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Design and Simulation of an 80,000 Tone/Year Capacity Plant for Aerosol Antiperspirant Deodorant Production

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Abstract

Antiperspirant deodorants are formulated products designed to minimize body odour and control sweating. The global antiperspirant market is growing rapidly because of the increasing awareness about personal hygiene, as well as the increase in the purchasing power of consumers. The world as we know it, is also fast evolving and as such, industries must adapt to the changing times and embrace better and more innovative approaches to problems. A prominent area of evolution in the chemical process industry is in plant design. In recent years, process simulation software tools have been developed and employed in favour of old traditional manual design methods due to their numerous advantages. Process simulation as a chemical design tool has come to stay as a hallmark in the chemical process industry. Design calculations to produce an 8 X 10^4 tone/year Aerosol Antiperspirant Deodorant have been carried out manually and then compared with Aspen HYSYS Simulated results. Aspen HYSYS is a Chemical Engineering design simulation software. The material and energy balances of the various units of the plant, the mechanical design, equipment sizing and cost estimation for the entire plant were also carried out manually and compared with Aspen HYSYS simulated results. Process control and instrumentation was done, and the plant layout was determined and discussed. Plant safety and environmental factors were also considered and discussed. It was found that both the manual and simulated results correlated perfectly, showing that the use of HYSYS is highly preferable in terms of flexibility of manipulating the variables, economics of man-hours and computational time saved.

Keywords :

Antiperspirant deodorants, Simulation, Aspen Hysys, Design, Variables

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1. INTRODUCTION

Throughout history, humans have always looked for ways to mask unpleasant body odour from various parts of their bodies and control sweat secretions for personal, social and aesthetic reasons. Having unpleasant body smells as a result of perspiration can prove to be an obstacle in social interactions and inter-relations. Hence the strong need for antiperspirant deodorants. At the end of the 19th century, chemists invented products that could help in preventing the formation of body odour. The earliest antiperspirant deodorants were in the form of pastes, which were applied to the underarm area. The first of such products to be trademarked and patented in the U.S was “Mum” in 1888(Green, 2004).It was however difficult to apply and very messy. By the late 1950s, people had started adopting aerosol technology for perfumes and other personal care products. In the early 1960s, the first aerosol antiperspirant deodorant, “Right Guard” by the Gillete Company was produced. Aerosols gained popularity among consumers due to their ease of use, as well as the fact that they allowed the user to apply the product without needing to touch the underarm area. By 1967, half of the antiperspirant deodorants sold in the United States were in aerosol form and accounted for a large percentage of all sales. They are still very popular and widely used today.

An antiperspirant deodorant is a formulated product that helps to minimize and control body odour and sweating. It does this by preventing the decomposition of sweat, which is relatively odourless until it is broken down by bacteria, and blocking the sweat glands (Everts, 2012).

Antiperspirants deodorants are also used on any part of the body where sweat would be inconvenient and unsafe, such as interfering with comfort, grip or vision.

The human skin contains two kinds of sweat glands. They are the apocrine and eccrine sweat glands. The eccrine sweat glands cover a very large area of the skin and secrete odourless, watery sweat. The apocrine sweat glands on the other hand, produce a heavier, oilier sweat made up of proteins, fatty acids and carbohydrates. This type of sweat is decomposed by bacteria found on the skin to produce compounds like trans-3-methyl-hexenoic acid that cause body odour. The apocrine glands are dormant until puberty sets in. This is the reason body odour often only becomes detectable at that time (Kuehl, 2003).

Antiperspirant deodorants work by preventing bacterial action on sweat on the skin and significantly reducing perspiration (Marc Praye, 2009). Aluminium-based compounds found in antiperspirant deodorants react with the electrolytes in the sweat to form a gel-like plug in the duct of the sweat glands. The plugs work in preventing the sweat gland from secreting sweat and are removed over time by the natural sloughing of the skin or by bathing.

Metal salts also found in antiperspirant deodorants also prevent sweat by interacting with the keratin fibrils in the sweat ducts. This action forms a plug which stops sweat from getting to the surface of the skin. They also have astringent properties which cause the pores on the skin to contract, further preventing sweat from reaching the surface of the skin (Draelos, 2001).

The global antiperspirant and deodorant market is growing as a result of the increasing awareness about personal hygiene, as well as the increase in purchasing power of consumers.

Europe currently represents the largest regional market for deodorants and along with the U.S, they collectively account for a major share of sales of deodorants on a global scale. The demand for deodorants in the U.S and Europe significantly dropped in 2009 as a result of economic slowdown that year. Asia-Pacific is coming up as the next fastest growing market for deodorants, with sales projected to grow at a compound annual rate of 4.6% over the analysis period. Rising levels of income in developing markets such as Asia-Pacific, Latin America, Middle East and African nations are also fuel growth opportunities for deodorants in the near future (Shahbandeh, 2019).

The global antiperspirants and deodorants markets are expected to garner revenue of USD70 Billion by 2024 and projected to record a Compound Annual Growth Rate of 3.5% during the forecast period of 2019 to 2024 (Sawant, 2019).

In order to keep pace with the increasing demand of antiperspirant deodorants in aerosol form, there will be need to produce more of the product at a faster rate, larger capacity manufacturing plants will be required and the existing smaller scale plants would require upgrading. Since majority of these small scale plants use batch reactors which were manually designed, upgrading them would require the use of process simulation packages to obviate the cumbersomeness of manual computations.

Robert (2016) developed an aerosol antiperspirant formulation which tackled the issue of proper deposition on the skin. According to the inventor, when regular aerosol antiperspirants are sprayed on target areas of the body, they are deposited as fine droplets. Some of these droplets are bounced off the skin while others are dispersed, thereby reducing the anti-wetness efficacy of such antiperspirant, and consequently, its overall effectiveness in reducing sweating and combating malodour. He thus invented a formulation containing at least one active antiperspirant deodorant, a silicone solvent, a bis-vinyl dimethicone/dimethicone copolymer, at least one fatty acid ester and at least one propellant. This formulation is believed to increase the deposition of active ingredients on target body areas leading to greater efficacy.

Mesurolle et al (2014) conducted a study which was aimed at exploring what amount of aluminum-based complexes (an active ingredient found in antiperspirants) could lead to the production of radiopague particles. Radiopague substances are found during mammogram sessions and they tend to look like micro-calcifications. The study was also aimed at finding out whether there was a relationship between the percentages of aluminum-based complexes used in antiperspirants and the presence of radiopague particles induced by antiperspirants. 43 antiperspirants containing aluminum-based complexes with percentages within a range of 16% to 25% were tested. Each of the antiperspirants was rubbed on a plastic shield and thereafter put on an ultrasound gel pad, the gel pad mimicking breast tissue. Results from the experiments showed that there was no significant relationship between the amounts of aluminum-based used in antiperspirant deodorants and the shape or density of the radiopague substances. It was also found that there was no significant relationship between the size or shape of the radiopague particles and the method of application of the antiperspirant.

Khandare et al (2017) carried out a study with the aim of formulating a herbal based deodorant. They sought to determine its efficacy at controlling body odour for up to 48 hours. The herbal based deodorant was formulated with the use of soxhleted alcohol extract of Neem, Methi and Curry. Testing was carried out on 8 subjects within the age range of 16 to 70 years. A panel of experts rated the intensity of body odour on a scale of 1 to 5, with 5 being very strong body odour and 1 being no body odour. The subjects were split into two groups. One group served as the control group tested with the deodorant formulation containing no herbal complex and perfume, while the other group was tested with the deodorant formulation containing herbal complex. The testing method included spraying of the formulated products on both armpits of the subjects once. The test lasted for 48 hours, with intensity of body odour recorded at 0, 12, 24, 36 and 48 hours respectively. The results were obtained by plotting a graph of the time in hours against the intensity of body odour for the two groups. It was found that the group tested with the herbal complex showed a much higher rating of long lasting protection from body odour, compared to the group tested without the herbal complex.

The activity of metal salts such as Aluminium and Zirconium salts in antiperspirants deodorants can be increased. This conditioning increases their efficiency in product formulations. It can be done by mixing the said salt with a non-aqueous liquid carrier in which the salt is suspended but insoluble. The mixture is then preserved at a temperature of 20-70°C and modified to an average particle size of 2 microns, wherein the increased efficiency is made possible by increasing the amount of smaller formations by 10% in relation to the starting salt (John et al, 2001). The non-aqueous liquid carrier can be selected from a group made up of mineral oils, cyclomethicones and low viscosity fatty esters.

There has been an ongoing debate regarding the use of bactericidal products in antiperspirant formulations that inhibit the growth of odour causing bacteria in areas of the body. These bactericidals don’t just kill the odour-causing bacteria in the target region; they kill the entire microbial flora present on the skin surface. Scientists worry that that causes changes in the skin’s natural pH and thus interfere with its natural defense functions. Yvonne et al (2004) proposed the formulation of an antiperspirant deodorant containing chitosan (deacetylated chitin). Chitosan is a linear polysaccharide made by treating chitin cells of shrimps and other crustaceans with an alkaline substance such as sodium hydroxide. The chitosan effectively replaces ingredients that would otherwise eliminate all microbial flora in the target region, not just the odour causing bacteria. Part of the production involves the addition of chitosan deodorizing preparations which are produced by weight and a portion of antiperspirant active ingredients in the range of 1-35% by weight, based on the total mass of the preparation.

However, a drawback to this invention lies in the fact that chitosan has a high degree of deacetylation of more than 80% in nano, micro or macro emulsions. This causes instability, phase separation, turbidity and water deposits. This is likely due to the tendency of chitosan to form undesirable emulsions with oils and lipids used during the product formulation.

In spite of the popularity in the use of aerosol antiperspirants, some users have reported negative physical reactions to some of the ingredients found in most brands. For example, dimethicone, a type of silicone mostly used in antiperspirant formulations may cause moderate itching and a stinging sensation in some persons. Other more severe side effects may include hives, difficulty breathing and chest tightness. Alan Passero et al (2015) developed an antiperspirant formulation containing no silicones (silicone-free). It is made up of an antiperspirant active, an absorbent oil selected from the group consisting of Aluminium Octenyl succinate starch, an ester, a suspending agent, and at least one propellant. This composition, according to the inventors, leaves a dry touch on the skin, provides lasting effectiveness, and is substantially free of silicone.

Most antiperspirant deodorants have aluminium salts as their main and active ingredients. However, some individuals have reported allergic reactions to the salt, as well as toxic build-up owing to clogged pores. This has led some researchers to develop Aluminium-free alternatives. Peter et al (2017) developed an aluminium-free antiperspirant formulation comprising an oil-in-water emulsion (made up of an emulsifier, a plant-based oil, a polyol and water) and an active ingredient which is zinc-based. Zinc salts were previously considered for use as the active ingredient, but from experimental procedures, it was found that zinc salts precipitate as hydroxides within the pH range of 6.5 to 8. This makes them behave erratically, thus being termed unreliable as antiperspirant actives. This irregular behavior was reported to be as a result of many factors, including the possible lack of hydrolysis conversion to relatively inactive carbonate or oxide.

2. Martials and Methods

2.1 Materials

The materials used for the production of aerosol antiperspirant deodorant are as follows;

i) Ingredients

Cyclomethicone, aluminium chlorohydrate, propylene glycol, triethanolamine, magnesium silicate, butylated hydroxytoluene, colour, fragrance, stearic acid and triclosan.

ii) Equipment

Equipment used include the following;

- Mixer
- Heat exchanger
- Continuous Stirred Tank Reactor
- Storage tank

2.2 Methods

In this section, the methodology used to develop the design parameters for the mixer and continuous stirred tank reactor will be outlined. The methodology will employ the material balance principle to develop the design parameters of mixer and batch reactor for the production of 80,000Tonnes/year of aerosol antiperspirant deodorant. The material balance principle is presented below;

$$\begin{bmatrix} Rate\ of \\ Accumulation\ of \\ materials\ within\ the \\ unit\ (mol/hr \end{bmatrix} = \begin{bmatrix} Rate\ of\ inflow\ of \\ materials\ into \\ the\ unit\ (\frac{mol}{hr}) \end{bmatrix} - \begin{bmatrix} Rate\ of outflow \\ of materials \\ from \\ the\ unit\ (mol/hr \end{bmatrix} \pm \begin{bmatrix} Rate\ of depletion \\ due\ to \\ chemical \\ reaction \\ (\frac{mol}{hr}) \end{bmatrix}$$

(2.1)

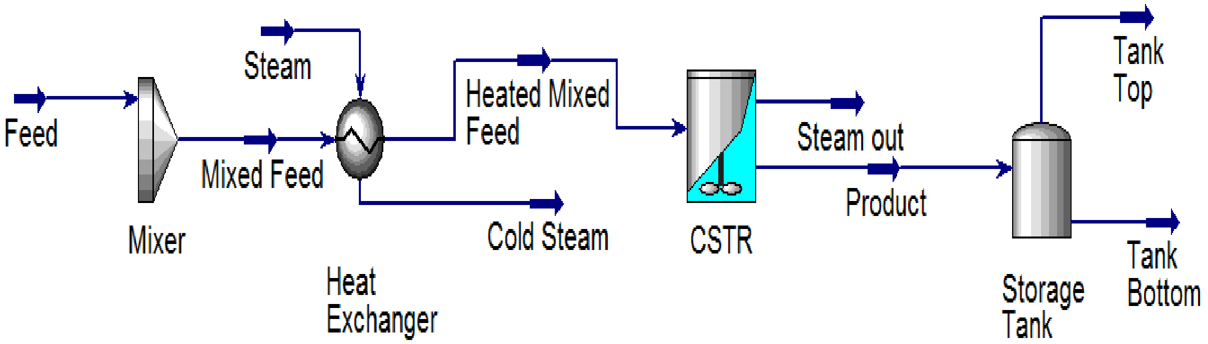


Figure 2.1: Process flow diagram of the HYSYS simulation

2.2.1 Development of mixer model

The function of the mixer is to obtain a homogenous system from the various ingredients so as to avoid by-products occurring as a result of unwanted or side reactions taking place.

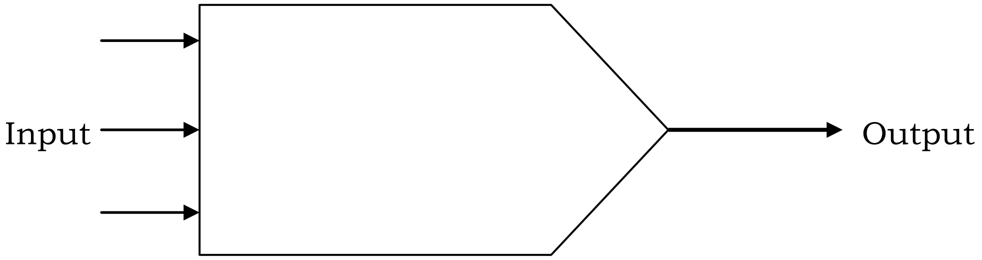


Fig 2.2: Schematic diagram of a mixer

2.2.2 Impeller-Generated Flow in the Mixer

The impeller-generated flow of materials in the mixer is represented by the equation below;

$$Q = F_L \times N \times D^3 \qquad (2.2)$$

Where;

Q = Impeller generated flow rate (m^3/s)

N = Number of rotations

D = Diameter of impeller (m)

F_L = Flow regime.

2.2.3 Power Required for the Mixer

The power required by the impeller for proper mixing which enhances mixing of ingredients to achieve a homogenous system is obtained with the following equation.

Hence, for turbulent regime, the equation is;

$$P = K_\rho \mu N^2 D^3 \qquad (2.3)$$

Where:

ρ = density of the fluid (kg/m^3)

K_p = laminar power constant

μ = Viscosity of the fluid (Ns/m^2)

N = Rotational speed (S^{-1})

D = Diameter of the impeller (m)

P = Power required (kW/m^3)

2.2.4 Time Required for Mixing

The time required to blend the system to within 5% of the final concentration is obtained using the following equation;

For turbulent regime, the equation is:

$$\theta_{95} = \frac{5.40}{P_0^{1/3}} \left(\frac{T}{D}\right)^2 \tag{2.4}$$

Also, for transitional regime:

$$\theta_{95} = \frac{34596}{P_0^{1/3} N^2 D^2} \left(\frac{\mu}{P}\right) \left(\frac{T}{D}\right)^2 \tag{2.5}$$

Then for laminar regime, the equation is:

$$\theta_{95} = \frac{896x10^3 k_P^{-1.69}}{N} \tag{2.6}$$

Note:

The transitional/turbulent boundary occurs at $P_0^{1/3} Re = 6404$

Also, the laminar/transitional boundary occurs at $P_0^{1/3} Re = 186$

2.2.5 Development of Continuous Stirred Tank Reactor model

The various terms in equation (2.1) are obtained mathematically as follows:

[Rate of accumulation of component *i*] = $V \frac{dC_i}{dt}$ (2.7)

Rate of input of component *i* = $V_O C_{iO} = F_{iO}$ (2.8)

Rate of output of component *i* = $V_O C_i = F_i$ (2.9)

Rate of depletion of component *i* = $(-r_i)V$ (2.10)

Substituting equations (3.7) to (3.10) into equation (3.1) gives:

$$V \frac{dC_i}{dt} = F_{iO} - F_i - (-r_i)V \tag{2.11}$$

Where: $V = the\ volume\ of\ reactor$

$F_{iO} = the\ initial\ molar\ flow\ rate\ of\ the\ gas$

$F_i = the\ final\ molar\ flow\ rate\ of\ the\ gas$

$(-r_i) = the\ rate\ of\ depletion\ of\ the\ gas$

$dC_i = is\ the\ concentration\ differential\ of\ the\ gas$

At steady state, the rate of accumulation $\frac{dC_i}{dt} = 0$ (2.12)

$$0 = F_{i0} - F_i - (-r_i)V \qquad (2.13)$$

Recall: $F_i = F_{i0} - F_{i0}X_i$ (2.14)

$$0 = F_{i0} - F_i - (-r_i)V \qquad (2.15)$$

Substituting (3.14) into (3.15)

$$0 = F_{i0} - (F_{i0} - F_{i0}X_i) - (-r_i)V \qquad (2.16)$$

$$0 = F_{i0} - F_{i0} + F_{i0}X_i - (-r_i)V \qquad (2.17)$$

Simplifying equation (3.17)

$$0 = F_{i0}X_i - (-r_i)V \qquad (2.18)$$

$$-F_{i0}X_i = -(-r_i)V \qquad (2.19)$$

Multiply through equation (3.19) by -1

$$F_{i0}X_i = (-r_i)V \qquad (2.20)$$

Writing equation (3.20) in terms of concentration

Recall: $F_{i0} = C_{io}V_o$ (2.21)

Substituting (3.20) into (3.21)

$$C_{io}V_oX_i = (-r_i)V \qquad (2.22)$$

Equation (2.22) is the basic model for the development of the design equations for the reactor.

2.2.6 Volume of Reactor

The volume of a reactor is a function of the diameter of the reactor and increases as the diameter increases. For a CSTR, the volume can be obtained from equation (2.19) as follows:

$$V = \frac{C_{io}V_oX_i}{(-r_i)} \qquad (2.23)$$

2.2.7 Height of Reactor

The height of reactor is also a very important dimensional parameter to be determined in the design of any process. It has a direct relationship with the volume of the reactor and tends to have same effect on the process as the volume. The height of the reactor also affects the cost of the reactor, hence the need to calculate the height of the system based on the basis of the design under consideration to avoid wastage and unnecessary costs. For the CSTR, assuming a cylindrical shape;

Recall: Volume of Cylinder is given as:

$$V = \frac{\pi D^2 H}{4} \qquad (2.24)$$

Making height (H) the subject of formula

$$H = \frac{4V}{\pi D^2} \tag{2.25}$$

2.2.8 Space Time

The space time is defined as the reaction time required to process one reactor volume of feed measured at specified condition. It is otherwise known as holding or mean residence time.

Mathematically stated:

$$\tau = \frac{V}{V_o} \tag{2.26}$$

2.2.9 Space Velocity

Space velocity is defined as the numbers of reactor volumes of feed at specified conditions which can be treated per unit time and is designated asS_v. It is the reciprocal of the space time.

Mathematically S_v is expressed as;

$$S_v = \frac{V_o}{V} \tag{2.27}$$

2.2.10 Heat Load

The heat load is a function of molar flow feed rate, the degree of conversion and heat of reaction and is expressed as;

$$Q = \Delta H_R^o F_{io} X_i \tag{2.28}$$

Substituting equation (2.21) into (2.28)

$$Q = \Delta H_R C_{io} V_o X_i \tag{2.29}$$

2.2.11 Heat Generated Per Unit Volume

$$q = \frac{\Delta H_R C_{io} V_o X_i}{V} \tag{2.30}$$

2.2.12 Heat Exchanger Design Equations

The relation governing heat transfer in heat exchanger is given by

$$Q = UA\Delta T \tag{2.31}$$

Where;

Q = Heat transfer per unit time, W,

U = the overall heat transfer coefficient, W/m^2 ^{o}C

A = Heat transfer area, m^2,

ΔT – Effluent temperature difference, ^{o}C,

For a liquid, heated or cooled (^{o}C,) the duty required to be performed by the following equation.

$$Q = mCp\Delta T \tag{2.32}$$

2.2.13 Simulation of Models Developed

The design models will be subjected to computer programming. The computer program developed will be used to compute and simulate the design parameters of the unit operations (mixer and batch reactor) in the plant for the production. The plant design will be done using Aspen HYSYS for the simulation of design parameters for suitable design specifications for the production of 80,000 Tonnes/year of aerosol antiperspirant deodorant.

2.3 Material Balance

Material balance is the most fundamental part of every process design. It ensures the determination of the quantity of raw materials required and the products produced. Balances over individual process units set the process stream flows, conditions and compositions. Material balances are good tools for checking performance against design. They help check instrument calibration and locate areas of material loss.

The loss of mass associated with the production of energy is significant only in nuclear reactions; energy and materials are always considered to be separately conserved in chemical reactions.

The general conservation equation for any process can be written as:

[Material out] = [Material in] + [Generation] – [Consumption] – [Accumulation]

For steady state processes, the accumulation term will be zero. Except in nuclear reactions, mass is neither generated nor consumed in the process. If there is no chemical reaction, the steady state balance reduces to:

[Material out] = [Material in]

A balance can be written for each separately identifiable species present, elements, compounds, radicals and for the total material.

The following conventions and streams shall be used for the various units and streams.

UNITS

U001 – Mixing unit

U002 – Heat Exchanger unit

U003 – CSTR unit

U004 – Storage tank unit

STREAMS

S1 – Feed Stream

S2 – Mixed feed stream
S3 – Steam stream
S4 – Heated mixed feed stream
S5 – Cold steam stream
S6 – Product stream
S7 – Tank bottom stream

2.3.1 Material Balance for mixing unit

$yAl_2Cl(OH)_5 = 0.45$

$yC_{12}H_7Cl_3O_2 = 0.2$

$yMgO.Si = 0.15$

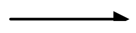


Fig. 3.3: Material Balance for mixing unit

$$Mole\ Fraction\ of\ component\ i = \frac{Moles\ of\ component\ \ i}{Total\ \ moles} \qquad (2.34)$$

The calculations for the mole fractions of the individual components are shown in appendix 1A.

Table 3.1: Material Balance Summary for Mixing Unit

Input (S1) Component	**Composition**	**Molar Flow (kgmol/hr)**	**Mass Flow (kg/hr)**	**Output (S2) Composition**	**Molar Flow (kgmol/hr)**	**Mass Flow (kg/hr)**
$Al_2Cl(OH)_5$	0.45	1003.95	4499.704	0.45	1003.95	4499.704
$C_{12}H_7Cl_3O_2$	0.2	446.2	1999.868	0.2	446.2	1999.868
MgO_3Si	0.15	334.65	1499.901	0.15	334.65	1499.901
$C_{10}H_{30}O_5Si$	0.12	267.72	1199.921	0.12	267.72	1199.921
$C_{18}H_{36}O_2$	0.01	22.31	149.990	0.01	22.31	149.990
$C_{15}H_{24}O$	0.015	33.465	549.986	0.015	33.465	549.986
$C_6H_{15}NO_3$	0.055	122.71	99.993	0.055	122.71	99.993
TOTAL	**1.000**	**2231.02**	**9999.364**	**1.000**	**2231.02**	**9999.364**

2.3.2 Material Balance for Heat Exchanger Unit

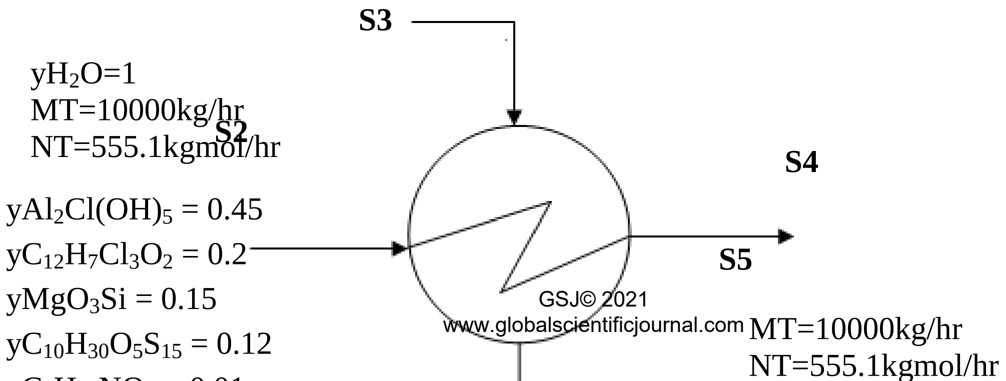
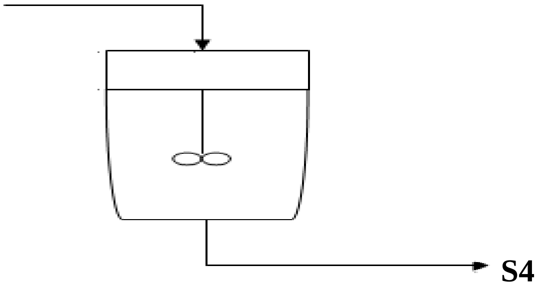


Fig 3.4: Material balance for heat exchanger unit

Table 3.2: Material Balance Summary for Heat Exchanger Unit

Input				**Input**			**Output**			**Output**		
S2				**S3**			**S4**			**S5**		
Component	**Composition**	**Molar Flow (kgmol/hr)**	**Mass Flow (kg/hr)**	**Composition**	**Molar Flow (kgmol/hr)**	**Mass Flow (kg/hr)**	**Composition**	**Molar Flow (kgmol/hr)**	**Mass Flow (kg/hr)**	**Composition**	**Molar Flow (kgmol/hr)**	**Mass Flow (kg/hr)**
$Al_2Cl(OH)_5$	0.45	1003.95	4499.704	-	-	-	0.45	1003.95	4499.704	-	-	-
$C_{12}H_7Cl_3O_2$	0.2	446.2	1999.868	-	-	-	0.2	446.2	1999.868	-	-	-
MgO_3Si	0.15	334.65	1499.901	-	-	-	0.15	334.65	1499.901	-	-	-
$C_{10}H_{30}O_5Si$	0.12	267.72	1199.921	-	-	-	0.12	267.72	1199.921	-	-	-
$C_{18}H_{36}O_2$	0.01	22.31	149.990	-	-	-	0.01	22.31	149.990	-	-	-
$C_{15}H_{24}O$	0.015	33.465	549.986	-	-	-	0.015	33.465	549.986	-	-	-
$C_6H_{15}NO_3$	0.055	122.71	99.993	-	-	-	0.055	122.71	99.993	-	-	-
H_2O	-	-	-	1	555	10001.1	-	-	-	1	555	10001.1
TOTAL	**1.000**	**2231.02**	**9999.364**	**1**	**555**	**10001.1**	**1.000**	**2231.02**	**9999.364**	**1**	**555**	**10001.1**

2.3.3 Material Balance for CSTR Unit



S4

$yAl_2Cl(OH)_5 = 0.45$

$yC_{12}H_7Cl_3O_2 = 0.2$

$yMgO_3Si = 0.15$

$yC_{10}H_{30}O_5S_{15} = 0.12$

$yC_6H_{15}NO_3 = 0.01$

$yC_{18}H_{36}O_2 = 0.015$

$yC\,H\,O = 0.055$

Fig 3.5: Material balance for CSTR Unit

From Material Balance;

Since the system is a single input, single output type of system, therefore S4=S6

Table 3.3: Material Balance Summary for CSTR Unit

Input				**Output**		
S4				**S6**		
Component	**Composition**	**Molar Flow (kgmol/hr)**	**Mass Flow (kg/hr)**	**Composition**	**Molar Flow (kgmol/hr)**	**Mass Flow (kg/hr)**
$Al_2Cl(OH)_5$	0.45	1003.95	4499.704	0.45	1003.95	4499.704
$C_{12}H_7Cl_3O_2$	0.2	446.2	1999.868	0.2	446.2	1999.868
MgO_3Si	0.15	334.65	1499.901	0.15	334.65	1499.901
$C_{10}H_{30}O_5Si$	0.12	267.72	1199.921	0.12	267.72	1199.921
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$C_{15}H_{24}O$	0.015	33.465	549.986	0.015	33.465	549.986
$C_6H_{15}NO_3$	0.055	122.71	99.993	0.055	122.71	99.993
TOTAL	**1.000**	**2231.02**	**9999.364**	**1.000**	**2231.02**	**9999.364**

2.3.4 Material Balance for Storage Tank

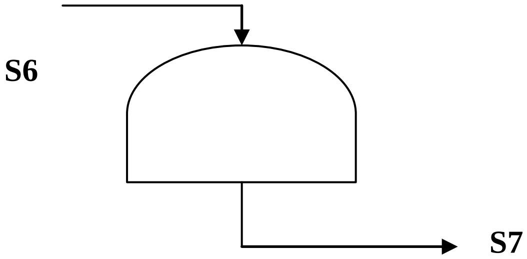


Fig 3.6: Material balance for storage tank

From material balance: Since the system is a single input single output system, S6=S7

Table 3.4 Material Balance Summary for Storage Unit

Input				**Output**		
S6				**S7**		
Component	**Composition**	**Molar Flow (kgmol/hr)**	**Mass Flow (kg/hr)**	**Composition**	**Molar Flow (kgmol/hr)**	**Mass Flow (kg/hr)**
$Al_2Cl(OH)_5$	0.45	1003.95	4499.704	0.45	1003.95	4499.704
$C_{12}H_7Cl_3O_2$	0.2	446.2	1999.868	0.2	446.2	1999.868
MgO_3Si	0.15	334.65	1499.901	0.15	334.65	1499.901
$C_{10}H_{30}O_5Si$	0.12	267.72	1199.921	0.12	267.72	1199.921
$C_{18}H_{36}O_2$	0.01	22.31	149.990	0.01	22.31	149.990
$C_{15}H_{24}O$	0.015	33.465	549.986	0.015	33.465	549.986
$C_6H_{15}NO_3$	0.055	122.71	99.993	0.055	122.71	99.993
TOTAL	**1.000**	**2231.02**	**9999.364**	**1.000**	**2231.02**	**9999.364**

2.4 Energy Balance

A general energy balance equation can be written as:

$$\begin{bmatrix} Rate\ of\ outflow \\ of\ energy \end{bmatrix} = \begin{bmatrix} Rate\ of\ inflow \\ of\ energy \end{bmatrix} + \begin{bmatrix} Rate\ of\ generation \\ of\ energy \end{bmatrix} - \begin{bmatrix} Rate\ of\ consumption \\ of\ energy \end{bmatrix} - \begin{bmatrix} Rate\ of\ accumulation \\ of\ energy \end{bmatrix} \qquad (3.35)$$

If there is no chemical reaction, equation (3.35) becomes;

$$\begin{bmatrix} Rate\ of\ generation \\ of\ energy \end{bmatrix} = \begin{bmatrix} Rate\ of\ consumption \\ of\ energy \end{bmatrix} = 0 \qquad (3.36)$$

If the system is a steady state process;

$$\begin{bmatrix} Rate\ of\ accumulation \\ of\ energy \end{bmatrix} = 0 \qquad (3.37)$$

Energy flow can be computed in terms of heat flow using the formula;

$$\dot{Q} = \dot{m}C\dot{p}_{mean}\ (T - T_{ref}) \qquad (3.38)$$

Where;

$\dot{Q}$=Heat flow rate in kJ/hr

m= Mass flow rate in kg/hr

Cp_{mean} = Mean specific heat capacity in kJ/kg°C

T= Temperature of the stream in °C

T_{ref} = Reference temperature of stream, sometimes assumed as zero.

2.4.1 Energy Balance for mixing unit

J=25°C
P=101.3Kpa
MT=10000kg/hr
Cp=211.12kJ/kg°C
Tref=0°C

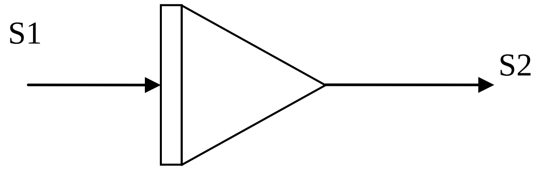


Fig 3.7: Energy balance for mixing unit

Table 3.5: Energy Balance Summary for Mixing Unit

	Input	**Output**
Stream	**S1**	**S2**
Temperature (°C)	25	25
Pressure (kPa)	101.3	101.3
Mass flow (kg/hr)	10000	10000
Cp_{mean} (kJ/kg°C)	211.12	211.12
Heat flow (kJ/hr)	-5.278×10^{7}	-5.278×10^{7}

2.4.2 Energy Balance for Heat Exchanger unit

S3

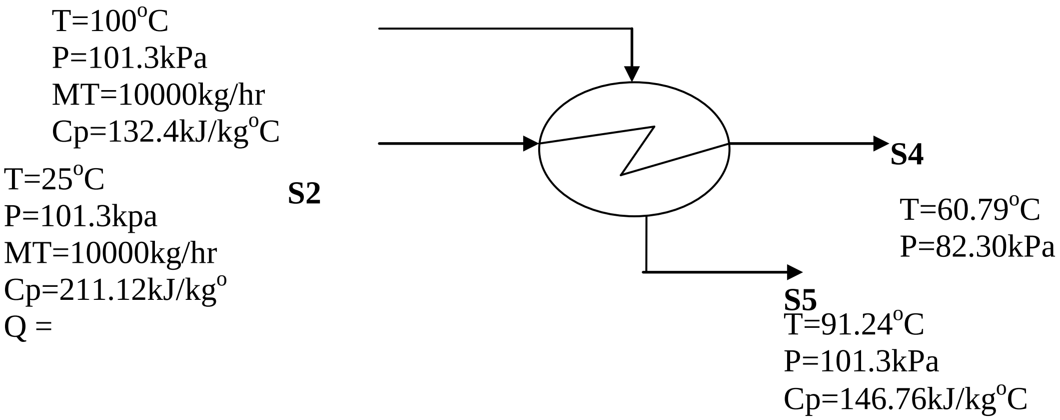
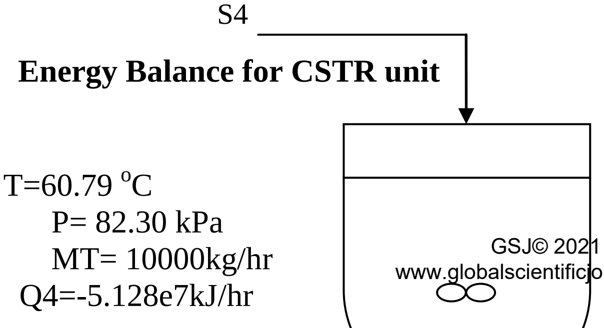


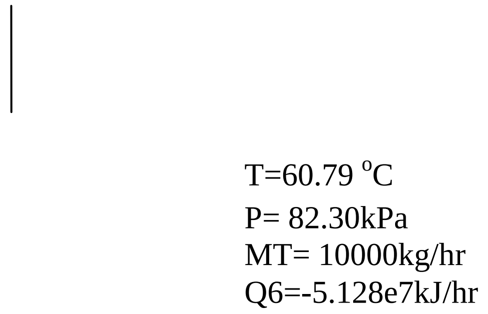
Fig 3.8: Energy balance for heat exchanger unit

Table 3.6: Energy Balance Summary for Heat Exchanger Unit

	Input	**Input**	**Output**	**Output**
Stream	**S2**	**S3**	**S4**	**S5**
Temperature(°C)	25	100	60.79	91.24
Pressure (kPa)	101.3	101.3	82.30	101.3
Mass flow rt (kg/hr)	10000	10000	-	146.76
Cpmean (kJ/kg°C)	211.12	132.4		
Heat Flow (kJ/hr)	-5.278e7	-1.324e8	-5.128e7	-1.339e8

2.4.3 Energy Balance for CSTR unit





From energy balance, Q4=Q6

Fig 3.9: Energy Balance for CSTR Unit

Table 3.7: Energy Balance Summary for CSTR unit

	Input	**Output**
Stream	**S4**	**S6**
Temperature(°C)	60.79	60.79
Pressure (kPa)	82.30	82.30
Mass flow rt (kg/hr)	10000	10000
Cp_{mean} (kJ/kg°C)	-	-
Heat Flow (kJ/hr)	-5.128e7	-5.128e7

2.4.4 Energy Balance for storage tank

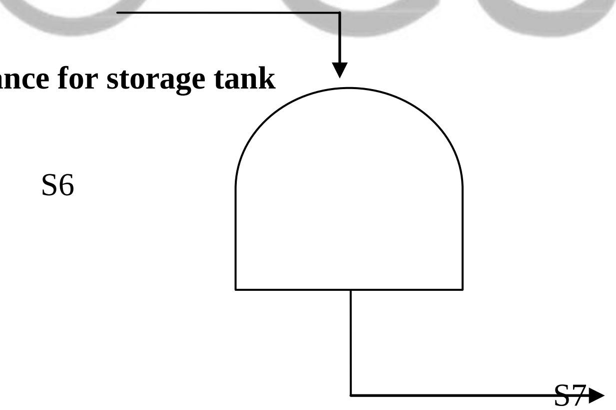


Fig 3.10: Energy balance for storage tank unit

Table 3.8: Energy Balance Summary for Storage Tank Unit

	Input	**Output**
Stream	**S6**	**S7**
Temperature(°C)	60.79	60.79
Pressure (kPa)	82.30	82.30

Mass flow rt (kg/hr)	10000	10000
Cpmean (kJ/kg^{o}C)	-	-
Heat Flow (kJ/hr)	-5.128e7	-5.128e7

2.5 Equipment Design/Sizing

2.5.1 Mixing Unit

Mixing units fitted with some form of agitator are the most commonly used type of equipment for blending and mixing. To design the mixer, we must be able to estimate the shaft power required to drive an agitator, which is given by the equation below:

$$N_p = KRe^b Fr^c \qquad (3.39)$$

where;

$$Re = Reynold's\ number = \frac{D^2 N\rho}{\mu} = \frac{\rho VD}{\mu}\ ;\ \ Fr = Froude\ number = \frac{DN^2}{g}$$

$$N_p\ = Power\ number = \frac{P}{D^5 N^3 \rho}$$

$$P = Shaft\ power$$

$$K = constant, depending\ on\ the\ agitator\ type, size\ and\ the\ tank\ geometry.$$

$$\rho = fluid\ density\ (kg/m^3)$$

$$\mu = Fluid\ viscosity(Ns/m^2)$$

$$N = Agitator\ speed\ in\ rev\ per\ second\ (S^{-1})$$

$$D = Agitator\ diameter\ (m)$$

$$g = acceleration\ due\ to\ gravity, 9.81\ m/s^2$$

For our design, based on information from the Chemical Engineering handbook (R.K Sinnot, 2005), the power range for mild agitator mixing is from 0.04 to 0.10 KW/m^3.

2.5.2 Heat Exchanger Unit

We are required to design a heat exchanger unit that will heat our feed stream from 25^{o}C to 60.79^{o}C, using steam as the heating medium. The flow rate of our feed is 10,000kg/hr. The temperature of the steam drops from 100^{o}C to 91.24^{o}C.

The calculations for the sizing and design are shown in appendix 2C.

3.5.3 CSTR Sizing

3.5.3.1 Estimation of diameter

$$D = \sqrt{\frac{4a}{\pi}} \qquad (3.40)$$

where D= Diameter

A= Cross sectional Area

This calculation is shown in Appendix 3D

3.5.3.2 Estimation of volume

$$V=\frac{\pi d^2 H}{4} \qquad (3.41)$$

Where;

V = Volume of CSTR

D= Diameter

H= Height of CSTR

Calculations are shown in appendix 3D

3.5.3.3 Estimation of space time

$$\tau = \frac{v}{v_o} \qquad (3.42)$$

Where;

$$\tau = Space\ time$$

$$v = volume\ of\ reactor$$

$$v_o = Volumetric\ flow\ rate$$

3.5.3.4 Estimation of space velocity

$$Sv = \frac{1}{\tau}$$

3.5.4 Storage Tank Sizing

3.5.4.1 Estimation of diameter

$$D = \sqrt{\frac{4a}{\pi}} \qquad (3.43)$$

Where;

D =Tank Diameter

A= Cross sectional Area

3.5.4.2 Estimation of volume

$$V=\frac{\pi d^2 H}{4} \qquad (3.44)$$

Where;

V = Volume of tank

D= Diameter of tank

H= Height of tank

2.6 Mechanical Design

This involves estimating the minimum wall thickness required to ensure that any vessel is sufficiently rigid to withstand its own weight, and any incidental loads. As a general guide the wall thickness of any vessel should not be less than the values given below, the values include a corrosion allowance of 2mm.

Table 3.9: Vessel diameter showing minimum required thickness

Vessel Diameter(m)	Minimum thickness(mm)
1	5
1 to 2	7
2 to 2.5	9
2.5 to 3.0	10
3.0 to 3.5	12

2.6.1 Mechanical Design of the Continuous Stirred Tank Reactor Unit

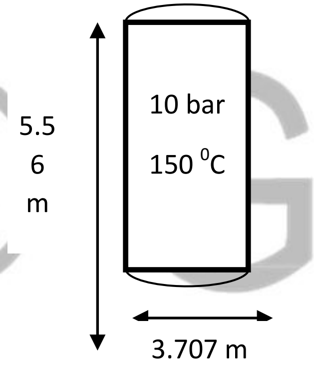


Fig 3.11: Schematic diagram showing mechanical design of a CSTR unit

2.6.2 Mechanical Design of the Storage Tank Unit

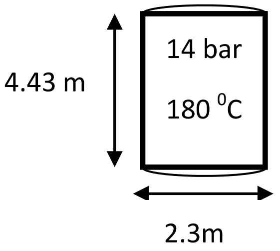


Fig 3.12: Schematic diagram showing mechanical design of a storage tank unit

2.7 Plant Instrumentation and Control

Instruments are provided to monitor the key process variables during plant operation. They may be incorporated in automatic control loops, or used for the manual monitoring of the process operation. They may also be part of an automatic computer data logging system. Instruments monitoring critical process variables will be fitted with automatic alarms to alert the operators to critical and hazardous situations.

It is desirable that the process variable to be monitored be measured directly. Often however, this is impractical and some dependent variable, that is easier to measure, is monitored in its place. For example, in the control of distillation columns, the continuous, on-line, analysis of the overhead product is desirable but difficult and expensive to achieve reliably. So temperature is often monitored as an indication of composition. The temperature instrument may form part of a control loop controlling, say, reflux flow; with the composition of the overheads checked frequently by sampling and laboratory analysis.

2.7.1 Instrumentation and Control Objectives

The primary objectives of the designer when specifying instrumentation and control schemes are:

1. Safe plant operation

(a) To keep the process variables within known safe operating limits.

(b) To detect dangerous situations as they develop and to provide alarms and automatic shut-down systems.

(c) To provide interlocks and alarms to prevent dangerous operating procedures.

2. Production rate

a) To achieve the design product output.

3. Product quality

a) To maintain the product composition within the specified quality standards.

4. Cost

a) To operate at the lowest production cost, commensurate with the other objectives.

These are not separate objectives and must be considered together. The order in which they are listed is not meant to imply the precedence of any objective over another, other than that of putting safety first. Product quality, production rate and the cost of production will be dependent on sales requirements. For example, it may be a better strategy to produce a better-quality product at a higher cost.

In a typical chemical processing plant, these objectives are achieved by a combination of automatic control, manual monitoring and laboratory analysis.

2.7.2 Typical Control Systems

2.7.2.1 Level Control

In any equipment where an interface exists between two phases (e.g. liquid, vapour), some means of maintaining the interface at the required level must be provided. This may be incorporated in the design of the equipment, as is usually done for decanters or by automatic control of the flow from the equipment. Figure 3.13 shows a typical arrangement for the level control at the base of a column. The control valve should be placed on the discharge line from the pump.

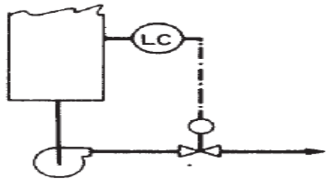


Figure 3.13: Level Control

2.7.2.2 Pressure Control

Pressure control will be necessary for most systems handling vapour or gas. The method of control will depend on the nature of the process. Typical schemes are shown in Figures 2.14a, b, c, d. The scheme shown in Figure 2.14a would not be used where the vented gas was toxic, or valuable. In these circumstances the vent should be taken to a vent recovery system, such as a scrubber.

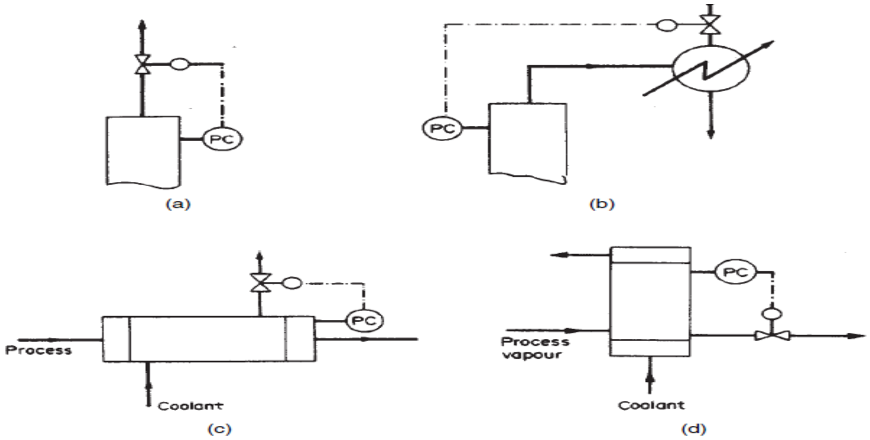


Fig. 2.14(a) pressure control by direct venting (b) Venting of non-condensable vapour after a condenser (c) condenser pressure control by controlling coolant flow (d) pressure control by varying the heat transfer area, area dependent on liquid.

2.7.2.3 Flow Control

Flow control is usually associated with inventory control in a storage tank or other equipment. There must be a reservoir to take up the changes in flow-rate. To provide flow control on a compressor or pump running at a fixed speed and supplying a near constant volume output, a by-pass control would be used, as shown in Figure 3.15.

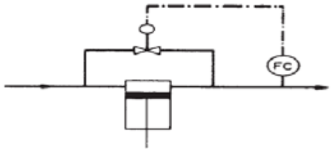


Figure 2:15:Flow Control

2.7.2.4 Temperature Control

The primary objective of temperature control is to keep the feed flow rate and composition at a desired temperature

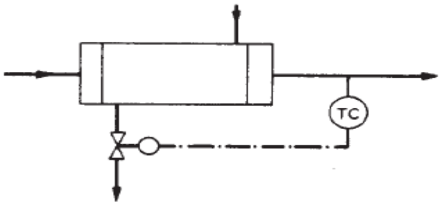


Figure 2.16: Temperature Control

2.7.2.5 CSTR Control

The schemes used for reactor control depend on the process and the type of reactor. If a reliable on-line analyzer is available and the reactor dynamics are suitable, the product composition can be monitored continuously and the reactor conditions and feed flows controlled automatically to maintain the desired product composition and yield. More often, the operator is the final link in the control loop, adjusting the controller set points to maintain the product within specification, based on periodic laboratory analysis. Reactor temperature will normally be controlled by regulating the flow of the heating or cooling medium. Pressure is usually held constant. Material balance control will be necessary to maintain the correct flow of reactants to the reactor and the flow of products and un-reacted materials from the reactor. A typical CSTR control scheme is shown in Figure 7.4 as having Temperature control (TC), Level control (LC) and Flow control (FC) configuration.

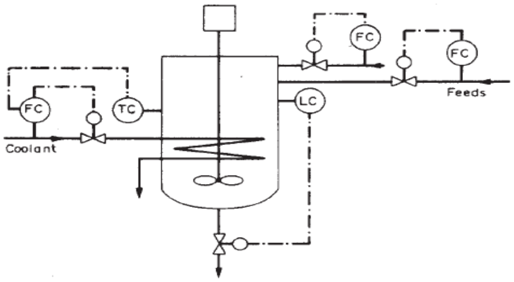
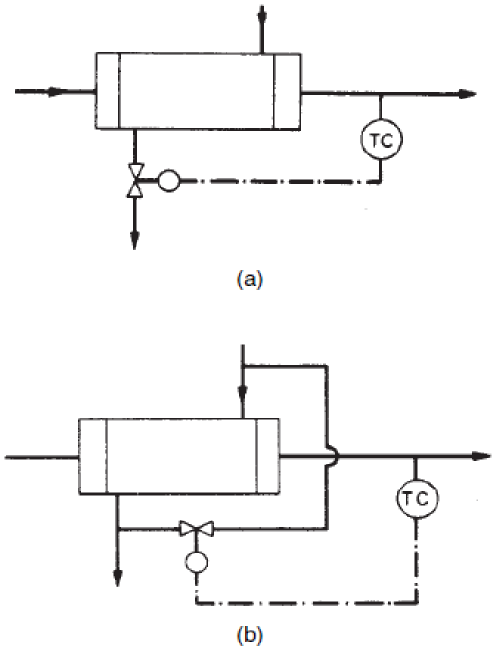


Fig 2:17: A Typical Stirred Tank Reactor Control Scheme, Temperature Cascade Control and Reagent Flow Control

2.7.2.6 Heat Exchanger Control

Figure 3.18ashows the simplest arrangement, the temperature being controlled by varying the flow of the cooling or heating medium. If the exchange is between two process streams whose flows are fixed, by-pass control will have tobe used, as shown in Figure 3.18b.



(a)

(b)

Fig 3:18: (a) Control of one fluid stream (b) By-pass control

2.8 Cost Estimation

2.8.1 Cost analysis for heat exchanger

The following were used for the cost analysis, which include:

i. Heat transfer area = 167m^2
ii. Material for construction = Stainless Steel (SS)
iii. Material factor for costing =

From Chemical Engineering Design Handbook (Coulson and Richardson, 2009), the equipment cost corresponding to a heat transfer area of 167m^2 = 300 x \$1000 = \$300,000

2.8.2 Cost Analysis for CSTR

The following parameters shall be used for the cost analysis of the CSTR;

Diameter = 3.707m

Area = 10.7928m^2

Volume = 60m^2

Height = 5.560m

Material factor for stainless steel = 2

Pressure factor for stainless steel = 1.1

Purchased cost = bare cost X material factor X pressure factor

2.8.3 Cost analysis for storage tank

The following parameters shall be used for the cost analysis of the storage tank:

Diameter = 3.707m

Area = 10.7928m^2

Volume = 60m^3

Height = 5.560m

Material factor for stainless steel clad = 1.5

Pressure factor for stainless steel clad = 1.4

Therefore, purchased cost = bare cost x material factor x pressure factor

Calculations for the costs for the storage tank are shown in Appendix 4D.

This section covers the process simulation of the plant using Aspen HYSYS. The units of the plants are given below.

Units

U001 – Mixing unit

U002 – Heat Exchanger unit

U003 – CSTR unit

U004 – Storage tank unit

Streams

S1 – Feed Stream

S2 – Mixed feed stream

S3 – Steam stream

S4 – Heated mixed feed stream

S5 – Cold steam stream

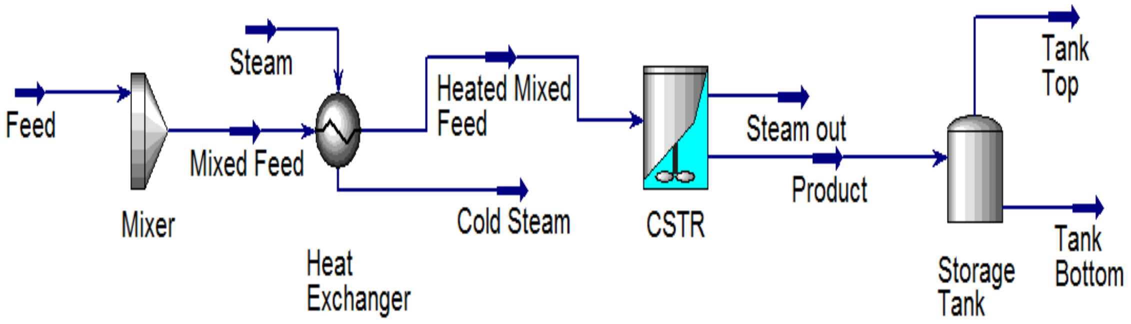
S6 – Product stream

S7 – Tank bottom stream

2.9 Process Description

Production of aerosol antiperspirant deodorants employs the CSTR process. Ingredients are combined together in a mixer and sent to a jacketed stainless steel reactor. Heat in the form of steam is applied to melt the ingredients during the mixing. The temperature is regulated carefully to avoid scorching the waxy ingredients. Once all the ingredients have been added, they are all blended until uniform. The concentrate is then sent to a storage tank and subsequently charged to a standard aerosol can. A valve is mounted and crimped on the can and the propellant ingredients are added under pressure.

The full process diagram of the HYSYS simulation is given below where the feed enters the mixer before it is sent to a heat exchanger in order to heat up the feed using steam. The heated product then enters the CSTR where the final product is formed and then sent to the storage tank.



3 RESULTS AND DISCUSSION

3.1 Material Balance Results

The various results of the material balance of the plant are presented in the following tables below and comparison is made between the HYSYS simulation and the manual calculation.

Table 3.1: Comparison of Material Balance Result of HYSYS Simulation with manual Calculation for mixing unit (U001)

Streams	Manual calculation	HYSYS simulation	Difference
Feed stream (S1)			
Mass flow rate (kg/hr)	9999.364	10000	0.636
Molar flow rate (kgmol/hr)	2231.02	2231	0.02
Mixed feed stream(S2)			
Mass flow rate (kg/hr)	9999.364	10000	0.636
Molar flow rate (kgmol/hr)	2231.02	2231	0.02

Table 3.1 shows the material balance result of the mixing unit which consist of one input stream (S1) and one output stream (S2). The table is also in agreement with the principles of conservation of mass which states that inflow of mass equals to outflow of mass, hence S1 = S2.

Table 3.2: Comparison of Material Balance Result of HYSYS Simulation with manual Calculation for Heat exchanger unit (U002)

Streams	Manual calculation	HYSYS simulation	Difference
Mixed feed stream(S2)			
Mass flow rate (kg/hr)	9999.36	10000	0.636
Molar flow rate (kgmol/hr)	2231.02	2231	0.02
Steam Stream			
Mass flow rate (kg/hr)	10000.10	10000	0.10
Molar flow rate (kgmol/hr)	555	555.1	0.10
Heated mixed feed			
Mass flow rate (kg/hr)	9999.364	10000	0.636
Molar flow rate (kgmol/hr)	2231.02	2231	0.02
Cold steam stream			
Mass flow rate (kg/hr)	10000	10000.1	0.10
Molar flow rate (kgmol/hr)	555.1	555	0.10

Table 3.2 shows the material balance result for the Heat exchanger unit which consist of two input streams been S2 and S3 as well two output streams been S4 and S5. The table is also in agreement with the principles of conservation of mass which states that inflow of mass equals to outflow of mass, hence S2+ S3 = S4 +S5.

Table 3.3: Comparison of Material Balance Result of HYSYS Simulation with manual CSTR unit (U003)

Streams	Manual calculation	HYSYS simulation	Difference

Heated mixed feed(S4)			
Mass flow rate (kg/hr)	9999.364	10000	0.636
Molar flow rate (kgmol/hr)	2231.02	2231	0.02
Product Stream (S6)			
Mass flow rate (kg/hr)	9999.364	10000	0.636
Molar flow rate (kgmol/hr)	2231.02	2231	0.02

Table 3.3 shows the material balance result of the mixing unit which consist of one input stream (S4) and one output stream (S6). The table is also in agreement with the principles of conservation of mass which states that inflow of mass equals to outflow of mass, hence S4 = S6.

Table 3.4: Comparison of Material Balance Result of HYSYS Simulation with manual Calculation for storage tank (U004)

Streams	Manual calculation	HYSYS simulation	Difference
Product Stream(S6)			
Mass flow rate (kg/hr)	9999.364	10000	0.636
Molar flow rate (kgmol/hr)	2231.02	2231	0.02
Tank bottom (S7)			
Mass flow rate (kg/hr)	9999.364	10000	0.636
Molar flow rate (kgmol/hr)	2231.02	2231	0.02

Table 3.1 shows the material balance result of the mixing unit which consist of one input stream (S6) and one output stream (S7). The table is also in agreement with the principles of conservation of mass which states that inflow of mass equals to outflow of mass, hence S6 = S7.

3.2 Energy Balance Result

The various results of the material balance of the plant are presented in the following tables below and comparison is made between the HYSYS simulation and the hand calculation.

Table 3.5: Comparison of Energy Balance Result of HYSYS Simulation with manual Calculation for Mixing unit (U001)

Streams

Feed stream (S1)			
Temperature (^oC)	25	25	0.00
Pressure (kPa)	101.3	101.3	0.00
Heat flow (kJ/hr)	-5.279E7	-5.278E7	1E7
Mixed feed stream(S2)			
Temperature (^oC)	25	25	0.00
Pressure (kPa)	101.3	101.3	0.00
Heat flow (kJ/hr)	-5.279E7	-5.278E7	1E7

Table 3.5 shows the Energy balance result of the mixing unit which consist of one input stream (S1) and one output stream (S2). The table is also in agreement with the principles of conservation of Energy which states that inflow of Energy equals to outflow of mass, hence S1 = S2.

Table 3.6: Comparison of Energy Balance Result of HYSYS Simulation with manual Calculation for Heat Exchanger (U002)

Streams	Manual calculation	HYSYS simulation	Difference
Mixed feed stream(S2)			
Temperature (^oC)	25	25	0.00
Pressure (kPa)	101.3	101.3	0.00
Heat flow (kJ/hr)	-5.279E7	-5.278E7	1E7
Steam Stream (S3)			
Temperature (^oC)	100	100	0.00
Pressure (kPa)	101.3	101.3	0.00
Heat flow (kJ/hr)	-5.278E7	-5.278E7	1E7
Heated Mixed feed(S4)			
Temperature (^oC)	60.79	60.79	0.00
Pressure (kPa)	82.30	82.30	0.00
Heat flow (kJ/hr)	-5.128E7	-5.130E7	2E7

Cold steam(S5)			
Temperature (^{o}C)	91.24	91.24	0.00
Pressure (kPa)	101.3	73.50	27.8
Heat flow (kJ/hr)	-1.339E8	-1.339E8	0.00

Table 3.6 shows the Energy balance result for the Heat exchanger unit which consist of two input streams been S2 and S3 as well two output streams been S4 and S5. The table is also in agreement with the principles of conservation of Energy which states that inflow of Energy equals to outflow of Energy, hence S2+ S3 = S4 +S5.

Table 3.7: Comparison of Energy Balance Result of HYSYS Simulation with manual Calculation for CSTR Unit (U003)

Streams	**Manual calculation**	**HYSYS simulation**	**Difference**
Heated Mixed feed(S4)			
Temperature (^{o}C)	60.79	60.79	0.00
Pressure (kPa)	82.30	82.30	0.00
Heat flow (kJ/hr)	-5.128E7	-5.130E7	2E7
Product Stream			
Temperature (^{o}C)	60.79	60.79	0.00
Pressure (kPa)	82.30	82.30	0.00
Heat flow (kJ/hr)	-5.128E7	-5.130E7	2E7

Table 3.7 shows the energy balance result of the mixing unit which consist of one input stream (S4) and one output stream (S6). The table is also in agreement with the principles of conservation of energy which states that inflow of energy equals to outflow of energy, hence S4 = S6.

Table 3.8: Comparison of Energy Balance Result of HYSYS Simulation with manual Storage Tank Unit (U004)

Streams	Manual calculation	HYSYS simulation	Difference
Heated Mixed feed(S4)			

Temperature (°C)	60.79	60.79	0.00
Pressure (kPa)	82.30	82.30	0.00
Heat flow (kJ/hr)	-5.128E7	-5.130E7	2E7
Tank Bottom (S7)			
Temperature (°C)	60.79	60.79	0.00
Pressure (kPa)	82.30	82.30	0.00
Heat flow (kJ/hr)	-5.128E7	-5.130E7	2E7

Table 3.8 shows the energy balance result of the mixing unit which consist of one input stream (S6) and one output stream (S7). The table is also in agreement with the principles of conservation of energy which states that inflow of mass equals to outflow of energy, hence S6= S7.

3.3 Sizing Results

Table 3.9: Comparison of Sizing Result of HYSYS Simulation with manual for Heat Exchanger Unit (U002)

Design/Sizing Item	HYSYS Simulation	Manual Calculation	% Deviation
Equipment Name	Shell and tube heat exchanger	Shell and tube heat exchanger	
Objective.	Heating the mixer effluent	Heating the mixer effluent	

Equipment Number	U-002	U-002	
Designer	ALEKIRI MAUREEN PG.2017/02868	ALEKIRI MAUREEN PG.2017/02868	
Type	Split ring floating head (two shell four tubes)	Split ring floating head (two shell four tubes)	
Utility	Brackish Water	Brackish Water	
Insulation	Foam Glass	Foam Glass	
Heat load Q (kw)	412	411.78	0.0
Heat transfer Area (m^2)	167	167.03	0.2
LMTD (°C)	52	51.55	0.2
U (W/m^2K)	780	799.3	0.1
Inlet temperature) °C)	61	60.79	0.0
Shell Diameter (mm)	476	476	0.0
Shell coefficient W/m^2C	3168	3168.4	0.2
Outlet temperature (°C)	40	40	0.0
Baffle spacing (25% cut)	95.2	95.2	0.0
Shell material	Carbon steel	Carbon steel	
Inlet temperature (°C)	25	25	0.0
Tube Diameter (mm od/id)	20/16	20/16	0.0
Tube length (m)	4.83	4.83	0.0
Pitch type	Triangular	triangular	
Outlet temperature (°C)	40	40	0.0
Number of Tubes	172	172.2	0.0
Tube material	Carbon alloy	Carbon alloy	
Pitch	25mm	25mm	0.0

Table 3.9 shows the sizing result of the various parameter of Heat exchanger having a maximum percentage deviation of 0.2%.

Table 3.10: Comparison of Sizing Result of HYSYS Simulation with manual for CSTR Unit (U003)

Design/Sizing Item	HYSYS Simulation	Manual Calculation	% Deviation
Flow Type			
Materials of Construction	Stainless steel	Stainless steel	
Column Height (m)	5.54	5.56	0.36
Column Diameter(m)	3.72	3.71	1.40
Cross Sectional Area(m^2)	10.80	10.79	1.30

Volume(m^3)	60.02	60.00	3.30
Space Time(hr)	0.08	0.09	1.33
Space Velocity(hr^{-1})	1.44	1.44	0.00
Thickness(mm)	21.60	21.59	1.67
Corrosion allowance(mm)	2.00	2.00	0.00

Table 3.10 shows the sizing result of the various parameter of CSTR having a maximum percentage deviation of 3.3%.

Table 3.11: Comparison of Sizing Result of HYSYS Simulation with manual calculation for storage tank Unit (U004)

Design/Sizing Item	HYSYS Simulation	Manual Calculation	% Deviation
Flow Type			
Materials of Construction	Stainless steel	Stainless steel	
Column Height (m)	5.54	5.56	0.36
Column Diameter(m)	3.72	3.70	1.40
Cross Sectional Area(m^2)	10.80	10.79	1.30
Volume(m^3)	60.02	60.00	0.00
Space Time(hr)	0.74	0.75	1.33
Space Velocity(hr^{-1})	1.35	1.33	1.50
Thickness(mm)	21.60	21.59	1.67
Corrosion allowance(mm)	2.00	2.00	0.00

Table 3.11 shows the sizing result of the various parameter of storage tank having a maximum percentage deviation of 1.67%.

3.4 Costing Result

Table 3.12: Comparison of Costing Result of HYSYS Simulation with manual Calculation for Heat Exchanger Unit (U002)

Parameter	Manual Calculation	HYSYS simulation	Difference
Heat transfer area (m^2)	167	168	1.00
Material for Construction	Stainless steel	Stainless Steel	
Material factor	1.0	1.0	0.00
Pressure factor	1.0	1.0	1.0
Equipment Cost ($)	30000	30000	0.0

Table 3.12 shows the costing for the Heat exchanger compared with that from HYSYS simulation having a purchased cost of $30000.

Table 3.13: Comparison of Costing Result of HYSYS Simulation with manual Calculation for CSTR Unit (U001)

Parameter	Manual Calculation	HYSYS Simulation	Difference
Bare cost ($)	36363.64	36363	0.64
Material for Construction	Stainless Steel	Stainless Steel	
Material factor	2	2	0.0
Pressure factor	1.1	1.1	0.00
Equipment Cost ($)	80000	80000	0.00

Table 3.13 shows the costing for the CSTR compared with that from HYSYS simulation having a purchased cost of $80000

Table 3.14: Comparison of Costing Result of HYSYS Simulation with Manual Calculation for Storage Tank Unit (U001)

Parameter	Manual Calculation	HYSYS simulation	Difference
Bare Cost ($)	42380	42380	0.00
Material for Construction	Stainless Steel	Stainless Steel	
Material factor	1.5	1.5	0.00
Pressure factor	1.4	1.4	0.00
Equipment Cost ($)	88999	89000	1.00

Table 3.14 shows the costing for the Heat exchanger compared with that from HYSYS simulation having a purchased cost of $89000 and $88999 for manual calculation.

4 Conclusion

This design project was aimed to bring forth an integrated detailed design of an 80,000ton/yr Aerosol Antiperspirant Deodorant Production Plant using Aspen HYSYS as a design tool and employing the CSTR method, comparing the design process to the manual design method.

This research covered several aspects of the plant's design, including a literature background on the production of aerosol antiperspirant deodorant. Rigorous material and energy balances were done throughout the plant manually and with the use of Aspen HYSYS. It was found that both methods yielded similar computational results, with a very small error margin.

Detailed equipment sizing and specification as well as mechanical design of the plant were also carried out on the following units: CSTR Unit [U003], Heat Exchanger Unit [U002] and finally Storage Tank Unit [U004]. These were also done manually and with the use of Aspen HYSYS. It was found that the results from both methods were close in value with a negligible error margin between the results.

The mechanical design to determine the thickness of vessels to withstand pressure was also considered as well as adding corrosion allowance. Both the manual and simulated approaches were employed and compared and it was found that the results were similar with a negligible error margin between them.

A full instrumentation and control for the various part of the plant such as pressure, temperature and flow control were also analyzed. A detailed cost estimation and economic evaluation was analyzed to determine the profitability of the plant before setting up.

The layout of the plant, safety and environmental consideration were considered so as not to pollute the environment as a result of the toxic waste from the flared gases. The final task was to simulate the process to obtain an optimized view of the plant's operations using Aspen HYSYS

REFERENCES

Abrutyn, Eric (2010). Antiperspirants and Deodorants. 10. 1002/9781444317657. Ch20.

Alan Passero, G. L. (2015). *Patent No. BR102015012612A2.* Brazil.

Bedalov, Zark (2020). Designing Plant Layout. 10.1002/9781119535003.ch4.

Benohanian, Antranik (2001). Antiperspirants and Deodorants. Clinics in Dermatology. 10.1016/S0738-081x(01)00192-4.

Benoit Mesurolle, Joan Ceccarelli, Igor Karp, Simon Sun, Mona El-Khoury (2013). Effects of Antiperspirant Aluminium Percent Composition and Mode of Application on Mock Microcalcifications in Mammography. *European Journal of Radiology*. 279-282. www.elsevier.com/locate/ejrad

Carlos Gonzalez (2017). *The Impact of Simulation and the Future of Manufacturing.* Retrieved from https://www.machinedesign.com/3d-priniting-cad (Accessed June,2020).

Coulson, J.M. & Richardson J.F. (2003). Chemical Engineering Design (Volume 6, 3rd Edition). Oxford: Butterworth-Heinemann.

D.P Morgan (2010). Chemical Plant Expansion. 10.1021/cen-v025n002.p078.

Darlenski, Razvigor and Fluhr, Joachim (2011). Antiperspirants and Deodorants. Practical Aspects of Cosmetic testing; How to Set up a Scientific Study in Skin Physiology. 217-226. 10.1007/978-3-642-05067-1.

Draelos, Z. (2001). Antiperspirants and the Hyperhidrosis Patient. *Dermatol Ther*, 220-224.

Epic Process Systems (2019). *Full Deodorant Process Plant Design and Conversion.* Retrieved from https://www.epicmodularprocess.com/case-studies/process-plant-design (Accessed March,2020).

Ernest E.L. (1997). Applied Process Design and Integration. England: Wiley and Sons Ltd.

Everts, S. (2012). What are deodorants and antiperspirants and how do they fight sweat. *C & EN* , 27.

Feroldi, R (2008). Deodorants and Antiperspirants: A guide for the Right Choice. Vol. 23. 10-11.

Green, J. (2004). The Apothecary: Elixirs, Remedies, and Tonics. In J. Green, *The Apothecary: Elixirs, Remedies, and Tonics* (p. 356). Rodal Books.

Grytch Robert. (2016). *Patent No. US9408799B2.* United States.

Hrastic I. & Jug Mario (2005). Antiperspirants and Deodorants. Farmaceutski Glasnik. 61. 557-570.

James, G.S. (2002). Chemical and Process Design Handbook. USA: McGraw-Hill.

John Brahms, J. C. (2001). *Patent No. HU0301196A.* Hungary.

Kakac, S. & Liu, Hongtan & Pramuanjaroenkij, Anchasa. (2020). Classification of Heat Exchangers. 10.1201/9780429469862-1.

Kuehl BL, Fiona K. (2003). Cutaneous Cleansers.

Laska, Michael & Clooney,Charles. (2002). Bioreactors, Continuous Stirred-Tank Reactors. 10.1002/0471250589.

Marc Praye, H. I. (2009). Handbook of Cosmetic Science and Technology. Informa Health Care.

Mark J. Dickson (2011). Process Understanding. For Scale up and Manufacture of Active Ingredients. 10.1002/9783527637140.ch10.

Moran Sean (2019). Stages of Process Plant Design. 10.1016/B978-0-12-814860-0.

Nunes, Leonel & Matias, Joao & Catalao, Joao (2018). Plant Design and Operation. 10.1016/B978-0-12-809462-4.

Peter R. Hilliard and J. S. (2017). *Patent No. CA3037566A1.* Canada.

Rauwendaal, Chris (2018). Instrumentation and Control. 10.3139/9781569906996.002.

Ray, Martyn & Sneesby, Martin (2020). Site Considerations: Site Selection and Plant Layout. 10.1201/9781003078234-6.

Ray, Subhabrata & Das, Gargi. (2020). Plant Instrumentation and Control. 10.1016/B978-0-12-814885-3.

Robin, S. (2005). Chemical Process Design and Integration. England: Wiley and Sons Ltd.

Safety Center (2010). Plant Design. 10.1002/9780470938270.

Sawant, A. (2019, July 15). *Antiperspirants and Deodorants Market Size Estimation; Business Statistics, Opportunities, Company Landscape, Latest Innovation, New Trends and Forthcoming Developments.* Retrieved from MarketWatch: https://www.marketwatch.com/press-release.

Screiber Joery (2009). Handbook of Cosmetic Science and Technology. Third Edition.

Scott H. Fogler (2010). Essentials of Chemical Reaction Engineering: Mole Balances. Retrieved from

https://www.informit.com/articles.

Sean Moran (2019). Applied Guide to Process and Plant Design. 33-62. 10.1016/B978-0-12-814860-0.

Shahbandeh, M. (2019). Size of the Global Antiperspirant and Deodorant Market 2012-2025. *Statista* .

Shen, Juanshu & Nardello-Rataj (2009). Deodorants and Antiperspirants. Chemistry of Underarms. Actualite Chimique.8-18.

Silverson Inc (2020). *Manufacture of Deodorants and Antiperspirants.* Retrieved from https://www.silverson.com/us/resource-library/.

Smith, P. (2011). Material and Energy Balances. 10.1007/978-1-4419-7662-8.

Stanley, M.W. (1990). Chemical Process Equipment: Design and Selection. USA: Butterworth-Heinemann.

Sunden, Bengt. (2000). Heat Transfer and Heat Exchangers. 10. 1002/0471238961.

Theodore, Louis & Dupont, Roberts & Ganesan, Kumar (2017). Process and Plant Design. 10.1002/9781119283706. ch8.

Vaibhav Khandare & Satish Sakhwade (2017). Formulation & Long Lasting Efficacy of Herbal Based Deodorant up to 48 hours by Sniff Test Method. *International Journal of Research in Financing and Marketing. Volume 7.* (2231-5985). 210-216.

Yvonne Cierpisz, H. F.-Z. (2004). *Patent No. DE102004049282A1*. Germany.