



INTERNATIONAL JOURNAL OF CREATIVE RESEARCH THOUGHTS (IJCRT)

An International Open Access, Peer-reviewed, Refereed Journal

MANUFACTURE OF GUANIDINE HCl AND GUANIDINE NITRATE

Pujita Sravya Sri. B, Sreenivas Matla, Pampana Anilkumar, Prof. K. V. Rao, P. Anil Kumar
 Student, Assistant Professor, Assistant Professor, Programme Director, Assistant Professor
 Department of Petroleum and Petrochemical Engineering,
 Jawaharlal Nehru Technological University Kakinada, Kakinada, India

Abstract: Guanidinium chloride and guanidine Nitrate are the halides of guanidine. Due to rapid growth in population and industrialization, worldwide Guanidinium chloride and guanidine Nitrate demand is increasing continuously. The production of Guanidinium chloride and guanidine Nitrate are completely industrial processes. The best cost effective and abundant productions of each compounds, Guanidinium chloride and guanidine Nitrate have been selected. This project entitled "Manufacture of Guanidinium chloride and guanidine Nitrate" is a detailed report on production of Guanidinium chloride and guanidine Nitrate. The material balances and energy balances for the process to be used are calculated and the heat of reactions and specific heats for the components are calculated for the process used.

Index Terms - Component, formatting, style, styling, insert.

Introduction

Guanidine HCl:

Guanidinium chloride or guanidine hydrochloride is that the complex salt of guanidine. Having a formula of CH_6ClN_3 . Guanidinium chloride crystallizes in orthorhombic area cluster. The crystal structure consists of network of Guanidinium cations and chloride anions coupled by $\text{N-H}\cdots\text{Cl}$ element bonds. It is a weak acid with a pka of thirteen.6. It exists as dry powder. Guanidinium chloride could be a robust chaotrope and one amongst the strongest denaturants employed in physiochemical studies of organic process. It additionally has the flexibility to decrease catalyst activity and increase the solubility of hydrophobic molecules. At high concentrations of guanidinium chloride (e.g., 6 M), proteins lose their ordered structure, and that they tend to become arbitrarily rolled, i.e. they are doing not contain any residual structure. However, at concentrations within the millimolar aim vivo, guanidinium chloride has been shown to "cure" particle positive yeast cells (i.e. cells exhibiting a particle positive makeup revert to a particle negative phenotype). This is often the results of inhibition of the Hsp104 chaperone macromolecule notable to play a crucial role in particle fiber fragmentation and propagation.

Guanidine Nitrate:

Guanidine nitrate is that the compound with the formula $[\text{C}(\text{NH}_2)_3]\text{NO}_3$. It additionally referred to as Guanidine mononitrate, Nitroguanidine it's a colorless, soluble salt. It is actually a compound comprised of guanidine ($\text{NH}_2\text{-C}(\text{NH})\text{-NH}_2$) and acid (HNO_3) radicals. every Guanidine nitrate molecule has 2 molecules of guanidine combined with one molecule of acid.

Takes some effort to ignite however once lit it burns with increasing vigor because the fireplace progresses. If contaminated with flammable materials it accelerates their burning. Prolonged exposure to fireside or heat might lead to associate degree explosion. Produces deadly oxides of gas throughout combustion.

II. PROCESS DESCRIPTION

Guanidine HCl:

This chapter includes the study of varied steps that are happening within the method technology used at the side of the reactions, temperatures and pressures of streams used together with the method flowchart that is shown in figure 2.1.

The present invention includes the subsequent technological processes of melting, dissolution, filtration, dehydration and crystallization. Thus, high-purity guanidine coordination compound is obtained. The current invention has the benefits of straightforward and sensible technology and cheap principle. The guanidine coordination compound ready by the tactic of the current invention has the benefits of fine quality and high purity of over 99.9%, and is greatly popular users.

Preparation technique of guanidine coordination compound includes the subsequent method flows:

- Melting, particularly swing dicyandiamide and salt in a very weight magnitude relation of one: 1.27 into a reaction kettle, and ending a melting reaction at 170- 230 °C to get a guanidine coordination compound crude product;
- dissolving, particularly dissolving the crude guanidine coordination compound into water at traditional temperature consistent with the proportion of one: one or 1.5: 1;

- filtering, and removing the raw materials and reaction by-products by a filtering method;
- dehydrating, particularly dehydrating the filtered mother liquor;
- Further:, adding dicyandiamide into the guanidine coordination compound obtained within the step d, permitting the guanidine coordination compound to enter a reaction kettle, performing arts a melting reaction for 3-4 hours at 170-230 °C, performing arts steps b, c, and d to get the guanidine coordination compound, and continuance the steps for multiple time and further: within the dissolving step, a base is more to the answer.

The method has easy and sensible method and cheap principle, and also the guanidine coordination compound ready by the tactic has sensible quality and high purity which may reach 99.9% and is well received by users.

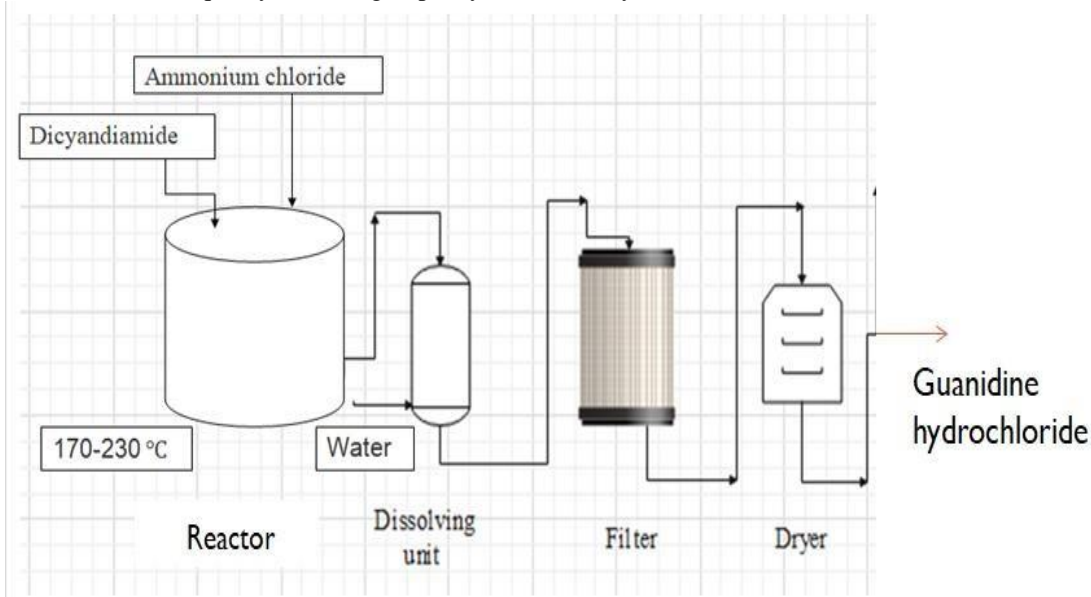


Fig2.1 Process Flow diagram

Guanidine Nitrate:

This chapter includes the study of varied steps that *are* happening within the method technology used at the side of the reactions, temperatures and pressures of streams used as well as the method multidimensional language that is shown in figure a 2.2.

This method for the assembly of guanidine nitrate from a mix of carbamide and nitrate within the presence of a catalyst containing silicium compound at an increased temperature, the initial mixture of carbamide and nitrate having a far more than nitrate and therefore the fashioned guanidine nitrate being separated off. Moreover the invention provides equipment for its performance.

It's already identified to pass a liquified mixture of carbamide and nitrate in an exceedingly molecular quantitative relation of 1:1 to 1:6, desirable 1:2 to 1:3, below traditional pressure and a temperature of approx. 175⁰C.-225⁰C. And desirable one hundred 90⁰C.- 200⁰C. Through a vertical column containing the catalyst and to isolate the fashioned guanidine nitrate in an exceedingly well-known manner to supply guanidine nitrate. During this method the unreacted nitrate and carbamide compositions are separated from the fashioned guanidine nitrate compound and mixed with recent initial material and once more skillful the catalyst. A most popular catalyst within the well-known method could be a gel of acid.

To obtain a high production rate as desired, there would be an opportunity to equip the reactor with an outsized range of parallel operated tubes however during this case every tube would need a dosing device of its own to ensure a fair output through every reactor tube. Even so it should rather be that with gradual exhaust of the catalyst it clogs any of the tubes for the passage of the soften at an early stage and so the passage of the soften through the opposite pipes is sped up and therefore the desired conversion and therefore the optimum yield don't seem to be obtained. Moreover the catalyst is incessantly enriched with triazines during this case and so additionally incessantly its activity is diminished.

Furthermore it's to be recognized that with the specified conversion temperatures of approx. 192⁰C., beside of the oxidisation of 8-9% carbamide, more and more triazines, notably ammeline and ammelide ar fashioned. The latter are nearly insoluble and canopy the catalyst surface and so its activity and therefore the reactivity of the mixture is significantly diminished so reducing the yield that might be obtained.

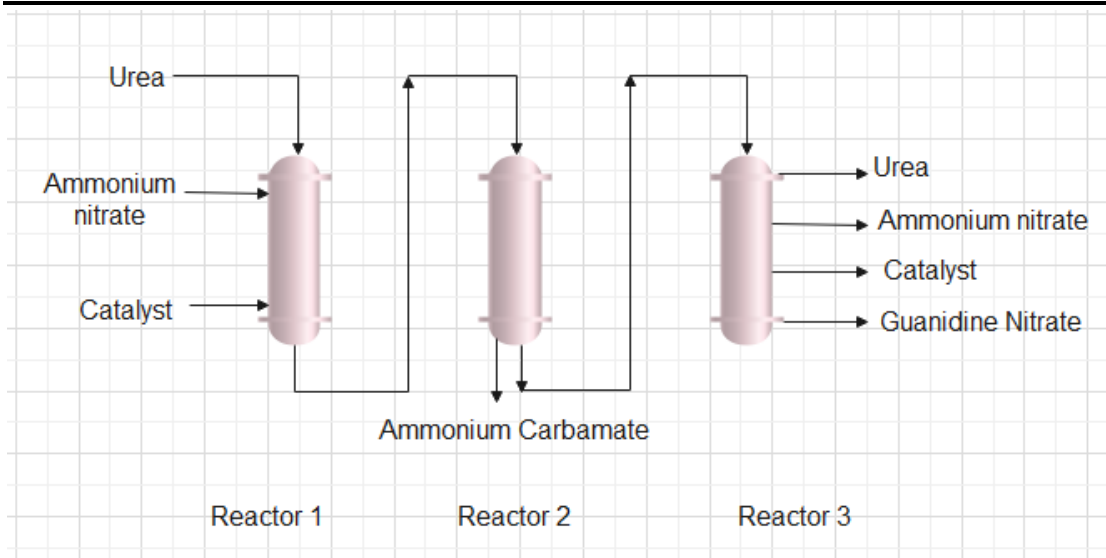


Fig2.2 Process flow diagram

III.MATERIAL BALANCES

Material balances are the basis of process design. A material balance taken over complete process will determine the quantities of raw materials required and products produced. Balances over the individual process until set the process stream flows and compositions.

The general conservation equation for any process can be written as

$$\text{Material in} = \text{Material out} + \text{Accumulation}$$

For a steady state process the accumulation term is zero. If a chemical reaction is taking place a particular chemical species may be formed or consumed. But if there is no chemical reaction, the steady state balance reduces to $\text{Material in} = \text{Material out}$

Material balance also useful tool for study of plant operation and trouble shooting. They can be used to check the performance against design to check instrument calibration and to locate the sources of material loss.

Guanidine HCl:

Material Balance around Reaction Kettle

Table 3.1 Material Balance around Reaction Kettle

Compound	Input		Output	
	Kg/hr	%	Kg/hr	%
Dicyandiamide	27.2	44	--	--
Ammonium Chloride	35.27	56	--	--
Guanidine Hydrochloride	--	--	62.99	100
Total	62.99	100	62.99	100

Material Balance around dissolving unit

Table 3.2 Material Balance around dissolving unit

Compound	Input		Output	
	Kg/hr	%	Kg/hr	%
Guanidine Hydrochloride	62.99	50	--	--
Water	62.99	50	--	--
Wet product	--	--	125.98	100
Total	100		125.98	100

Material Balance around Dryer

Table 3.3 Material Balance around Dryer

Compound	Input		Output	
	Kg/hr	%	Kg/hr	%
Wet product	125.98	100	--	--
Water	--	--	44.09	34.9
Dry product	--	--	81.887	65.1
Total	125.98	100	125.98	100

Guanidine Nitrate:

Material Balance around Reactor 1

Table 3.4 Material Balance around Reactor 1

Compound	Input Kg/hr		Output Kg/hr	
		%		%
Urea	600	27.2	480	21.8
Ammonium Nitrate	1200	54.6	1130	51.3
Catalyst	400	18.2	400	18.18
Guanidine Nitrate	--	--	190	8.6
Total	2200	100	2200	100

Material Balance around Reactor 2

Table 3.5 Material Balance around Reactor 2

Compound	Input		Output Kg/hr	
	Kg/hr	%		%
Urea	1080	38.5	330	11.7
Ammonium Nitrate	1130	40.3	650	23.2
Catalyst	400	14.2	400	14.2
Guanidine Nitrate	190	6.7	890	31.7
Ammonium Carbamate	--	--	530	18.9
Total	2800	100	2800	100

Material Balance around Reactor 3

Table 3.6 Material Balance around Reactor 3

Compound	Input		Output	
	Kg/hr	%	Kg/hr	%
Urea	930	32.4	60	2.0
Ammonium Nitrate	650	22.6	420	14.6
Catalyst	400	13.9	400	13.9
Guanidine Nitrate	890	31.0	1990	69.3
Total	2870	100	2870	100

IV. ENERGY BALANCES

The First law of natural philosophy states that energy will neither be created nor be destroyed. Within the method style energy balances square measure created to work out the Energy necessities of the method. The following may be a systematic energy balance performed for every unit of the method. Assumptions:

- The system is Associate in Nursing open system at steady state.
- Steam is employed for heating functions.
- Wherever cooling is needed, standard water is employed. Equations used for calculation
General equation,

$$Q - W_s = \Delta H + \Delta E_k + \Delta E_p$$

However, based on the assumption made, the above equation is reduced to the form of:

$$Q = \Delta H = mC_p\Delta T$$

Equation heat capacity,

$$C_p = A + BT + CT^2 + DT^3 .$$

Estimation of specific heat capacity:

The Rowlinson-Bondi equation was used to estimate specific heat capacity (C_p) for pure component fatty acids. The equation, as quoted in Reid , is as follows:

$$(C_p - C_p^\circ)/R = 1.45 + 0.45 * (1 -)^{-1} + 0.25 \omega [17.11 + 25.2 (1 - Tr)^{1/3} Tr^{-1} + 1.742(1 -)^{-1}].$$

Where

C_p is the liquid specific heat capacity,

C_p° is the ideal gas specific heat capacity, R is the universal gas constant, Tr is the reduced temperature,

ω (Appendix II) is the acentric factor.

C_p° is calculated using the method of Rihany and Doraisamy

Guanidine HCl

Energy Balance around reaction kettle

Table 4.1 Energy Balance around reaction kettle

Compound	Flowrate(Kg/h)		Temperature(K)	Cp (KJ/Kg.K)
	Input	Output		
Dicyandiamide	27.2	--	298	1.572
Ammonium Chloride	35.27	--	298	1.403
Guanidine Hydrochloride	-	62.49	473	10.95

Heat gained (Q)= $m \cdot C_p \cdot dt = 308415.2301$ KJ/hr

Energy Balance around dissolving unit

Table 4.2 Energy Balance around dissolving unit

Compound	Flowrate(Kg/hr)		Temperature(K)	Cp (KJ/Kg.K)
	Input	Output		
Guanidine Hydrochloride	62.994	--	473	10.95
Water	62.994	--	298	4.18
Wet product	--	125.98	298	10.95

Heat gained (Q)= $m \cdot C_p \cdot dt = 6349.51$ KJ/hr

Energy Balance around dryer

Table 4.3 Energy Balance around dryer:

Compound	Flowrate(Kg/hr) Input Output	Temparat ure(K)	Cp(KJ/Kg.K)
Wet product	125.98	-- 298	10.95
Water	44.09	-- 298	4.18
Dry product	81.887	298	10.95

$$\text{Heat Losss (Q)} = m \cdot C_p \cdot dt = -89243.49 \text{ KJ/hr}$$

Guanidine Nitrate:

Energy Balance around Reactor 1

Table 4.4 Energy Balance around Reactor 1

Compound	Input Kg/hr T	Output Kg/hrT	Cp KJ/kg.K
Urea	600 298	480 459	2.49
AmmoniumN itrate	1200 298	1130 459	0.2
Catalyst	400 298	400 459	1.13
Guanidine Nitrate	-- --	190 459	1.059

$$\text{Heat Required (Q)} = m \cdot C_p \cdot dt = 300726.1 \text{ KJ/hr}$$

Energy Balance around Reactor 2

Table 4.5 Energy Balance around Reactor 2

Compoun d	Input Kg/hr	Output Kg/hr	T kelvin	Cp KJ/kgk
Urea	1080	330	459	2.49
Ammoniu m Nitrate	1130	650	459	0.2
Catalyst	400	400	459	1.13
Guanidine Nitrate	190	890	459	1.059
Ammoniu m Carbamate	--	530	459	2.59

$$\text{Heat required (Q)} = m \cdot C_p \cdot dt = 759484.80 \text{ KJ/hr}$$

Energy Balance around Reactor 3

Table 4.6 Energy Balance around Reactor 3

Compound	Input Kg/hr	Output Kg/hr	T kelvin	Cp KJ/kg k
Urea	930	60	459	2.49
Ammonium Nitrate	650	420	459	0.2
Catalyst	400	400	459	1.13
Guanidine Nitrate	890	1990	459	1.059

Heat Loss (Q)= m*Cp*dt = -51536.01 KJ/hr

V.SPECIFIC EQUIPMENT DESIGN

Guanidine HCl:

Volume of reactor	147.02 m ³
Diameter of reactor	4.99 m
Wall thickness	0.014 m
Volume of liquid content	110.268 m ³
Height of liquid level	7.49 m
Impeller diameter	1.66 m
Speed of impeller	57.5 rpm
Power requirement of impeller	72.43 hp

Guanidine Nitrate:

Volume of reactor	1025 m ³
Diameter of reactor	9.54 m
Volume of liquid content	769 m ³
Height of liquid level	14.32 m
Stirrer diameter	2.385 m
Stirrer length	12.73 m
Wall thickness	0.024 m
Power requirement	2.92W

VI. PLANT COST ESTIMATION

As the final process-design stage is complete, it becomes attainable to create correct price estimation as a result of elaborate instrumentation specification and definite plant facility data square measure offered. Direct worth quotation supported elaborate specification will then be obtained from varied makers. However work ought to proceed to the ultimate stages before prices square measure thought-about and value estimate ought to be created through out all the first stages of the look once complete specifications aren't offered. Analysis of prices within the preliminary style is alleged predesign price estimation. Such estimation ought to be capable of providing a basis for company management to come to a decision if additional capital ought to be invested with within the project.

A capital investment is needed to any process, and determination of the mandatory investment is a vital a part of a plant style project. the full investment for any method consists of the physical instrumentation and facilities within the plant and

the assets for cash that should be offered to pay salaries keep raw materials and product reachable and handle alternative special things requiring an on the spot forged out lay.

CAPITAL INVESTMENTS

Before associate degree complex may be place into operation, great amount of cash should be provided to buy and install the mandatory machinery and instrumentation, land and repair facilities should be obtained and also the plant-must be erected. Complete with all pipe controls hostel services. Additionally it's necessary to own cash offered for payment of expenses concerned within the plant operation. The capital required to produce the mandatory producing and plant facilities is named the fastened capital investment whereas the mandatory for the operation of the plant is termed because the assets investment Working Capital Investment: The capital which is necessary for the operation of the plant working capital investment.

Fixed Capital Investment:

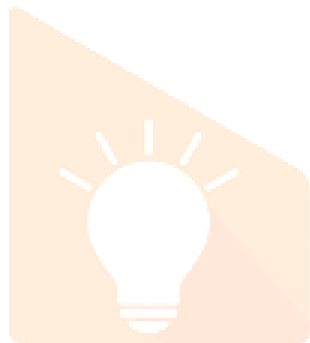
The capital needed to supply necessary and plant facilities is called fixed capital investment. The fixed capital investment classified in to two sub divisions.

- Direct Cost
- Indirect Cost

Direct Cost

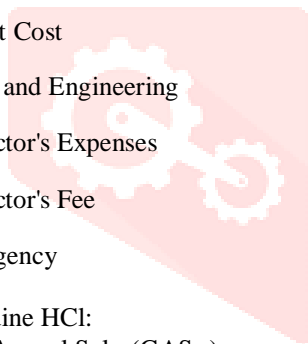
The direct cost items are incurred in the construction of the plant in addition to the cost of equipment.

- Purchased Equipment
- Purchased Equipment Installation
- Instrumentation and Control
- Piping
- Electrical Equipment and Materials
- Building (Including Services)
- Yard Improvement
- Services Facilities



Indirect Cost

- Land
- Design and Engineering
- Contractor's Expenses
- Contractor's Fee
- Contingency



Guanidine HCl:

• Gross Annual Sales(GAS)	=US \$25000000
• Total Direct Cost	= US \$39500000
• Total Indirect cost	= US \$ 7500000
• Fixed Capital Investment	= US \$25000000
• Total Capital Investment	= US \$28750000
• Total production cost	= US \$ 17825000
• Gross profit	= US \$ 7175000
• Net profit	= US \$ 5022500
• Pay out time	= 5 years
• % Return	=17.46%

Guanidine Nitrate:

• Gross Annual Sales(GAS)	= US \$252000000
• Total Direct Cost	= US \$398160000
• Total Indirect cost	= US \$75600000
• Fixed Capital Investment	= US \$252000000
• Total Capital Investment	= US \$289800000
• Total production cost	= US \$179676000
• Gross profit	= US \$72324000
• Net profit	= US \$50626800
• Pay out time	= 5 years
• % Return	=17.46%

CONCLUSION:

From this, we conclude by saying that, the Guanidine HCL and nitrate have a variety of properties and applications in the field of science which led to many researches on it. Guanidine hydrochloride is the hydrochloride salt of guanidine. Having a molecular formula of CH_6CN_3 . Guanidinium chloride crystallizes in orthorhombic space group. The crystal structure consists of Guanidinium cations and chloride anions linked by $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds. Guanidine nitrate is essentially a compound comprised of guanidine ($\text{NH}_2-\text{C}(\text{NH})-\text{NH}_2$) and nitric acid (HNO_3) radicals. Each Guanidine nitrate molecule has two molecules of guanidine combined with one molecule of nitric acid. The material balances and energy balances for the process to be used are calculated and the heat of reactions and specific heats for the components are calculated for the process used. The plant location and layout are selected in a way that the availability of raw materials possibility. Such that the cost used in the transportation will be reduced. Also the cost estimates for the plant construction have been done.

REFERENCES:

1. Peter Schalke, Rodenbach; Langer Manfred, Karlstein; Klaus Huthmacher, Gelnhausen, all of Fed. Rep. of Germany 73) Assignee: Degussa Aktiengesellschaft, Frankfurt am Main, Fed. Rep. of Germany 21 Appl. No.: 237,728 22 Filed: Feb. 24, 1981
2. Yanxing Qi , Haixiang Gao , Min Yang , Chun-Gu Xia & Jishuan Suo (2003) Synthesis of Guanidine Derivatives and Molecular Recognition, Synthetic Communications, 33:7, 1073-1079, DOI: 10.1081/SCC-120017128
3. George F. Wright, Toronto, Ontario, Canada, a signor to The Honorary Advisory Council for Scientific and Industrial Research, Ottawa, Ontario, Canada, a corporation of Canada.
4. Patented Aug. 12, 1941 PRODUCTION OF GUANIDINE NITRATE William H. Hill, Mount Lebanon, Pa., and Robert C. Swain, Riverside, and Joseph H. Paden, Glenbrook, Conn., assignors to American Cyanamid Company, New York, N. Y., a corporation of Maine No Drawing.
5. MANUFACTURE OF GUARDINE NITRATE Elwyn Roberts, Eisham, London, and Thomas Martin, Waltham Cross, England, assignors to Minister of Aviation in Her Majesty's Government of the United Kingdom of Great Britain and Northern Ireland, London, England Filed May 5, 1959, Ser. No. 81.218 Claims priority, application Great Britain May 6, 1958.

