1430.459	201.808
1-Nonene	C ₉ H ₁₈	66.6 to 147.9	6.95777	1437.862	205.814
<i>n</i> -Octane	<i>n</i> -C ₈ H ₁₈	52.9 to 126.6	6.91874	1351.756	209.100
<i>i</i> -Octane	<i>i</i> -C ₈ H ₁₈	41.7 to 118.5	6.88814	1319.529	211.625
1-Octene	C ₈ H ₁₆	44.9 to 122.2	6.93637	1355.779	213.022
<i>n</i> -Pentane	<i>n</i> -C ₅ H ₁₂	13.3 to 36.8	6.84471	1060.793	231.541
<i>i</i> -Pentane	<i>i</i> -C ₅ H ₁₂	16.3 to 28.6	6.73457	992.019	229.564
1-Pentanol	C ₅ H ₁₂ O	74.7 to 156.0	7.18246	1287.625	161.330
1-Pentene	C ₅ H ₁₀	12.8 to 30.7	6.84268	1043.206	233.344
Phenol	C ₆ H ₆ O	107.2 to 181.8	7.13301	1516.790	174.954
1-Propanol	C ₃ H ₈ O	60.2 to 104.6	7.74416	1437.686	198.463
2-Propanol	C ₃ H ₈ O	52.3 to 89.3	7.74021	1359.517	197.527
Propionic acid	C ₃ H ₆ O ₂	72.4 to 128.3	7.71423	1733.418	217.724
Propylene oxide	C ₃ H ₆ O	-24.2 to 34.8	7.01443	1086.369	228.594
Pyridine	C ₅ H ₅ N	67.3 to 152.9	7.04115	1373.799	214.979
Styrene	C ₈ H ₈	29.9 to 144.8	7.06623	1507.434	214.985
Toluene	C ₇ H ₈	35.3 to 111.5	6.95805	1346.773	219.693
1,1,1-Trichloroethane	C ₂ H ₂ Cl ₃	-5.4 to 16.9	8.64344	2136.621	302.769
1,1,2-Trichloroethane	C ₂ H ₂ Cl ₃	50.0 to 113.7	6.95185	1314.410	209.197
Trichloroethylene	C ₂ HCl ₃	17.8 to 86.5	6.51827	1018.603	192.731
Vinyl acetate	C ₄ H ₆ O ₂	21.8 to 72.0	7.21010	1296.130	226.655
Water*	H ₂ O	0 to 60	8.10765	1750.286	235.000
Water*	H ₂ O	60 to 150	7.96681	1668.210	228.000
<i>m</i> -Xylene	<i>m</i> -C ₈ H ₁₀	59.2 to 140.0	7.00646	1460.183	214.827
<i>o</i> -Xylene	<i>o</i> -C ₈ H ₁₀	63.5 to 145.4	7.00154	1476.393	213.872
<i>p</i> -Xylene	<i>p</i> -C ₈ H ₁₀	58.3 to 139.3	6.98820	1451.792	215.111

Table B.5 Properties of Saturated Steam: Temperature Table*

T(°C)	P(bar)	\hat{V} (m ³ /kg)		\hat{U} (kJ/kg)		\hat{H} (kJ/kg)		
		Water	Steam	Water	Steam	Water	Evaporation	Steam
0.01	0.00611	0.001000	206.2	zero	2375.6	+0.0	2501.6	2501.6
2	0.00705	0.001000	179.9	8.4	2378.3	8.4	2496.8	2505.2
4	0.00813	0.001000	157.3	16.8	2381.1	16.8	2492.1	2508.9
6	0.00935	0.001000	137.8	25.2	2383.8	25.2	2487.4	2512.6
8	0.01072	0.001000	121.0	33.6	2386.6	33.6	2482.6	2516.2
10	0.01227	0.001000	106.4	42.0	2389.3	42.0	2477.9	2519.9
12	0.01401	0.001000	93.8	50.4	2392.1	50.4	2473.2	2523.6
14	0.01597	0.001001	82.9	58.8	2394.8	58.8	2468.5	2527.2
16	0.01817	0.001001	73.4	67.1	2397.6	67.1	2463.8	2530.9
18	0.02062	0.001001	65.1	75.5	2400.3	75.5	2459.0	2534.5
20	0.0234	0.001002	57.8	83.9	2403.0	83.9	2454.3	2538.2
22	0.0264	0.001002	51.5	92.2	2405.8	92.2	2449.6	2541.8
24	0.0298	0.001003	45.9	100.6	2408.5	100.6	2444.9	2545.5
25	0.0317	0.001003	43.4	104.8	2409.9	104.8	2442.5	2547.3
26	0.0336	0.001003	41.0	108.9	2411.2	108.9	2440.2	2549.1
28	0.0378	0.001004	36.7	117.3	2414.0	117.3	2435.4	2552.7
30	0.0424	0.001004	32.9	125.7	2416.7	125.7	2430.7	2556.4
32	0.0475	0.001005	29.6	134.0	2419.4	134.0	2425.9	2560.0
34	0.0532	0.001006	26.6	142.4	2422.1	142.4	2421.2	2563.6
36	0.0594	0.001006	24.0	150.7	2424.8	150.7	2416.4	2567.2
38	0.0662	0.001007	21.6	159.1	2427.5	159.1	2411.7	2570.8
40	0.0738	0.001008	19.55	167.4	2430.2	167.5	2406.9	2574.4
42	0.0820	0.001009	17.69	175.8	2432.9	175.8	2402.1	2577.9
44	0.0910	0.001009	16.04	184.2	2435.6	184.2	2397.3	2581.5
46	0.1009	0.001010	14.56	192.5	2438.3	192.5	2392.5	2585.1
48	0.1116	0.001011	13.23	200.9	2440.9	200.9	2387.7	2588.6
50	0.1234	0.001012	12.05	209.2	2443.6	209.3	2382.9	2592.2
52	0.1361	0.001013	10.98	217.7	2446	217.7	2377	2595
54	0.1500	0.001014	10.02	226.0	2449	226.0	2373	2599
56	0.1651	0.001015	9.158	234.4	2451	234.4	2368	2602
58	0.1815	0.001016	8.380	242.8	2454	242.8	2363	2606
60	0.1992	0.001017	7.678	251.1	2456	251.1	2358	2609
62	0.2184	0.001018	7.043	259.5	2459	259.5	2353	2613
64	0.2391	0.001019	6.468	267.9	2461	267.9	2348	2616
66	0.2615	0.001020	5.947	276.2	2464	276.2	2343	2619
68	0.2856	0.001022	5.475	284.6	2467	284.6	2338	2623

*From R. W. Haywood, *Thermodynamic Tables in SI (Metric) Units*, Cambridge University Press, London, 1968. \hat{V} = specific volume, \hat{U} = specific internal energy, and \hat{H} = specific enthalpy. Note: kJ/kg \times 0.4303 = Btu/lb_m.

(continued)