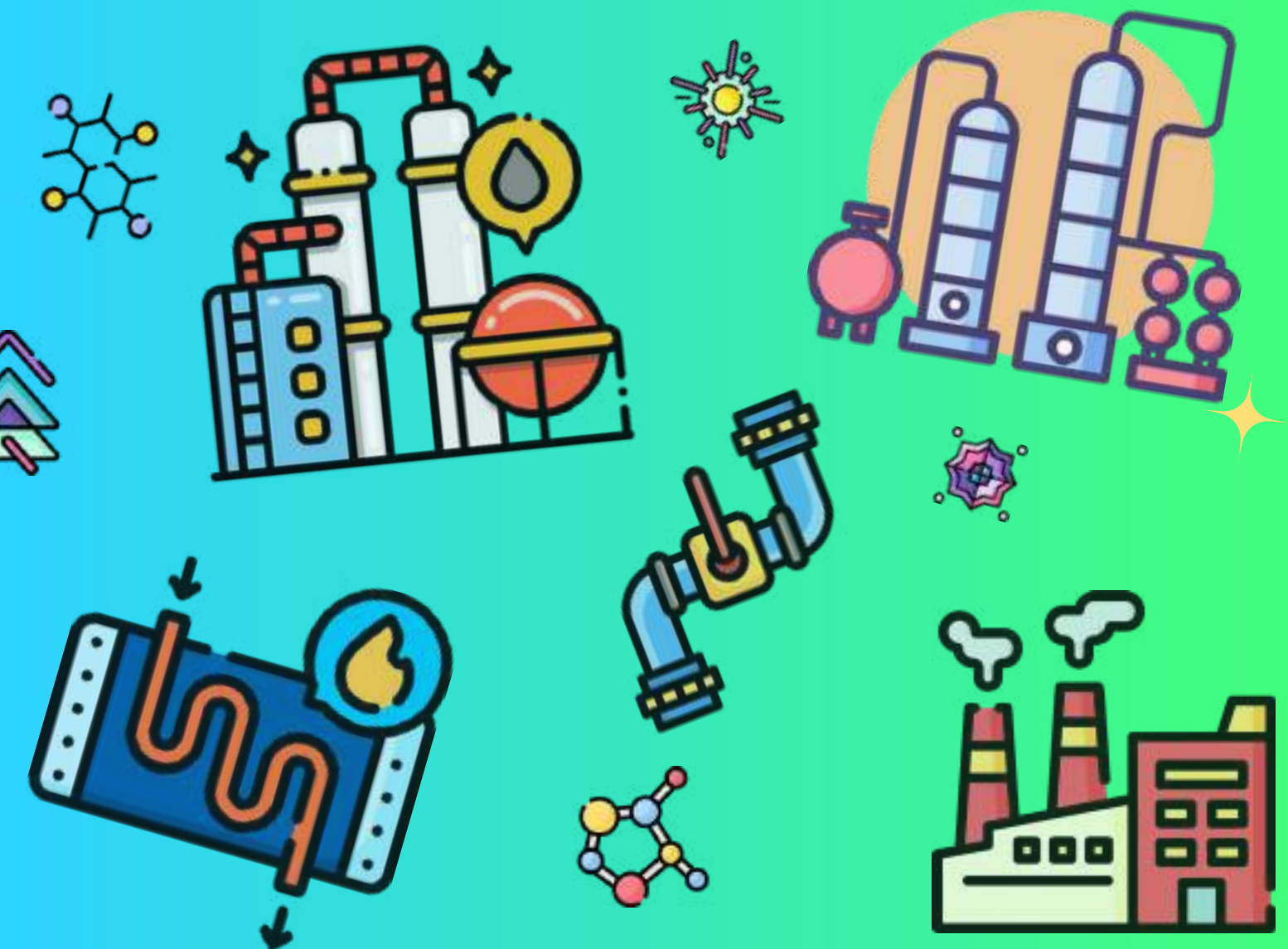# CHEMEVO

DEPARTMENT OF CHEMICAL ENGINEERING

2019 - 2020

SRI VENKATESWARA COLLEGE OF ENGINEERING
AUTONOMOUS - AFFILIATED TO ANNA UNIVERSITY

>>> VISION

To be a leader in Higher Technical Education and Research by providing state-of-the-art facilities to transform the learners into global contributors and achievers.

>>> MISSION

To develop SVCE as a "CENTRE OF EXCELLENCE", offering Engineering Education to men and women at Undergraduate and Postgraduate degree levels, bringing out their total personality, emphasising ethical values and preparing them to meet the growing challenges of the industry and diverse societal needs of our nation.

DEPARTMENT OF CHEMICAL ENGINEERING

>>> VISION

To be a leader in Chemical Engineering Education and Research by providing balanced learning and fostering research to enable the learners to meet the challenges of process industries and societal needs.

>>> MISSION

1. To produce graduates practicing Chemical Engineering professionally and ethically.
2. To produce Chemical Engineering graduates contributing to the betterment of society in the competitive global environment.
3. To focus on the development of Chemical Engineers to foster innovation through proficiency and effective communication.

ABOUT THE DEPARTMENT

The Department of Chemical Engineering was started in the year 1994. The Department currently offers a 4-year B.Tech and 2-year M.Tech programmes in Chemical Engineering. The Department has been recognized as a Research Centre for Ph.D. Programmes by Anna University from 2011. The Undergraduate programme is approved by AICTE and accredited by National Board Accreditation (NBA), AICTE, New Delhi. The Department has taken several Strategic Initiatives to fulfill the ever-growing local and global demands in allied Chemical Engineering streams. All the laboratories contain state-of-the-art infrastructure facilities for academic and research needs and are fully equipped with the latest equipment and advanced software packages like ANSYS FLUENT, ASPEN-HYSYS, PROSIM and MATLAB. In addition, the Department has a CTS-sponsored Process Modeling and Simulation Laboratory and an exclusive, industrial-grade "Distributed Control System" (DCS) in the Process Control Laboratory. The Department has qualified & experienced faculty and staff members, who possess a deep commitment to nurturing the next generation's education and consistently pursue excellence in all areas of their expertise. The Department is also engaged in research activities in the wide areas of Chemical Engineering, Environmental Engineering, Fuel Cell Chemistry, Process Control and other related areas. The Department organizes a National Level Technical Symposium "PANSOPHY" every year and also organizes STTP/FDP/Seminars/ Workshops periodically.

MESSAGE FROM THE SECRETARY

Dr. M. Sivanandham
SECRETARY

Chemical Engineering is a field that has continuously contributed to the betterment of society and industries through innovations and advancements. In today's world, where sustainability and environmental consciousness are paramount, the role of Chemical Engineers becomes even more critical. These professionals play a crucial role in developing processes and technologies that are both efficient and eco-friendly. As the Secretary of SVEHT, I am delighted to announce that the Department of Chemical Engineering is launching a e-magazine dedicated to this dynamic field. This magazine will serve as a platform to showcase the ground-breaking research, projects, and achievements of our esteemed faculty members and talented students. It will provide insights into the latest developments in Chemical Engineering, including cutting-edge technologies, sustainable practices, and their applications in various industries. I am confident that this e-magazine will not only disseminate valuable knowledge but also ignite a passion for research and innovation among our readers. I extend my heartfelt appreciation to the editor and the entire editorial team for their efforts in bringing this initiative. Their dedication and hard work will undoubtedly make this e-magazine a tremendous success.

Secretary

MESSAGE FROM THE PRINCIPAL

Dr. S. Ganesh Vaidyanathan
PRINCIPAL

In the realm of scientific and technological progress, Chemical Engineering stands tall as a discipline that has revolutionized numerous industries, touching every aspect of modern life. It is with immense pride and enthusiasm that I extend my heartfelt congratulations to the Department of Chemical Engineering on the launch of their much-awaited magazine. This magazine comes at a time when the world is seeking innovative solutions to address global challenges, and the Department of Chemical Engineering has consistently been at the forefront of such endeavours. The magazine promises to be a valuable resource, providing valuable insights into the latest research, developments, and breakthroughs in the field of Chemical Engineering. It will be a testament to the relentless pursuit of excellence by our faculty and students. My heartfelt appreciation goes to the faculty members and students for their dedication and hard work in bringing this magazine. May this magazine illuminate minds, spark innovation, and reaffirm the vital role of Chemical Engineering in shaping a sustainable and prosperous future for all.

Principal

MESSAGE FROM HEAD OF THE DEPARTMENT

Dr. N. Meyyappan
HEAD OF THE DEPARTMENT

The Department of Chemical Engineering at SVCE has been a pioneer in providing exemplary education and fostering a research-driven environment since its inception. As the Head of the Department, it fills me with immense pride to introduce our exclusive magazine dedicated to showcasing the exceptional work and accomplishments of our students and faculty members. Chemical Engineering is a domain that constantly evolves to address the ever-changing needs of society. Our department has been committed to staying at the forefront of these developments, equipping our students with not only theoretical knowledge but also practical skills and problem-solving capabilities. This magazine serves as a testament to our commitment to academic excellence and innovation. Through this magazine, we aim to offer readers a glimpse into the diverse research areas explored by our students and faculty. It will feature cutting-edge projects, sustainable solutions, and novel technologies that have the potential to impact industries and improve lives. "CHEMEVO" will not only inspire researchers and professionals but also engage a broader audience, raising awareness about the significance of Chemical Engineering in addressing global challenges. I would like to extend my heartfelt gratitude to the entire editorial team for their tireless efforts in making this magazine a reality.

Head of the Department

FROM THE EDITOR

S. Mohana Murali

"Surely we have a responsibility to leave for future generations a planet that is healthy and habitable by all species."
– Sir David Attenborough

Salutations to my dear readers,

Since the world is becoming ever more industrialized, the rate of energy consumption, waste generation, and usage of resources have also skyrocketed with an increase in emissions. As chemical engineers, we have the power and the skills to satisfy human needs sustainably and for that, we need to be aware of what is happening currently. CHEMEVO is a combined effort of the members of Chemical Engineering department which sheds knowledge on current research technologies in addressing the key issues faced by the world. Being an editor of CHEMEVO, I feel immense pleasure in expressing my indebtedness to the head of department, faculty in-charge and all our thinkers and writers who dedicated their invaluable time in developing this magazine. As readers, if you feel any new topics to be discussed or want to showcase your ideas, we welcome you to provide valuable suggestions in improving "CHEMEVO" and making it a great success.

FACULTY IN-CHARGE

Dr. N. P. Kavitha
ASSISTANT PROFESSOR / CHE

BEST STUDENT CHAPTER AWARD - AMBUJA WINNER

2019 - 2020

PANICKKER AWARD WINNER

Mr. N. N. Harish Kumar
2019 - 2020

SREE HAREEHARA SUDHAN EDUCATIONAL TRUST AWARD WINNER

Ms. Haarini Ramesh

2019 - 2020

DUBASI BALAKRISHNA DORA AWARD WINNER

Ms. I. Harini

2019 - 2020

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2019 - 2020

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S. Yadhunand

Yagna Madhavan

An eco-friendly approach to synthesizing nanoparticles and its potential use in water treatment.

INTRODUCTION

Research in nanotechnology has grown exponentially over the past decade, with nanoparticles finding applications in various fields, particularly in biotechnology and medicine. Their unique properties, resulting from the reduced size in the nanometer range, have sparked significant interest among scientists and scholars worldwide. Nanoparticles exhibit altered physicochemical, magnetic, electronic, and conducting properties, making them versatile for a wide range of applications. Moreover, their increased surface-to-volume ratio enhances interactions with solutions and microbes, providing significant advantages in various domains.

Notably, nanoparticles have been traditionally synthesized through physical and chemical methods, involving concentrated reductants and stabilizing agents, which often raise environmental concerns due to high radiation exposure. To overcome these limitations, researchers have embraced green synthesis, a bottom-up approach that integrates nanotechnology with principles of green chemistry. In this method, plant extracts or microbial strains act as bio-reducing agents, eliminating the need for harmful chemicals and energy-intensive processes.
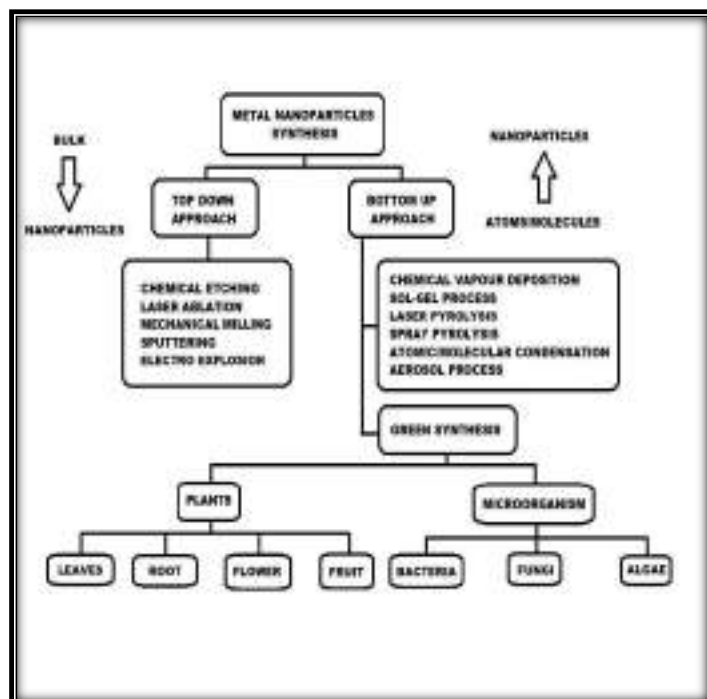
Of all the green synthesis approaches, using plant extracts as bio-reducing agents has shown remarkable promise. Plant-based methods offer several advantages over microorganism-based processes, such as simplified production procedures and relatively shorter production times. The combination of compounds present in plant extracts, including alkaloids,

polyphenols, sugars, and proteins, effectively acts as both capping and reducing agents during nanoparticle synthesis.
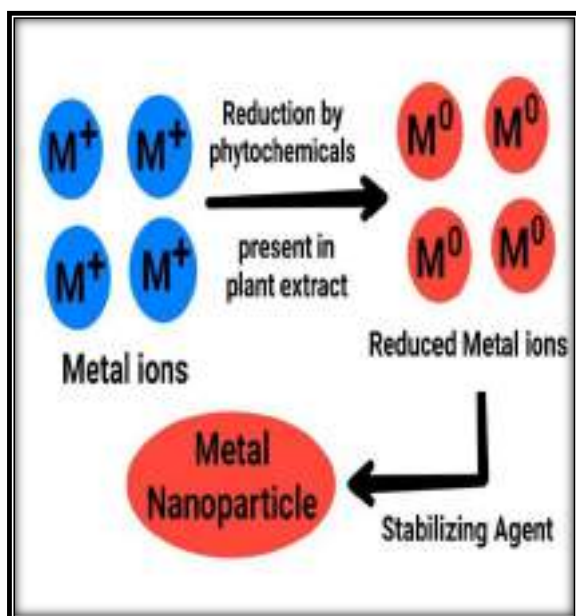
Among the various metal oxide nanoparticles that can be synthesized through green synthesis, Copper Oxide (CuO) nanoparticles have garnered significant attention. CuO nanoparticles possess numerous properties, including temperature stability, superconductivity, photocatalytic, photothermal, and photoconductive abilities. Their high surface-to-volume ratio enhances interactions with microbes, making them effective antimicrobial agents. When in nanoparticle form, copper exhibits increased antimicrobial efficiency compared to its bulk counterpart.

Given the widespread application of Copper Oxide nanoparticles, researchers have also explored their potential in reducing heavy metal ion concentrations. This has crucial implications for water treatment, as heavy metals like Nickel (Ni) often contaminate water sources due to industrial and agricultural waste. The bioaccumulation of heavy metals in living organisms poses severe environmental and health risks, underscoring the urgency to develop effective removal methods.

In light of these considerations, there was a research project undertaken by our team that experimented with synthesizing CuO nanoparticles using clove extract as a bio-reducing and capping agent. This study seeks to provide a characterization of the synthesized nanoparticles and assess their efficiency in reducing heavy metal concentrations in contaminated water solutions.

Materials and Methods

The research begins by preparing clove extract, utilizing the buds of the Myrtaceae family. The clove powder is washed with deionized water and activated at a specific temperature, yielding a dark brown liquid after filtration. This clove extract serves as the bio-reducing and capping agent in the CuO nanoparticle synthesis. CuO

nanoparticles are synthesized through a series of simple steps. Copper sulphate solutions are mixed with the clove extract at various ratios, and the mixture is allowed to react for 24 hours. The completion of the reaction is indicated by the color change from dark brown to sea green. Subsequently, the solution is left to settle, and the nanoparticles are washed multiple times with deionized water. The resulting slurry is dried in a hot air oven, producing powdered nanoparticles.

To determine the optimal synthesis conditions, five samples are prepared, each with a different ratio of extract to CuSO4 solution and varying concentrations. UV-Vis Spectral Analysis is carried out to identify the wavelength range between 200-300 nm, where CuO nanoparticles exhibit surface plasmon absorption. FESEM analysis further confirms the morphology and size of the nanoparticles, which are found to be spherical with an average size of 200-400 nm CuO Nano. particles

Table 1: UV-Vis analysis of CuO samples at different ratios

Ratio (CuSO$_4$.5H$_2$O)	CuSO$_4$ solution Concentration (M)	Wavelength (λ)(nm)	Absorbance (A)
1:10	0.1	200	0.383
1:10	0.01	200	0.310
1:2	0.0001	232	1.296
5:1	0.1	258	0.654
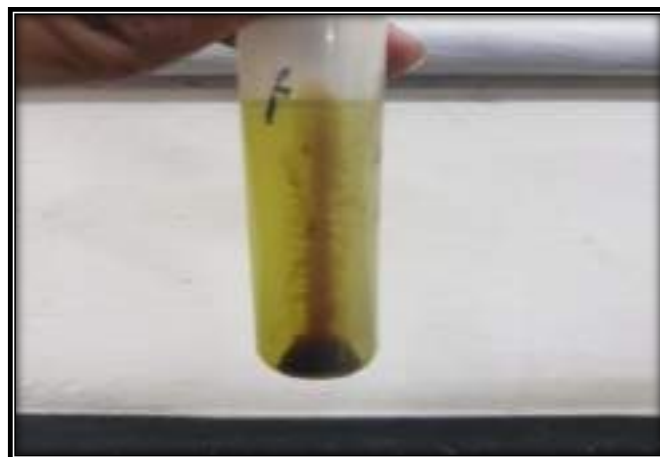
Centrifuged Mixture

CuO Nano. particles

Potential application in water treatment

Having successfully synthesized CuO nanoparticles, the research project explores their application in removing heavy metals from water, with Nickel (Ni) as the target metal. By varying the dosage of CuO nanoparticles, pH, and contact

time, the researchers assess their efficiency in reducing Ni concentration in a solution. AAS (Atomic Absorption Spectroscopy) is employed to measure the extent of metal removal. The results demonstrate that CuO nanoparticles effectively remove Nickel from water, with the highest removal percentage achieved at higher pH values. A basic solution is more favorable for CuO nanoparticles' adsorption of heavy metals, which aligns well with the typical pH range of water. Using just 0.05 grams of CuO nanoparticles per 100 ml of Nickel solution, an impressive 89.5% removal is achieved, highlighting their potential as efficient adsorbents.

Conclusion and Analysis

The research project showcases the successful green synthesis of CuO nanoparticles using clove extract as a bio-reducing and capping agent. This eco-friendly approach offers economic and safe nanoparticle production, avoiding the use of harmful chemicals and energy-intensive processes. The characterized CuO nanoparticles exhibit promising properties, including a spherical morphology and an average size of 200-400 nm.

The applications of CuO nanoparticles in heavy metal removal are particularly noteworthy. Through efficient adsorption,

CuO nanoparticles effectively reduce Nickel (Ni) concentrations in water solutions, with an impressive removal percentage of 89.5% achieved under optimal conditions results indicate that a basic solution with a contact time of 65 minutes and 0.05 grams of nanoparticles per 100 ml of Ni solution yields the highest removal efficiency. This demonstrates the potential of CuO nanoparticles for environmental remediation, addressing the growing concern of heavy metal contamination in water sources.

The significance of this research lies in the potential environmental and health implications. Heavy metal contamination poses serious risks to ecosystems and human health, making effective removal methods crucial. CuO nanoparticles offer a promising solution for mitigating heavy metal pollution in water, contributing to environmental protection and ensuring the safety of water resources.

However, the study is not without limitations. Further research is needed to explore the regeneration and recyclability of CuO nanoparticles after their initial use as adsorbents. Ensuring their long-term efficiency and sustainability would enhance their practical application in real-world scenarios.

In conclusion, the research project successfully demonstrates the green synthesis of CuO nanoparticles using clove extract and their efficient application in heavy metal removal. The findings highlight the potential of CuO nanoparticles as a valuable tool for water treatment and environmental remediation. With further investigation and development, CuO nanoparticles hold the promise of contributing to a cleaner and healthier environment

Yagna m

TREATMENT OF HYDROGEN SULPHIDE

Fossil fuels have occupied a major position in every man's life. The everyday energy demand is met by the combustion of fossil fuels. As a result of gasification, there is a wide release of poisonous greenhouse gases (GHC) like CO_2, CO, H_2S, NOx, Sox and Hg. These gases along with the particulates and water vapour is referred to as 'Flue gas'. Flue gas emissions contribute not only to air pollution and also it affects the regular life cycle of the globe. So, it is highly important to take into account these gas emissions. This could be achieved in any of the following ways:

1) By releasing the gases into atmosphere by the industries within prescribed pollution control limits,

2) Collecting and treating the excess polluting gases by using separation techniques,

3) Separation of elements from gaseous compounds and use in energy storage applications,

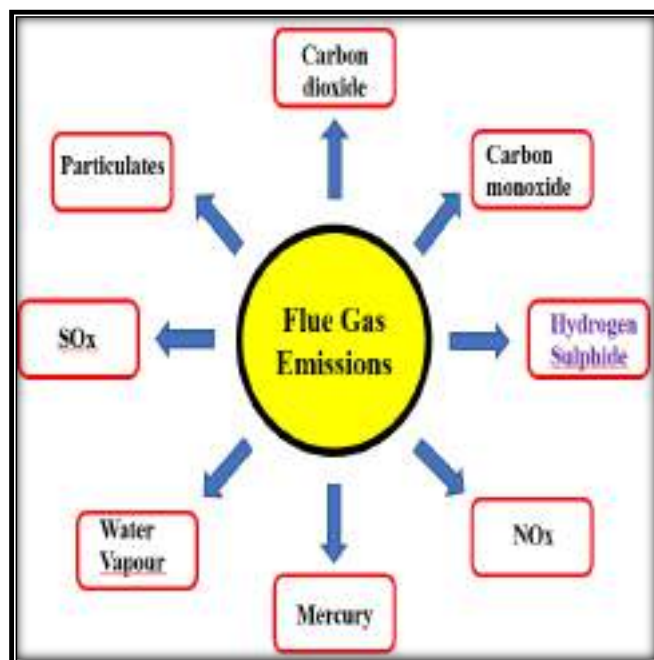4) Conversion of gases into other useful products.

Fig 1. Schematic representation of Flue gas emissions

Upon considering the aforementioned gas emissions, hydrogen sulphide should be taken with at most concern because if it is not treated properly, it can even lead to death at times.

Hydrogen sulphide

Hydrogen sulphide production is highly devoted to oil and gas industries as the crude petroleum processing liberates hydrogen sulphide enormously either during the initial or final stage. Hydrogen sulphide is also liberated during biomass gasification. It is lethal and corrosive in nature. In low concentrations it has

pungent odour and it is odourless at high concentrations. It disturbs the water cycle and causes damage to the environment and living organisms by causing acid rain when it gets oxidized to sulphur dioxide. It also poisons industrial catalysts and also pipe lines gets corroded during the transportation.

Treatment methods

Claus process is the oldest and traditional method for the treatment of Hydrogen sulphide. In this process there are two units: amine unit and Claus unit. In the amine unit H_2S and CO_2 are separated from the sour gas. In Claus unit at the temperature of 900 to 1300℃ the conversion of sour gas into elemental sulphur along with its derivatives takes place via Claus process. Claus unit comprises of thermal stage and catalytic stage.

Emerging methods

Based on the principle of removal the removal techniques are classified as

1. Dry methods and
2. Wet methods.

Dry methods

Treating hydrogen sulphide by dry methods includes

➢ Plasma removal,

➢ Ozonation,

➢ Photocatalytic oxidation,

➢ Photo-decomposition

➢ Membrane separation and

➢ Adsorption.

Wet methods

The removal of hydrogen sulphide by mainly includes

➢ Biological method,

➢ Complex absorption,

➢ Alkali absorption,

➢ Catalytic oxidation,

➢ Ionic liquid absorption

➢ Chemical oxidation and

➢ Electrolysis.

Our work

We aim to overcome the drawbacks of traditional method-Claus process by indirect electrolysis followed by post scrubbing with anode and cathode as graphite, reference electrode as calomel at basic pH and operation temperature below 100℃.

- Naveen kumar

Amine Absoprtion Of CO$_2$ – A Simulation Study using Aspen Plus

.Arun Prem Anand, Asssistant Professor, Department of Chemical Engineering, SVCE

Introduction:

Due to the green house effects, there is an increase in the global warming. Recent researches are focused mainly on the removal of CO$_2$ related techniques. Also, one of the most polluting gas in the world is carbon di oxide which is emitted to the atmosphere by human activities. In developing countries like India, 75 percent of electricity is being generated by the combustion of coal. This leads to the release of CO$_2$ in the atmosphere. There are many methods for capturing CO$_2$. The two main classifications of capturing technologies are pre-combustion and post-combustion processes. Among this, capturing of CO2 by Monoethanolamine (MEA) can be used frequently because it can be operated at atmospheric conditions.

Literature Survey:

Stefano et al modelled the CO$_2$ capturing process by RateFrac. The design consisted of absorption column, stripper and heat exchanger. The solvent contained 30 % MEA (monoethanolamide) in water. The RadFrac absorbed model was integrated with the help of FORTRAN. The thermodynamic model used here was Electrolyte-NRTL. Many sensitivity analyses were done based on solvent rate,

height of column, HSS (heat stable salt) loading, pressure in stripping column, and temperature of stripper and absorber. The solvent should flow slightly higher than the normal. The height of packing should be more for better mass transfer. Acid should be added to the solvent for better absorption. The stripper should operate at normal atmospheric pressure. Alie et al, 2004 optimized the operating variables in amine loading and temperature of MEA into the columns. Flue gases of different CO$_2$ concentration from gas turbine, coal plant and cement plant were studied. The author modelled the different unit operations and the decoupled system and compared the results with the integrated flow sheets. The study mainly focused on the overall recovery, purity of CO$_2$ etc. As number of trays increased in absorption column, flow rate of MEA was reduced in that column.

Jassem et al, 2006 designed various methods and compared the results of those methods. The column used here was designed with the help of RateFrac. In the process, 4 modes of stripper modifications were done and the

results were compared. The types of stripper are simple stripper, ii) stripper with vapour recompositing (at the stripper, the CO_2 was entering into multistage compressor as high-pressure gas and bottoms from stripper was used to remove heat of CO_2 i.e. bottoms used to recover the heat of condensation). iii) Multi-pressure stripping (In this, the stripper was connected with the series of compressors for regulating the stripper pressure). iv) Multi-pressure stripping with vapour recompositing. (This was the combination of the 2nd and 3rd design). For various optimization cases; nearly 20 cases were studied for the different CO_2 removal methods. Alie et al, 2006 simulated the coal power plant integrated with the CO_2 capturing techniques. Since the process of CO_2 capturing was integrated, the heat energy used in the CO_2 capturing can be bought from the coal power plant heat recovery systems. i.e., the heat from the coal power plant can be utilised for the capturing techniques. The sensitivity analysis done for the various design parameters such as absorption and stripping column height, stripper reboiler pressure and temperature etc., the heat (Q) of reboiler can be minimised for the maximum power output of plant. The heat sources can be recycled within the CO_2 capturing process which improves thermal efficiency compared to the heat supplied from the external source. Abu-Zara et al, 2006 studied the technical

parameters using the RADFRAC subroutine. The scope of optimization was to find the various concentration of MEA in absorber, CO_2 removal, pressure in stripper etc. A minimum circulation flow rate was expected for the best thermal energy requirement. The concentration of MEA increased for the lower thermal energy requirement. High pressure was maintained in the stripping column for better mass transfer to occur i.e., the CO_2 mass transfer. The temperature of lean solvent entering the absorption should be maintained at optimum condition i.e., not too high or low. Another optimization study was also done based on the thermal energy requirements. Oexmann et al, 2008 designed the process of capturing CO_2 using piperazine promoted potassium carbonate (K_2CO_3/PZ) solution. Many sensitivity analyses were done on solvent loading in absorber and stripper and pressure studies in stripper. Also, for various solvent concentrations, the efficiency of the product was studied. The optimum lean loading should be maintained.Also, for the different CO_2 – lean rich loading, the composition and flow rates were studied. The pressure inside the stripper should be maintained below the ambient temperature. The investment cost for columns were reduced compared to using MEA solvent. Plaza et al, 2009 simulated the CO_2 capturing process as same as the pilot plant specifications. The column were designed with

the help of RateSep. The comparative study was done between the pilot scale and ASPEN PLUS simulation and the result matched the same with slight deviations. Optimization study was done for the simulation work. Instead of stripper, three stage adiabatic flashes were introduced and the efficiency of the process increased compared to the normal stripper column used. The study of the design of absorber was also done. By introducing the intercooling system, the CO_2 removal was increased and also the size of packing in absorption column decreased. Zhang et al, 2009 modelled using rate-based process instead equilibrium stage modelling. The parameters for the simulation was taken from the pilot plant in Austin. The modelling was done with the help of RateSep. More than 48 cases for 24 operating condition for the comparison of pilot scale and simulations were done. The optimization techniques such as different modelling approaches, film discretization etc., were also studied. The results of simulations matched with the pilot plant data.

Rochelle et al, 2009 developed a dynamic based rate model using Aspen Custom Modeler. Many assumptions were considered for this modelling. Many sensitivity analyses were made such as adjusting packing height, solvent loading in stripper and absorber. Two control strategy systems were studied. i) Constant lean loading in stripper ii) Constant flow rate of rich lean solution in stripper. The results of the both cases varied and the results were compared. The liquid residence time will be the dominant factor in the reboiler which operated in dynamic conditions. Dave et al, 2009 did a comparative study by using different solvents and different solvent compositions. The various solvents included ammonia solution, Methyl-ethanolamine, MDEA, Amino Methyl Propanol. The CO_2 from the flue gases leaving from coal fired power plant was taken into consideration. The results of various solvent compositions were discussed and compared. If the concentration of ammonia solution is more, which indicates that the ammonia loses in the vapour phases and also it forms precipitation in the absorber. The process conditions and energy requirements were similar to both ammonia and MEA based solvent processes. By the usage of AMP, it required lesser energy requirement for the process. Mark B. Shiflett et al, 2010 modelled an ionic liquid that can reduce the energy losses by 16% compared to a commercial MEA process which involved simple absorption and stripping configurations. The choice of the ionic liquid, 1-butyl-3-methylimidazolium acetate, was not optimized but was chosen based on chemical absorption behaviour. Engineering design indicated that the investment for the ionic liquid process

would be 11% lower than the amine-based process and provided a 12% reduction in equipment footprint. Modelling indicated that the IL process can reduce the energy losses by 16% compared to the MEA process. G. Pellegrini et al, 2010 compared MEA and DGA to ammonia with respect to their capability to capture CO_2 from a flue gas stream. The ammonia process captured CO_2 by formation of stable salts, which were separated from the solvent stream by filtration or sedimentation. Energy requirements were greatly reduced. Energy was required for the reduction of ammonia emissions. Simulation of all processes was carried out with Aspen Plus. Comparative flowsheet simulations for the CO_2 capture performance of three different solvents were carried out. It showed that ammonia was a better absorbent. Low concentrations of ammonia in the solution for CO_2 removal was a good compromise between high removal efficiency and low ammonia losses with the exhaust gas stream. David H. van Wagener et al, 2011 worked with several configurations with Aspen Plus with MEA to determine the most useful method for arranging process units. The configurations included multi-stage flash, multi-pressure columns, and advanced stripping columns. Using a higher number of pressure stages, packing in place of equilibrium flashes, and vapor recompression were good methods to reduce the overall equivalent work

requirement, but the most significant improvement was seen with an overheated column. More pressure stages yielded better performance due to more reversible operation. The baseline simple stripper required 35.0 kJ/mol CO_2 at its optimum lean loading of 0.39. The Interheated column configuration demonstrated the best performance, with equivalent and minimum amount of work requirement. Moioli et al, 2011 studied based on the different stripper configurations for the energy saving scheme. The novel procedure had been followed for the simulation work. The various configurations included basic novel process, the double column for stripper and mutipressure column stripper. In the double column configuration, the two-stripper column was present and each reboiler operated at different pressures. In the mutipressure column, the stripper was fitted with the compressor to compress the CO_2 at the upper zone. At the high pressure, CO_2 was removed from water and it was separated at a higher concentration. Various energy saving parameters for the different configurations was compared based on reboiler duty, compression work, and equivalent work per unit time etc. Each configuration showed best results for different parameters.

Hill Wong et al, 2011 studied the various types of dynamic control strategies in the novel CO_2 capturing techniques. The entire process was

simulated using Aspen Dynamics. Control systems such as valves at the top of absorber, lean MEA solution stream, CO_2 exit, make up water stream were setup. The dynamic study for non-disturbances and disturbances such as step input etc., at various places was given and studied. Many optimization techniques such as water makeup, disturbances in the flue gases i.e., step input at the feed, the solvent loading, flow rate and makeup water parameters affected the efficiency of CO_2 removal. The dynamic results showed the successful CO_2 removal ratio and optimum lean loading in the process. By the changing the set point in the reboiler via optimizing control procedure, the minimum energy consumption can be adjusted in the process. Noorlisa Harun et al, 2012 worked on a dynamic MEA absorption process model and it had been developed to predict the dynamic behaviour of the CO_2 capture process. The dynamic model was used to study the transient response of the MEA absorption process to changes in the flue gas flow rate and the reboiler heat duty. Changes in flue gas flow rate and reboiler heat duty were the key process variables that affected lean loading, liquid to gas ratio and percentage of CO_2 removal. The proposed model was validated using an Aspen Plus steady-state simulation. Dynamic behaviour of the CO_2 capture process during the course of the dynamic operation of a power plant was studied by incorporating the input changes in the flue gas flow rate and reboiler heat duty. Victor Darde et al, 2012 worked with the performance of the CO_2 capture process using aqueous ammonia. Two process configurations had been tested and a thorough sensitivity analysis of the main process parameters was performed to analyse their effects on the heat and electricity requirements. The heat requirement was found to be in the same range as the values reported recently for advanced amine processes. The Chilled Ammonia Process was a promising option for post combustion CO_2 capture. The main process parameters had an effect on the heat requirement in both the CO_2 desorber and the NH_3 stripper and on the global electricity consumption. Stevens et al, 2012 used the K_2CO_3 (Potassium Carbonate) solution as the solvent for absorption of CO_2. Due to the poor kinetics of MEA absorption, it acted as the promotor which improved the rate of the reaction. The study was done in a wetted wall column, which allowed the direct contact between gas and liquid. Thus, for the addition of various concentrations of MEA into K_2CO_3 solution, which in turn increased the pH of the solvent. Hence the overall rate of CO_2 absorption increased. For the solvents K_2CO_3 and MEA, both results were compared and also the results for the K_2CO_3 and pilot scale plant results were studied. Also, many kinetic studies were done for promotors such as piperazine,

MEDA, DEA, AMP etc., and the results for activation energy for the reaction between the solvent and CO_2, pre exponential factor, rate constant etc., were noted.

Duan et al, 2012 improvised the process by combining the separation of CO_2 and generation of energy from it. By introducing various types of CO_2 compressor system, Absorption Heat Transformer, Absorption Heat Pump models etc., increased the efficiency of the process. This process was integrated with the coal power plant and it contained 2 different types of integration. Many energy generating studies were done based on addition of throttling valve near the turbine region, addition of steam turbine generator, heat recovery systems for the overall process etc. The comparative study of the various simulation works and the real time pilot plant was done. The former worked and all were based on the optimization of the lean solvent, energy consumption etc. This study showed that during the removal of CO_2 process, the energy generated will reduce the energy consumption of overall process. Rochelle et al, 2014 simulated the process by developing various advance stripper configurations. The solvent used in the process MEA and Piperazine of various concentrations were studied. The stripper configuration included simple stripper, Cold Rich Bypass (in this some of the cold rich solvent entered into the top of stripper), Rich Exchange Bypass (a heat exchanger was connected in the exit CO_2 steam so that the latent heat of the steam can be recovered), Interheated stripper (in this another heat exchanger was connected to the former method and this solution from the middle of stripper entered into the heat exchanger and thus solvent entered into the next stage), reboiler stripper with rich heat exchanger, flash stripper, flash with cold bypass, flash with rich bypass, and flash with combination of above two. These were the various types of configurations of strippers. For the different types of feeds and also for various concentrations the results were studied. The reboiler with bypass and heat exchanger showed good performance with reduced energy losses. Also, Flash stripper with bypass and heat exchanger showed the greater potential with low capital cost. S.M. Nazmul Hassan et al, 2014 worked on several methods with respect to the validity and performance of MEA based CO_2 capture process for cement plants. Design and costing of CO_2 capture from cement plant flue gas was similar to design and costing of capturing CO_2 from power plant flue gases by using MEA based CO_2 absorption process. Cement produces large quantities of heat to satisfy parasitic heat requirements of MEA process; at nominal load, about 36 MW is available from the St. Mary's process. To decide

what is the best operating condition for the CO_2 capture process for cement plants, not only the minimum capture cost should be considered, but also the maximum steam that can be supplied and the maximum annual cost per year that can be paid. Erik et al, 2014 compared the simulation of CO_2 using different tools; Aspen Plus and Aspen Hysys. For the different configurations of the strippers the results were compared. The equilibrium model used in Aspen Hysys was amine package with non-ideal gases. For the calculations, both rate-based approach and Murphee efficiency were used. Three methods of CO_2 modelling was done (Novel process, vapour recompression, vapour recompression with split stream). Results for the 4 different simulation tools were used and were compared with 4 different types of stripper. The vapour recompression process suited best for the minimum energy consumption in CO_2 absorption process.

Kangkang Li et al, 2015 presented improvements to post combustion capture processes (PCC) based on aqueous MEA. First, a rate-based model of the CO_2 capture process from flue gas by aqueous MEA was developed using Aspen Plus, and was validated against results from PCC pilot plant trials. Important process parameters were MEA concentration, lean CO_2 loading, lean temperature, and stripper pressure were optimized. In their study,

combination of pilot-plant trials and process modelling had demonstrated that a validated rate-based model was effective to evaluate and improve the MEA-based CO_2 capture process. The simulation results of absorber model were in agreement with the experimental results in terms of CO_2 loading in the rich solvent, temperature profiles along the column and CO_2 absorption rate, while the stripper model provided a good prediction of stripper parameters including temperature profiles along the stripper column, CO_2 product composition, and solvent regeneration duty. Kang kang Li et al, 2016 investigated the techno-economic performance of CO_2 capturing techniques. The Aspen Cost modeler was used for the evaluation of the Capital cost investment etc. Many optimization studies including heat exchanger optimization and flow process modifications were studied. The process modifications included absorber intercooling system, rich split process, modified rich split, stripper inter heating. Optimized parameters were reboiler duty, temperature, CO_2 purity, stripper pressure, lean loading temperature etc., also many sensitivity analyses were done on the economic parameters and technical driven parameters. Various improvements were done in order to reduce the capital cost.

Bao-Hong Li et al, 2016 worked on an improved rate-based model of a CO_2 capture process by aqueous MEA solution with Aspen Plus V8.0 software. The improved model was built on the basis of an example model coming along with Aspen Plus V8.0, and the thermodynamic model of ENRTL-RK was adopted. The washing section of the absorption column was strictly modelled by a separate column, and the error on mass balance of MEA was greatly reduced. First, the washing section of the absorption column was strictly modelled by a separate column. Next, the model was validated by the recently published pilot-scale experiment results of the absorption of CO2 by MEA solution. It accurately predicted the experimental profiles of the temperature and the concentration of CO2 in the liquid phase, and obviously much better than the recently reported model with accuracy of ±8%. Annaland et al, 2020 Optimized various parameters of the solvent for reducing the total cost of CO_2 capturing. The results were compared with a real time pilot scale plant. The study of solvent properties such as viscosity, density, surface tension, heat capacity, thermal conductivity, volatility, enthalpy studies etc., were done for the process. An artificial solvent consisting of all the former cases at optimum level was assumed and simulated. The results were also compared with the real time process and the process with MEA. An increased solvent

viscosity, decreased solvent volatility, reduced heat capacity etc., were investigated for an improved cost-efficient process. Mahsa Amirkhosrow et al, 2020 developed a rate-based model of desorber column in CO_2 capture process by MEA solution was performed using Aspen Plus. The effect of flow model on rate-based modelling of desorber was also studied and a proper flow model was chosen. Results indicated the good performance of optimum model in prediction of temperature and concentration profiles along the desorber column and low errors in prediction of several variables in outlet streams with respect to experimental data. The study of combinations of different reaction kinetics and mass transfer correlations resulted in an optimal model for the desorber .

2. Simulation of MEA based CO_2 capturing

2.1 Process Flow Sheet

The flue gas from the coal power plant (FLUEGAS) is entering into the absorption column's (ABSOR) bottom portion and the MEA (LEAN-IN) is entering the column at the top portion. The flow rate should be lesser for a better contacting time. MEA absorbs the CO_2 present in the flue gas and it exits as a bottom product. The remaining flue gas with some small quantity of CO_2 (VENTGAS) will escape from the top of the column. Now this bottom product (RICH-MEA) is entering into the heat exchanger for getting pre-heated before

entering into the flash drum for separation. The hot fluid being utilised for heat exchanger operation is from bottom product of the flash drum. Thus, the lean (RICH-IN) is heated up and enters into the flash drum. The flash drum is operated at a very low pressure and thus the CO_2 from the lean is separated and it exits at the top. The bottom product which doesn't contain CO_2, which is at a higher temperature, enters as the hot fluid in the heat exchanger which losses its heat and it enters into the mixer. Thus, some mixture of MEA (MAKE-UP) is added to the mixer section and it enters into the absorption column as LEAN-IN. Column and the accuracy of this model had an acceptable error range. The results indicated that the kinetic model had more impact on desorber prediction than the mass transfer correlation; this means that a good prediction of desorber column is highly dependent on temperature dependent correlations.

2.3 Study of individual equipment(s):

2.3.1 Absorption column:

In this simulation, RADFRAC column of 12 stages was used. Stages and calculations were done based on equilibrium type modelling. Since the column is mentioned as an absorption column, there is no reboiler and condenser being used. The flue gas entered above the 1st stage and the LEAN-IN liquid entered on the 12th stage. The pressure in the column was maintained at 1 atm.

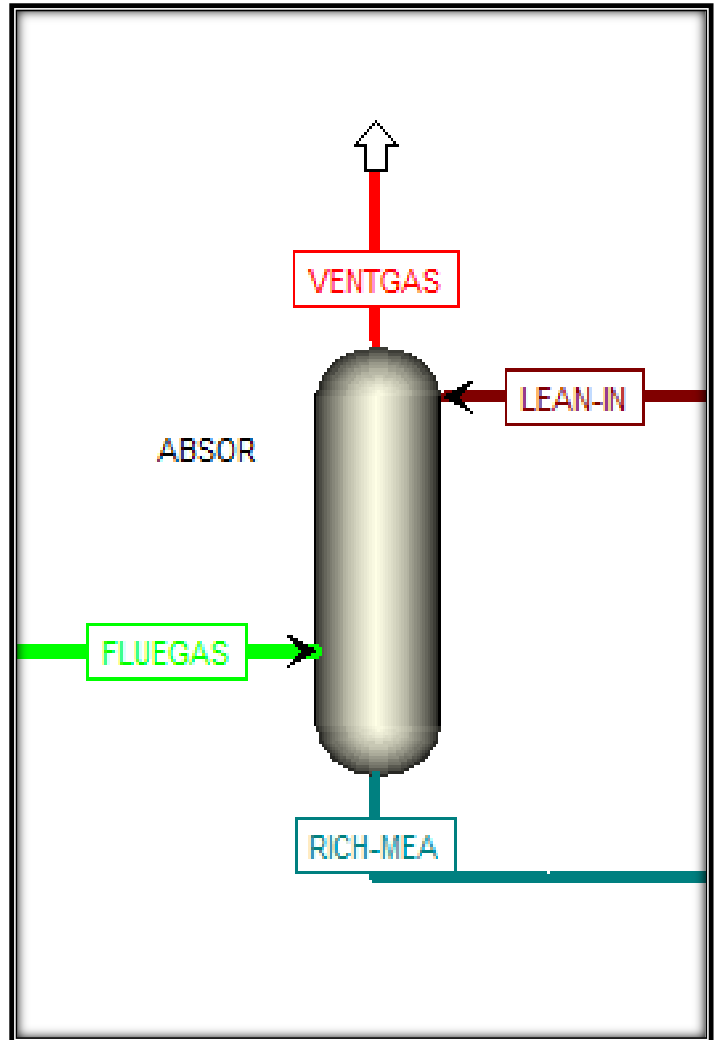The vent gas leaves the column at the 1st stage and the RICH-MEA leaves the column at the 12th stage .

FIGURE 1: Typical Absorption column design.

2.2 Selection of model:

The simulation was done using ASPEN Plus. Since we used amine as a solvent, E-NRTL thermodynamic model was used.

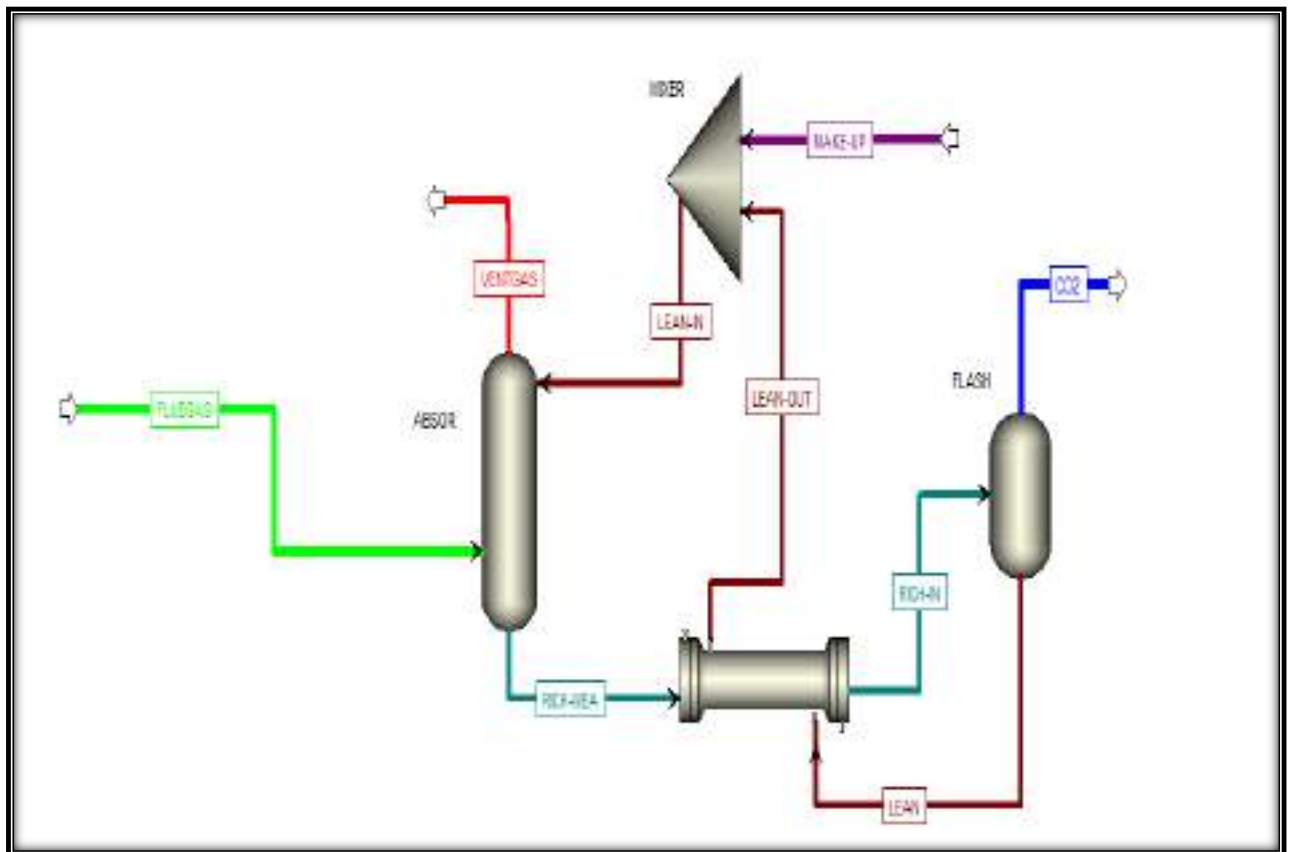| Absorber	
Model type	RADFRAC
Calculation type	Equilibrium
Number of Stages	25
Condenser type	none
Reboiler type	none
Reflux ratio	none

FIGURE 2: Process Flow Diagram

2.3.2 Heat exchanger

The heat exchanger used in this simulation was shortcut-type heat exchanger. The counter current operation was used in this heat exchanger. The calculation was based on the design mode. The minimum temperature approach was set to be 75°C.
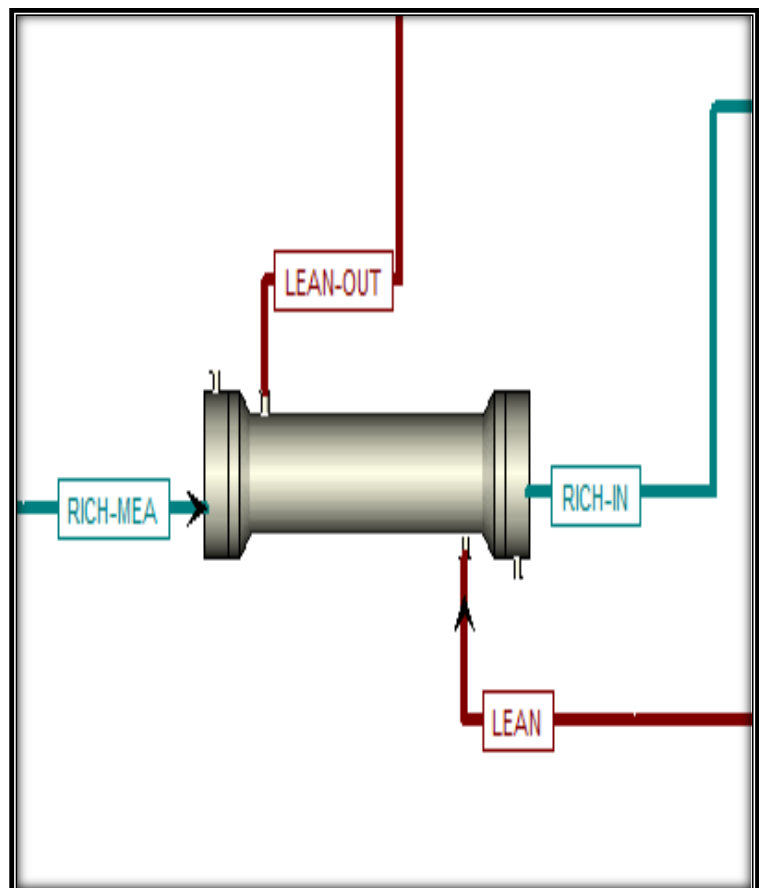
2.3.3 Flash drum:

The flash drum was operated at a temperature of 120°C and pressure 0.2 bar. The convergence parameters were set to a minimum of 30 iterations. In this, CO2 escapes as a vapor at the top and the LEAN leaves at bottom at a higher temperature. This heat was used for heating the input of flash drum
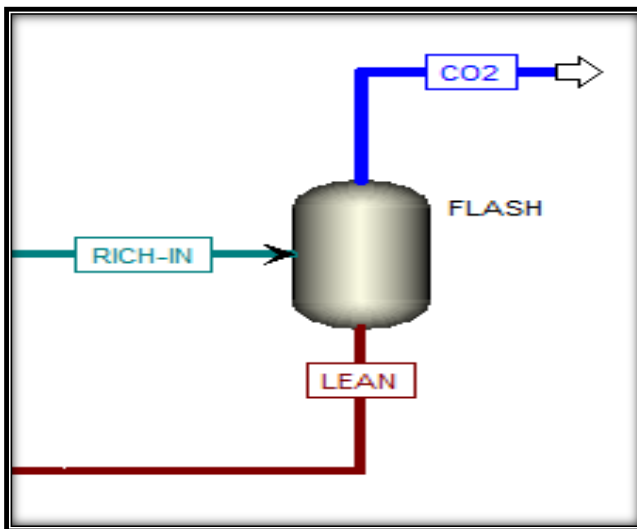

FIGURE 4: Typical Flash Drum design.

Conclusion:

The CO$_2$ from flue gas is almost removed and only small fraction of CO$_2$ is again entering into the LEAN MEA solution stream. The results are discussed in table 2 which indicates that the CO$_2$ is completely removed from the flue gas and thus the CO$_2$ - free flue gas is sent for further removal of SO$_2$ and other components. The flowrate is kept very low for better contacting time between the solvent and the flue gases. Also, the number of stages is reduced for reducing the

expenditure of the column. The operating conditions of the entire process except the flash drum is under atmospheric pressure. This process can be further improvised by changing the flash drum and setting some other stripping equipments or by adding compressors for the pressure reducing conditions, etc. Furthermore, many control valves are incorporated so that dynamic studies in the processes can be analysed. Many sensitivity analysis and Various temperature, pressure, flow rate profiles can be studied. Also, some properties such as energy savings, separation factors, vapour compositions can be studied and modified.

Material						
Stream Name	Units	FLUEGAS	VENTGAS	RICH-MEA	RICH-IN	CO2
Phase		Vapor Phase	Vapor Phase	Liquid Phase	Liquid Phase	Vapor Phase
Temperature	C	85	67.295	67.295	67.295	120
Pressure	bar	1.01325	1.01325	1.01325	1.01325	0.2
Mole Flows	kmol/hr	100	147.606	55.393041	55.393041	12.96135
CO2	kmol/hr	14	1.574	12.426	12.426	11.523
H2O	kmol/hr	5	62.9286	1.3073	1.3073	0.9995
MEA	kmol/hr	0	0.0313212	40.7327	40.7327	0.0026
N2	kmol/hr	75	74.2222	0.777813	0.777813	0.32256
O2	kmol/hr	6	5.85077	0.149228	0.149228	0.11369
Mole Fractions		1	0.917749881	0.5387669	0.5387669	0.15285294
CO2		0.14	0.0148263	0.13242	0.13242	0.12658
H2O		0.05	0.0492758	0.0139316	0.0139316	0.010214
MEA		0	0.000333781	0.383683	0.383683	0.00732664
N2		0.75	0.790964	0.00732664	0.00732664	0.00732664
O2		0.06	0.06235	0.00140566	0.00140566	0.00140566

TABLE 2: Stream Table Results

Analysis of NO$_X$ Reduction Catalysis using Pt-based HC-SCR Catalysts for various O$_2$ inlet conditions

Abstract:

The reduction of NOx emissions has become a significant challenge in the automotive industry due to its detrimental impact on air quality and human health. Catalytic converters play a vital role in reducing NOx emissions, and the choice of catalyst is crucial for effective NOx reduction. In this study, we performed microkinetic modelling using the CHEMKIN software to compare the performance of Pt and Ag catalysts for NOx reduction. Two papers, Ravikeerthi et al and Mantri et al, were modelled to understand their respective mechanisms. Additionally, we investigated the NOx reduction using a hydrocarbon-based selective catalytic reduction with a Pt/Alumina-based catalyst (Vishnu et al). Our results provide valuable insights into the catalytic behaviour of Pt and Ag catalysts and offer recommendations for optimizing NOx reduction in automotive applications

Introduction:

NOx emissions from internal combustion engines contribute significantly to air pollution and environmental degradation. Catalytic converters, containing noble metal catalysts, have been widely employed to reduce NOx emissions through selective catalytic reduction (SCR) processes. In this study, we focused on comparing Pt and Ag catalysts for their efficacy in NOx reduction. We also investigated the role of hydrocarbon-based selective catalytic reduction with a Pt/Alumina-based catalyst.

Methodology:

Microkinetic modelling using the CHEMKIN software was performed on the two papers, Ravikeerthi et al and Mantri et al, to understand the mechanisms and kinetics involved in NOx reduction. The simulation results were compared to experimental data to validate the accuracy of the models. Additionally, a similar microkinetic simulation was conducted for Vishnu et al, which utilized a hydrocarbon-based selective catalytic reduction with a Pt/Alumina-based catalyst.

Results and Discussion:

The microkinetic modelling of Pt and Ag catalysts for NOx reduction revealed significant differences in their performance. Pt catalyst demonstrated higher NO conversion at lower temperatures, making it suitable for use in reducing environments. On the other hand, Ag catalyst showed superior performance in oxidizing conditions due to its resistance to catalyst poisoning. The results indicated that the choice of motivation depends on the prevailing oxygen conditions and the specific requirements of the application.

In the case of hydrocarbon-based selective catalytic reduction, our simulations showed that the use of propane (C_3H_6) as the reducing agent led to successful NOx reduction. The NO conversion was higher at higher temperatures, indicating the importance of elevated temperatures for efficient removal. Our results also demonstrated the formation of N_2 as the primary product, signifying good selectivity towards N_2 production.

Conclusion:

The comparative analysis of Pt and Ag catalysts for NOx reduction revealed their respective strengths and weaknesses in different oxygen conditions. Pt catalyst showed better performance in reducing environments, while Ag catalyst exhibited better resistance to catalyst poisoning in oxidizing conditions. The hydrocarbon-based selective catalytic reduction with a Pt/Alumina-based catalyst proved to be effective in NOx reduction, particularly at higher temperatures.

Future Work:

In the future, experimental validation of the microkinetic models is essential to obtain accurate parameters for both Pt and Ag catalysts. Additionally, the simulation of Ag/Alumina-based catalysts with a similar reaction mechanism as Vishnu et al would provide valuable insights into the potential of Ag as an alternative catalyst for NOx reduction. This would aid in developing optimized catalytic conditions and selecting the most suitable catalyst for NOx reduction in automotive applications.

In conclusion, this study offers valuable insights into the catalytic behaviour of Pt and Ag catalysts for NOx reduction and highlights the importance of oxygen conditions and temperature in achieving efficient NOx reduction. Further research and experimental validation are necessary

to establish the practical applicability of Ag catalysts in NOx reduction processes.
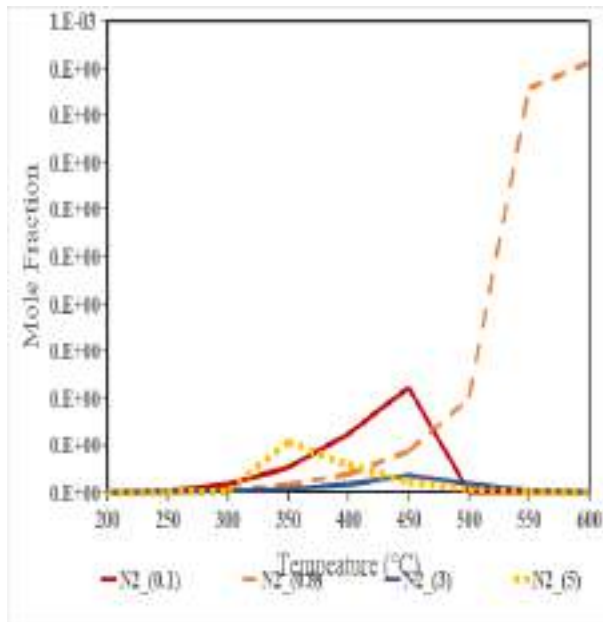

Figure 1: N₂ Mole Fraction vs reactor temperature for varying oxygen inlet concentrations viz., 0.1%, 0.8%, 3% and 5% resp. for Pt.
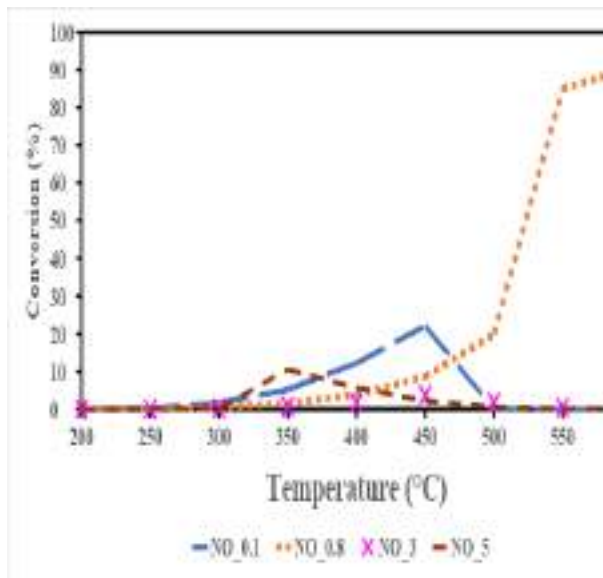

Figure 2: NO conversion vs Reactor Temperature for varying O₂ inlet concentration
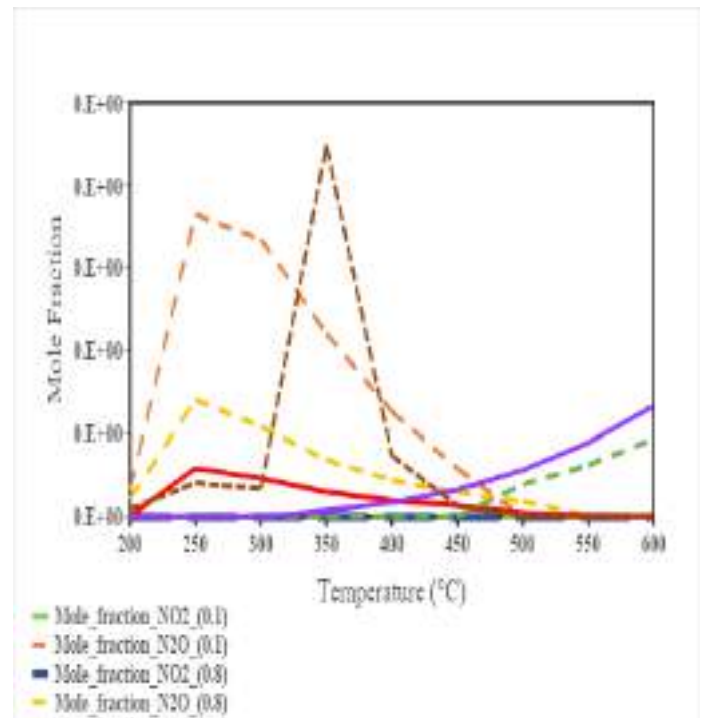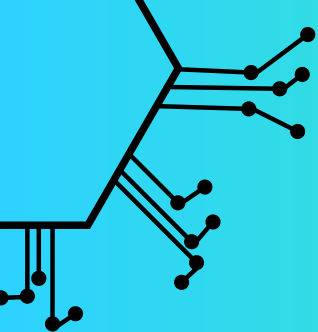
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Figure 3: N₂O and NO₂ mole fraction vs Reactor Temperature for different O₂ inlet.

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