Simulation and Optimization of Carbonating Tower for Better Yield and Efficiency

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Certificate

This is to certify that work in this thesis has been carried out by **Mohib ur Rahman, Hamza Khan and Ahmed Osama** and completed under my supervision in School of Chemical and Materials Engineering, National University of Sciences and Technology, H-12, Islamabad, Pakistan.

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Dedication

This thesis is dedicated to our parents and our family
for their endless love, support and
encouragement

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We would like to acknowledge and thank our project supervisor, Dr. Iftikhar Ahmad for his efforts in guiding and supporting us towards the completion of our project. His guidance was very vital for us in the fulfilment of the requirements of the project within the set project timeline.

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Abstract

Currently, the production of Soda Ash at ICI Ltd is 1000 tons per day, and the thermal efficiency of the carbonating tower is nearly 70%. This project aims at increasing the yield of sodium bicarbonate from the carbonating tower and also at improving the efficiency of the tower. For the simulation purpose Aspen PLUS has been utilized.

Carbonating tower comprises of two portions, in one of them the main reaction is taking place and in the other cooling boxes are present in order to assist the crystallization process. For increase in production, the CO_2 content in the tower needs to be increased and the O_2 content in the inlet needs to decrease which depends on the coke to limestone ratio in the kiln from where the carbonating tower receives most of its CO_2. Also, the amount of unreacted CO_2 being wasted needs to be reduced. For improving the efficiency of the carbonating tower, the main focus is on the operating parameters of the tower which include the outlet temperature of the tower magma. To reduce this temperature, a change of cooling medium from water to ammonia has been proposed.

Table of Contents

Certificate i

Acknowledgement iii

Abstract iv

Table of Contents v

List of figures: ix

Abbreviations: x

Chapter - 1 1

Introduction 1

  1.1 Soda Ash: 1

  1.2 Solvay process: 2

Chapter - 2 3

Theoretical Background 3

  2.1 Yield 3

  2.2 Efficiency 3

  2.3 Crystallization 4

  2.4 Structure of a Carbonating Tower 5

Chapter - 3 6

Soda Ash at ICI 6

  3.1 Raw Materials 6

    3.1.1 SALT 6

    3.1.2 LIMESTONE 6

    3.1.3 COKE 7

3.1.4 AMMONIA ... 7

3.1.5 OTHERS ... 7

3.2 Plant overview – ICI Soda Ash ... 9

3.3 Carbonating Tower ... 10

3.3.1 Details of accessories and equipment ... 12

3.3.2 Process overview and description: ... 15

3.3.3 Theoretical Aspects: ... 17

Chapter - 4 ... 20

Material Balance ... 20

4.1 Calculations ... 21

4.1.1 CVL: ... 21

4.1.2 TE (Top Entry): ... 25

4.1.3 BE (Bottom Entry): ... 27

4.1.4 Magma: ... 30

4.1.5 Tower Exit Gas: ... 34

Chapter - 5 ... 38

Energy Balance ... 38

5.1 Calculations: ... 38

5.1.1 CVL ... 38

5.1.2 TE ... 40

5.1.3 BE ... 41

5.1.4 Magma ... 43

5.1.5 Tower Exit Gas ... 44

5.1.6 Overall Energy Balance ... 46

Chapter - 6 ... 47

Yield Improvement 47
6.1 Recommendations:..47
6.1.1 Calculations:..47
Chapter - 7..50
Efficiency Improvement..50
7.1 Current Efficiency..50
7.2 Increasing Efficiency 51
7.2.1 Recommendation: 52
7.3 Revised energy balance..52
7.3.1 Magma 52
7.3.2 Overall Energy Balance 54
Chapter – 8 55
Simulation 55
8.1 Component list 56
8.2 Property package..57
8.3 Simulation Environment 58
Chapter - 9..66
HSE Aspects and HAZOP Study..66
9.1 Health, safety and environment aspects:..66
9.2 HAZOP Study..67
9.2.1 Safety of the Personnel: 68
9.2.2 HAZOP 70
Table 9.2.3 - HAZOP on transfer of cooling water to cooling boxes:.....................72
Table 9.2.4 - HAZOP on ammonia running through the plant: 73
Table 9.2.5 - HAZOP on transfer of reactants to the tower:...................................74

Chapter – 10 75

Conclusion 75

10.1 Calculating mass flowrate for ammonia as cooling medium replacement 75

References: 77

Plagiarism Report 78

List of figures:

Fig No.	*Description*	*Page*
Fig 3.1	Plant overview ICI Soda Ash	8
Fig 3.2	Construction of Carbonating Tower	10
Fig 4.1	Overview of the material balance	20
Fig 8.1	Molecule Editor	55
Fig 8.2	Component list	56
Fig 8.3	Aspen Plus Method Assistant	57
Fig 8.4	Property method selection	57
Fig 8.5	CVL Specifications	58
Fig 8.6	CVL Flash Options	59
Fig 8.7	TE Specifications	59
Fig 8.8	TE Flash Options	59
Fig 8.9	BE Specifications	60
Fig 8.10	BE Flash Options	60
Fig 8.11	Reactor Specifications	61
Fig 8.12	Reaction Set	61
Fig 8.13	Cooler Specifications	62
Fig 8.14	Cooler Pressure drop	63
Fig 8.15	CW Specifications	63
Fig 8.16	CW Flash Options	64
Fig 8.17	Control Panel	64

Abbreviations:

- CVL = Carbonated VAT Liquor
- TE = Top Entry
- BE = Bottom Entry
- TW Exit Gas = Tower Washer Exit Gas
- CW = Cooling Water
- CWR = Cooling Water Return
- ρ = Density
- wt% = Weight percent
- mol% = Molar percent
- kg = Kilogram
- m = Meter
- h = Hour
- kmol = Kilo mole
- ΔH = Enthalpy change
- Q = Heat flow
- C_p = Specific heat capacity
- T = Temperature
- HSE = Health, Safety and Environment
- HAZOP = Hazards and operability

Chapter - 1

Introduction

1.1 Soda Ash:

Soda Ash (sodium carbonate-Na_2CO_3) is a white anhydrous powder used in several industries as raw material. Some of these include the glass, chemicals, detergents and soap industries.

Soda Ash is crystalline, odourless and white. It is water soluble and insoluble in acetone, alcohol and ether. It is hygroscopic and absorption of water in humid conditions can cause its alkalinity to decrease.

There are two main grades of soda ash available, dense soda ash and light soda ash. The difference in these two grades is only in the physical characteristics like shape and size of particles and bulk density, which can influence the angle of repose and flow characteristics. The bulk density of dense soda ash is around 950 to 1100 kg/m^3 and it is preferred in the manufacturing of glass as the light soda ash causes froth to be formed in the melt. The bulk density of light soda ash is around 520 to 600 kg/m^3 and is mainly used in the detergent and chemical industries. The remaining physical and chemical properties are common for both the grades of soda ash. [1]

Soda Ash can mainly be produced by two processes:

- Le Blanc Process
- Solvay Process

The process being used by ICI is the Solvay process.

1.2 Solvay process:

The Solvay process was developed by an industrial chemist from Belgium, Ernest Solvay. His method involved using ammonia to convert sodium chloride to sodium carbonate.

The following is the overall reaction of the Solvay process:

$$2NaCl + CaCO_3 \rightarrow Na_2CO_3 + CaCl_2 \qquad (1.2.1)$$

This reaction is not possible directly so it is carried out through a series of intermediate steps.

Limestone ($CaCO_3$) is first decomposed in a kiln to produce CO_2. This CO_2 is used in later steps.

$$CaCO_3 \rightarrow CaO + CO_2 \qquad (1.2.2)$$

Ammonia is absorbed into brine to form ammoniated brine. This acts as an intermediate and helps in the reacting brine with CO_2 as they are unable to react on their own. Ammoniated brine reacts with CO_2 to first form ammonium carbonate ($(NH_4)_2CO_3$) and then from further reaction to form ammonium bicarbonate (NH_4HCO_3).

$$NaCl + H_2O + NH_3 + CO_2 \rightarrow (NH_4)_2CO_3 + H_2O + NaCl \qquad (1.2.3)$$

$$(NH_4)_2CO_3 + H_2O + CO_2 \rightarrow 2NH_4HCO_3 \qquad (1.2.4)$$

Sodium bicarbonate ($NaHCO_3$) is then produced by reacting ammonium bicarbonate with NaCl. Ammonium chloride (NH_4Cl) is also produced.

$$2NH_4HCO_3 + 2NaCl \rightarrow 2NaHCO_3 + 2NH_4Cl \qquad (1.2.5)$$

The sodium bicarbonate crystals are then filtered out and decomposed at a high temperature to give out CO_2 and produce sodium carbonate (Na_2CO_3) crystals as the final product.

$$2NaHCO_3 \rightarrow Na_2CO_3 + H_2O + CO_2 \qquad (1.2.6)$$

Chapter - 2

Theoretical Background

2.1 Yield

Yield is the quantity of product produced from a chemical reaction. There are three types of yields that can be calculated, the theoretical yield, the actual yield and the percentage yield.

The theoretical yield is the amount of product that is to be produced according to the stoichiometric ratios of the reactants. Calculations for the theoretical yield are based on the amount of limiting reactant present at the start of the reaction.

The actual yield is the actual amount of product that is produced when the reaction takes place. Stoichiometric ratios are not considered for this. The difference in the theoretical yield and the actual yield is due to a number of reasons. Energy losses, impure reactants, variations in reaction conditions, side reactions, and unwanted products are some of the reasons for a lower actual yield.

The actual yield and the theoretical yield can be compared by calculating the percentage yield.

$$Percentage\ yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\%$$

It is important that the units of the actual and the theoretical yield are kept consistent while calculating the percentage yield. [2]

2.2 Efficiency

In literal terms, efficiency is the ability to produce some desired result with the minimum wastage of resources available. The resources could be raw material, time, cost or energy. There are number of forms of efficiencies that can be calculated to measure how efficient a process is.

Thermal efficiency considers and compares the thermal energy provided to the work that is produced from the provided energy. It tells us how much of the heat has been successfully utilized and how much of it has been lost to the surroundings.

Reaction efficiency takes into account the chemical reaction taking place. It gives a comparison between the amount of reactants provided and the amount of product produced.

Absorption efficiency will be the efficiency of absorption taking place in an absorption column. The factors that are considered to calculate this efficiency are the amount of the gas to be absorbed at the inlet of the column and the amount of that gas at the exit of the column. For example, in the case of absorption of CO_2, the efficiency will be calculated by considering the amount of CO_2 present in the inlet stream of the column and the amount of CO_2 that remained in the outlet stream of the column. [3]

2.3 Crystallization

Crystallization is the phenomenon where solid particles are formed either directly from vapor or from liquid melt. It results in the formation of pure crystals from a solution that is impure. The mixture of the crystals formed and the mother liquor is known as the magma.

The most important objectives of crystallization include purity and high yield. Uniformity of the size of crystals and a properly developed crystalline structure are also very important objectives and are vital in the further processing of the product crystals.

There are several factors that contribute to the final structures and purity of crystals. Mechanical disturbances have a negative impact on the crystallization process. Crystal growth occurs by the deposition of molecules on a pre-existing structure in an orderly fashion. Abrupt changes in the environment caused by agitation or vibration can hinder the crystal development.

Time is another important factor. Letting crystals grow over a long period of time is best for the quality of the crystal. Fast crystallization results in the quality of the crystals being poor.

In case of cooling crystallization, the best result is obtained when the cooling is done slowly. Gradual decrease in temperature gives enough time for the solute molecules to settle in an orderly manner around the growing crystal. Sudden cooling will result in the crystal structure being non-uniform. The molecules won’t have enough time to settle properly. [4]

2.4 Structure of a Carbonating Tower

According to a US Patent Document produced in 1978, a carbonating tower is a hollow casing used to produce the magma of sodium bicarbonate. It contains plates that are perforated and are arranged one over another. The carbonating tower is divided into the absorption compartments and the cooling compartments. These compartments communicate through overflow pipes. The absorption compartments contain flat discs with openings that allow gas flow to occur. Different shapes can be used for the openings and may contain toothed caps that help in distributing the gas in the magma. The cooling compartments are responsible for controlling the temperature of the magma. Cooling pipes are present in which the circulation of cooling liquid occurs. The bottom of the tower contains pipes that are responsible for feeding the gas and the removal of the product magma. The top of the tower contains pipes for the entry of ammoniated brine and for the exit of the waste gas. The flow of gas and solution is counter-current in nature. [5]

Chapter - 3

Soda Ash at ICI

ICI Pakistan Limited's Soda Ash Works is located at Khewra in the northern part of Punjab at the foot hills of salt ranges. The Soda Ash plant is located at the area where salt and limestone, the two main raw materials of the process are abundant. Installed capacity of plant in 1948 was 18000 tonnes per annum, the first extension of plant was raised to almost 33000 tonnes per annum by 1966. The second extension of plant was commissioned in 1980 raising the plant capacity to 81000 tonnes per annum. By the end of 1994, plant's capacity was and is 191000 tonnes per annum.

3.1 Raw Materials

3.1.1 SALT

Salt, NaCl, is found in abundance in the mountain ranges surrounding Khewra. Rock salt varies in composition and is, therefore, dissolved in water to form brine of the required compositions in basins. On average, the salt is 85 % NaCl. The rock salt is mined by a number of mining companies, but ICI's main supplier is Pakistan Mineral Development Corporation (PMDC).

3.1.2 LIMESTONE

Limestone is burnt in the kilns for the production of unslaked lime, which is in turn dissolved in water to produce milk of lime. It is abundantly available from limestone rocks situated situated 4-10 km from Khewra. Small quantities of limestone, known as gorge stone, are collected from gorge area. Apart from the gorge area, ICI also owns two quaries, Dandot and Tobar.

Limestone has the following average specifications:

Calcium Carbonate ($CaCO_3$)	90-92%
Magnesium Carbonate ($MgCO_3$)	0.8-1.0%

Calcium Sulphate ($CaSO_4$)	0.1-0.3%
Silica Oxides (SiO_3)	3-4%
Other Oxides	3-4%

Limestone of 2.5”-5” diameter size is used in the kilns. The suitability of limestone is determined by the contents of $CaCO_3$, $MgCO_3$ and silicious matter. Excessive quantity of silicious tends to form fusible clinker blocking the kiln or attacking the kiln lining.

3.1.3 COKE

Coke is an expensive raw material used to generate CO_2 gas for the process. It has a calorific value of about 6500 calories per gram and contains about 17% ash. Coke of 1.25”-2.5” diameter is used in the kilns. Pakistan Steel, Karachi, is the sole supplier of Coke to the ICI Soda Ash Business.

Typical Chemical analysis of a Coke sample shows:

Ash	17%
Moisture (H_2O)	1%
Volatile Matters	2%
Fixed Carbon	80%

3.1.4 AMMONIA

Ammonia used in the Solvay process to facilitate absorption of carbon dioxide into brine. It is mostly recovered in the gas form in the distiller and the process condensate distiller (PCD). However, make-up ammonia of about 7 kgs per ton of Soda Ash produced has to be added. Ammonia is obtained from fertilizer plants in 5 ton cylinders.

3.1.5 OTHERS

Other material used for the production of Soda Ash are Sui Gas/Furnace oil as fuel, and water.

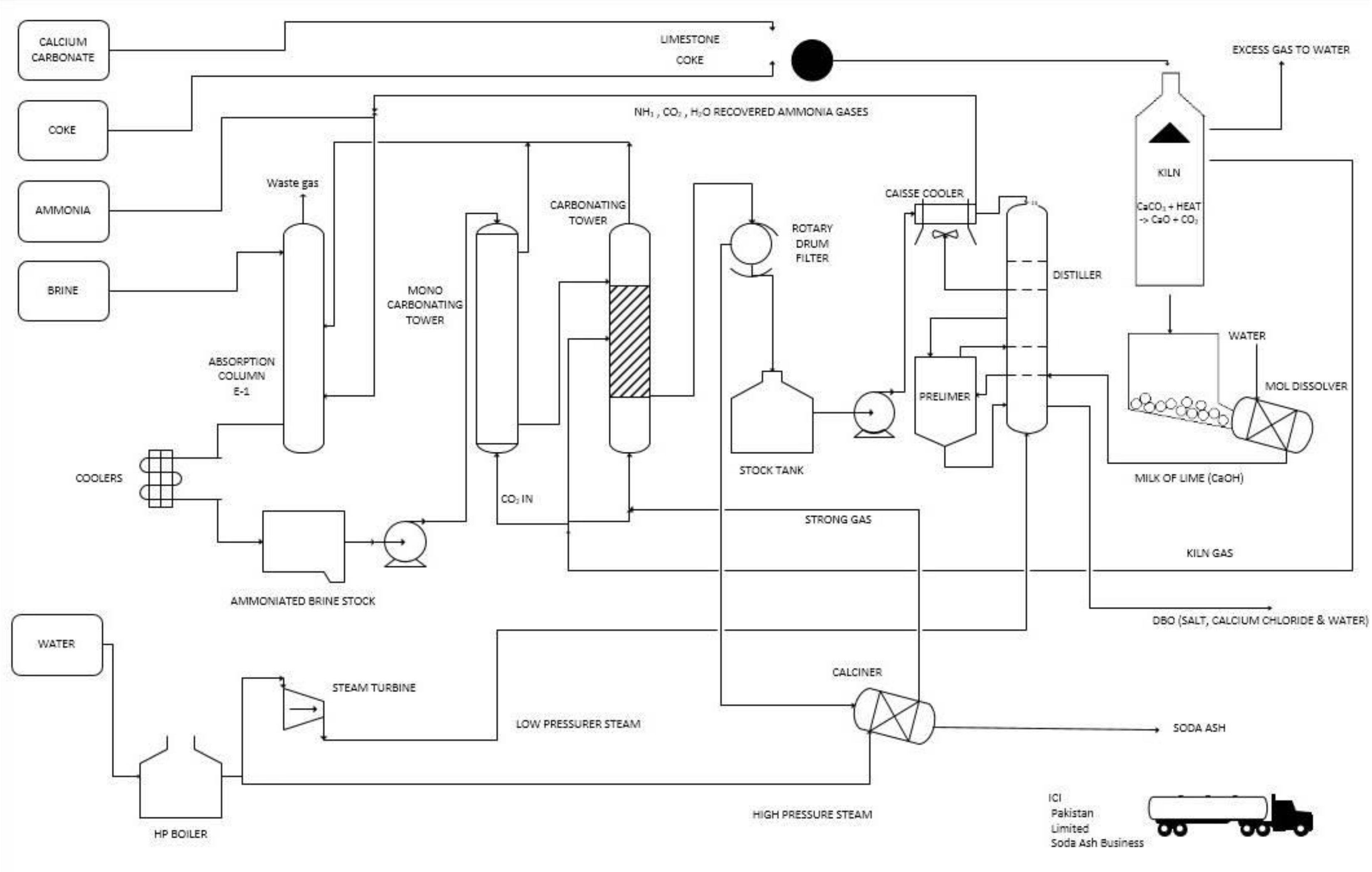


Fig 3.1 – Plant overview ICI Soda Ash

3.2 Plant overview – ICI Soda Ash

The manufacture of Soda Ash by the Solvay process has been practiced for over a century. The basic chemistry of the process is straightforward but its application into a large industrial unit is very complex. Very briefly, the problem is to get the two ions of Salt (NaCl) and the two ions of limestone ($CaCO_3$) to change places to give sodium carbonate (Na_2CO_3) and calcium choride ($CaCl_2$). This cannot be done directly and ammonia has to be used as a recoverable ‘cyclical carrying agent’ to carry carbon dioxide.

Process technology includes burning of limestone with coke in kilns. This causes the stone to be decomposed into two components, burnt lime (CaO) and carbon dioxide gas (CO_2). Both of these components are used later in the process.

Secondly, ammonia gas is absorbed in brine. This liberates a considerable amount of heat which must be removed. After cooling, the ammoniated brine is pumped into the top of a series of towers called Solvay Towers, whereby carbon dioxide gas is introduced which carbonates the ammoniated brine. A magma is produced which comprises sodium bicarbonate ($NaHCO_3$) in crystal form and ammonium chloride (NH_4Cl) in solution. There is liberation of a considerable amount of heat during carbonation which is removed by water-cooled tubes at the bottom of the towers.

The sodium bicarbonate, which is in the form of a wet cake, is then fed into large rotary driers or calciners where heat decomposes the sodium bicarbonate to give the product, sodium carbonate, with the evolution of carbon dioxide gas and water. The carbon dioxide gas is cooled, washed, and added to the gas from the kilns for reabsorption in the Carbonating Towers.

Calcium oxide obtained from the kiln is slaked in water and the milk of lime is used to recover ammonia gas in the distillers, and for the purification of brine.

Discharge of the distillers, called Distiller Blow Off (DBO), forms the major part of the plant waste which is disposed of in an environmentally safe manner.

The overall enthalpy change for the process is -46.84 Kcal., i.e. the process is exothermic by nature, and requires fine temperature control for optimum crystal growth in the carbonating towers.

3.3 Carbonating Tower

The unit operation that is the main focus of our project is the carbonating tower.

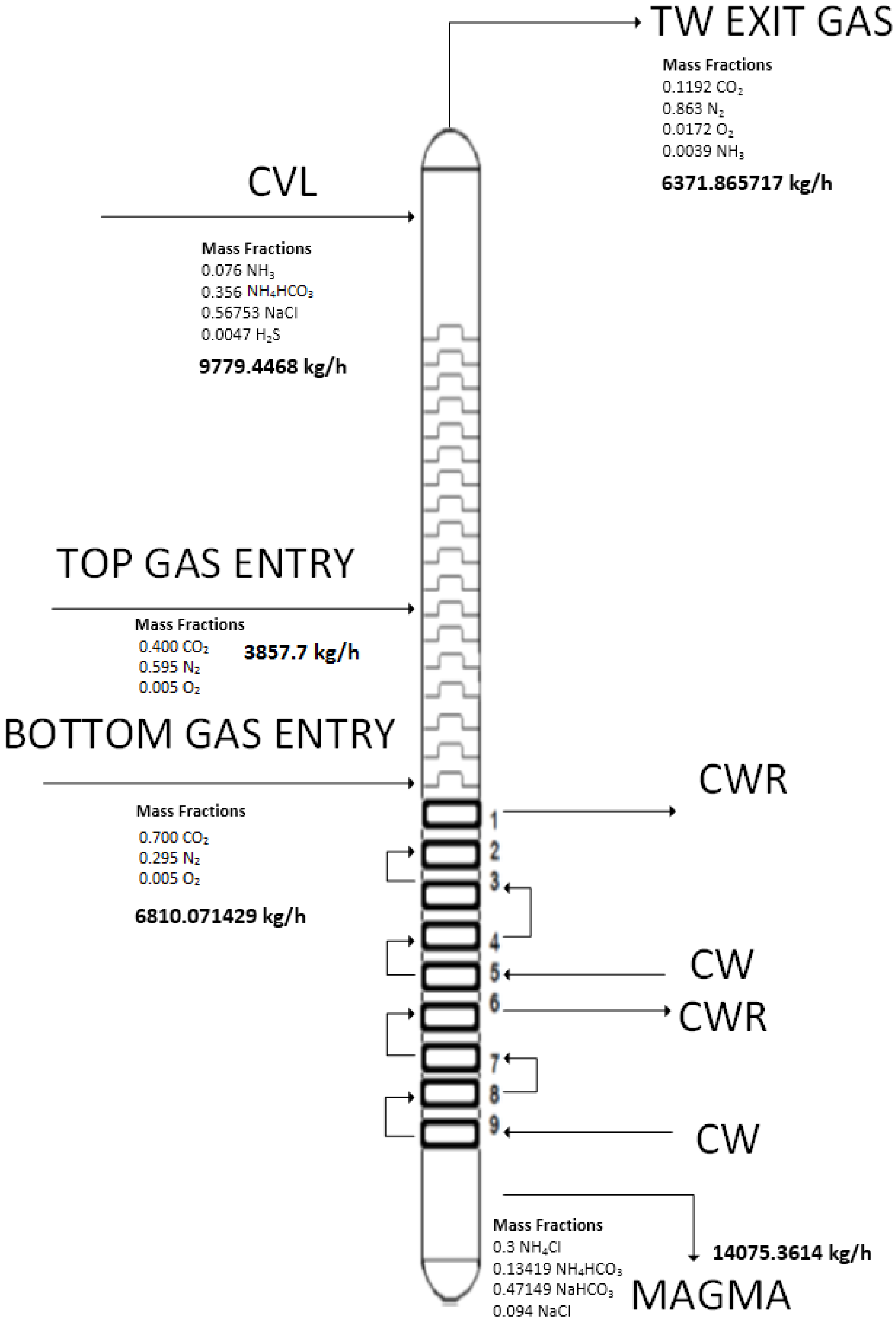


Fig 3.2 – Construction of Carbonating Tower

The carbonating tower is divided into two sections, the absorption section and the cooling section. The absorption section consists of trays of the bubble cap type containing a single bubble cap. The trays increase the contact area of the feed solution and the CO_2 gas. They also increase the residence time of the reactants and thus increasing the absorption taking place. The reaction taking place is of the chemisorption type in which CO_2 absorbs into the solution and then chemical reaction takes place. There are a total of 26 reaction chambers in one carbonating tower.

The cooling section consists of cooling boxes which have cooling pipes running through them. The cooling fluid used is water which enters at atmospheric temperature. The cooling is a very vital part of the carbonation process. There are a total of 9 cooling boxes in one carbonating tower which ensure proper crystallization of the sodium bicarbonate crystals.

The process fluid that enters the carbonating tower from the top is called the Carbonated Vat Liquor (CVL). It is liquor that results from the absorption of ammonia into brine forming ammoniated brine in the absorbers and the subsequent absorption of low concentration CO_2 in the monocarbonating towers. CVL that enters the carbonating towers contains NH_3, $(NH_4)_2CO_3$, and NaCl.

The CVL from the monocarbonating tower comes into intimate contact with carbon dioxide, from two sources. The primary source of carbon dioxide being the kiln gas, 40% CO_2 called the Top Entry (TE) and the secondary source is the strong gas coming from the decomposition reactions in the calciner, 70% CO_2 called the Bottom Entry (BE).

Basically, the reaction is carried out in enclosed vessels by blowing the carbon dioxide gas into the CVL. However, the reaction being exothermic, the liquor temperature must be closely controlled so that proper sodium bicarbonate crystals growth takes place, the maximum quantity of carbon dioxide is absorbed, and ammonia is retained in solution. This situation is explained by the following reactions,

$$(NH_4)_2CO_3 + CO_2 + H_2O \rightarrow 2NH_4HCO_3 \qquad (3.3.1)$$

$$NH_4HCO_3 + NaCl \rightarrow NaHCO_3 + NH_4Cl \qquad (3.3.2)$$

Both these reactions can be written as one overall reaction:

$$(NH_4)_2CO_3 + 2NaCl + CO_2 + H_2O \rightarrow 2NaHCO_3 + 2NH_4Cl \quad (3.3.3)$$

When the CVL is initially carbonated it has a high affinity for carbon dioxide and so the lower strength kiln gas is used. However, as the reaction proceeds, higher strength gas is required and a mixture of the two sources of CO_2 is used, making a CO_2 concentration of 70%. The final temperature of the liquor is important to make sure that the maximum quantity of sodium bicarbonate has been precipitated. The temperature is maintained using an intricate water circulation system. The top, middle and draw temperatures are 60, 45 and 25˚C respectively.

The magma containing the solid sodium bicarbonate in suspension is then drawn off and the solids recovered by filtration. Due to deposition of sodium bicarbonate, ammonium bicarbonate and ammonium carbonate on the inside of towers a cleaning routine is carried out every 72 hours, during which ammoniated Vat Liquor is circulated in the towers to dissolve the scale. The scaling on the inside of the towers reduces the inner volume of the reaction and cooling chambers. Even though the reduction in volume is quite small but it greatly affects the efficiency of the absorption taking place in the tower. The scaling that takes place on the cooling tubes present also puts a negative impact on the efficiency of the carbonating tower. Scale present on cooling tubes greatly reduces the heat transfer taking place. With reduction in the cooling efficiency, proper crystal formation is hindered and the efficiency of the carbonating tower reduces.

3.3.1 Details of accessories and equipment

Following major units constitute this operation:

- Carbonating Towers
- Gas Compressors
- Top Entry Scrubbers

- Bottom Entry Scrubbers
- Tower liquor circulation (TLC) System
- Bleed on and Bleed off circulation system
- Cooling System

Carbonating Towers

Carbonating tower or Solvay Tower is the main unit of Solvay process. It is a tall vertical vessel of cast iron cylindrical sections or rings of about 6ft diameter and 81ft height. Each tower has 9 cooling boxes. Top three cylinders of towers are hollow below which 35 passette plate compartments are present. Out of 35, 26 compartments have an opening of 26” diameter, whereas the remaining 9 compartments have an opening of 17” diameter. These nine compartments have cooling boxes in them – each cooling box has 88 tubes in it through which cooling water flows.

Reaction between ammoniated and partially carbonated brine with carbon dioxide gas takes place in the carbonating tower. Cooling boxes facilitate the temperature control in the middle and bottom section of the tower to drive the reaction in forward direction as well as increasing the size of crystals for efficient filtration. Sodium bicarbonate along with ammonium chloride is discharged from the bottom in the form of Magma.

Currently, there are fifteen Carbonating Towers for the manufacture of sodium bicarbonate at our site. These towers are divided into three sets. Each set consists of five towers, four towers are on making and one tower is on cleaning duty. On a making duty, one tower has the capacity to produce 82-85 tons per day soda ash.

Gas Compressors

Carbon dioxide gas is introduced at two locations i.e., at tower middle known as “top entry” and at tower bottom known as “bottom entry”. Top entry is introduced at a pressure of 17-19 psig whereas bottom entry at 34-36 psig. The bottom entry contains mixed gas i.e. kiln gas plus strong gases from calciners. The top entry is basically compressed kiln gas. Screw compressors for top entry and bottom entry serve the purpose of compressing the gases to desired pressure.

Top Entry & Bottom Entry Scrubbers and Coolers

Top entry scrubbers serve the purpose of cooling the compressed gas to desired temperature for better absorption and reaction as compression results in increasing the temperature of discharge gas. Cooling water is used as cooling medium. These scrubbers are packed with 2” ceramic rings. Cooling water is showered from the top which comes in contact with the gas and decreases its temperature.

The basic difference between gas cooler and scrubber is that of design as both serve the same purpose. In gas scrubbers, there is direct contact between gas and the cooling medium and random packing provides the intimate contact for effective cooling, whereas, gas coolers are of shell and tube type. Gas is in the tube side whereas water in shell side.

TLC Circuit

Once a tower has completed 72 hours of operation, it is put on cleaning duty. A close circulation of liquor is established within the tower. The liquor in the cleaning tower is circulated in a way that the circulating pump draws the liquor from the cleaning tower’s bottom or top and pumps it back to the top or bottom of the tower.

There are two types of circulations done during the cleaning operation of the tower:

Upward circulation: The liquor is pumped from bottom to top.

Downward circulation: The liquor is pumped from top to bottom.

The cleaning is carried out in the following order:

-	1st upward circulation:	4 hrs.
-	1st downward circulation:	4 hrs.
-	2nd upward circulation:	4 hrs.
-	2nd downward circulation:	4 hrs.

Bleed On & Bleed off system

Bleed on & Bleed off system consists of following items:

- Bleed on Pumps
- Bleed on & bleed off vessels

During cleaning of a tower, vat liquor is introduced into the tower as it has more capacity to dissolving bicarbonate deposited on the internal surfaces of the tower. A fresh stream of vat liquor from stocks is called bleed on. An equal amount of liquor is bled off from the tower to vats is known as bleed off.

Vat liquor from stocks is pumped to bleed on vessels via bleed on pumps. Normal bleed on flow at one set is in the range of 50 – 66 m3/hr.

Cooling Water system

Cooling water is used for the temperature control and its flow is regulated in two different sets of cooling boxes. Upper set consists of four cooling water boxes and is used for control of middle temperature. Bottom set consists of five cooling water boxes for draw temperature control. Cooling water from cooling water header splits into individual streams for each tower. Cooling water in the upper stream enters from the 6th box and leaves from the 9th cooling box and joins the return header. Similarly, lower stream enters at 1st box and leaves from the 5th box and joins the common return header.

Magma Distribution & Tundish system

Magma leaving the tower is routed to magma tundishes, which are essentially small open tanks providing buffer to rotary drum filters.

3.3.2 Process overview and description:

CVL enters the tower from top whereas, carbon dioxide gas enters at two locations, one (TE) almost in the middle of the tower (41-42% concentration) while the other enters at the bottom which is mixed gas of Kilns and Calciners (70-72% concentration). As this gas rises in tower, reaction takes place, i.e. sodium bicarbonate starts to form. The gas rises up through the gas risers of Passette plates while the CVL flows down through the same opening of the plates. The liquor and gas come in contact at the top portion above the entrance of top entry gas. Ammonium carbonate in CVL is converted to ammonium bicarbonate which ultimately gives sodium bicarbonate. Sodium bicarbonate begins to separate out from the solution as the reaction proceeds and the size of crystal continues to grow as the temperature is gradually reduced from top zone to draw. The magma is drawn through the draw main line.

The temperature gradient in the tower is very important factor for the bicarbonate crystals to grow larger towards the bottom as the liquor descends. Most part of the bicarbonate formation is completed in upper part of tower. Gradual cooling is started from the middle towards bottom portions of the tower. This cooling is carried out according to certain temperature curve for maximum crystal growth. The liquor is finally collected in a magma trough from where it goes to filters.

Cooling water is used for the temperature control and its flow is regulated in two different sets of cooling boxes. Upper stream consists of four cooling water boxes and is used for control of middle temperature. Bottom stream consists of five cooling water boxes for draw temperature control.

In the making towers it is very important that steady conditions are maintained for better efficiency of the plant. The bottom entry pressure is maintained at 34-36 psig and top entry pressure is maintained at 17-19 psig. Gases after being compressed in the screw compressors, delivered into the top entry and bottom entry scrubbers. Cooling water is sprayed from the top, to cool the gases (i.e., the temperature of the gases is controlled by the cooling water) and to remove the carry overs.

There is a certain level of water maintained at the bottom of the scrubbers. If more water is poured i.e., if the level is increased then it would block the gas inlet point coming from compressor, this will exert back pressure on the compressor, leading to tripping in worst cases. The scrubbers are packed with 2in. Polypropylene rings.

Flow of the gases is adjusted according to the plant rate. The bottom entry contains mixed gas i.e. kiln gas plus gases from Calciners. The top entry gases consist of kiln gases alone. The percentage of carbon dioxide in the mixed gas should be about 71-72%. Any variation in tower height will disturb backpressure on compressors and will disturb towers performance.

Tower Changeover:

After a cycle of continuous operation, tower needs to be cleaned because the cooling tubes become coated with precipitated bicarbonate after 3 days of operation (making). This condition results in increase in the percentage of carbon dioxide in waste gases and in the increase in draw temperature, since the cooling water in unable to absorb the heat generated in the tower by chemical reaction. In the worst case, the magma at the draw comes out, not in smooth, continuous stream, but in broken jets, and considerable carbon dioxide gas foam appears in the draw liquor. In such cases tower is put on cleaning duty. During cleaning, gas supply to the tower is cut off along with the cooling water completely. Liquor present in the tower is circulated for 16 hours in two alternate cycles of 4 hours upward and 4 hours downward circulation. During circulation, vat liquor is also introduced alternatively through draw main and 10th cylinder from top temperature point. Equal quantity of liquor is bled off through bleed off main. Vat liquor dissolves the bicarbonate as well as maintains the temperature of tower liquor at around 60-65 °C. At the end of cleaning cycle carbonates of vat liquor and bleed off liquor are checked. Equal carbonates at in an out would indicate good cleaning. For every four towers on making cycle, there is always one tower at cleaning cycle.

3.3.3 Theoretical Aspects:

Assuming excess surface area is available at all times for CO_2 absorption, the driving force for absorption is given by the difference between the CO_2 partial pressure and the CO_2 vapor pressure. The absorption of CO_2 into the partially ammoniated brine is kinetically controlled, and is slow at low temperatures. At higher temperatures the faster absorption rate is counteracted by a fall in the driving force due to increase in CO_2 vapor pressure. The most efficient absorption of CO_2 occurs, therefore, at intermediate temperatures.

As the liquor enters the tower, it is under-saturated in CO_2 and increasingly rapid absorption takes place as the temperature rises. Once the liquor becomes supersaturated with sodium bicarbonate, nucleation occurs but, due to increasing solubility of sodium bicarbonate as the liquor rises in temperature, little further crystallization takes place and

CO_2 absorption slows to a rate sufficient to maintain a saturated solution. As the effect of cooling section is felt and liquor temperature begins to fall, the rate of absorption rises to a maximum.

The temperature profile determines the crystallization occurring in the tower. There is a rapid increase in sodium bicarbonate supersaturation at the top of cooling section due to (i) cooling of existing solution and (ii) rapid absorption of CO_2. These factors will give a rapid increase in crystallization either as growth on existing crystals or as new crystals, the latter case leading to a fall in bicarbonate quality. McCabe's law states that the mean growth rate of a crystal is directly proportional to the crystal surface area. Ideally, nucleation should occur high in the tower to produce a set number of crystals which will have the correct total surface area required to satisfy the supersaturation at all points in the tower. If too many nuclei are formed, there will be an excess of crystal surface area present, resulting in a small sized product which would be difficult to filter. If too few nuclei are formed, the total surface area will be too small at the top of cooling section and a second nucleation will occur giving a product containing a large number of fines, which again would be difficult to filter. Since, the variation in crystal growth rate with temperature is small, the important factors become the residence time of the crystals in the cooling section and the rate of cooling.

In tower operation, temperature regulation is very essential. The temperature gradient in the towers is controlled by controlling the cooling water flow to cooling boxes in such a way that the bicarbonate crystals will grow larger and larger towards the bottom as the liquor descends and is cooled.

The lowest temperature is of course to be found at the draw at the bottom as cooling is arranged counter-currently. Various statements appear in the text books for the best draw temperatures, such as 30° C, 36° C, etc. Practice does not confirm these statements. With a well-constructed apparatus and good cooling facilities, as low a draw temperature as 22° C. has been found advantageous. The temperature for draw liquor is primarily limited by the cooling capacity with the cooling water available, rather than by the desirability of working at a certain temperature for chemical reasons. The formation of good crystals in the column depends upon:

a) High concentrations of ammonia and sodium chloride in the cooled ammoniated brine with a proper ratio between the two titers

b) Rich carbon dioxide gas properly cooled

c) High reaction temperature at a point about two-thirds of the height of the column above the base

d) Gradual cooling from this point down, ending with thorough cooling with as much cooling water as possible as the draw point is reached

This is consistent with the theory of crystallization. In a solution containing high concentrations of reacting constituents, sodium chloride, ammonia and carbon dioxide, the ionic concentrations are such that the solubility product of the desired compound is quickly exceeded and the sparingly soluble substance (in this case sodium bicarbonate) is precipitated in solid form. So when the reaction occurs at a high temperature i.e., when the precipitation, as of sodium bicarbonate, takes place in the hot condition, the crystals grow as the liquor is gradually cooled. Finally, cooling the mother liquor to a low temperature for drawing helps to throw as much of the substance out of the solution as possible. Thus a good conversion ratio, “percent decomposition” and good crystals for filtration and washing operations are simultaneously affected. Furthermore, as the draw liquor is exposed to the air during filtration, the loss of ammonia by exposure is reduced.

Chapter - 4

Material Balance

The following figure gives an overview of the material balance as applied on the carbonating tower on the current running parameters at ICI Soda Ash. Detailed calculations follow the figure.

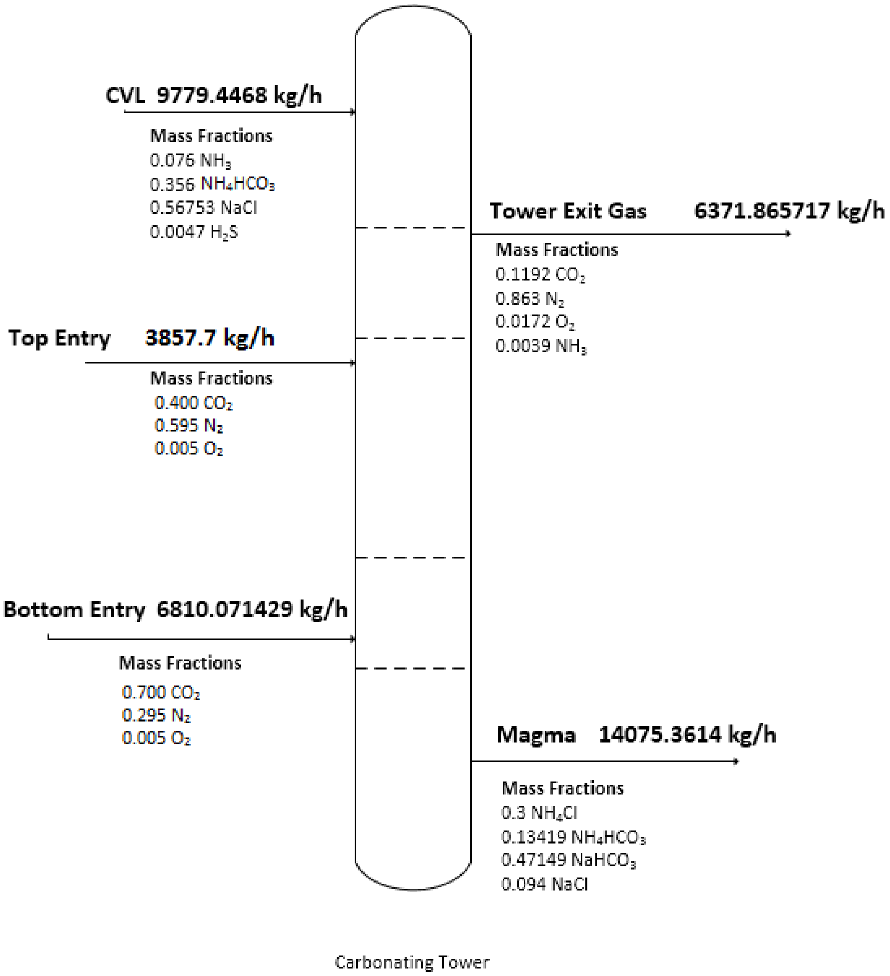


Fig 4.1 – Overview of the material balance

4.1 Calculations

The carbonating tower consists of 3 inlet streams: CVL (Carbonated VAT Liquor), TE (Top Entry) and BE (Bottom Entry); and it has 2 outlet streams: Magma and Tower Exit Gas.

4.1.1 CVL:

Given Data:

Volumetric Flowrate = 21.96 m^3/h

Density $_{NH3}$, ρ_{NH3} = 3.4 kg/m^3

Density $_{NH4HCO3}$, $\rho_{NH4HCO3}$ = 158.4 kg/m^3

Density $_{NaCl}$, ρ_{NaCl} = 252.72 kg/m^3

Density $_{H2S}$, ρ_{H2S} = 0.21 kg/m^3

By addition, the total density of the CVL stream will be:

Density $_{Total}$, ρ_{Total} = 445.33 kg/m^3

Mass composition:

To calculate the mass composition of the stream the following equation will be applied on each of the component of the stream:

$$wt\% = \frac{\rho i}{\rho total}$$

NH_3 composition

wt% NH_3 = 3.4/445.33

wt% NH_3 = 0.076

NH_4HCO_3 composition

wt% NH_4HCO_3 = 158.4/445.33

wt% NH_4HCO_3 = 0.36

NaCl composition

wt% NaCl = 252.72/445.33

wt% NaCl = 0.567

H_2S composition

wt% H_2S = 0.21/445.33

wt% H_2S = 0.00047

<u>Total mass flowrate:</u>

Total mass flowrate is calculated using the formula:

$$Total\ mass\ flowrate = Volumetric\ flowrate \times Total\ density$$

Total mass flowrate = 21.96 x 445.33

Total mass flowrate = 9779.44 kg/h

<u>Individual mass flowrates:</u>

Individual mass flowrate of each component is calculated using the following equation:

$$Individual\ mass\ flowrates = Total\ mass\ flowrate\ \times mass\ composition$$

NH_3 mass flowrate

NH_3 mass flowrate = 9779.44 x 0.076

NH_3 mass flowrate = 743.23 kg/h

NH_4HCO_3 mass flowrate

NH_4HCO_3 mass flowrate = 9779.44 x 0.356

NH_4HCO_3 mass flowrate = 3481.7 kg/h

NaCl mass flowrate

NaCl mass flowrate = 9779.44 x 0.567

NaCl mass flowrate = 5550.13 kg/h

H_2S mass flowrate

H_2S mass flowrate = 9779.44 x 0.00047

H_2S mass flowrate = 4.596 kg/h

Individual molar flowrates:

Individual molar flowrate of each component is calculated using the following equation:

$$Moles = \frac{Mass\ in\ kg}{Molar\ mass}$$

NH_3 molar flowrate

NH_3 molar flowrate = 743.23/17

NH_3 molar flowrate = 43.72 kmol/h

NH_4HCO_3 molar flowrate

NH_4HCO_3 molar flowrate = 3481.7/79

NH_4HCO_3 molar flowrate = 44.069 kmol/h

NaCl molar flowrate

NaCl molar flowrate = 5544.94/58.5

NaCl molar flowrate = 94.87 kmol/h

H_2S molar flowrate

H_2S molar flowrate = 4.59/34

H_2S molar flowrate = 0.135 kmol/h

Total molar flowrate:

Total molar flowrate is the sum of all the individual component molar flowrates.

Total molar flowrate = 182.798 kmol/h

Molar composition:

Individual component molar composition is calculated using the following formula:

$$Individual\ molar\ composition = \frac{Individual\ molar\ flowrate}{Total\ molar\ flowrate}$$

NH_3 molar composition

mol% NH_3 = 43.72/182.798

mol% NH_3 = 0.239

NH_4HCO_3 molar composition

mol% NH_4HCO_3 = 44.069/182.798

mol% NH_4HCO_3 = 0.241

NaCl molar composition

mol% NaCl = 94.87/182.798

mol% NaCl = 0.519

H_2S molar composition

mol% H_2S = 0.135/182.798

mol% H_2S = 0.00074

4.1.2 TE (Top Entry):

Given Data:

Volumetric flowrate = 1180.63 m^3/h

Mass composition:

wt% CO_2 = 0.40

wt% N_2 = 0.595

wt% O_2 = 0.005

Density CO_2 , ρ_{CO2} = 1.307 kg/m^3

Total density:

The total density of the stream is calculated using the formula:

$$wt\% = \frac{\rho i}{\rho total}$$

$Density_{total}$, ρ_{total} = 1.307/0.40

$Density_{total}$, ρ_{total} = 3.26 kg/m^3

Total mass flowrate:

Total mass flowrate is calculated using the formula:

$$Total\ mass\ flowrate = Volumetric\ flowrate \times Total\ density$$

Total mass flowrate = 1180.63 x 3.26

Total mass flowrate = 3857.71 kg/h

Individual mass flowrates:

Individual mass flowrate of each component is calculated using the following equation:

$$Individual\ mass\ flowrates = Total\ mass\ flowrate\ \times mass\ composition$$

CO_2 mass flowrate

CO_2 mass flowrate = 3857.71 x 0.40

CO_2 mass flowrate = 1543.08 kg/h

N_2 mass flowrate

N_2 mass flowrate = 3857.71 x 0.595

N_2 mass flowrate = 2295.34 kg/h

O_2 mass flowrate

O_2 mass flowrate = 3857.71 x 0.005

O_2 mass flowrate = 19.29 kg/h

Individual molar flowrates:

Individual molar flowrate of each component is calculated using the following equation:

$$Moles = \frac{Mass\ in\ kg}{Molar\ mass}$$

CO_2 molar flowrate

CO_2 molar flowrate = 1543.08/44

CO_2 molar flowrate = 35.07 kmol/h

N_2 molar flowrate

N_2 molar flowrate = 2295.34/28

N_2 molar flowrate = 81.98 kmol/h

O_2 molar flowrate

O_2 molar flowrate = 19.29/32

O_2 molar flowrate = 0.602 kmol/h

Total molar flowrate:

Total molar flowrate is the sum of all the individual component molar flowrates.

Total molar flowrate = 117.6 kmol/h

Molar composition:

Individual component molar composition is calculated using the following formula:

$$Individual\ molar\ composition = \frac{Individual\ molar\ flowrate}{Total\ molar\ flowrate}$$

CO_2 molar composition

mol% CO_2 = 35.07/117.6

mol% CO_2 = 0.298

N_2 molar composition

mol% N_2 = 81.98/117.6

mol% N_2 = 0.696

O_2 molar composition

mol% O_2 = 0.603/117.6

mol% O_2 = 0.00512

4.1.3 BE (Bottom Entry):

Given Data:

Volumetric flowrate = 1423 m^3/h

Mass composition:

wt% CO_2 = 0.70

wt% N_2 = 0.295

wt% O_2 = 0.005

Density CO_2 , $\rho_{CO2} = 3.35$ kg/m^3

Total density:

The total density of the stream is calculated using the formula:

$$wt\% = \frac{\rho i}{\rho total}$$

Density$_{total}$, ρ_{total} = 3.35/0.70

Density$_{total}$, ρ_{total} = 4.78 kg/m^3

Total mass flowrate:

Total mass flowrate is calculated using the formula:

$$Total\ mass\ flowrate = Volumetric\ flowrate \times Total\ density$$

Total mass flowrate = 1423 x 4.78

Total mass flowrate = 6810.07 kg/h

Individual mass flowrates:

Individual mass flowrate of each component is calculated using the following equation:

$$Individual\ mass\ flowrates = Total\ mass\ flowrate\ \times mass\ composition$$

CO_2 mass flowrate

CO_2 mass flowrate = 6810.07 x 0.70

CO_2 mass flowrate = 4767.05 kg/h

N_2 mass flowrate

N_2 mass flowrate = 6810.07 x 0.295

N_2 mass flowrate = 2008.97 kg/h

O_2 mass flowrate

O_2 mass flowrate = 6810.07 x 0.005

O_2 mass flowrate = 34.05 kg/h

<u>Individual molar flowrates:</u>

Individual molar flowrate of each component is calculated using the following equation:

$$Moles = \frac{Mass\ in\ kg}{Molar\ mass}$$

CO_2 molar flowrate

CO_2 molar flowrate = 4767.05/44

CO_2 molar flowrate = 108.34 kmol/h

N_2 molar flowrate

N_2 molar flowrate = 2008.97/28

N_2 molar flowrate = 71.75 kmol/h

O_2 molar flowrate

O_2 molar flowrate = 34.05/32

O_2 molar flowrate = 1.064 kmol/h

<u>Total molar flowrate:</u>

Total molar flowrate is the sum of all the individual component molar flowrates.

Total molar flowrate = 181.15 kmol/h

<u>Molar composition:</u>

Individual component molar composition is calculated using the following formula:

$$Individual\ molar\ composition = \frac{Individual\ molar\ flowrate}{Total\ molar\ flowrate}$$

CO_2 molar composition

mol% CO_2 = 108.34/181.15

mol% CO_2 = 0.598

N_2 molar composition

mol% N_2 = 71.75/181.15

mol% N_2 = 0.396

O_2 molar composition

mol% O_2 = 1.064/181.15

mol% O_2 = 0.00587

4.1.4 Magma:

Given Data:

Density $_{NH4Cl}$, ρ_{NH4Cl} = 174.3 kg/m^3

Density $_{NH4HCO3}$, $\rho_{NH4HCO3}$ = 77.9 kg/m^3

Density $_{NaHCO3}$, ρ_{NaHCO3} = 273.7 kg/m^3

Density $_{NaCl}$, ρ_{NaCl} = 54.6 kg/m^3

By addition, the total density of the Magma stream will be:

Density $_{Total}$, ρ_{Total} = 580.5 kg/m^3

Mass composition:

To calculate the mass composition of the stream the following equation will be applied on each of the component of the stream:

$$wt\% = \frac{\rho i}{\rho total}$$

NH_4Cl composition

wt% NH_4Cl = 174.3/580.5

wt% NH_4Cl = 0.30

NH_4HCO_3 composition

wt% NH_4HCO_3 = 77.9/580.5

wt% NH_4HCO_3 = 0.134

$NaHCO_3$ composition

wt% $NaHCO_3$ = 273.7/580.5

wt% $NaHCO_3$ = 0.471

NaCl composition

wt% NaCl = 54.6/580.5

wt% NaCl = 0.094

Total mass flowrate:

Since chlorine is present only in the CVL stream and the Magma stream, a chlorine balance can be used to calculate the mass flowrate of the magma. The chorine balance is as follows, where X is the mass flowrate of magma:

$$9779.44 \times 0.567 = x \times 0.3 + x \times 0.094$$

X=14075.36 kg/h

Total mass flowrate = 14075.36 kg/h

Individual mass flowrates:

Individual mass flowrate of each component is calculated using the following equation:

$$Individual\ mass\ flowrates = Total\ mass\ flowrate\ \times mass\ composition$$

NH_4Cl mass flowrate

NH_4Cl mass flowrate = 14075.36 x 0.30

NH_4Cl mass flowrate = 4226.24 kg/h

NH_4HCO_3 mass flowrate

NH_4HCO_3 mass flowrate = 14075.36 x 0.134

NH_4HCO_3 mass flowrate = 1888.83 kg/h

$NaHCO_3$ mass flowrate

$NaHCO_3$ mass flowrate = 14075.36 x 0.471

$NaHCO_3$ mass flowrate = 6636.39 kg/h

NaCl mass flowrate

NaCl mass flowrate = 14075.36 x 0.094

NaCl mass flowrate = 1323.88 kg/h

Individual molar flowrates:

Individual molar flowrate of each component is calculated using the following equation:

$$Moles = \frac{Mass\ in\ kg}{Molar\ mass}$$

NH_4Cl molar flowrate

NH_4Cl molar flowrate = 4226.24/52.5

NH_4Cl molar flowrate = 80.50 kmol/h

NH_4HCO_3 molar flowrate

NH_4HCO_3 molar flowrate = 1888.83/79

NH_4HCO_3 molar flowrate = 23.91 kmol/h

$NaHCO_3$ molar flowrate

$NaHCO_3$ molar flowrate = 6636.39/84

$NaHCO_3$ molar flowrate = 79.005 kmol/h

NaCl molar flowrate

NaCl molar flowrate = 1323.88/58.5

NaCl molar flowrate = 22.63 kmol/h

Total molar flowrate:

Total molar flowrate is the sum of all the individual component molar flowrates.

Total molar flowrate = 206.04 kmol/h

Molar composition:

Individual component molar composition is calculated using the following formula:

$$Individual\ molar\ composition = \frac{Individual\ molar\ flowrate}{Total\ molar\ flowrate}$$

NH_4Cl molar composition

mol% NH_4Cl = 80.50/206.04

mol% NH_4Cl = 0.391

NH_4HCO_3 molar composition

mol% NH_4HCO_3 = 23.91/206.04

mol% NH_4HCO_3 = 0.116

$NaHCO_3$ molar composition

mol% $NaHCO_3$ = 79.005/206.04

mol% $NaHCO_3$ = 0.383

NaCl molar composition

mol% NaCl = 22.63/206.04

mol% NaCl = 0.110

4.1.5 Tower Exit Gas:

Given Data:

Density $_{CO2}$, ρ_{CO2} = 0.152 kg/m^3

Density $_{N2}$, ρ_{N2} = 1.100 kg/m^3

Density $_{O2}$, ρ_{O2} = 0.022 kg/m^3

Density $_{NH3}$, ρ_{NH3} = 0.0005 kg/m^3

By addition, the total density of the Tower Exit Gas stream will be:

Density $_{Total}$, ρ_{Total} = 1.2745 kg/m^3

Mass composition:

To calculate the mass composition of the stream the following equation will be applied on each of the component of the stream:

$$wt\% = \frac{\rho i}{\rho total}$$

CO_2 composition

wt% CO_2 = 0.152/1.2745

wt% CO_2 = 0.119

N_2 composition

wt% N_2 = 1.1/1.2745

wt% N_2 = 0.863

O_2 composition

wt% O_2 = 0.022/1.2745

wt% O_2 = 0.0172

NH_3 composition

wt% NH_3 = 0.0005/1.2745

wt% NH_3 = 0.00039

Total mass flowrate:

Since the mass flowrates of all the other streams are known, the total mass flowrate of the Tower Exit Gas can be calculated by applying an overall material balance on the carbonating tower. The overall material balance is as follows, where x is the mass flowrate of the tower exit gas:

$$9779.44 + 3857.7 + 6810.07 = x + 14075.36$$

x = 6371.86 kg/h

Total mass flowrate = 6371.86 kg/h

Individual mass flowrates:

Individual mass flowrate of each component is calculated using the following equation:

$$Individual\ mass\ flowrates = Total\ mass\ flowrate\ \times mass\ composition$$

CO_2 mass flowrate

CO_2 mass flowrate = 6371.86 x 0.119

CO_2 mass flowrate = 759.92 kg/h

N_2 mass flowrate

N_2 mass flowrate = 6371.86 x 0.863

N_2 mass flowrate = 5499.45 kg/h

O_2 mass flowrate

O_2 mass flowrate = 6371.86 x 0.0172

O_2 mass flowrate = 109.99 kg/h

NH_3 mass flowrate

NH_3 mass flowrate = 6371.86 x 0.00039

NH_3 mass flowrate = 2.499 kg/h

Individual molar flowrates:

Individual molar flowrate of each component is calculated using the following equation:

$$Moles = \frac{Mass\ in\ kg}{Molar\ mass}$$

CO_2 molar flowrate

CO_2 molar flowrate = 759.92/44

CO_2 molar flowrate = 17.27 kmol/h

N_2 molar flowrate

N_2 molar flowrate = 5499.45/28

N_2 molar flowrate = 196.4 kmol/h

O_2 molar flowrate

O_2 molar flowrate = 109.99/32

O_2 molar flowrate = 3.44 kmol/h

NH_3 molar flowrate

NH_3 molar flowrate = 2.499/17

NH_3 molar flowrate = 0.147 kmol/h

Total molar flowrate:

Total molar flowrate is the sum of all the individual component molar flowrates.

Total molar flowrate = 217.26 kmol/h

Molar composition:

Individual component molar composition is calculated using the following formula:

$$Individual\ molar\ composition = \frac{Individual\ molar\ flowrate}{Total\ molar\ flowrate}$$

CO_2 molar composition

mol% CO_2 = 17.27/217.26

mol% CO_2 = 0.079

N_2 molar composition

mol% N_2 = 196.4/217.26

mol% N_2 = 0.904

O_2 molar composition

mol% O_2 = 3.44/217.26

mol% O_2 = 0.0158

NH_3 molar composition

mol% NH_3 = 0.147/217.26

mol% NH_3 = 0.0006768

Chapter - 5

Energy Balance

The overall energy balance is as follows:

$$\Delta H_{reaction} = \Delta H_{products} - \Delta H_{reactants}$$

In the above equation,

$$\Delta H_{products} = Q_{magma} + Q_{TWexitgas}$$

and,

$$\Delta H_{reactants} = Q_{CVL} + Q_{TE} + Q_{BE}$$

where,

$$Q = \dot{m}\, C_p \Delta T$$

5.1 Calculations:

5.1.1 CVL

Given data:

T = 42˚C

T_{ref} = 25˚C

NH_3

m = 743.23 kg/h

C_p at 42˚C = 2.17 kJ/kmol.K

C_p at 25˚C = 2.164 kJ/kmol.K

Avg C_p = 2.167 kJ/kmol.K

Q = m x Cp x ΔT

Q = 743.23 x 2.167 x 17

Q = 27380.12 kJ/h

NH_4HCO_3

m = 3481.48 kg/h

C_p at 42˚C = 1.924 kJ/kmol.K

C_p at 25˚C = 1.913 kJ/kmol.K

Avg C_p = 1.9185 kJ/kmol.K

Q = m x Cp x ΔT

Q = 3481.48 x 1.9185 x 17

Q = 113546.83 kJ/h

NaCl

m = 5550.13 kg/h

C_p at 42˚C = 0.86 kJ/kmol.K

C_p at 25˚C = 0.853 kJ/kmol.K

Avg C_p = 0.8565 kJ/kmol.K

Q = m x Cp x ΔT

Q = 5550.13 x 0.8565 x 17

Q = 80812.66 kJ/h

H_2S

m = 4.596 kg/h

C_p at 42˚C = 1.01 kJ/kmol.K

C_p at 25˚C = 1.003 kJ/kmol.K

Avg C_p = 1.0065 kJ/kmol.K

Q = m x Cp x ΔT

Q = 4.596 x 1.0065 x 17

Q = 78.646 kJ/h

Total heat of stream

Total Q is the sum of all the Qs of the individual components calculated above.

Q_{CVL} = 221818.2778 kJ/h

5.1.2 TE

Given data:

T = 45˚C

T_{ref} = 25˚C

CO_2

m = 1543.083 kg/h

C_p at 45˚C = 0.8697 kJ/kmol.K

C_p at 25˚C = 0.8507 kJ/kmol.K

Avg C_p = 0.8602 kJ/kmol.K

Q = m x Cp x ΔT

Q = 1543.083 x 0.8602 x 20

Q = 26547.21 kJ/h

N_2

m = 2295.34 kg/h

C_p at 45˚C = 1.0418 kJ/kmol.K

C_p at 25˚C = 1.0410 kJ/kmol.K

Avg C_p = 1.0414 kJ/kmol.K

Q = m x Cp x ΔT

Q = 2295.34 x 1.0414 x 20

Q = 47807.27 kJ/h

O_2

m = 19.288 kg/h

C_p at 45˚C = 0.92275 kJ/kmol.K

C_p at 25˚C = 0.9196 kJ/kmol.K

Avg C_p = 0.921175 kJ/kmol.K

Q = m x Cp x ΔT

Q = 19.288 x 0.921175 x 20

Q = 355.36 kJ/h

Total heat of stream

Total Q is the sum of all the Qs of the individual components calculated above.

Q_{TE} = 74709.83 kJ/h

5.1.3 BE

Given data:

T = 30˚C

T_{ref} = 25˚C

CO_2

m = 4767.05 kg/h

C_p at 30˚C = 0.8646 kJ/kmol.K

C_p at 25˚C = 0.8507 kJ/kmol.K

Avg C_p = 0.85765 kJ/kmol.K

Q = m x Cp x ΔT

Q = 4767.05 x 0.85765 x 5

Q = 20442.302 kJ/h

N_2

m = 2008.97 kg/h

C_p at 30˚C = 1.0416 kJ/kmol.K

C_p at 25˚C = 1.0410 kJ/kmol.K

Avg C_p = 1.0413 kJ/kmol.K

Q = m x Cp x ΔT

Q = 2008.97 x 1.0413 x 5

Q = 10459.7 kJ/h

O_2

m = 34.05 kg/h

C_p at 30˚C = 0.92234 kJ/kmol.K

C_p at 25˚C = 0.9196 kJ/kmol.K

Avg C_p = 0.92097 kJ/kmol.K

Q = m x Cp x ΔT

Q = 34.05 x 0.92097 x 5

Q = 156.80 kJ/h

Total heat of stream

Total Q is the sum of all the Qs of the individual components calculated above.

Q_{BE} = 31058.8 kJ/h

5.1.4 Magma

Given data:

T = 30˚C

T_{ref} = 25˚C

NH_4Cl

m = 4226.24 kg/h

C_p at 30˚C = 1.73 kJ/kmol.K

C_p at 25˚C = 1.5719 kJ/kmol.K

Avg C_p = 1.65095 kJ/kmol.K

$Q = m \times Cp \times \Delta T$

Q = 4226.24 x 1.65095 x 5

Q = 34886.60 kJ/h

NH_4HCO_3

m = 1888.83 kg/h

C_p at 30˚C = 1.917 kJ/kmol.K

C_p at 25˚C = 1.913 kJ/kmol.K

Avg C_p = 1.915 kJ/kmol.K

$Q = m \times Cp \times \Delta T$

Q = 1888.83 x 1.913 x 5

Q = 18085.63 kJ/h

$NaHCO_3$

m = 6636.39 kg/h

C_p at 30˚C = 1.0475 kJ/kmol.K

C_p at 25˚C = 1.043 kJ/kmol.K

Avg C_p = 1.04525 kJ/kmol.K

Q = m x Cp x ΔT

Q = 6636.39 x 1.04525 x 5

Q = 34683.45 kJ/h

NaCl

m = 1323.88 kg/h

C_p at 30˚C = 0.855 kJ/kmol.K

C_p at 25˚C = 0.853 kJ/kmol.K

Avg C_p = 0.854 kJ/kmol.K

Q = m x Cp x ΔT

Q = 1323.88 x 0.854 x 5

Q = 5652.98 kJ/h

Total heat of stream

Total Q is the sum of all the Qs of the individual components calculated above.

Q_{MAGMA} = 93308.66 kJ/h

5.1.5 Tower Exit Gas

Given data:

T = 45˚C

T_{ref} = 25˚C

CO_2

m = 759.92 kg/h

C_p at 45˚C = 0.8697 kJ/kmol.K

C_p at 25˚C = 0.8507 kJ/kmol.K

Avg C_p = 0.8602 kJ/kmol.K

Q = m x Cp x ΔT

Q = 759.92 x 0.8602 x 20

Q = 13073.74 kJ/h

N_2

m = 5499.45 kg/h

C_p at 45˚C = 1.0418 kJ/kmol.K

C_p at 25˚C = 1.0410 kJ/kmol.K

Avg C_p = 1.0414 kJ/kmol.K

Q = m x Cp x ΔT

Q = 5499.45 x 1.0414 x 20

Q = 114542.597 kJ/h

O_2

m = 109.99 kg/h

C_p at 45˚C = 0.92275 kJ/kmol.K

C_p at 25˚C = 0.9196 kJ/kmol.K

Avg C_p = 0.921175 kJ/kmol.K

Q = m x Cp x ΔT

Q = 109.99 x 0.921175 x 20

Q = 2026.38 kJ/h

NH_3

m = 2.4997 kg/h

C_p at 45˚C = 2.172 kJ/kmol.K

C_p at 25˚C = 2.164 kJ/kmol.K

Avg C_p = 2.168 kJ/kmol.K

Q = m x Cp x ΔT

Q = 2.4997 x 2.168 x 20

Q = 108.39 kJ/h

Total heat of stream

Total Q is the sum of all the Qs of the individual components calculated above.

$Q_{TWexitgas}$ = 129751.109 kJ/h

5.1.6 Overall Energy Balance

$$\Delta H_{reaction} = \Delta H_{products} - \Delta H_{reactants}$$

Where,

$$\Delta H_{products} = Q_{magma} + Q_{TWexitgas}$$

$\Delta H_{products}$ = 223059.77 kJ/h

and,

$$\Delta H_{reactants} = Q_{CVL} + Q_{TE} + Q_{BE}$$

$\Delta H_{reactants}$ = 327586.92 kJ/h

Therefore,

$\Delta H_{reaction}$ = -104527.15 kJ/h which shows the energy taken by the cooling water of the tower.

Chapter - 6

Yield Improvement

One of the main objectives of this project is the increase of the yield from the carbonating tower. There are some issues in the carbonating tower which, if worked on, can increase the yield from the carbonating tower.

Oxygen coming along with carbon dioxide in TE and BE streams forms deposits of sodium carbamate on the walls of the carbonating towers on reaction with ammonia and brine. These deposits decrease the contact area between CO_2 and NH_4HCO_3, thus decreasing efficiency and yield.

6.1 Recommendations:

There are two recommendations to counter the negative effects that oxygen has on the reactions taking place in the carbonating tower.

Currently, cleaning is performed after every 72 hours to remove the scaling present inside the tower. This time needs to be decreased to 48 hours so that a lot of scale is not accumulated.

Secondly, the coke to limestone ratio which is fed to the kiln to produce CO_2 needs to be adjusted. Currently, the ratio fed is 0.08 due to which 0.5% O_2 is found in the streams going to the carbonating tower as the coke acts as a limiting reactant in its reaction with oxygen and the excess oxygen leaves in the TE and BE streams.

Increasing this ratio up to 0.085 or above will minimize O_2 percentage in the inlets of the carbonating towers while minimizing scaling and increasing yield.

6.1.1 Calculations:

This can be shown by the following calculations:

All calculations are based per hour.

O_2 in TE = 19.28 kg O_2

Mol O_2 = 19.28/32

Mol O_2 = 0.602 kmol O_2

$$C + O_2 \rightarrow CO_2$$

1 kmol of O_2 requires 1 kmol of C for complete reaction.

0.602 kmol of O_2 requires 0.602 kmol of C for complete reaction.

Mass of C = 0.602 x 12

Mass of C = 7.224 kg C

The elemental analysis of coke shows the following composition:

C = 80%

O = 16%

S = 1%

H = 1%

So,

7.224 kg of C = 7.224/0.8 = 9.03 kg of coke

i.e. 9.03 kg of additional coke is required to use up the amount of O_2 that is currently leaving the kiln into the carbonating tower. Under current conditions, 80 kg of coke is being used per hour.

Hence,

80 + 9.03 = 89.03 kg of coke will efficiently burn to give 0% oxygen in outlets of kiln.

89.03 kg coke/1000 kg limestone = 0.08903 (ratio of coke to limestone)

Now as to change the ratio as per stoichiometric calculations,

9.03/2 = 4.515 kg of coke

4.515 x 0.8 = 3.612 kg of C

Moles of C = 3.612/12 = 0.301 kmol C

0.301 kmol of C requires 0.301 kmol of O_2

Mass O_2 = 0.301 x 32 = 9.632 kg of O_2 consumed

In TE we have 19.28 kg of O_2, so

19.28 – 9.632 = 9.648 kg O_2 left

And for CO_2 in TE:

0.301 x 44 = 13.244 kg of CO_2 extra production

The revised composition of the TE stream going into the carbonating tower will be:

CO_2 = 1543.08341 + 13.244

CO_2 = 1556.32741 kg/h

O_2 = 9.648 kg/h

N_2 = 2295.336572 kg/h

Similarly for the BE stream the revised composition will be:

CO_2 = 4767.05 + 13.244

CO_2 = 4780.294 kg/h

O_2 = 34.05 – 9.632

O_2 = 24.418 kg/h

N_2 = 2008.97 kg/h

Chapter - 7

Efficiency Improvement

7.1 Current Efficiency

The thermal efficiency of the carbonating tower can be calculated using the following formula:

$$Efficiency = \frac{Q_C}{Q_H} = \frac{Products}{Cooling\ water}$$

NaCl:

$$Q = m\ C_p \Delta T_1 - m\ C_p \Delta T_2$$

Q = 1500 x 0.8565 x (70-25) – 1323.88480 x 0.854 x (30-25)

Q = 52160.76 kJ/h

NH_4HCO_3:

$$Q = m\ C_p \Delta T_1 - m\ C_p \Delta T_2$$

Q = 2000 x 1.918 x (70-25) – 1888.813 x 1.915 x (30-25)

Q = 154534.376 kJ/h

$NaHCO_3$:

$$Q = m\ C_p \Delta T_1 - m\ C_p \Delta T_2$$

Q = 6460 x 1.048 x (70-25) – 6636.393 x 1.04525 x (30-25)

Q = 269970.15 kJ/h

NH_4Cl:

$$Q = m\, C_p \Delta T_1 - m\, C_p \Delta T_2$$

Q = 4000 x 1.80 x (70-25) – 4226.245 x 1.05 x (30-25)

Q = 289133.479 kJ/h

<u>*Efficiency:*</u>

$$Efficiency = \frac{Q_C}{Q_H} = \frac{Products}{Cooling\ water}$$

Where,

$Q_C = Q_{Products} = Q_{NaHCO3} + Q_{NH4Cl}$

$Q_H = Q_{CoolingWater} = Q_{NaCl} + Q_{NH4HCO3} + Q_{NaHCO3} + Q_{NH4Cl}$

Efficiency = 559103.63/765798.77 x 100%

Efficiency = 73%

This is the thermal efficiency of the carbonating tower on the current operating parameters.

7.2 Increasing Efficiency

Now suppose we aim to increase the efficiency to 81%. The outlet temperature required for the magma to get this efficiency can be calculated as shown below.

$$0.81 = \frac{Q_C}{Q_H} = \frac{Products}{Cooling\ water}$$

$$Q = m\, C_p \Delta T_1 - m\, C_p \Delta T_2$$

Q_C = (32400 – 6973.3042 T + 34866.5212) + (304653.6 – 6936.689 T + 34683.4489)

Q_C = 740153.0042 – 13909.993 T

Q_H = (32400 – 6973.3042 T + 34866.5212) + (304653.6 – 6936.689 T + 34683.4489) + (172620 – 3617.1247 T + 18085.6238) + (57813.75 – 1130.5976 T + 5652.988)

Q_H = 952375.9311 – 18657.71535 T

∴

$$0.81 = \frac{740153.0042 - 13909.993\ \mathrm{T}}{952375.9311 - 18657.71535\ \mathrm{T}}$$

T = 26 ºC

The outlet temperature of the magma should be 26 ºC to achieve an efficiency of 81%.

7.2.1 Recommendation:

Currently, water is being used as a cooling medium to cool the magma being produced. The cooling water reduces the outlet temperature to 30 ºC.

To bring the outlet temperature down to 26 ºC, we recommend the use of ammonia, NH_3, as a cooling medium.

The changes that this will cause on the energy balance are shown below.

7.3 Revised energy balance

Since the energy of only the magma stream will be affected, the detailed calculations for the magma stream are shown.

7.3.1 Magma

Given data:

T = 26˚C

T_{ref} = 25˚C

NH_4Cl

m = 4226.24 kg/h

C_p at 26˚C = 1.62 kJ/kmol.K

C_p at 25˚C = 1.5719 kJ/kmol.K

Avg C_p = 1.59595 kJ/kmol.K

Q = m x Cp x ΔT

Q = 4226.24 x 1.59595 x 1

Q = 6744.876 kJ/h

NH_4HCO_3

m = 1888.83 kg/h

C_p at 26˚C = 1.914 kJ/kmol.K

C_p at 25˚C = 1.913 kJ/kmol.K

Avg C_p = 1.9135 kJ/kmol.K

Q = m x Cp x ΔT

Q = 1888.83 x 1.9135 x 1

Q = 3614.29 kJ/h

$NaHCO_3$

m = 6636.39 kg/h

C_p at 26˚C = 1.044 kJ/kmol.K

C_p at 25˚C = 1.043 kJ/kmol.K

Avg C_p = 1.0435 kJ/kmol.K

Q = m x Cp x ΔT

Q = 6636.39 x 1.0435 x 1

Q = 3614.29 kJ/h

NaCl

m = 1323.88 kg/h

C_p at 26˚C = 0.8533 kJ/kmol.K

C_p at 25˚C = 0.853 kJ/kmol.K

Avg C_p = 0.85315 kJ/kmol.K

Q = m x Cp x ΔT

Q = 1323.88 x 0.85315 x 1

Q = 1129.47 kJ/h

Total heat of stream

Total Q is the sum of all the Qs of the individual components calculated above.

Q_{MAGMA} = 18413.72 kJ/h

7.3.2 Overall Energy Balance

$$\Delta H_{reaction} = \Delta H_{products} - \Delta H_{reactants}$$

Where,

$$\Delta H_{products} = Q_{magma} + Q_{TWexitgas}$$

$\Delta H_{products}$ = 148164.8255 kJ/h

and,

$$\Delta H_{reactants} = Q_{CVL} + Q_{TE} + Q_{BE}$$

$\Delta H_{reactants}$ = 327586.92 kJ/h

Therefore,

$\Delta H_{reaction}$ = -179422.0987 kJ/h which shows the energy taken by the cooling water of the tower.

Chapter – 8

Simulation

Simulation of the whole process in the Carbonating tower was originally decided to be performed in ASPEN HYSYS. Due to unavailability of few components in Aspen HYSYS, ASPEN PLUS was opted instead.

In Aspen PLUS there is an option to create a component by drawing its molecular structure. Ammonium Carbonate wasn't available in Aspen Properties of Components.

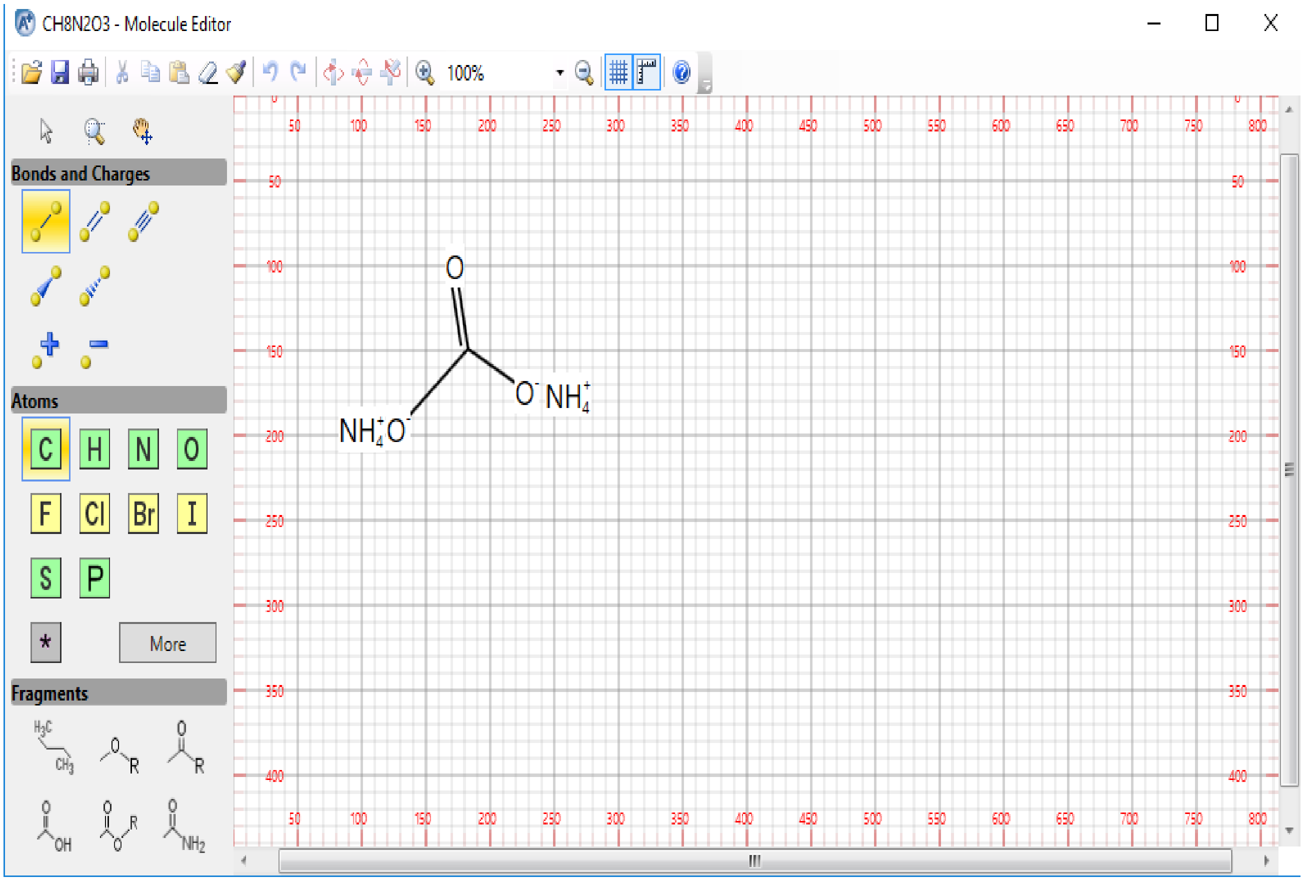


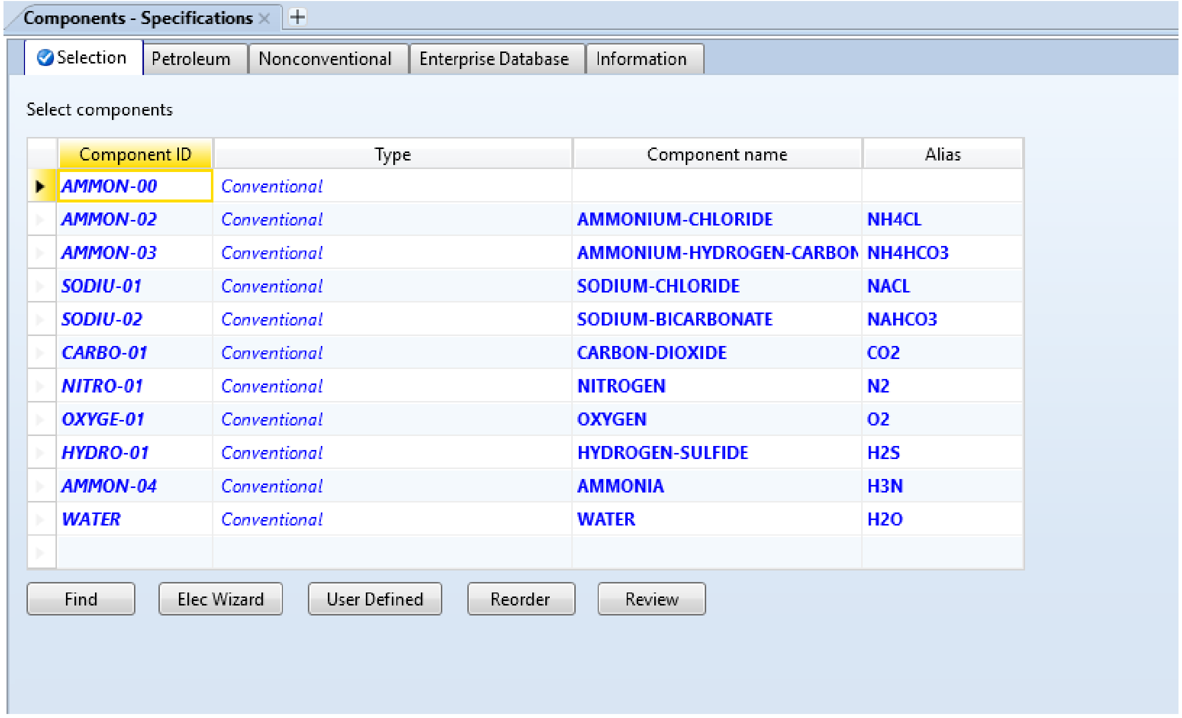
Fig 8.1 – Molecule Editor

All the properties of Ammonium Carbonate were achieved and then the modeling in ASPEN PLUS was started.

8.1 Component list

According to the data provided, 11 components were required which are as follows:

Ammonium Carbonate	$(NH_4)_2CO_3$	AMMON-00
Ammonium Chloride	(NH_4Cl)	AMMON-02
Ammonium Bicarbonate	(NH_5CO_3)	AMMON-03
Ammonia	(NH_3)	AMMON-04
Sodium Chloride	(NaCl)	SODIU-01
Sodium Bicarbonate	$(NaHCO_3)$	SODIU-02
Carbon dioxide	(CO_2)	CARBO-01
Nitrogen	(N_2)	NITRO-01
Oxygen	(O_2)	OXYGE-01
Hydrogen Sulfide	(H_2S)	HYDRO-01
Water	(H_2O)	WATER



Select components

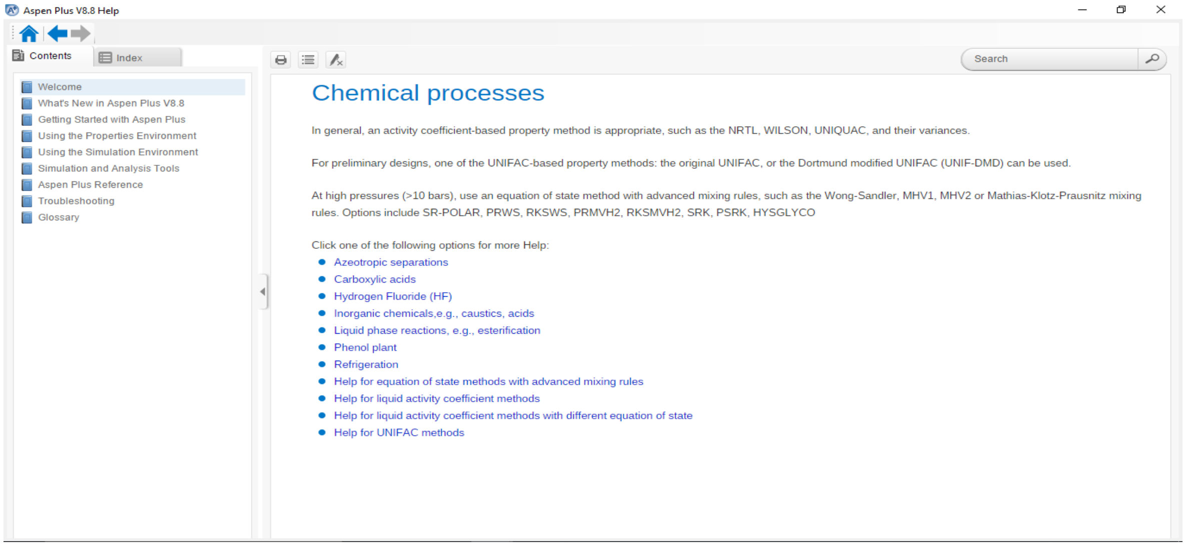
Component ID	Type	Component name	Alias
AMMON-00	Conventional		
AMMON-02	Conventional	AMMONIUM-CHLORIDE	NH4CL
AMMON-03	Conventional	AMMONIUM-HYDROGEN-CARBON	NH4HCO3
SODIU-01	Conventional	SODIUM-CHLORIDE	NACL
SODIU-02	Conventional	SODIUM-BICARBONATE	NAHCO3
CARBO-01	Conventional	CARBON-DIOXIDE	CO2
NITRO-01	Conventional	NITROGEN	N2
OXYGE-01	Conventional	OXYGEN	O2
HYDRO-01	Conventional	HYDROGEN-SULFIDE	H2S
AMMON-04	Conventional	AMMONIA	H3N
WATER	Conventional	WATER	H2O

Fig 8.2 – Component list

8.2 Property package

Property package is chosen according to the components and the operating conditions. NRTL was used as the property package for the process and STEAMNBS for cooling water purpose.

With the help of Method Assistant, Chemical system was defined as the process type and NRTL, WILSON, UNIQUAC and their variances were shown as the available property package. NRTLD was selected for the process.



Chemical processes

In general, an activity coefficient-based property method is appropriate, such as the NRTL, WILSON, UNIQUAC, and their variances.

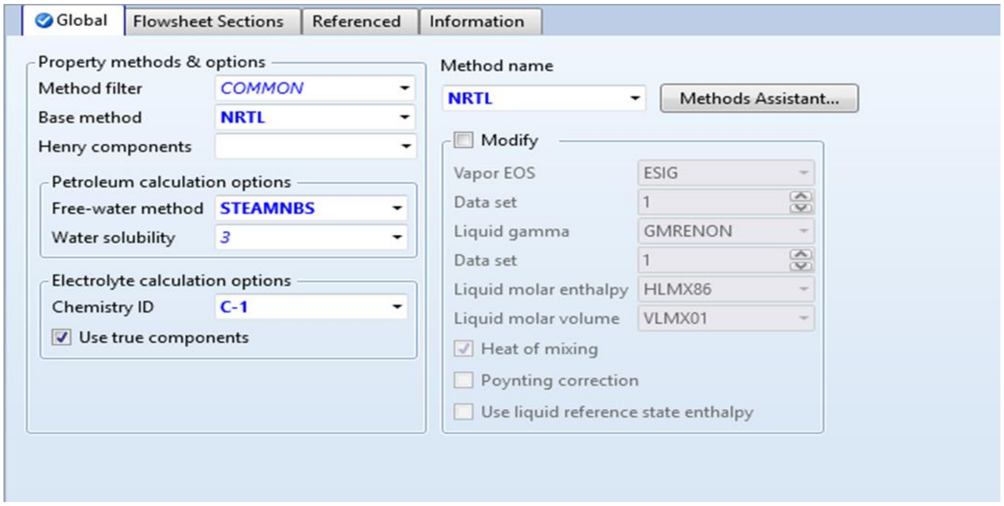
For preliminary designs, one of the UNIFAC-based property methods: the original UNIFAC, or the Dortmund modified UNIFAC (UNIF-DMD) can be used.

At high pressures (>10 bars), use an equation of state method with advanced mixing rules, such as the Wong-Sandler, MHV1, MHV2 or Mathias-Klotz-Prausnitz mixing rules. Options include SR-POLAR, PRWS, RKSWS, PRMVH2, RKSMVH2, SRK, PSRK, HYSGLYCO

Click one of the following options for more Help:

- Azeotropic separations
- Carboxylic acids
- Hydrogen Fluoride (HF)
- Inorganic chemicals,e.g., caustics, acids
- Liquid phase reactions, e.g., esterification
- Phenol plant
- Refrigeration
- Help for equation of state methods with advanced mixing rules
- Help for liquid activity coefficient methods
- Help for liquid activity coefficient methods with different equation of state
- Help for UNIFAC methods

Fig 8.3 – Aspen Plus Method Assistant



Property methods & options
Method filter: COMMON
Base method: NRTL
Henry components:

Petroleum calculation options
Free-water method: STEAMNBS
Water solubility: 3

Electrolyte calculation options
Chemistry ID: C-1
☑ Use true components

Method name: NRTL

☐ Modify
Vapor EOS: ESIG
Data set: 1
Liquid gamma: GMRENON
Data set: 1
Liquid molar enthalpy: HLMX86
Liquid molar volume: VLMX01
☑ Heat of mixing
☐ Poynting correction
☐ Use liquid reference state enthalpy

Fig 8.4 – Property method selection

8.3 Simulation Environment

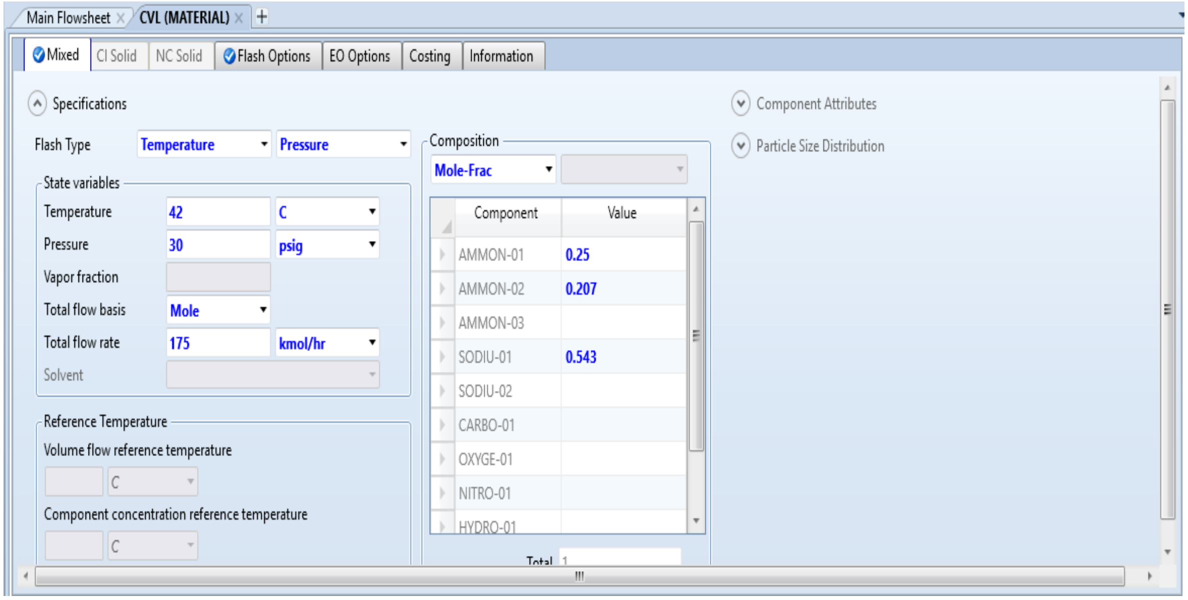
Simulation Environment was then activated. The carbonating tower is a tall vertical vessel in which reaction and cooling is taking place. In ASPEN PLUS, the model of a carbonating tower was not available.

A strategy was devised in which the reaction chamber in carbonating tower was considered as a reactor and for cooling purpose a heat exchanger was applied which acts as a cooler.

Firstly, all the input streams to reactor were defined. There are 3 input stream of reactor in total named as:

1. Carbonated VAT liquor (CVL)
2. Top Entry (TE)
3. Bottom Entry (BE)

- **Carbonated VAT Liquor**



Flash Type: Temperature, Pressure

State variables

Temperature: 42 C

Pressure: 30 psig

Vapor fraction:

Total flow basis: Mole

Total flow rate: 175 kmol/hr

Solvent:

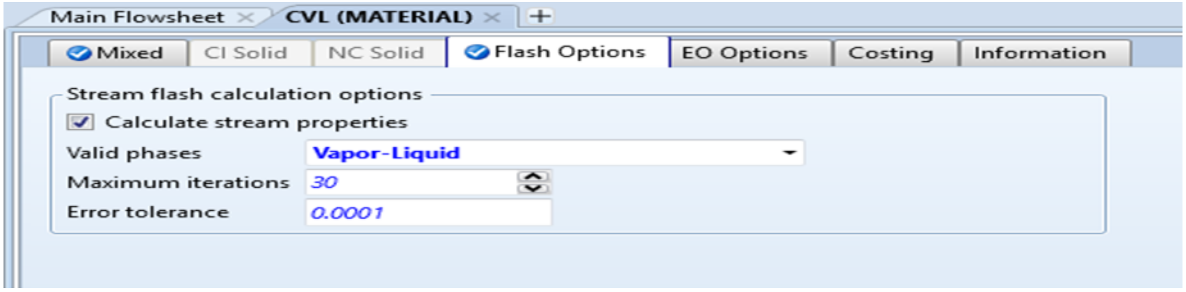
Composition: Mole-Frac

Component	Value
AMMON-01	0.25
AMMON-02	0.207
AMMON-03	
SODIU-01	0.543
SODIU-02	
CARBO-01	
OXYGE-01	
NITRO-01	
HYDRO-01	

Total 1

Fig 8.5 – CVL Specifications

This shows the Conditions of this stream including Temperature, Pressure, Flow rate, and Composition. The Flash option shows the phase of the material stream

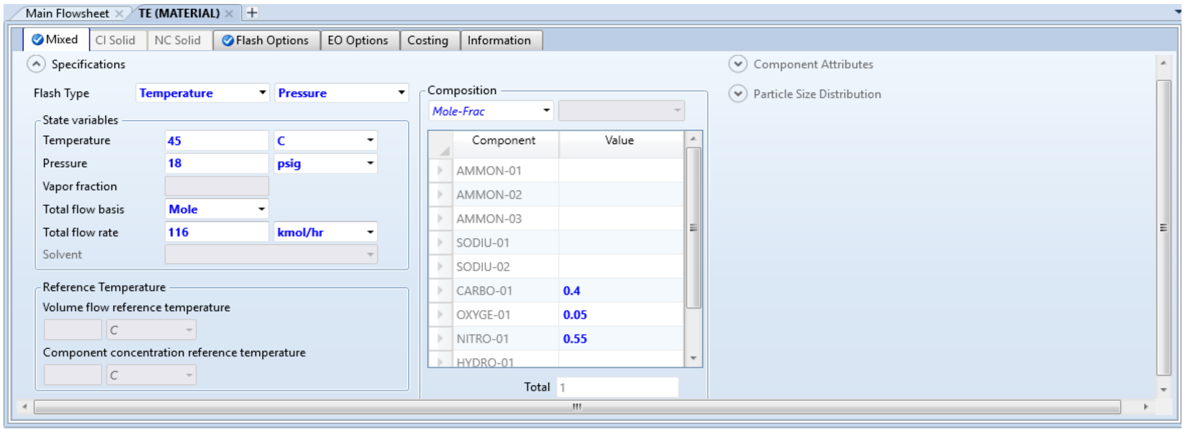


☑ Calculate stream properties
Valid phases: Vapor-Liquid
Maximum iterations: 30
Error tolerance: 0.0001

Fig 8.6 – CVL Flash Options

- **Top Entry**

This shows the Conditions of this stream including Temperature, Pressure, Flow rate, and Composition.

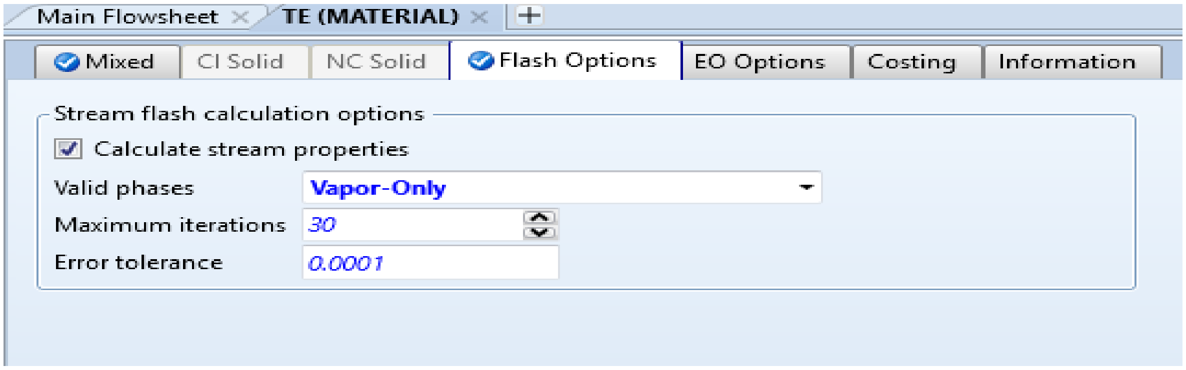


Flash Type: Temperature, Pressure
Temperature: 45 C
Pressure: 18 psig
Vapor fraction:
Total flow basis: Mole
Total flow rate: 116 kmol/hr
Solvent:
Volume flow reference temperature: C
Component concentration reference temperature: C
Mole-Frac

Component	Value
AMMON-01	
AMMON-02	
AMMON-03	
SODIU-01	
SODIU-02	
CARBO-01	0.4
OXYGE-01	0.05
NITRO-01	0.55
HYDRO-01	

Total 1

Fig 8.7 – TE Specifications

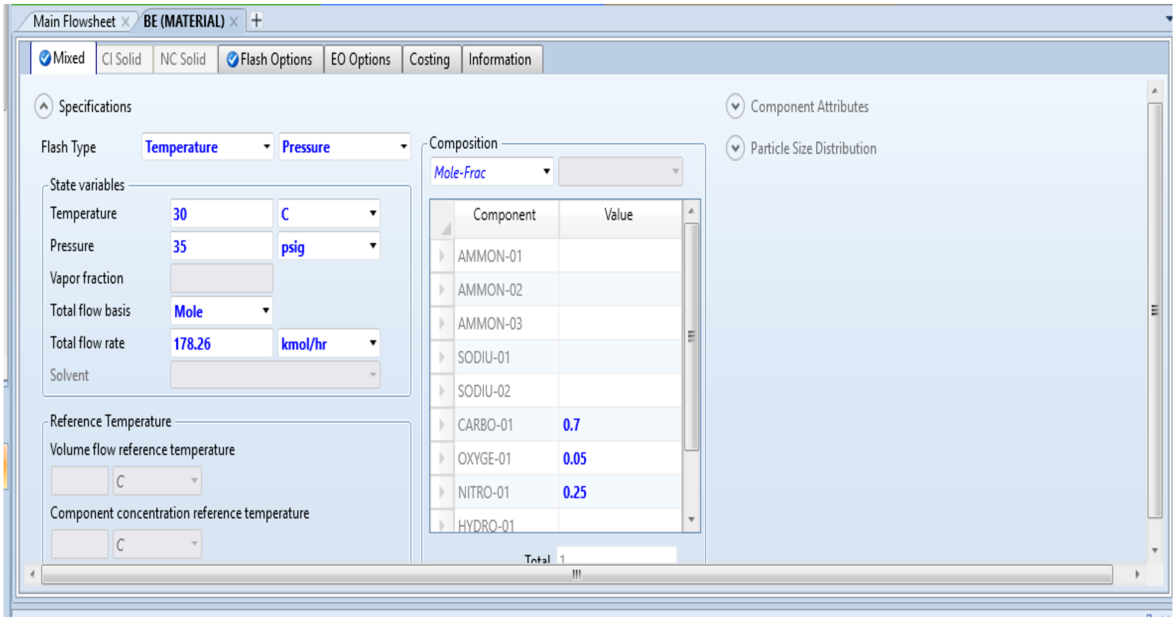


☑ Calculate stream properties
Valid phases: Vapor-Only
Maximum iterations: 30
Error tolerance: 0.0001

Fig 8.8 – TE Flash Options

- **Bottom Entry**

The stream conditions are specified as below along with the valid phase:



Flash Type: Temperature, Pressure

State variables

Temperature: 30 C

Pressure: 35 psig

Vapor fraction:

Total flow basis: Mole

Total flow rate: 178.26 kmol/hr

Solvent:

Reference Temperature

Volume flow reference temperature: C

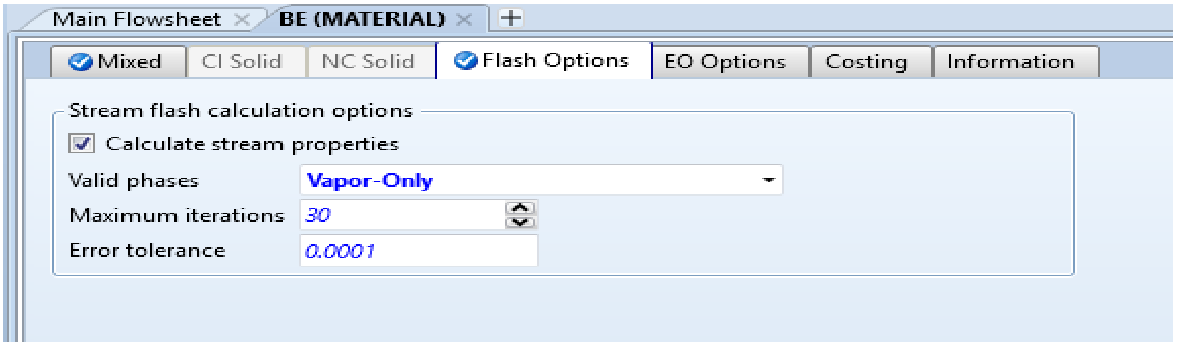
Component concentration reference temperature: C

Composition: Mole-Frac

Component	Value
AMMON-01	
AMMON-02	
AMMON-03	
SODIU-01	
SODIU-02	
CARBO-01	0.7
OXYGE-01	0.05
NITRO-01	0.25
HYDRO-01	

Total: 1

Fig 8.9 – BE Specifications



Stream flash calculation options

☑ Calculate stream properties

Valid phases: Vapor-Only

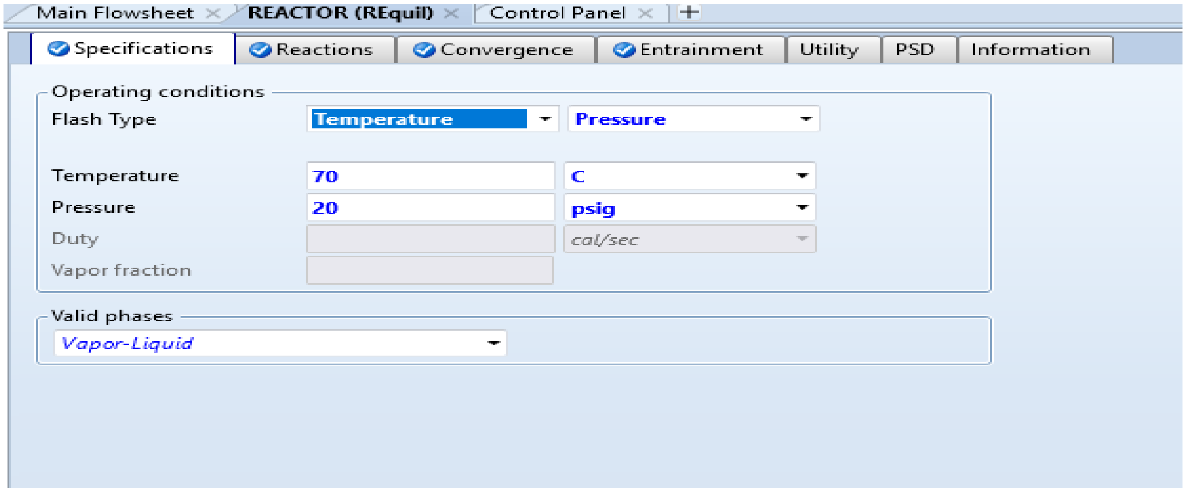
Maximum iterations: 30

Error tolerance: 0.0001

Fig 8.10 – BE Flash Options

After specifying the inlet streams, a simple reactor was selected known as Equilibrium Reactor (REquill).

The temperature and pressure conditions are inserted to this reactor. The temperature provided is high because this is the maximum temperature to which the reaction will go.



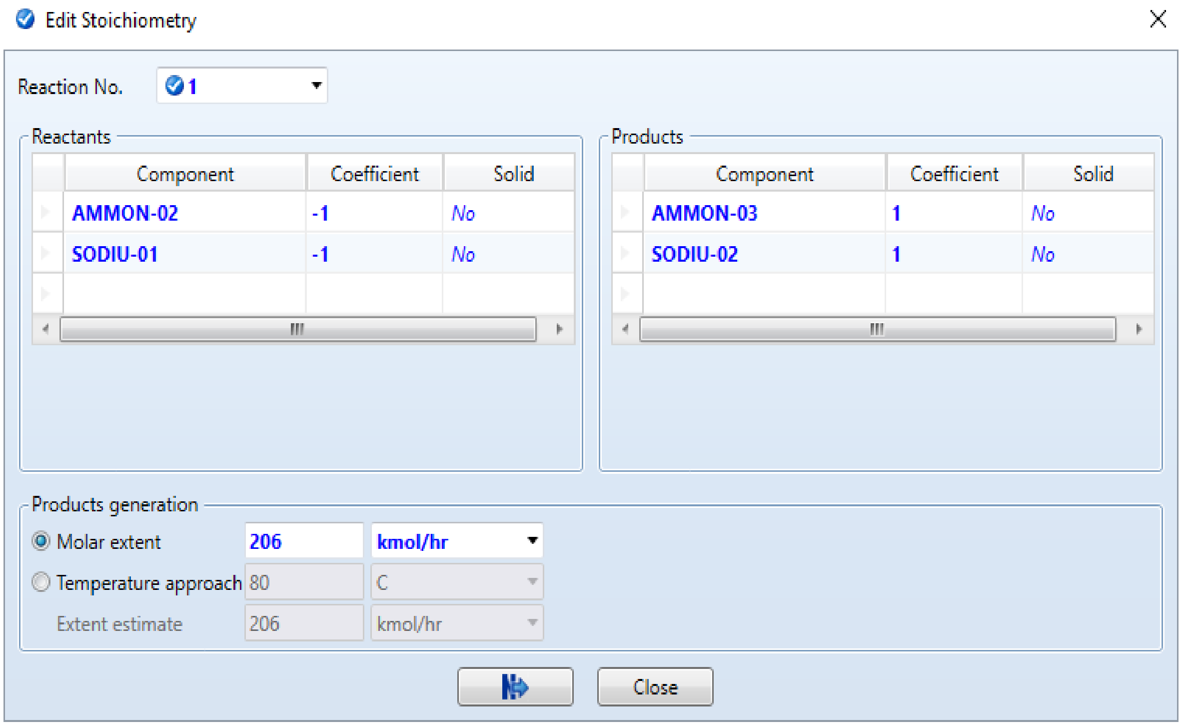
Operating conditions

Flash Type	Temperature	Pressure
Temperature	70	C
Pressure	20	psig
Duty		cal/sec
Vapor fraction		

Valid phases: Vapor-Liquid

Fig 8.11 – Reactor Specifications

After providing the conditions, the reaction in the reactor was set which involves Sodium Chloride and Ammonium Bicarbonate as reactants and Sodium Bicarbonate and Ammonium Chloride as products.



Reaction No. 1

Reactants

Component	Coefficient	Solid
AMMON-02	-1	No
SODIU-01	-1	No

Products

Component	Coefficient	Solid
AMMON-03	1	No
SODIU-02	1	No

Products generation

● Molar extent	206	kmol/hr
○ Temperature approach	80	C
Extent estimate	206	kmol/hr

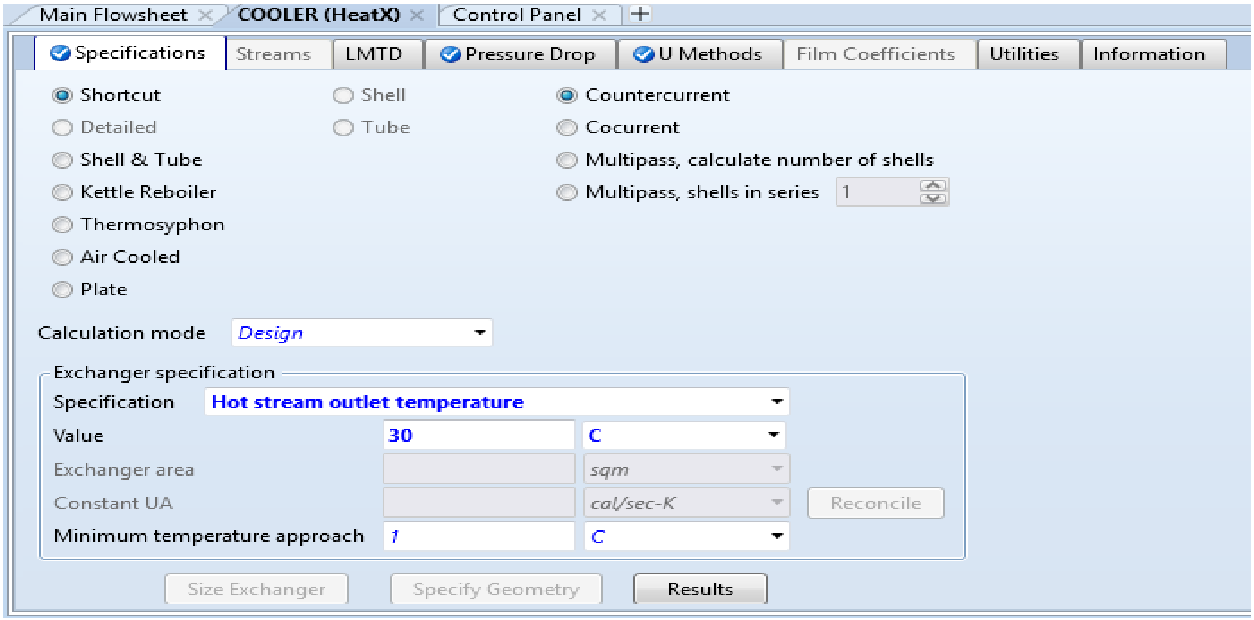
Fig 8.12 – Reaction Set

The outlets of this reactor are two streams named as

- Product
- TW Exit Gas

Product mainly contains the main product, by product and unreacted components. In TW Exit Gas stream, Carbon Dioxide, Oxygen and Nitrogen are present.

A General Heat Exchanger was then inserted for the purpose of cooling and cooling water stream (CW) was introduced as cooling agent. Shortcut Model Fidelity was selected with counter current flow direction. The desired outlet temperature of product was around 300C.



● Shortcut
○ Detailed
○ Shell & Tube
○ Kettle Reboiler
○ Thermosyphon
○ Air Cooled
○ Plate

○ Shell
○ Tube

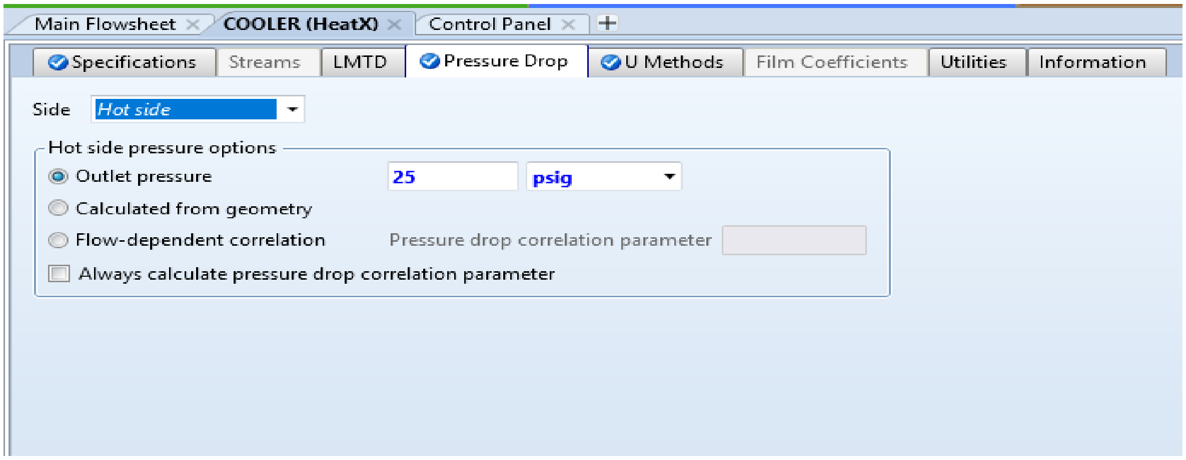
● Countercurrent
○ Cocurrent
○ Multipass, calculate number of shells
○ Multipass, shells in series 1

Calculation mode: Design

Exchanger specification
Specification: Hot stream outlet temperature
Value: 30 C
Exchanger area: sqm
Constant UA: cal/sec-K
Minimum temperature approach: 1 C

Fig 8.13 – Cooler Specifications

Pressure drop across the cooler is considered to be as minimum as possible so almost the similar outlet pressure of product stream is selected for MAGMA stream.



Side: Hot side

Hot side pressure options

● Outlet pressure 25 psig

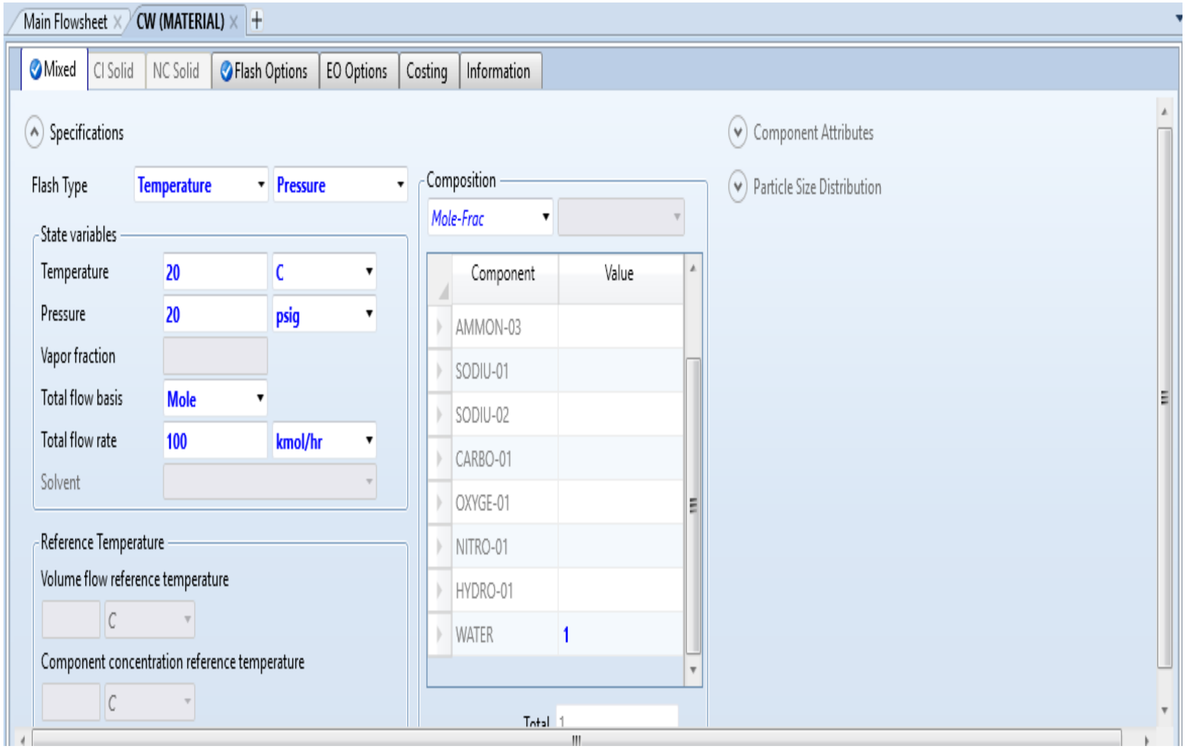
○ Calculated from geometry

○ Flow-dependent correlation — Pressure drop correlation parameter

☐ Always calculate pressure drop correlation parameter

Fig 8.14 – Cooler Pressure drop

After this the operating parameters were entered on the last inlet stream that is CW (cooling water) stream entering into heat exchanger.



Flash Type: Temperature, Pressure

State variables

Temperature: 20 C

Pressure: 20 psig

Vapor fraction:

Total flow basis: Mole

Total flow rate: 100 kmol/hr

Solvent:

Reference Temperature

Volume flow reference temperature: C

Component concentration reference temperature: C

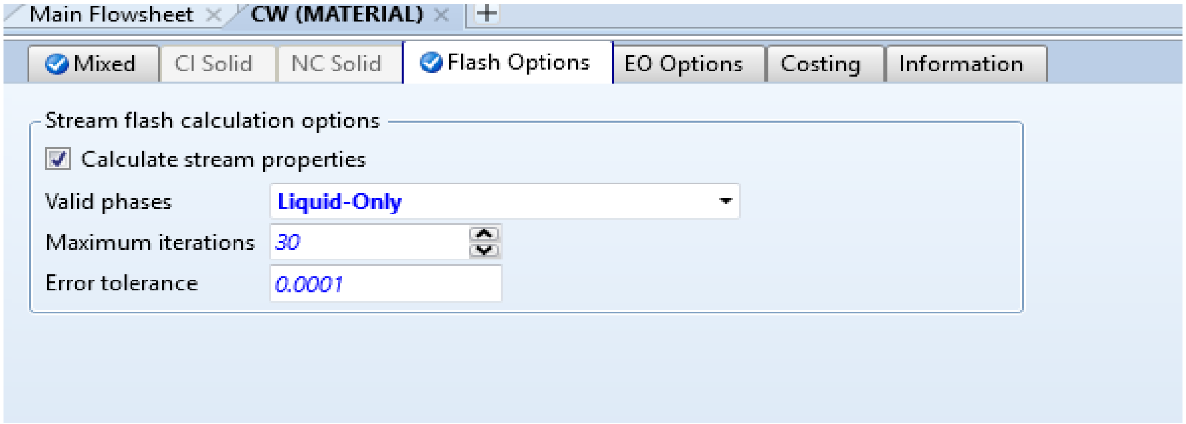
Composition: Mole-Frac

Component	Value
AMMON-03	
SODIU-01	
SODIU-02	
CARBO-01	
OXYGE-01	
NITRO-01	
HYDRO-01	
WATER	1

Total: 1

Fig 8.15 – CW Specifications

The liquid phase is the valid phase in the Flash Option



Stream flash calculation options

☑ Calculate stream properties

Valid phases: Liquid-Only

Maximum iterations: 30

Error tolerance: 0.0001

Fig 8.16 – CW Flash Options

After completing all the input specification for all streams and blocks. Simulation was run, which gave few warnings like

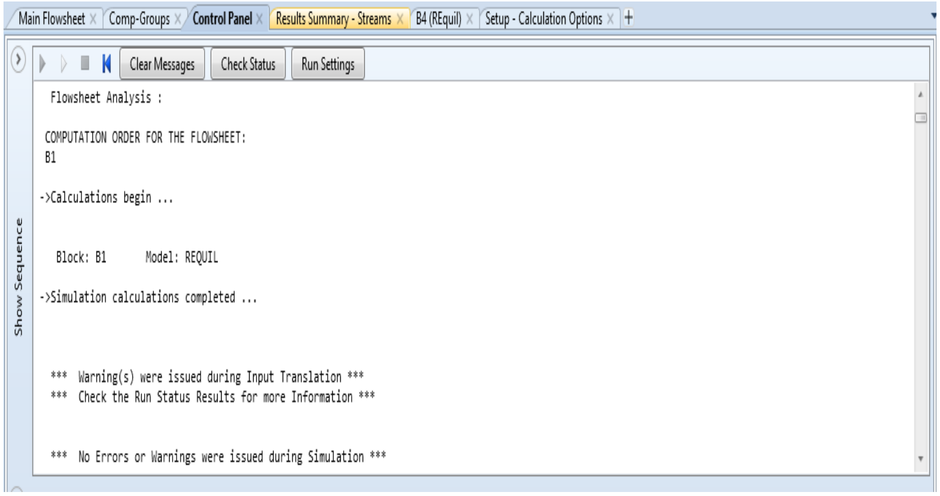
“** WARNING

DGFORM of AMMON_02 is not specified

the flash calculation will not be completed”

Such warnings are removed by providing heat of formation of that particular component in parameters tab and adding a pure new parameter which is scalar. DGFORM is added as new parameter and the component and its heat of formation is entered into the cell.

Again running the simulation provided the full results without any error.



```
 Flowsheet Analysis :

COMPUTATION ORDER FOR THE FLOWSHEET:
B1

->Calculations begin ...


  Block: B1       Model: REQUIL

->Simulation calculations completed ...



 ***  Warning(s) were issued during Input Translation ***
 ***  Check the Run Status Results for more Information ***


 ***  No Errors or Warnings were issued during Simulation ***
```

Fig 8.17 – Control Panel

The complete results were obtained at the end in the form of table as shown below:

Heat and Material Balance Table									
Stream ID		BE	CVL	CW	CWR	MAGMA	PRODUCT	TE	TWEXIT
From					COOLER	COOLER	REACTOR		REACTOR
To		REACTOR	REACTOR	COOLER			COOLER	REACTOR	
Phase		VAPOR	MIXED	LIQUID	LIQUID	MIXED	LIQUID	VAPOR	VAPOR
Substream: MIXED									
Mole Flow	kmol/hr								
AMMON-01		0.0	43.75000	0.0	0.0	0.0	0.0	0.0	0.0
AMMON-02		0.0	36.22492	0.0	0.0	23.89600	23.89600	0.0	0.0
AMMON-03		0.0	7.72218E-5	0.0	0.0	80.50480	80.50480	0.0	0.0
SODIU-01		0.0	95.02492	0.0	0.0	22.61880	22.61880	0.0	0.0
SODIU-02		0.0	7.72218E-5	0.0	0.0	78.98040	78.98040	0.0	0.0
CARBO-01		124.7820	0.0	0.0	0.0	0.0	0.0	46.40000	17.38080
OXYGE-01		8.913000	0.0	0.0	0.0	0.0	0.0	5.800000	3.476160
NITRO-01		44.56500	0.0	0.0	0.0	0.0	0.0	63.80000	196.4030
HYDRO-01		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER		0.0	0.0	100.0000	100.0000	0.0	0.0	0.0	0.0
Total Flow	kmol/hr	178.2600	175.0000	100.0000	100.0000	206.0000	206.0000	116.0000	217.2600
Total Flow	kg/hr	7025.257	9162.373	1801.528	1801.528	14152.21	14152.21	4014.908	6378.091
Total Flow	l/min	21636.42	10635.51	31.10342	31.94829	16029.85	1031.873	22626.81	34985.96
Temperature	C	30.00000	42.00000	20.00000	49.00000	50.00000	50.00000	45.00000	45.00000
Pressure	bar	3.426415	3.081677	2.392201	2.392201	2.736939	3.426415	2.254306	2.736939
Vapor Frac		1.000000	.4570003	0.0	0.0	.5000000	0.0	1.000000	1.000000
Liquid Frac		0.0	.5429997	1.000000	1.000000	.5000000	1.000000	0.0	0.0
Solid Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-65771.84	-95549.77	-69096.47	-68495.83	-34247.91	-1.5686E+5	-37447.56	-7381.059
Enthalpy	cal/gm	-1668.905	-1824.987	-3835.437	-3802.096	-498.5137	-2283.250	-1081.947	-251.4246
Enthalpy	cal/sec	-3.2568E+6	-4.6448E+6	-1.9193E+6	-1.9027E+6	-1.9597E+6	-8.9758E+6	-1.2066E+6	-4.4545E+5
Entropy	cal/mol-K	-.3689825	68.75979	-39.27201	-37.57445	-23.77357	-33.86872	.8513587	-.7552921
Entropy	cal/gm-K	-9.3626E-3	1.313302	-2.179928	-2.085699	-.3460488	-.4929941	.0245977	-.0257278
Density	mol/cc	1.37315E-4	2.74239E-4	.0535846	.0521676	2.14184E-4	3.32728E-3	8.54444E-5	1.03499E-4
Density	gm/cc	5.41160E-3	.0143581	.9653428	.9398145	.0147144	.2285846	2.95734E-3	3.03841E-3
Average MW		39.41017	52.35642	18.01528	18.01528	68.70005	68.70005	34.61127	29.35695
Liq Vol 60F	l/min	159.1202		30.08333	30.08333			103.5451	193.9328

Table 8.1 – Aspen PLUS Heat and Material Balance

Chapter - 9

HSE Aspects and HAZOP Study

9.1 Health, safety and environment aspects:

Following is some information related to HSE aspects of Towers:

Hazards

- Ammonia
- Steam

Ammonia

- Flammable gas
- Toxic, if inhaled
- Causes severe skin burns & eye damage
- Corrosive to the respiratory tract

Precautions for Ammonia

- Operators must wear goggles while collecting samples
- They must use rubber sucker with pipette while taking samples
- Gas mask must be used while operating ammonia cylinder
- PPEs compliance must be observed i.e. gloves, proper clothing, eye protection must be used while sieves, pumps, PHEs changeovers

Steam

- Causes severe skin burns

Precautions for Steam

- Avoid touching hot surfaces

- Wear proper clothing, i.e. full sleeves
- Use gloves while operating valves

First aid measures for Ammonia

Inhalation	Remove victim to uncontaminated area. Call a doctor. Apply artificial respiration if breathing stopped
Skin contact	In case of contact, immediately flush affected areas with plenty of water for at least 15 minutes while removing contaminated clothing and shoes
Eye contact	Immediately flush eyes thoroughly with water for at least 15 minutes

Suitable Extinguishing Media:

Carbon dioxide, Dry chemical, Water spray or fog.

9.2 HAZOP Study

Any association has a lawful commitment to shield the wellbeing and welfare of its workers and the overall population. Security is likewise a decent business. The great administration requirements expected to guarantee safe operation will beyond any doubt result in effective operation.

The sheltered operation of a process relies on the built of the machinery and on great working practice. It is essential that every administrator knows about the working of the material in his procedure range, that he knows the risks to his own and to other individuals wellbeing, or fire and blast threat, and that he knows defensive measures to take.

To consider the wellbeing of any procedure, the following points must be considered.

- Identification of the hazards.
- Control of the hazards.
- Control of the process.
- Limitations of the loss.

9.2.1 Safety of the Personnel:

Prevention:

The best assurance of the wellbeing of the individual is to avoid the event of any unsafe circumstances. Under typical conditions, there will be no gases, vapor, fluid or chemicals released in the environment.

At the point when a break is created, it ought to be ceased or repaired on the double. On the off chance that this ought not be conceivable, different means must be connected to forestall spreading, to counteract mischance to work force and to keep away from harm to hardware.

Health Hazards:

At the point when a man harmed by the outer contact, inward breath or oral infusion of the poisonous substance, the medical aid directions for that compound must be taken without a moment's delay. Consequently, it is most essential that all individuals know about these medical aid guidelines.

Protective equipment:

At the point when the defensive gear is important it must be utilized appropriately. The hardware chosen must be suited for the reason and the individual utilizing the defensive gear must be comfortable with it. All defensive hardware for the wellbeing of individual must be kept in great working conditions at record-breaking.

Eye protection:

Goggles and face shields will be given to every administrator. He should be comfortable with the area and the utilization of eye shower and security showers should be done.

Respiratory protection:

All gases other than air are destructive to people when breathed in adequate fixation. Dangerous gases might be named either suffocating or bothering.

Suffocating gases might bring about death by displacing air in lungs or by responding with O_2 conveyed in the blood. e.g., H_2S, CO_2, Smoke. Disturbing gases might bring about harm or passing by suffocation as well as both inner and consuming (e.g. Cl_2, SO_2, HF).

To guard against the inhalation of harmful gases the operator should,

- Score a gas test certification showing the gas conditions of the atmosphere (vessel).
- Avoid standing on the side of an opening where escaping gas will be blown towards him.
- Provide ventilation.
- Wear the gas mask when required.

Foot Protection:

It is prescribed to utilize shoes of ideal cowhide with an implicit steel toe top. Whenever important, boot of unique substance safe material can be put on.

Head Protection:

Security must be forever utilized inside the plant, particularly repairing is being made and there is plausibility devices and materials mishap.

Skin and Hand protection:

Suits made of engineered elastic or other endorsed material might be worn when finish body insurance is essential, gloves made of manufactured elastic or other affirmed material ought to be worn to ensure the hands. In the event of extreme releases just legitimately secured individual ought to stay in the territory.

9.2.2 HAZOP

Introduction:

A HAZOP think about distinguishes risks and Operability issues. The idea includes researching how the plant may go astray from the outline purpose. On the off chance that, during the time spent distinguishing issues amid a HAZOP examine, an answer winds up plainly clear, it is recorded as a major aspect of the HAZOP result; in any case, mind must be taken to abstain from attempting to discover arrangements which are not all that evident, on the grounds that the prime goal for the HAZOP is issue recognizable proof. Despite the fact that the HAZOP study was the created to supplement encounter based practices when another outline or innovation is included, its utilization has a few specialists with various foundations can cooperate and recognize a larger number of issues when cooperating than when working independently and joining their outcomes.

Hazard:

Any operation that could possibly cause a release of toxic, flammable or explosive chemicals or any action that could result in injury to personal or harm to the environment.

Operability:

Any operation inside the design envelope that would cause a shutdown that could possibly lead to a violation of environmental, health or safety regulations or negatively impact profitability.

When to perform a HAZOP?

The HAZOP study ought to ideally be completed as right on time in the outline stage as could be allowed, to have impact on the plan. Then again; to do a HAZOP we require a fairly total outline. As a bargain, the HAZOP is generally done as a last check when the definite outline has been finished. A HAZOP study may likewise be directed on a current office to distinguish adjustments that ought to be executed to decrease hazard and Operability prepare.

Success or failure of HAZOP:

The success or failure of the HAZOP depends on several factors

- The completeness and accuracy of drawings and other data used as a basis for the study.
- The technical skills insights of the team.
- The ability of the team to use the approach as an aid to their imagination in visualizing deviations, causes, and consequences.
- The ability of the team to concentrate on the more serious hazards which are identified.
- The process is systematic and it is helpful to define the terms that are used.

Study nodes:

The locations (on piping and instrumentation drawings and procedures) at the process parameters are investigated for deviation.

Intention:

The intention defines how the plant is expected to operate in the absence of deviations at the study nodes. This can take a number of forms and can either be descriptive or diagrammatic; e.g. flow sheets, line diagrams, P&IDs.

Deviations:

These are departures from the intention which are discovered by systematically applying the guide words (e.g. more pressure).

Causes:

These are the reasons why deviations might occur. Once a deviation has been shown to have a credible cause, it can be treated as a meaningful deviation. These cause can be hardware failures, human errors, an unanticipated process state (e.g., change of composition), external disruptions (e.g. loss of power), etc.

Consequences:

These are the results of the deviations should they occur (e.g. release of toxic materials). Trivial consequences, relative to the study objective, are dropped.

Guide words:

These are straightforward words which are utilized to qualify or evaluate the aim with a specific end goal to direct and strengthen the conceptualizing procedure thus find deviations. The guide words appeared in Table are the ones frequently utilized as a part of a HAZOP; a few associations have made this rundown particular to their operations, to manage the group all the more rapidly to the regions where they have already discovered issues. Each guide word is connected to the procedure factors at the point in the plant which is being analyzed.

Table 9.2.3 - HAZOP on transfer of cooling water to cooling boxes:

	Guide Words	**Parameter**	**Deviation**	**Causes**	**Consequences**
1	No	Flow	No flow	Control Valve struck closed, Water supply failed , Control Valve is Fail to close,	Temperature increases, by-product formation
2	More	Flow	More flow	Control Valve is fail to open	Reaction temperature can’t be maintained
3	Less	Flow	Less flow	Control Valve is partially opened	Diminished cooling and possible runaway
4	Reverse	flow	Reverse flow	Failure of water supply causes reverse flow	Diminished cooling and possible runaway

Table 9.2.4 - HAZOP on ammonia running through the plant:

	Guide Words	**Parameter**	**Deviation**	**Causes**	**Consequences**
1	No	Flow	No flow	Control Valve struck closed, Ammonia supply failed , Control Valve is Fail to close,	Reaction ceases.
2	More	Flow	More flow	Control Valve is fail to open	Excess ammonia, resulting in possible leakage and hazards.
3	Less	Flow	Less flow	Control Valve is partially opened	Low product formation.
4	Reverse	flow	Reverse flow	Failure of ammonia supply causes reverse flow	Disturbs process lines and may result in leakage.

Table 9.2.5 - HAZOP on transfer of reactants to the tower:

	Guide word	Parameter	Deviation	Cause	Consequences
1	No	Flow	No flow	Pump failure	Reaction rate and conversion decrease
2	Less	Flow	Less flow	Valve partially closed	Reaction rate and conversion decrease
3	More	Flow	More flow	Control system failure.	Reactor overflows

Chapter – 10

Conclusion

As a conclusion to our Final Year Project, we are putting forward the following recommendations to increase the yield and efficiency of the carbonating tower at ICI Soda Ash.

Currently, cleaning is performed after every 72 hours to remove the scaling present inside the tower. This time needs to be decreased to 48 hours so that a lot of scale is not accumulated.

Secondly, the coke to limestone ratio which is fed to the kiln to produce CO_2 needs to be adjusted. Currently, the ratio fed is 0.08 due to which 0.5% O_2 is found in the streams going to the carbonating tower as the coke acts as a limiting reactant in its reaction with oxygen and the excess oxygen leaves in the TE and BE streams.

Increasing this ratio up to 0.085 or above will result in more coke being available to react with O_2 and will minimize O_2 percentage in the inlets of the carbonating towers while minimizing scaling and increasing yield. CO_2 production will also increase as a result.

Lastly, water is being used as a cooling medium to cool the magma being produced. The cooling water reduces the outlet temperature to 30 ºC.

To bring the outlet temperature down to 26 ºC, we recommend the use of ammonia, NH_3, as a cooling medium. The reason for using ammonia is that it has a higher specific heat capacity and thus can take up more energy with a little change its own temperature. Also, it is one of the raw materials for the reaction taking place so it is readily available without additional cost of buying.

10.1 Calculating mass flowrate for ammonia as cooling medium replacement

$$Q = m\, C_P\, \Delta T$$

For cooling water

Q = -181520.6134 kJ/h

C_p = 4.18 kJ/kg.K

ΔT = 1° C

$$m = Q/(C_P \, \Delta T)$$

m = 43425.98 kg/h

As the cooling water enters from two entries in the cooling section

So,

m = 43425.98 / 2

m = 21712.99 kg/h

Alternatively with NH_3 as a cooling medium,

$$Q = m \, C_P \, \Delta T$$

C_p = 4.6 kJ/kg.K

$$m = Q/(C_P \, dT)$$

m = 39461.00 kg/h

NH_3 will enter from two entries in the cooling section

So,

m = 39461.00 / 2

m = 19730.50 kg/h

References:

[1] D. D.G., "Design of Soda Ash Process Plant," 2008.

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[4] McCabe, Smith and Harriot, Unit Operations of Chemical Engineering.

[5] V. I. Panov and A. Tkach, "Carbonating Tower for producing sodium bicarbonate magma". United States Patent 4,066,416, 3 January 1978.

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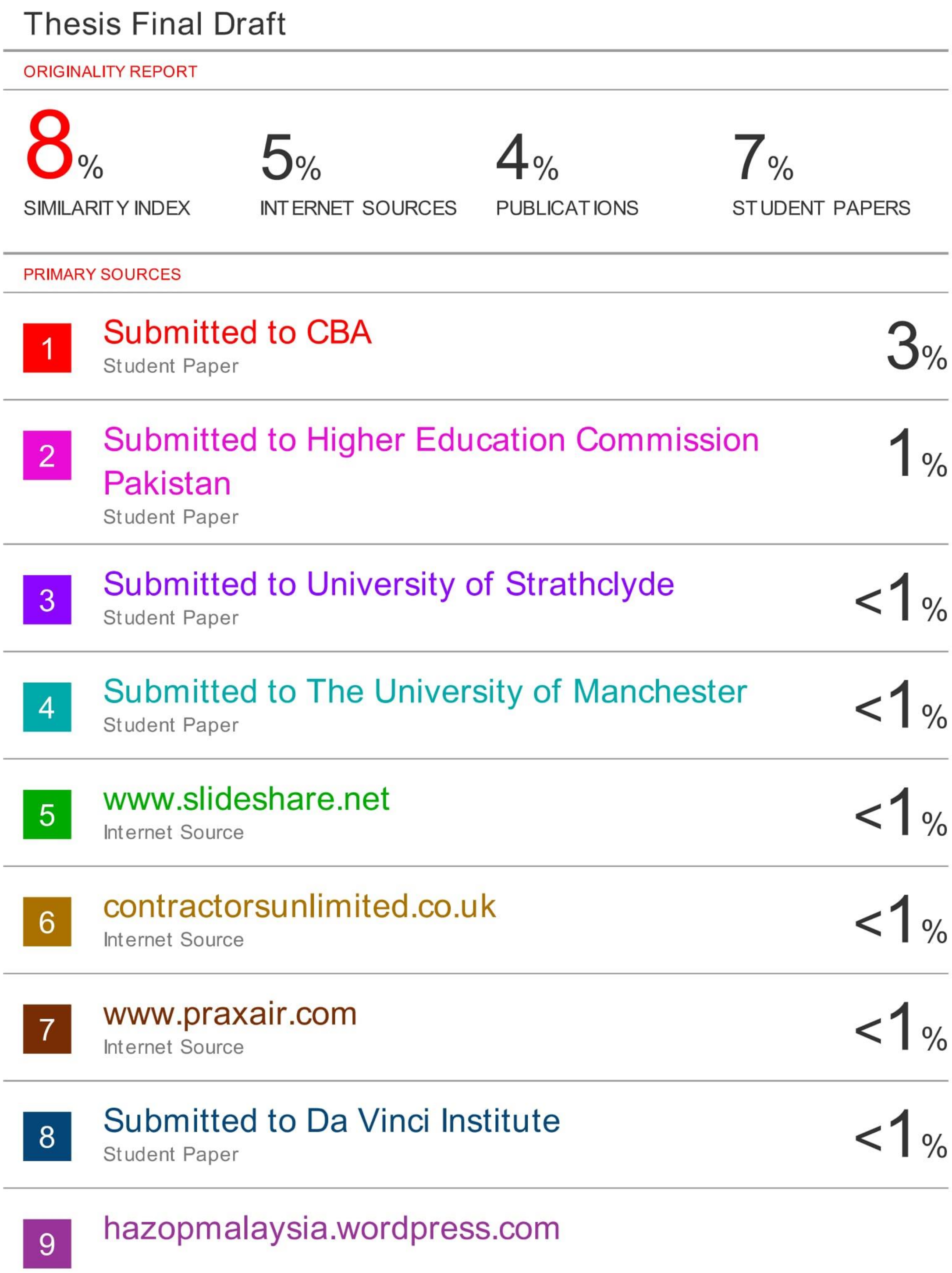

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