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Mass Balance Mathematical Model

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Discovering Thoughts, Inventing Future



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CHEMICAL ENGINEERING

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Chemical Warehouse 101: Establishing a Functional Chemical Storage Facility from Scratch

By Hussain I. Al Hussain

Abstract- This paper provides a foundational guide to establishing a chemical warehouse from ground up, focusing on essential elements such as site selection, regulatory compliance, infrastructure, safety protocols, and operational workflows. The aim is to present a concise, practical introduction not only for engineers and project managers, but also for warehousing companies, logistics service providers, and entrepreneurs planning to enter the chemical storage industry.

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Chemical Warehouse 101: Establishing a Functional Chemical Storage Facility from Scratch

Hussain I. Al Hussain

Abstract- This paper provides a foundational guide to establishing a chemical warehouse from ground up, focusing on essential elements such as site selection, regulatory compliance, infrastructure, safety protocols, and operational workflows. The aim is to present a concise, practical introduction not only for engineers and project managers, but also for warehousing companies, logistics service providers, and entrepreneurs planning to enter the chemical storage industry.

INTRODUCTION BACKGROUND AND LITERATURE REVIEW

The importance of chemical warehouse safety and efficiency has been well-documented in both regulatory and academic literature. Studies have highlighted the risks of chemical mismanagement, including fire hazards, toxic exposure, and environmental contamination (Zhao et al., 2018; OECD, 2021). Regulations such as the OSHA Hazard Communication Standard (HCS) and the NFPA's classification system provide detailed guidelines, yet the practical implementation often varies widely between facilities. Third-party warehousing and logistics services are increasingly used in the chemical industry to improve compliance and operational efficiency.

Furthermore, recent advancements in warehousing technologies, such as the integration of IoT-based monitoring and predictive analytics, are beginning to reshape operational standards (Jarašūnienė et al., 2023). However, there remains a lack of cohesive literature that consolidates these developments into a step-by-step framework accessible to both technical and non-technical audience. This paper aims to address that gap by synthesizing regulatory principles, industry best practices, and modern tools into an actionable guide for various stakeholders in the chemical storage ecosystem.

The safe and efficient storage of chemicals is vital across multiple industries. From pharmaceuticals to manufacturing, a well-organized warehouse minimizes risk while maximizing accessibility and compliance. Mismanagement in chemical storage can lead to catastrophic accidents, environmental harm, and regulatory penalties. This paper introduces six (6) key

considerations and steps to establish a chemical warehouse tailored to safety and operational standards, serving as an introductory yet comprehensive blueprint for warehousing organizations, logistics providers, and engineering professionals alike.

I. SITE SELECTION AND DESIGN

Selecting an appropriate site is critical to both safety and logistics. Factors to consider include:

- *Location:* Choose a site away from residential zones but accessible via major transportation routes (road, rail, or port). Proximity to emergency services and ease of containment in case of a spill or leak should also be assessed.
- *Zoning and Environmental Considerations:* Ensure the area is zoned for hazardous material storage and assess environmental risks such as flood zones or seismic activity. Environmental impact assessments (EIAs) may be required.

Layout Design: The layout should provide distinct zones for different chemical classes, with buffer zones and barriers to prevent cross-contamination. It should include:

- Designated areas for flammable liquids, corrosives, oxidizers, and toxic materials.
- Ventilation systems designed to reduce accumulation of hazardous vapors.
- Clearly marked emergency exits and access routes for fire and medical services.
- Spill containment features integrated into the floor plan.

II. REGULATORY COMPLIANCE

Compliance with environmental protection regulations is equally essential. The U.S. Environmental Protection Agency (EPA) provides guidance on hazardous waste management, secondary containment systems, and stormwater runoff under laws such as the Resource Conservation and Recovery Act (RCRA) and the Clean Water Act (CWA). Warehouses must comply with spill prevention, control, and countermeasure (SPCC) regulations when handling threshold quantities of hazardous substances (EPA, 2024).

Compliance with international and local regulations is non-negotiable. Key frameworks include:

- The Occupational Safety and Health Administration (OSHA) regulations (29 CFR 1910.1200) for hazard communication (OSHA, 2023).
- National Fire Protection Association (NFPA) Code 400 for hazardous materials (NFPA, 2023).
- Globally Harmonized System (GHS) for chemical classification and labeling.

Facilities must maintain updated permits, conduct periodic inspections, and ensure documentation (e.g., SDSs) is readily accessible to staff and regulators. A compliance matrix or checklist is highly recommended to track ongoing obligations and ensure ongoing and full compliance with regulatory requirements.

III. INFRASTRUCTURE AND EQUIPMENT

The infrastructure must be engineered to support safe storage and handling:

- *Spill Response Kits:* Each storage zone should be equipped with clearly marked spill kits. These should include absorbent pads, neutralizers, and containment pallets designed for the specific chemicals stored. Spill kits must be maintained in accessible locations and inspected regularly to ensure readiness for minor leaks or incidental spills.
- *PPE Storage Cabinets:* Designated cabinets must be installed near work zones to store personal protective equipment (PPE). PPE requirements should be determined based on the chemical hazard classification and material compatibility. At a minimum, PPE kits should include chemical-resistant gloves, safety goggles, face shields, coveralls, and respirators. Cabinets should be clearly marked, easily accessible, and regularly inspected for completeness and condition.
- *Emergency Safety Systems:* The facility must be equipped with emergency shower and eyewash stations in accordance with ANSI/ISEA Z358.1 standards. These should be located near areas where hazardous chemicals are handled to provide immediate decontamination in the event of accidental exposure.
- *Drainage System:* Design the floor with a chemical-resistant drainage system capable of containing and directing spills to a containment sump. The drainage plan must also comply with EPA spill containment and stormwater runoff requirements under the Clean Water Act (EPA, 2024). This helps prevent environmental contamination and facilitates cleanup.
- *Emergency Lighting:* Install battery-powered emergency lights that activate during power

outages, ensuring safe navigation toward exits and safety equipment.

- *Fire Protection:* Install sprinklers, extinguishers, and smoke detectors rated for chemical environments. Class D fire extinguishers may be required for combustible metals.
- *Storage Systems:* Use corrosion-resistant, ventilated shelving. Flammable chemicals should be housed in explosion-proof cabinets and bonding/grounding should be installed to prevent static discharge.
- *Climate Control:* Some chemicals require temperature and humidity control to prevent degradation or hazards. For example, organic peroxides and isocyanates must be stored below specific temperature thresholds with humidity mitigation.
- *Signage:* Display clear, standardized signage for all hazardous materials stored in the facility. This includes symbols and labels for corrosive, flammable, toxic, reactive, and environmentally hazardous substances, consistent with GHS and NFPA standards. Signage should be prominently posted on doors, storage cabinets, and individual containers.

Additionally, install safety awareness posters in visible areas such as entryways, locker rooms, and near handling zones to reinforce key procedures like spill response, PPE usage, and emergency actions. These posters can also be referenced and reinforced through employee training programs. Access to PPE should be immediate and accompanied by training.

IV. SAFETY AND RISK MANAGEMENT

Proactive safety planning reduces liability and improves response time:

- *Training:* Employees must be trained on chemical hazards, safe handling, and emergency response. Refresher training should be conducted semi-annually, and competency should be verified through assessments. Training should also include hands-on exercises for using spill kits, including identifying appropriate absorbents and deploying containment pallets. Employees should be familiar with minor spill containment techniques and understand the escalation protocol for larger incidents, in accordance with OSHA HAZWOPER and EPA SPCC guidelines. Additionally, organizations seeking structured training may consider enrolling employees in certified courses. One example is the OSHA HAZWOPER training provided by the OSHA Education Center, which includes modules on chemical spill response and safety protocols (OSHA Education Center, 2024). Other reputable providers include the National Safety Council (NSC), Hazmat School, and Global

HazMat, all of which offer in-person and online training aligned with SPCC and OSHA standards.

- *Emergency Response Plan:* Must include evacuation procedures, contact lists, and spill containment protocols. Periodic drills should simulate real scenarios. Coordination with local emergency responders is encouraged.
- *Storage Protocols:* Store chemicals based on compatibility matrices (e.g., acids separate from bases) and segregate by flammability, toxicity, and reactivity. Use of color-coded labeling systems and QR-linked SDS access can enhance clarity. Guidelines from the National Research Council's 'Prudent Practices in the Laboratory' recommend grouping chemicals by hazard class, ensuring proper ventilation, and maintaining separation between incompatible substances (National Research Council, 2011).

Step-Up Recommendation: Consider integrating mobile apps for on-the-go hazard reporting and digitized incident logs. These tools increase responsiveness and support real-time safety oversight without requiring full-scale simulation technologies. Notable examples include iAuditor by SafetyCulture, which enables real-time hazard reporting and inspection tracking, and ChemAlert Mobile, a chemical management app that provides QR-access to SDS and safety protocols. These tools enhance situational awareness and help standardize incident documentation.

V. OPERATIONAL PROCEDURES

Smooth operations depend on well-documented procedures:

- *Inventory Control:* Employ systems like barcode or RFID to monitor stock levels, expiration dates, and usage logs. Include monitoring of chemical shelf life to ensure expired substances are flagged and removed from circulation. Implement first-expire-first-out (FEFO) protocols.
- *Receiving and Dispatch:* Inspect all incoming materials for integrity and verify documentation. Outgoing shipments must be labeled and packaged per transport regulations (e.g., DOT, ADR).
- *Maintenance:* Periodic calibration of sensors, inspection of containment units, HVAC servicing, and review of SDSs should be scheduled. Maintain an up-to-date master material list that documents all chemicals on-site, their hazard classifications, storage requirements, and expiration dates. This list should be reviewed and updated regularly in coordination with inventory audits. Maintenance logs should be digitized for traceability.

VI. ADVANCED ENHANCEMENTS AND COST FEASIBILITY

While not part of minimum regulatory requirements, several modern practices can significantly enhance the performance and safety of a chemical warehouse.

- *Digital Tools and Automation:* Warehouse Management Systems (WMS) improve visibility and accuracy in inventory tracking. IoT sensors can monitor temperature, humidity, and leakage in real time, enabling early intervention. AI-powered analytics can predict demand trends, flag compliance risks, and optimize space allocation (Boston Consulting Group, 2022).
- *Cost Considerations and Feasibility:* Establishing a chemical warehouse involves significant capital and operating expenses. Capital expenditures (CapEx) include land acquisition, structural upgrades for fire safety, temperature control systems, and installation of regulatory-compliant fixtures. Operating expenditures (OpEx) include utility costs, employee training, PPE replenishment, insurance, and periodic third-party audits.

CONCLUSION

Starting a chemical warehouse requires strategic planning, regulatory awareness, and a safety-first mindset. This guide serves as a starting point; while further expansion and customization would depend on warehouse size, function, and chemical type. Future revisions may include real-world case studies or digital simulation tools to further contextualize warehouse implementation strategies. With increasing environmental and safety expectations, integrating smart technologies and strict compliance protocols will be key to long-term operational success. Whether the initiative is led by a private enterprise, a logistics firm, or an internal industrial team, a standardized and proactive approach to chemical warehousing is essential.

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Optimizing Water Networks through Regeneration-Reuse and Regeneration-Recycle Approaches for Multiple Contaminants

By Azza Mohamed Khalifa, Nadia Ali Elsayed & Mostafa Awad

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Abstract- Effective water management is crucial for industrial operations to minimize freshwater consumption and wastewater discharge. This paper presents a comprehensive approach for optimizing water network design in the presence of multiple contaminants. The proposed methodology incorporates regeneration, reuse, and regeneration-recycle strategies to achieve optimal water usage and contaminant removal. The effectiveness of the proposed approach is demonstrated through case studies involving industrial processes with diverse contaminant profiles. The results show significant reductions in freshwater consumption and wastewater generation compared to conventional designs. By comparing a water network design without any regeneration methods to one that incorporates regeneration techniques, it is evident that the amount of freshwater required is significantly higher in the network without regeneration. The inclusion of regeneration strategies, such as reuse and regeneration-recycle, allows for the treatment and recirculation of process water streams, thereby reducing the demand for costly and resource-intensive freshwater intake.

Keywords: *contaminant removal, mathematical modeling, optimization algorithms, regeneration methods, water network minimization.*

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Azza Mohamed Khalifa ^α, Nadia Ali Elsayed ^σ & Mostafa Awad ^ρ

Abstract- Effective water management is crucial for industrial operations to minimize freshwater consumption and wastewater discharge. This paper presents a comprehensive approach for optimizing water network design in the presence of multiple contaminants. The proposed methodology incorporates regeneration, reuse, and regeneration-recycle strategies to achieve optimal water usage and contaminant removal. The effectiveness of the proposed approach is demonstrated through case studies involving industrial processes with diverse contaminant profiles. The results show significant reductions in freshwater consumption and wastewater generation compared to conventional designs. By comparing a water network design without any regeneration methods to one that incorporates regeneration techniques, it is evident that the amount of freshwater required is significantly higher in the network without regeneration. The inclusion of regeneration strategies, such as reuse and regeneration-recycle, allows for the treatment and recirculation of process water streams, thereby reducing the demand for costly and resource-intensive freshwater intake.

The key difference lies in the ability of the regeneration-based network to efficiently manage contaminant levels and enable the reutilization of water within the system. Without regeneration, the water network would need to rely solely on freshwater makeup to dilute contaminants, leading to higher freshwater consumption. In contrast, the regeneration-enabled network can selectively remove contaminants and reintroduce the treated water back into the process, significantly decreasing the overall freshwater requirements, for example, The paper's first case study demonstrates that the fresh water consumption in the processes without regeneration is 112.9 tons per hour. However, by implementing regeneration in the same processes, the fresh water consumption decreases to 59.7 tons per hour. This comparison highlights the significant advantages of incorporating regeneration strategies into water network design. By optimizing the integration of treatment technologies and water recirculation pathways, industrial facilities can achieve substantial reductions in freshwater usage and minimize their environmental impact through more sustainable water management practices. This work provides a valuable decision-making tool for industrial water system designers and managers, facilitating the implementation of advanced water minimization techniques and promoting the adoption of circular economy principles in water resource management.

Keywords: contaminant removal, mathematical modeling, optimization algorithms, regeneration methods, water network minimization.

1. INTRODUCTION

Water network minimization is a crucial strategy for enhancing the efficiency and sustainability of water distribution systems. By optimizing water consumption and reducing losses, this approach ensures the effective management of our precious water resources. This process is essential for achieving a balance between water supply and demand, conserving water, and mitigating the environmental impact of water distribution systems. Through the implementation of water network minimization, communities can enjoy a reliable water supply, promote water conservation, and work towards a more sustainable future[1].

The concept of the circular economy underscores the importance of minimizing the utilization of fresh resources through the implementation of the 3R strategies: reduce, reuse, and recycle. In Malaysia, water consumption is predominantly driven by domestic and industrial activities, accounting for over 50% of the total water usage. consumption. Therefore, it is imperative to implement measures to decrease water usage in these areas, as the wastewater generated can be regenerated, reused, or treated, thereby reducing the reliance on freshwater resources[2].

The research focus on wastewater minimization has gained considerable attention due to the critical importance of water conservation and the imperative to decrease the discharge of wastewater. The integration of water systems plays a pivotal role in achieving substantial reductions in both the consumption of fresh water and the discharge of wastewater by implementing practices such as wastewater reuse and regeneration recycling [3].

Wastewater treatment plants (WWTPs) play a crucial role in removing pollutants from water to meet water quality standards and regulations. The increasing significance of adhering to environmental standards and the inefficiencies resulting from inadequate designs and practices underscore the need for systematic tools for WWTP design[4]. The objective of wastewater management is to establish measures for environmental

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protection while considering economic and social concerns.

Minimizing water consumption in the process industry is crucial to reduce operating costs and minimize aqueous emissions to the environment[5]. Improving the efficiency of water use in the process industry can be achieved through process changes or upgrades that facilitate reduced water requirements for water-using operations. These individual process modifications can contribute to the reduction of water consumption at the site level. However, it is unlikely to achieve significant water savings through such focused investigations, as they are often limited to particular equipment or subsystems within the plant.

To fully realize the potential for water savings and maximize the efficiency of water usage in the plant, a holistic approach is required. This approach allows for system-wide analysis of water systems as a whole and supports the integrated management of water across the entire site. The key concept of this integrated water management is to maximize the reusability of water between water-using operations. The reusability of water can be improved by collecting water discharged from water-using operations and feeding it to other operations. The extent to which contaminated water can be reused depends on the acceptability of the contaminated water for each individual operation and the arrangement of water mixing between freshwater or other less-contaminated water from other operations. The reusability of contaminated water, as well as the acceptability of reused water for the operation, can be enhanced by regenerating contaminated water through effluent treatment processes and reusing (or recycling) it in other operations[6].

The loop breaking technique and explained how that technique can be adapted with restrictions on the flow rate used for each process as well as water losses[7]. A novel graphical method that presents a supply and demand composite and shows concentration versus flow rate[8]. Finding the global optimum of a problem rather of a local one was a challenge for nonlinear mathematical programming techniques, especially when dealing with problems with numerous variables[9]. A new graphical approach, they discussed how to distribute the quality of the waste water that needs to be processed while also allocating fresh water as efficiently as possible[10]. A novel method for creating water utilization networks in process plants that minimize the use of fresh water and utilities[11]. The concentration potential conceptions of the streams serve as the foundation for regeneration recycle water network with internal mains[12]. In order to maximize water reuse, a new methodical design approach has been developed for the simultaneous management of energy and water systems [13].

In practice, finding the most appropriate manner of reusing water between operations can be

complex, as a large number of mixing and reusing options are available for the water systems. Since the early 1990s, various design methodologies have been proposed to systematically investigate water reuse and its implementation into a water network, primarily based on the concept of a limiting water profile.

This design philosophy has been successfully and widely applied to various industrial sectors, demonstrating the benefits of using an integrated and system-wide analysis in the design and operation of water systems. The successes lie in the methodological convenience and advantages associated with the use of a limiting water profile. The synthesis of water networks is made solely with the manipulation of information related to water conditions (i.e., water flowrate and concentration), while process streams and their conditions are not involved during the targeting and design of water networks. This simplification allows for a common, but powerful, basis for the integrated design framework of water-using operations, even though the mass transfer mechanisms for water use may not be the same across all operations. Another advantage of using this integrated method is the ability to target the theoretical maximum potential of water savings.

Three types of industrial applications:

There are three primary industrial applications for wastewater reuse: cooling towers and HVAC systems, industrial processes and manufacturing, and energy production[14].

In industrial settings, wastewater can be used as a cost-effective and sustainable water source for heating, cooling, and ventilation processes. The treated wastewater can function as a cooling agent, decreasing freshwater intake and reducing energy consumption. Reusing wastewater in cooling towers and HVAC systems can improve system efficiency, minimize maintenance costs, and decrease the risk of scaling and corrosion.

However, it is crucial to ensure appropriate treatment and disinfection of the wastewater before using it in these systems. This is necessary to prevent microbiological growth and minimize potential health risks. Proper system design, maintenance, and operation are essential to optimize performance and safety.

Wastewater can also be utilized in energy production applications. One approach is to use the treated wastewater as a cooling source, which can drive turbines to generate electricity. Alternatively, the wastewater can serve as a feedstock for biofuel production.

II. PROBLEM STATEMENT

Design and optimize an integrated water minimization and regeneration network for an industrial

manufacturing facility with the following objectives and requirements[15]:

a) *Objectives*

Minimize freshwater intake from municipal sources by 50% or more through water reuse and regeneration.

Maximize water recovery from process drainages, wastewater streams, and other sources.

Minimize life cycle costs including capital expenses, operational costs, and water/wastewater utilities.

b) *Requirements*

Provide sufficient water supply to meet all process and non-potable fixture demands.

Regenerated water must meet quality standards for intended end uses such as cooling tower makeup, landscape irrigation, wash down, etc.

System must comply with all applicable health, safety, and environmental regulations.

The optimized solution should achieve the stated objectives through effective integration of reuse, regeneration, and minimization strategies to reduce the plant's water usage, costs, and environmental impacts.

c) *Methodology*

The procedure essentially consists of the four steps listed below, omitting the regeneration process[16]:

- *Step1:* Determine the fresh water processes (FWPs), which their inlet concentration is zero
- *Step2:* Calculation of the limiting concentration of the regeneration processes which don't take fresh water only

$$\text{Lim CR} = C_0 \cdot (1 - \text{RR}) \quad (1)$$

Where Lim CR is limiting concentration of regeneration, C_0 is outlet concentration of process and RR is the removal ratio.

➤ *Step3:* Allocation of source and demand

1. Allocation of processes according to (CPD), if the CPD for a process equal zero, it will take fresh water only. When multiple source streams are available, we should priorities/ the reuse of one source over the others. Equation 1 displays the source stream with the highest quasi allocation ratio value first[17],[18],[19].

$$R_{i,j} = \min k = 1, 2, 3, \dots, NC \left(\frac{D_{limj,k}}{C_{Si,k}} \right) \quad (2)$$

Where, $R_{i,j}$ is the limiting quasi-allocation from S_i to D_j

2. When S_i is the allocation to D_j , Reuse critical contaminant is defined as the concentration that reaches the limiting value before any other.

3. The source with the next-highest quasi-allocation amount should be selected if one source is unable to fully meet the demand.
4. Calculate the mass load for demand and source at a definite reuse key contaminant by equations:

$$MD = FD \cdot C_i \quad (3)$$

$$MS = FS \cdot C_0 \quad (4)$$

There are three cases for mass load,

- a. If $MS = MD$, the source provides all the water to meet the demand.
- b. If $MS > MD$, the source provides the amount of water where $MS = MD$, and the remaining demand is met using fresh water.
- c. If $MS < MD$, the source provides all its water, and the remaining demand is met using the source with the next highest $R_{i,j}$ value.

$$WR = (MD / CS_{OUT}) \quad (5)$$

Step4: After allocation, determine the updated concentrations at the intake and output for each process[20], as follows:

$$CN_{i,I} = (C_{0,I} \cdot MN) / M_0 \quad (6)$$

$$CN_{i,O} = C_{0,O} - (C_{0,I} - CN_{i,I}) \quad (7)$$

Where, C_0 is the outlet concentration, WR is the water required for each process, RKC is the reuse key contaminant, $CN_{i,I}$ is new inlet concentration, $C_{0,I}$ is the old inlet focus, Old mass load is M_0 , and new mass load is MN , $CN_{i,O}$ is new outlet concentration, $C_{0,O}$ is old outlet concentration.

- Basically, the method consists of seven steps described in the following using regeneration method.

Step1: Determine the fresh water processes (FWPs), which their inlet concentration is zero.

Step2:

1. Determine the processes which feed the regeneration process by water (BP), and processes which take water from a regeneration process (AP)
2. Calculate the limiting concentration of the regeneration processes which don't take fresh water only
3. Determine type of processes:
4. Calculate the average of limiting concentration of regeneration
 - If the concentration of contaminant lower than the average of limiting concentration take ϕ sign
 - If the contaminant concentration is at least as high as the limiting concentration average take η sign
 - If $\phi > \eta$ the process called below process (BP)

- If $\eta > \phi$ the process called above process (AP)

Step3:

Using CPD values to determine the order in which processes should execute determining CPD for (BP+FW) process by using equation [14], [12], $CPD(Dj) =$

$$\sum_{i=1}^{Ns} \min k = 1, 2, 3, \dots NC \left(\frac{CD \lim i, k}{CSi, k} \right)$$

➤ Step4: Design procedure of water using networks, the design steps are as follows:

- 1) Allocation of processes according to order of priority factor (CPD), if the CPD for a process equal zero, it will take fresh water only. We should choose which source should be reused first when there are multiple streams of sources accessible. Equation 1 displays the source stream with the highest quasi allocation ratio value first.
 - 2) When a source S_i is allocated to a demand D_j , the concentration of the "reuse key contaminant" (RKC) reaching the limiting value first will be considered the RKC for the S_i - D_j pair.
 - 3) If the demand cannot be fully met by a single source, another source with the next highest "quasi-allocation amount" ($R_{i,j}$) value should be used to supplement the demand.
 - 4) The mass load calculations.
- Step5: After allocation, the updated concentrations at the intake and output of each process are calculated.
- Step6: Calculation of inlet regeneration concentration by using equation:

$$C^{o reg} = \sum_i (F_{si}^{lim} C_{reg,s}^{lim}) / \sum_i F_{si}^{lim} \quad (8)$$

Step7: The design procedure is then repeated from step 4 to optimize the water use network.

III. ALGORITHM

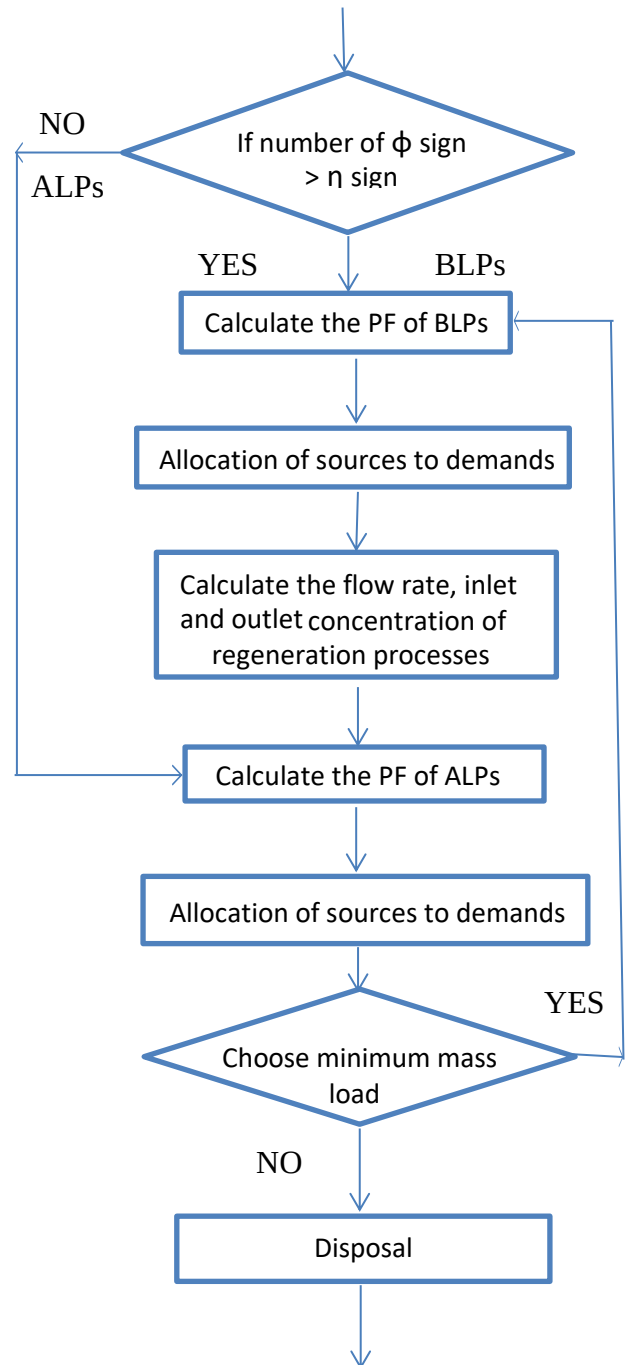


Fig. 3.1: Water network minimization flow chart

IV. CASE STUDY

This case study is taken from [21] with the data shown in table (2.2), including 5 processes, 3 contaminants and the removal ratio for regeneration is (0.99.9%, 0).

Table 4.1: Limiting data for example (1)

Process	Contaminant	Cin (ppm)	Cout(ppm)	Fmax (T/hr)
P1	A	0	15	50
	B	0	400	
	C	0	35	
P2	A	20	120	34
	B	300	12500	
	C	45	180	
P3	A	120	220	56
	B	20	45	
	C	200	9500	
P4	A	0	20	8
	B	0	60	
	C	0	20	
P5	A	50	150	8
	B	400	8000	
	C	60	120	

In this particular example, we consider a water network comprising five processes, and each process involves three contaminants. Our objective is to design a water network that demonstrates the reduction of fresh water usage through two different methods: one without regeneration and the other with regeneration by using removal ratio. Furthermore, we will conduct a thorough comparison between these two approaches to assess their effectiveness and efficiency.

According to network without regeneration:

Based on the determined order of processes (P1, P2, P3, P4, P5, P6), the allocation of process P2 and P3 requires a fresh water requirement of 8.5T/hr and 46.4T/hr, respectively. The determination of the recycle and keep concentration (RKC) in process 4 is denoted as (B) in S4 after choosing between S1 and S4, calculated using equation (3). Subsequently, equations (4) and (5) are employed to obtain the values. It is observed that the mass source (S4) is lower than the mass demand (D3). In this situation, S4 provides all the water to D3, while D3 will obtain water from other sources, specifically S1, indicating a requirement of 1.6 T/hr of water from S1 to D3, as determined by equation (6). The total amount of fresh water required is 46.4 T/hr. By utilizing equations (7) and (8), the new inlet and outlet concentrations can be calculated as follows: $CN,I = (3.29, 20, 3.86)$ ppm and $CNO = (103.29, 45, 9303.86)$. Within process 5, two sources, S1 and S3, are present. Applying equation (3), source S1 is selected with an assigned RKC of B. Equations (4) and (5) are then used to determine the corresponding values. The analysis reveals that the mass source (S1) exceeds the mass demand (D5), indicating a requirement of 8 T/hr of water to be transferred from S1 to D2, as determined by equation (6). By employing equations (7) and (8), the new inlet and outlet concentrations can be calculated as follows: $CN,I = (15, 400, 31.25)$ ppm and $CNO = (115, 8000, 91.25)$.

Within process 2, three sources, S1, S3, and S5, are present. Applying equation (3), source S1 is selected with an assigned RKC of B. Equations (4) and (5) are then used to determine the corresponding values. The analysis reveals that the mass source (S1) exceeds the mass demand (D2), indicating a requirement of 25.5 T/hr of water to be transferred from S1 to D2, as determined by equation (6).

By employing equations (7) and (8), the new inlet and outlet concentrations can be calculated as follows: $CN,I = (15, 400, 31.25)$ ppm and $CNO = (115, 8000, 91.25)$.

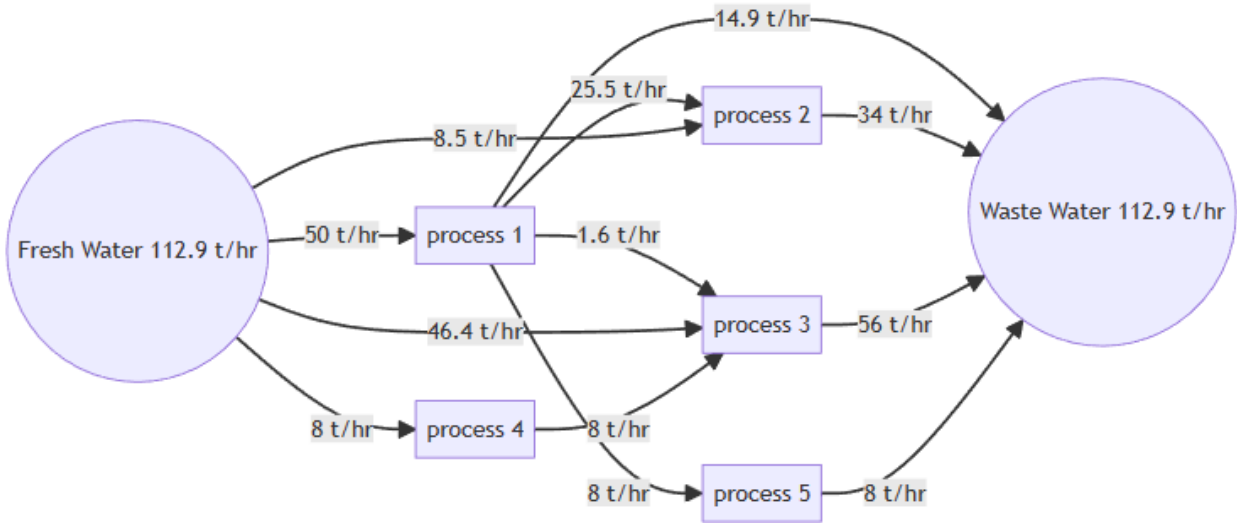


Fig. 4.1: Network design without regeneration

According to network with regeneration:

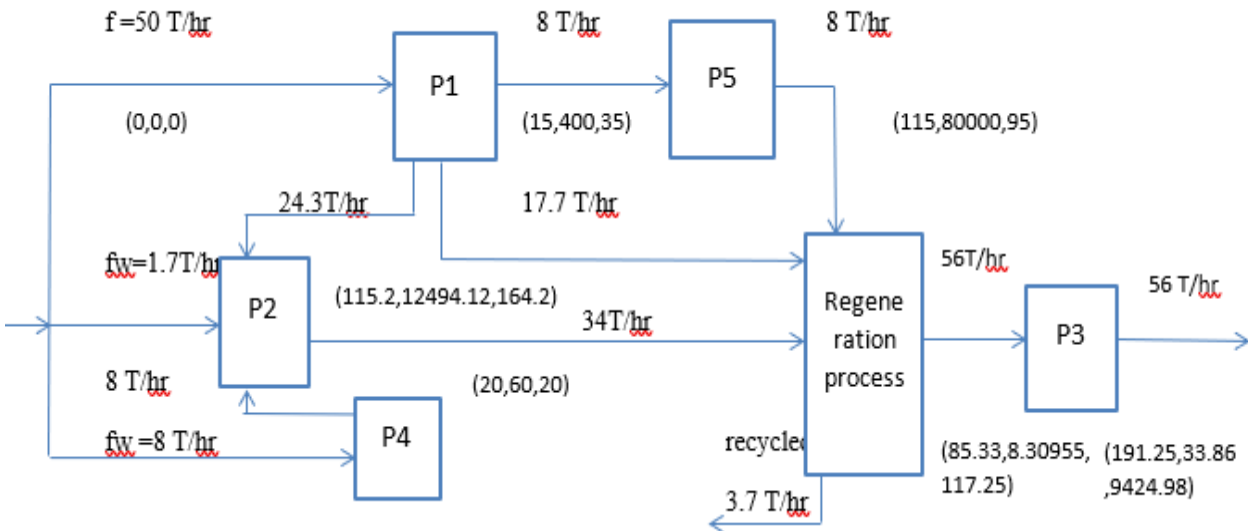


Fig. 4.2: The final water network design with regeneration

Table 4.2: Comparison table between using regeneration method and without regeneration method

	With using regeneration method	Without regeneration method
Fresh water(t/hr)	59.7	112.9

Table 4.3: Comparison between Different Methods for Example (2)

	Liu Z.Y.et al (2009b)	Our paper
Frsh water consumption	60.2	59.7
Method	Linear programming	Systematic approach(Regeneration recycle)

V. CASE STUDY

Shows limiting data taken from [22]. In Table 5, The removal ratio values for the regeneration unit to remove contaminants A, B, C are all 90%.

Table 5.1: Limiting data for example (2)

Process	Contaminant	Cin (ppm)	Cout(ppm)	Mass Load(g.hr ⁻¹)	F (T/Hr)
P1	A	300	500	180	0.9
	B	5000	11000	750	0.13
	C	1500	3000	100	0.07
P2	A	10	200	3610	19
	B	0	500	250	0.5
	C	0	1000	800	0.8
P3	A	10	1000	6000	6.06
	B	0	2000	15000	7.5
	C	0	3500	10000	2.86
P4	A	100	400	2000	6.67
	B	50	2000	800	0.41
	C	1000	3500	1000	0.4
P5	A	100	350	3000	12
	B	50	1800	1900	1.09
	C	1000	3500	2100	0.84
P6	A	85	350	3800	14.34
	B	300	6500	1100	0.18
	C	200	1000	2000	2.5

According to network without regeneration:

Based on the determined order of processes (P2, P6, P5, P4, P1, P3), the allocation of process P2 and P3 requires a fresh water requirement of 18.02 T/hr and 7.5 T/hr, respectively. The determination of the recycle and keep concentration (RKC) in process 6 is denoted as (C) in S2, calculated using equation (3). Subsequently, equations (4) and (5) are employed to obtain the values. It is observed that the mass source (D6) is lower than the mass demand (S2), indicating a requirement of 2.868 T/hr of water from S2 to D6, as determined by equation (6). The total amount of fresh water required is 11.47 T/hr. By utilizing equations (7) and (8), the new inlet and outlet concentrations can be calculated as follows: $CN,I = (38, 100, 200)$ ppm and $CNO = (303, 6300, 1000)$.

Within process 5, two sources, S2 and S6, are present. Applying equation (3), source S2 is selected with an assigned RKC of B. Equations (4) and (5) are then used to determine the corresponding values. indicating a requirement of 1.2 T/hr of water to be transferred from S2 to D5, as determined by equation (6). By employing equations (7) and (8), the new inlet and outlet concentrations can be calculated as follows: $CN,I = (19, 50, 100)$ ppm and $CNO = (269, 1800, 2600)$.

Within process 4, three sources, S2, S6, and S5, are present. Applying equation (3), source S2 is selected with an assigned RKC of B. Equations (4) and (5) are then used to determine the corresponding values. indicating a requirement of 0.667 T/hr of water to be transferred from S2 to D4, as determined by equation (6).

By employing equations (7) and (8), the new inlet and outlet concentrations can be calculated as

follows: $CN,I = (19, 50, 100)$ ppm and $CNO = (319, 2000, 2600)$.

Within process 1, three sources, S2, S6, S4, and S5, are present. Applying equation (3), source S2 is selected with an assigned RKC of C. Equations (4) and (5) are then used to determine the corresponding values. indicating a requirement of 0.9 T/hr of water to be transferred from S2 to D1, as determined by equation (6).

By employing equations (7) and (8), the new inlet and outlet concentrations can be calculated as follows: $CN,I = (190, 500, 1000)$ ppm and $CNO = (390, 6500, 2500)$.

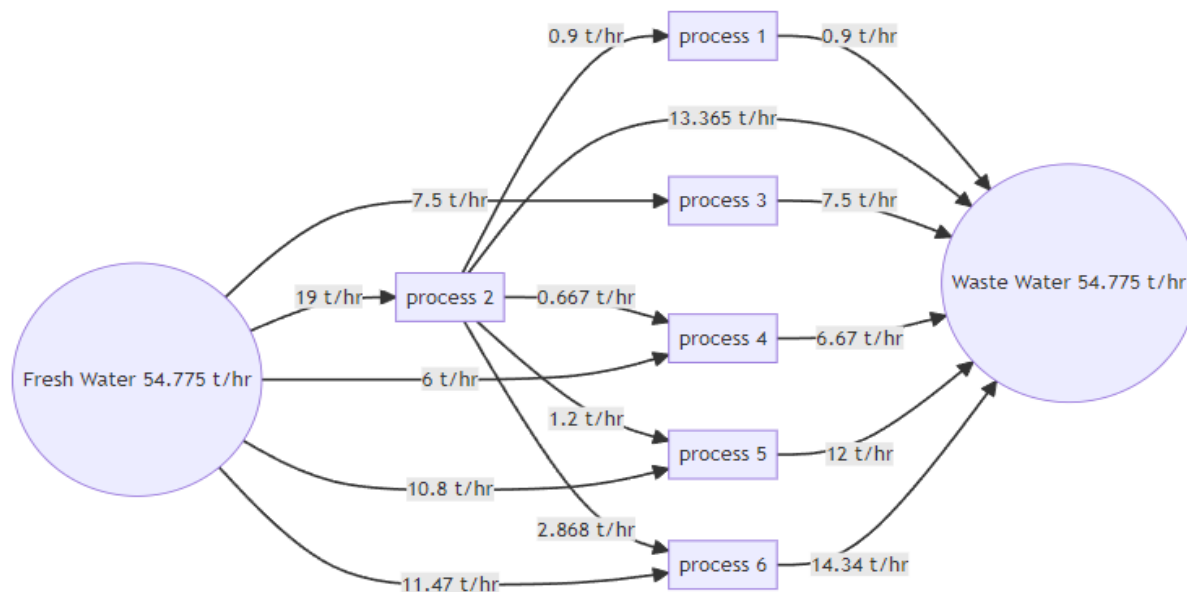


Fig. 5.1: Network design without regeneration

According to network with regeneration:

Table 5.2: Limiting data for limiting data for example (1)

Processes	Contaminants	Inlet conc (ppm)	Outlet conc(ppm)
P5	A	19	269
	B	50	1800
	C	100	2600
P6	A	37.62	302.62
	B	100.07	6300.07
	C	200	1000
P4	A	6	306
	B	50	2000
	C	31.48	2531.48
P1	A	36.69	236.69
	B	284.4	6284.4
	C	146.79	1646.79

Table 5.3: Inlet and outlet concentrations for regeneration-recycle method

Processes	Contaminants	Inlet conc (ppm)	Outlet conc(ppm)
P5	A	6.67	256.67
	B	50	1800
	C	31.67	2531.67
P6	A	36.93	301.93
	B	280.33	6480.33
	C	179.2	979.2
P4	A	6	306
	B	50	2000
	C	31.48	2531.48
P1	A	33.33	233.33
	B	266.67	6266.67
	C	166.67	1666.67

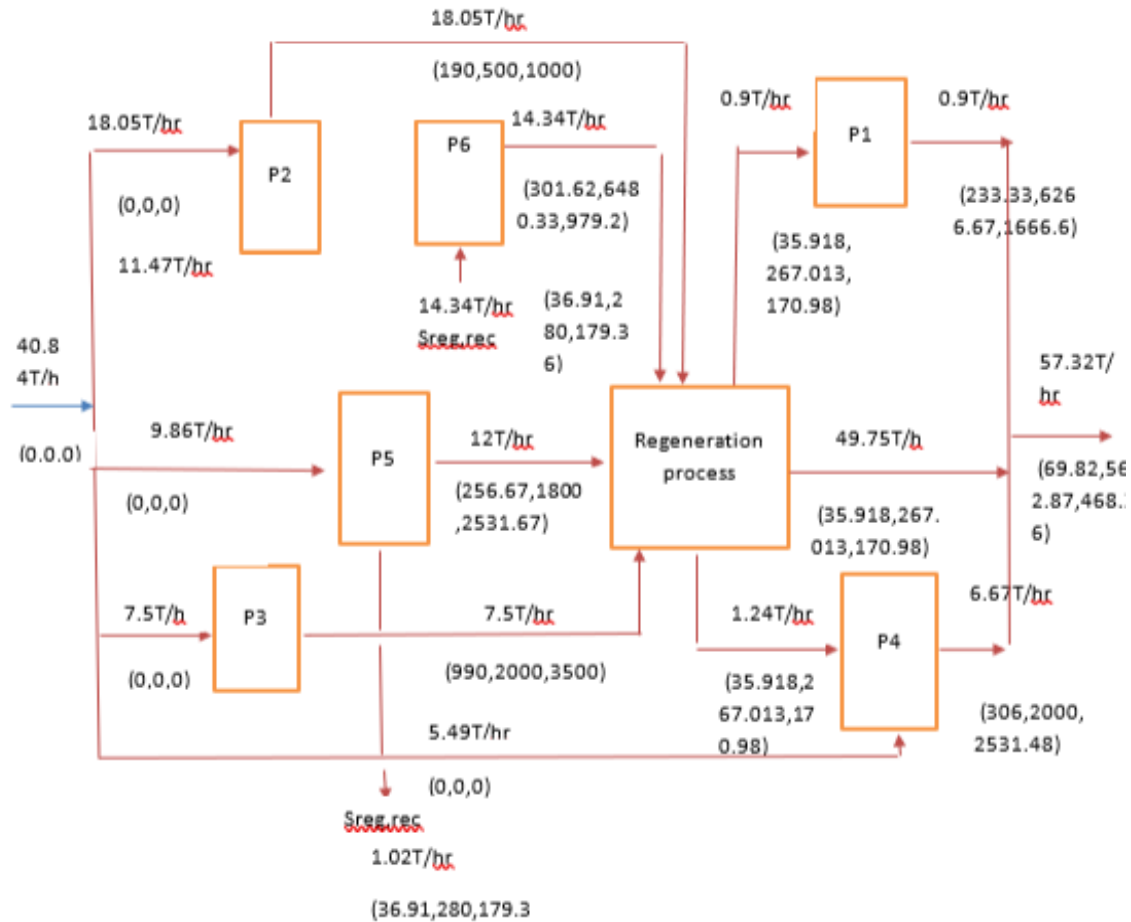


Fig. 5.2: The final water network design with regeneration

Table 5.4: Comparison table between using regeneration method and without regeneration method

	With using regeneration method	Without regeneration method
Fresh water(t/hr)	40.84	54.7775

Table 5.5: Comparison between Different Methods for Example (2)

	Zhaao H.P et al (2015)	Our paper
Frsh water consumption	53.826	40.84
Method	Linear programming	Systematic approach (Regeneration recycle)

VI. RESULT AND DISCUSSION

The optimization results of first case show that: Using equations (1) and (2), we can determine whether each process is an ABLP or a BLP. Processes P1, P4, P2, and P5 are identified as BLPs, while P3 is an ALP. By calculating the priority factor, we can establish the order of the processes as follows: P1, P4, P2, P5. For P1 and P4, fresh water is required as their inlet concentrations are zero and equal to 45 T/hr and 8 T/hr, respectively. Regarding P2, equation (3) is utilized to determine that the RKC is A for source S4. In this case, MD (mass demand) is greater than MS (mass source), indicating that all the water in S4 will be allocated to D2,

amounting to 8 T/hr. S1 is selected as the source for P2, and the RKC is determined as B, resulting in a fresh water requirement of 2.2 T/hr. The old and new mass loads are calculated using equations (4) and (5), respectively. The new inlet and outlet concentrations are determined using equations (7) and (8) as $C_{in} = (15.2, 294.12, 29.2)$ and $C_{out} = (115.2, 12494.12, 164.2)$. For P5, S1 is chosen as S4 has been consumed. Hence, the RKC is B. The new and old mass loads are calculated, and the new inlet and outlet concentrations are obtained as $(15, 400, 35)$ and $(115, 8000, 95)$. The inlet and outlet regeneration calculations from equation (8) are $(85.53, 8309.55, 117.25)$ and $(85.53, 8.30955, 117.25)$.

For P3, the RKC is determined as A from Sreg, and since MD is greater than MS, all the water from Sreg will be allocated to the demand, amounting to 59.7 T/hr. This value exceeds 56 T/hr, so there will be remaining water from Sreg. The old and new mass loads are calculated, and the new inlet and outlet concentrations are determined as (91.25, 8.86, 124.98) and (191.25, 33.86, 9424.98). By determining the minimum mass load, we can identify whether stream S3 or Sreg will be recycled. In this case, the stream from Sreg will be recycled. After repeating all the steps and calculating the inlet and outlet concentrations, it is observed that there is no need to recycle Preg because BLPs do not require any water from that recycled stream.

The optimization results of second case show that: Using equations (1) and (2), we can determine whether each process is an ABLP or a BLP. Processes P2, P3, P5, and P6 are identified as BLPs, while P1 and P4 are an ALP. By calculating the priority factor, we can establish the order of the processes as follows: P2, P3, P5, P6. For P2 and P3, fresh water is required as their inlet concentrations are zero and equal to 18.05 T/hr and 7.5 T/hr, respectively. For P5 equation (3) is utilized to determine that the RKC is B for source S2. In this case, Ms (mass demand) is greater than Md (mass source), Water required from S4 is 1.2T/hr.

S2 is selected as the source for P6, and the RKC is determined as c, water required from S2 is 2.87 T/hr. calculating inlet and outlet regeneration calculation by using equation(9).

$C_{in\ reg} = (369.07, 2800, 1793.6)$ and $c_{out\ reg} = (36.91, 280, 179.36)$

For P4, the RKC is determined as B from Sreg, and since Ms is greater than Md, water required from sreg=1.18 T/hr, so there will be remaining water from Sreg.

For P1, the RKC is determined as A from Sreg, water required from sreg=7.31 T/hr, but we need only 0.9T/hr.

Recycled the stream which have minimum mass load, calculate ALPS mass load. We recycled the stream which has minimum mass load but that process has low flow rate near to be neglect, so we will take P reg.

So we will repeat steps from determining priority factor, we can establish the order of the processes as follows: P2, P3, P5, P6. For P2 and P3, fresh water is required as their inlet concentrations are zero and equal to 18.05 T/hr and 7.5 T/hr, respectively. For P5 equation (3) is utilized to determine that the RKC is B for source Sreg. In this case, Ms (mass demand) is greater than Md (mass source), Water required from Sreg is 2.14T/hr.

Sreg is selected as the source for P6, and the RKC is determined as B, water required from Sreg is

15.36 T/hr. calculating inlet and outlet regeneration calculation by using equation(9).

$C_{in\ reg} = (351.98, 2670.13, 1709.8)$ and $c_{out\ reg} = (35.198, 267.013, 170.98)$

For P4, the RKC is determined as B from Sreg, and since Ms is greater than Md, water required from sreg=1.24 T/hr, so there will be remaining water from Sreg. The old and new mass loads are calculated.

For P1, the RKC is determined as A from Sreg, water required from sreg=7.67 T/hr, but we need only 0.9T/hr.

VII. CONCLUSION

The primary aim of this study was to develop an optimized water network design that minimizes freshwater consumption through the strategic integration of regeneration, reuse, and regeneration recycle methodologies. By considering the presence of multiple contaminants within the industrial process, the proposed approach addresses the complex challenge of water management in a comprehensive manner.

The results of this work clearly demonstrate the benefits of adopting the advanced water network optimization techniques presented. Compared to a conventional water network design without any regeneration strategies, the inclusion of regeneration, reuse, and regeneration-recycle methods leads to significant reductions in freshwater intake requirements.

The optimization framework allows for the identification of the most cost-effective and environmentally sustainable water network configuration, Balancing the trade-offs between freshwater consumption, wastewater discharge, and the capital and operational costs of the water treatment infrastructure is a key challenge in optimizing water management in industrial processes. This requires carefully evaluating the various options and their implications. The ability to selectively remove contaminants and recirculate the treated water within the process is the key driver behind the superior performance of the regeneration-based water network.

This research provides industrial facilities with a valuable decision-support tool for designing and implementing water networks that minimize freshwater usage and promote the principles of a circular economy. By adopting the strategies outlined in this study, organizations can enhance their overall water sustainability, reduce their environmental footprint, and contribute to the responsible management of this critical natural resource.

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Variations in the Concentration of CO₂ in Associated Gases: Evaluation of the Performance of a Conditioning Process with Turboexpander

By Leandro Vargas, Andrea Gonzalez & Giovanni Morales

Abstract- Herein we disclose an evaluation of the performance of a Turboexpander unit for the conditioning of associated gasses with different CO₂ contents. The performance evaluation was carried out by the comparison of the results from a simulation in Aspen Hysys v10 with the specifications established in the national gas transportation policy for natural gas (RUT). The Turboexpander unit was designed for the conditioning of an associated gas defined by the scenario of medium production for the Valle Medio del Magdalena, according to the prospects of the Mining and Energy Planning Unit (UPME). The conditioning unit considered the sections: stabilization, sweetening, dehydration, and separation by distillation. Similarly, the range for CO₂ content variation was defined between 3 - 12% mol, based on enhanced recovery (EOR) pilots of air injection and CO₂ injection. The results of the simulations showed an adequate performance of the Turboexpander unit for the conditioning of associated gasses with up to 6% mol of CO₂ contents, fulfilling the quality parameters of the RUT.

Keywords: turboexpander, gas transportation policy, associated gas, carbon dioxide, valle medio del magdalena, Aspen Hysys.

GJRE-C Classification: LCC: TP761, TP359



Strictly as per the compliance and regulations of:



Variations in the Concentration of CO₂ in Associated Gases: Evaluation of the Performance of a Conditioning Process with Turboexpander

Variaciones en la concentración de CO₂ en gases asociados: Evaluación del desempeño de un proceso de acondicionamiento con Turboexpander

Leandro Vargas ^α, Andrea Gonzalez ^σ & Giovanni Morales ^ρ

Resumen- Este documento presenta una evaluación de los desempeños de una unidad con Turboexpander, en el acondicionamiento de gases asociados con diferentes contenidos de CO₂. La evaluación de los desempeños fue efectuada por comparación de los resultados de una simulación desarrollada en Aspen Hysys v10 y las especificaciones establecidas en el Reglamento Único de Transporte de Gas Natural (RUT). Para esto, la unidad fue diseñada para el acondicionamiento del gas asociado definido por el escenario medio de producción de la cuenca del Valle Medio del Magdalena, según prospectivas de la Unidad de Planeación Minero-Energética; la unidad de acondicionamiento consideró las secciones: estabilización, endulzamiento, deshidratación y separación por destilación. De igual manera, el intervalo de variación de contenido de CO₂ entre 3 y 12% mol fue establecido, con base en reportes de literatura de pilotos de recobro mejorado (EOR) por inyección de aire e inyección de CO₂. Los resultados de las simulaciones mostraron un desempeño adecuado de la unidad con Turboexpander, en el acondicionamiento de gases asociados con concentraciones de CO₂ de máximo 6% mol, cumpliendo los parámetros de calidad estipulados en el RUT. Asimismo, los resultados de las simulaciones muestran que el perfil de temperatura en la torre de absorción, de la sección de endulzamiento, es alterado cuando se tratan gases con mayor contenido de CO₂. Esta alteración del perfil de temperatura en la torre de absorción conduciría al bajo desempeño en el retiro de CO₂. Lo anterior sugiere rediseños en la sección de endulzamiento o cambio de la respectiva tecnología, con lo cual, los gases tratados puedan cumplir los parámetros de calidad especificados en el RUT.

Palabras claves: turboexpander, RUT, gas asociado, dióxido de carbono, Valle Medio del Magdalena, Aspen Hysys.

Abstract- Herein we disclose an evaluation of the performance of a Turboexpander unit for the conditioning of associated gasses with different CO₂ contents. The performance evaluation was carried out by the comparison of the results from a simulation in Aspen Hysys v10 with the specifications established in the national gas transportation policy for natural gas (RUT). The Turboexpander unit was designed for the conditioning of an associated gas defined by the scenario of

medium production for the Valle Medio del Magdalena, according to the prospects of the Mining and Energy Planning Unit (UPME). The conditioning unit considered the sections: stabilization, sweetening, dehydration, and separation by distillation. Similarly, the range for CO₂ content variation was defined between 3 - 12% mol, based on enhanced recovery (EOR) pilots of air injection and CO₂ injection. The results of the simulations showed an adequate performance of the Turboexpander unit for the conditioning of associated gasses with up to 6% mol of CO₂ contents, fulfilling the quality parameters of the RUT. Likewise, the simulation results showed that the temperature profile in the absorption tower (sweetening section) changed when gasses with CO₂ contents greater than 6% mol were treated. This temperature profile change appeared to be responsible for poor CO₂ removal performance. The foregoing would suggest adjustments for the sweetening section or a shift of the respective technology in order to fulfill the quality parameters specified in the RUT.

Keywords: turboexpander, gas transportation policy, associated gas, carbon dioxide, valle medio del magdalena, Aspen Hysys.

1. INTRODUCCIÓN

El gas natural y la gasolina son productos de importancia en la canasta energética nacional, utilizados en diferentes sectores como el residencial, industrial, transporte y electricidad. El gas asociado de los yacimientos de crudo puede ser acondicionado para su uso como gas natural; adicionalmente, un flujo de gasolina natural es derivado como un subproducto. El acondicionamiento del gas asociado permite la disminución de contaminantes y líquidos condensables, a niveles adecuados para su aprovechamiento como fuente de energía térmica. Estos niveles están definidos en el Reglamento Único de Transporte de Gas Natural (Resolución CREG-071 de 1999 y su modificación posterior del año 2019).

Dentro de los contaminantes a retirar del gas asociado se encuentra el CO₂. Este gas es conocido por su participación en el cambio climático. El accionar del CO₂ en el aire impide la salida de calor de las capas

bajas de la atmósfera (efecto invernadero), lo cual ha generado un aumento progresivo en la temperatura promedio de la superficie del planeta (Osborn *et al.*, 2021). Debido a esta problemática, los gobiernos se han comprometido con la disminución en las emisiones de CO₂. En Colombia, el sector minero energético ha propuesto una meta de disminución en emisiones de 11,2 millones de toneladas de CO₂ equivalentes para el año 2030.

El retiro del contenido de CO₂ en los procesos de acondicionamiento de gas (endulzamiento), es usualmente realizado por absorción con monoetanolamina (MEA) (Elbashir *et al.*, 2019; Mokhatab & Poe, 2012); la MEA gastada es regenerada por calentamiento para su recirculación en el proceso. Posteriormente, el gas endulzado es sometido a un enfriamiento, que puede ser aplicado con un Turboexpander, para una posterior separación de los líquidos condensables, por medio de destilación fraccionada a baja temperatura (Mokhatab & Poe, 2012). Es importante anotar que, Colombia tiene instalada una importante cantidad de unidades de acondicionamiento de gases con Turboexpander (Martínez, 2018). Recientemente, Camacho (2021) desarrolló un análisis técnico-económico para la implementación de una unidad Turboexpander de acondicionamiento del gas asociado generado en el Valle Medio del Magdalena, considerando las proyecciones de producción definidas por la UPME (2018). Los resultados reportados por este autor indican factibilidad técnico-económica en la implementación de la unidad Turboexpander. Lo anterior manifiesta posibilidades futuras en el país, de nuevas unidades de acondicionamiento, basadas en Turboexpander.

Por otra parte, la aplicación de métodos de recobro mejorado (EOR, *enhanced oil recovering*) ha aumentado la producción de crudo (Jiang *et al.*, 2022; Mokheimer *et al.*, 2019), principal contribuyente del mercado energético mundial actual (Baumeister *et al.*, 2020). Uno de estos métodos EOR, basado en inyección de gases, ha conducido al aumento de la concentración de CO₂ en el gas asociado (Barbosa *et al.*, 2012; Escobar, 2006; Jiang *et al.*, 2022). Por consiguiente, se han realizado seguimientos a pilotos EOR de inyección de gases, implementados en diferentes yacimientos del país. Análisis cromatográfico de gases han reportado aumentos en los niveles de CO₂, hasta 12% mol en el gas asociado del campo Chichimene, por aplicación de EOR con inyección de aire (Díaz Molina *et al.*, 2019), y hasta 19% mol en el gas asociado del campo San Fernando, por aplicación de EOR por inyección de CO₂ (Díaz *et al.*, 2018). Este aumento en el contenido de CO₂, en gases asociados de pozos sujetos a EOR, puede ser progresivo en la respectiva ventana de operación (Marinov, 2015).

Este incremento en los contenidos de CO₂ afecta los desempeños resultantes de un proceso de

acondicionamiento de gas, especialmente en las etapas de endulzamiento y de recuperación de líquidos (Langé & Pellegrini, 2016; Rufford *et al.*, 2012). En la etapa de endulzamiento, una elevación en el contenido de CO₂ conduciría a un aumento en los requerimientos energéticos de la regeneración del absorbente (Langé & Pellegrini, 2016; Rufford *et al.*, 2012). Por su parte, los contenidos de CO₂ pueden afectar el equilibrio de fases en la etapa de separación de los hidrocarburos líquidos (Rufford *et al.*, 2012). Además, la presencia de CO₂ puede conducir a la formación de hidratos, a ciertas condiciones de presión y temperatura, ocasionando taponamiento en las líneas de flujo (Carroll, 2003).

Ante esta situación de incremento en los contenidos de CO₂, la mayoría de la literatura consultada dirige la atención en la proposición de alternativas de retiro simultáneo de líquidos condensables junto con el CO₂ (Arinelli *et al.*, 2019; Luyben, 2013; Maqsood *et al.*, 2014). Sorpresivamente, un número escaso de documentos reportaron análisis de los desempeños de las plantas con Turboexpander ante aumentos en el contenido de CO₂ en el gas asociado. Getu *et al.* (2013) compararon, por simulación con Aspen Hysys, los desempeños de diferentes procesos de separación de líquidos condensables en gases asociados con concentraciones de CO₂ de hasta 3.65% mol. Los autores mostraron factibilidad técnica en los procesos de retiro de líquidos (incluyendo Turboexpander) para las diferentes concentraciones analizadas, mencionando que las mayores recuperaciones de etano fueron obtenidas en los gases con menores concentraciones de CO₂. De igual manera, El-Husseiny *et al.* (2021) analizaron las variaciones energéticas del acondicionamiento con Turboexpander para gases asociados con concentraciones de CO₂ hasta 3.91% mol. Los autores reportaron factibilidad en el proceso de acondicionamiento para las diferentes concentraciones. Los trabajos de Getu *et al.* (2013) y El-Husseiny *et al.* (2021) presentan la característica de análisis para bajas concentraciones de CO₂; sin embargo, en unidades Turboexpander instaladas, esta condición de bajas concentraciones de CO₂ puede cambiar con los requerimientos de aplicación de EOR por inyección de gases. Asimismo, estos autores omiten los análisis de los perfiles de temperatura en las torres de endulzamiento y de separación de líquido. Estos análisis pueden ayudar en la explicación de los desempeños del proceso de acondicionamiento.

Las variaciones en los contenidos de CO₂ pueden conducir al incumplimiento de los requisitos mínimos para el transporte y la venta del gas, acondicionado en una determinada unidad. Un gas que no cumple con el RUT conlleva a pérdidas económicas y a contaminación ambiental; usualmente este gas es quemado en teas (Elehinafe *et al.*, 2022; Petri *et al.*, 2018). Lo anterior podría ser evitado con la predicción

de los desempeños de las unidades de acondicionamiento, previo al tratamiento de los gases asociados. Una predicción de los desempeños de las unidades instaladas conduciría a la selección de la unidad con mayor efectividad, en el acondicionamiento de un gas con determinado contenido de CO₂.

Considerando la problemática planteada, el presente documento expone un análisis sobre el desempeño de una unidad Turboexpander en el acondicionamiento de gases asociados con diferentes contenidos de CO₂. El análisis fue desarrollado considerando las proyecciones de producción de la UPME (2018) y los resultados de una simulación en Aspen Hysys v10.

II. METODOLOGÍA

El flujo de gas asociado correspondió al definido en el escenario medio de producción para la Cuenca del Valle Medio del Magdalena, según las proyecciones de la UPME (2018). Este escenario estableció un flujo promedio de 11,8 MMSCFD al año 2044. Por su parte, la composición de los gases en este

escenario fue asumida como la típica de los gases producidos en los campos Bonanza y Lisama de ECOPETROL S.A (Camacho, 2021); una característica de los gases en estos campos es la ausencia de H₂S (Camacho, 2021; SÁCHICA, 2012), lo cual facilita el respectivo proceso de endulzamiento. La Tabla 1 resume las condiciones de entrada y la composición del gas asociado.

La Tabla 2 compara la composición y las propiedades del gas asociado con los requisitos solicitados por el RUT. Según esta tabla, la composición de agua y de CO₂, así como el contenido de líquidos condensables (definido por el punto *Cricondentherm*) se encuentran fuera de especificación para el transporte y la comercialización del gas asociado; con lo anterior, el gas asociado requiere del respectivo acondicionamiento. Las secciones consideradas en el diseño estándar y en la simulación del proceso de acondicionamiento fueron: estabilización, endulzamiento, deshidratación y enfriamiento con Turboexpander, con una posterior separación por destilación.

Tabla 1: Condiciones y composición del gas asociado (Camacho, 2021)

Flujo, MMSCFD	11,8
Temperatura, °F	99,8
Presión, psi	500
Metano, % mol	77,06
Etano, % mol	7,20
Propano, % mol	4,87
n-butano, % mol	1,78
i-butano, % mol	1,59
n-Pentano, % mol	0,41
i-Pentano, % mol	0,57
2,2-Mpropano, % mol	0,03
n-Hexano, % mol	0,50
n-Heptano, % mol	0,12
n-Octano, % mol	0,04
n-Nonano, % mol	0,01
n-Decano, % mol	0,01
H ₂ O, % mol	0,21
Oxígeno, % mol	0,03
Nitrógeno, % mol	1,66
CO ₂ , % mol	3,91

Tabla 2: Verificación de la composición y las propiedades del gas asociado con los requerimientos del RUT (en paréntesis)

Componente	Gas de entrada (RUT)
H ₂ O, mg/m ³	58669,5 (<97)
O ₂ , % vol.	0,03 (<0,1)
N ₂ , % vol.	1,66 (<3)
Inertes, % vol.	5,60 (<5)
CO ₂ , % vol.	3,91 (<2)
H ₂ S, mg/m ³	0,00 (<6)
Poder calorífico, MJ/m ³	41,02 (35,4 – 42,8)
<i>Cricondentherm</i> , °F	114,0 (<45)

El paquete termodinámico Peng-Robinson fue utilizado para la mayoría de las corrientes y equipos en

la simulación; este paquete ha reportado resultados concordantes con diferentes datos de procesamiento

de hidrocarburos simples (Poe & Mokhatab, 2017). Por su parte, el paquete termodinámico "Acid Gas – Chemical Solvents" fue seleccionado para la sección de endulzamiento; este paquete aplica cálculos basados en el modelo NRTL en reacciones en fase acuosa, necesarias para el cálculo riguroso del proceso de absorción con MEA (Irina & Watanasiri, 2015). También, el paquete termodinámico "Glycol Package" fue definido para la sección de deshidratación; el "Glycol Package" aplica la ecuación de estado TST (Tsu-Sim-Tassone) en la determinación del equilibrio de fases, con resultados consistentes para la mezcla agua-TEG (trietilenglicol) (Hasan *et al.*, 2020).

Por otro lado, los equipos de proceso estándar fueron especificados con base en los trabajos de Benitez *et al.* (2015), Camacho (2021), Elbashir *et al.* (2019), Kherbeck & Chebbi (2015), Mokhatab *et al.* (2019), Mokhatab & Poe (2012) y Tristancho (2017). Para la etapa de estabilización, donde se aplica un tratamiento inicial, los equipos definidos fueron dos separadores *flash*, un compresor y un calentador. La sección de endulzamiento considera una absorción con MEA al 20% molar a 120°F y 847 psi, en una torre de 10 platos y de diámetro de 2,3 ft; es importante mencionar que la temperatura fue definida para una mayor absorción, a partir de pruebas con la simulación. También, la sección de endulzamiento considera una recuperación de MEA gastada, en una torre de destilación de 5 platos y diámetro de 3,9 ft.

La sección de deshidratación utiliza una solución de TEG al 99% p/p, en una torre de absorción con 20 platos y diámetro de 4,9 ft. El TEG gastado es recuperado en una torre de destilación de 5 platos, operando a presión atmosférica. El gas dulce y seco es enviado a la sección de enfriamiento con Turboexpander (criogenización). En esta sección, el gas es recibido por un enfriador, disminuyendo su temperatura hasta -31°F; el enfriamiento a esta temperatura conduce a una mayor recuperación de etano. Después del enfriador, la sección consideró dos torres de destilación para la generación del gas acondicionado, un flujo de etano y un flujo de GLP. La primera torre es llamada como demetanizadora, la cual es definida a una presión de 450 psia y temperaturas de -139°F en el tope hasta 85°F en el fondo de la torre, con un diseño de 17 platos y un diámetro de 4,9 ft. La segunda torre se denomina desetanizadora y es configurada con 28 platos, diámetro de 4,9 ft y operada a presiones en el rango de 200 a 210 psi y temperaturas desde -11°F en el tope hasta 130°F en el fondo de la torre. El diagrama de proceso (PFD) diseñado en Aspen Hysys es presentado en la Figura 1. En esta figura se definen las propiedades de los flujos principales de entrada y salida de la unidad, así como las secciones codificadas en el PFD.

Con el PFD desarrollado, un total de cinco (5) simulaciones fueron ejecutadas, considerando

diferentes concentraciones de CO₂ en el gas asociado. La Tabla 3 presenta las concentraciones del gas asociado para cada simulación; la simulación No 1 corresponde al caso base, con la composición de la Tabla 1. Las concentraciones de metano, del gas asociado del caso base, fueron ajustadas para la consecución de las composiciones mostradas en la Tabla 3. El gas de la simulación No 5 presenta una composición de CO₂ cercana a la máxima del gas asociado del campo Chichimene (EOR por inyección de aire), reportada por Díaz Molina *et al.* (2019). Por otro lado, cada simulación fue ejecutada, considerando las mismas especificaciones y condiciones de operación de los equipos, definidas anteriormente.

Tabla 3: Variación del contenido de CO₂ en el gas de entrada

No. Simulación	1	2	3	4	5
Metano % mol	77,0	75,1	73,3	71,4	69,5
Etano % mol	7,2	7,2	7,2	7,2	7,2
C ₃ + % mol	9,9	9,9	9,9	9,9	9,9
H ₂ O % mol	0,21	0,21	0,21	0,21	0,21
O ₂ % mol	0,03	0,03	0,03	0,03	0,03
N ₂ % mol	1,66	1,66	1,66	1,66	1,66
CO ₂ % mol	3,91	5,79	7,68	9,58	11,4

Nota: La simulación No 1 corresponde al caso base (Tabla 1).

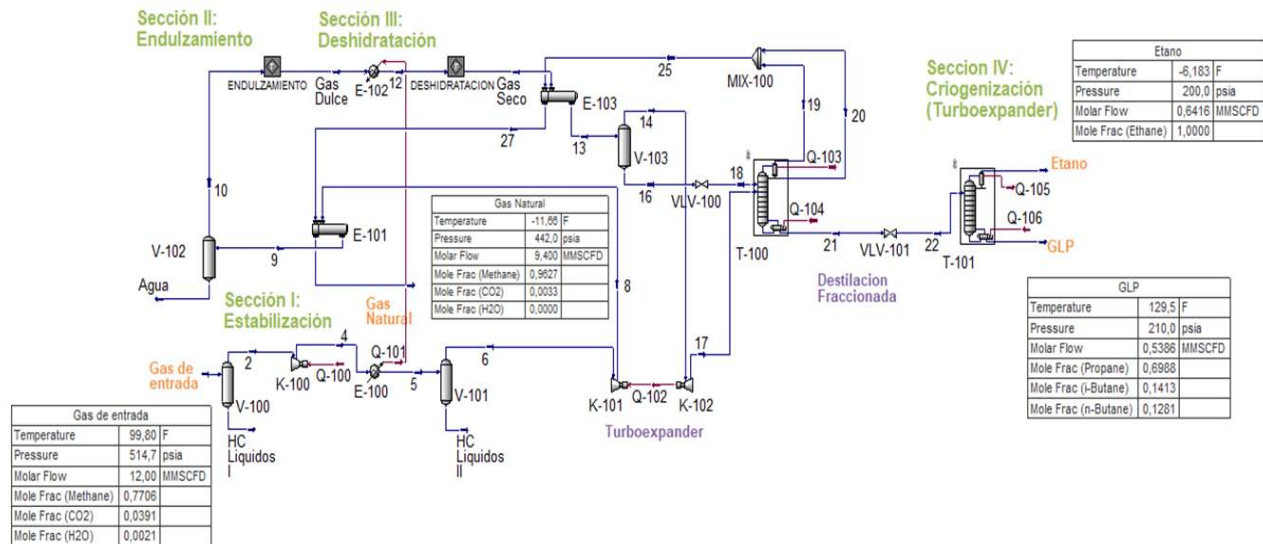


Figura 1: Diagrama de flujo en Aspen HYSYS del proceso de tratamiento de gas asociado

III. RESULTADOS Y DISCUSIÓN

a) Validación simulación para el caso base

El PFD de la simulación desarrollada en Aspen Hysys v10 es mostrado en la Figura 1. La simulación reportó convergencia con las composiciones del caso base. La Tabla 4 reporta las características del gas de salida de cada sección de la simulación. Según esta tabla, el proceso diseñado alcanza una disminución en el contenido de CO₂ al valor de 0,28% mol, en el gas de salida de la sección de endulzamiento. Para la sección de deshidratación, la simulación muestra una disminución en la concentración de agua, en el gas de salida, al valor de 53,8 mg/m³. La Tabla 4 resume las propiedades del gas de salida, reportadas por la simulación, en cada una de las secciones de la unidad. Según esta tabla, los valores obtenidos por la simulación presentan los mismos órdenes de magnitud que los resultados de Camacho (2021). De igual manera, las variables operacionales obtenidas por la simulación, para las diferentes secciones, (Tabla 4) coinciden con diferentes reportes de literatura (ver Chebbi *et al.*, 2010; Getu *et al.*, 2013; Swaidan, 2016; Tristancho, 2017).

Asimismo, una de las variables más importantes dentro del proceso criogénico con un Turboexpander corresponde a la recuperación de etano. El proceso Turboexpander de una sola etapa está diseñado para obtener recuperaciones en el rango 70-80% (Bogoya & Díaz, 2014; Chebbi et al., 2010); el proceso exhibe posibilidades de maximización, según el caso, a valores por encima del 90% (Chebbi et al., 2010; Kherbeck & Chebbi, 2015). Los resultados de la simulación con el caso base, de producción de gas asociado de la cuenca del Valle medio del Magdalena, indican una recuperación de etano del 74,3%, lo cual se encuentra dentro del rango reportado anteriormente.

Con base en la coincidencia entre los valores de la simulación con lo reportado en la literatura y con la recuperación de etano, es posible afirmar que la simulación desarrollada reproduce los valores de operación industrial para el proceso de acondicionamiento de gases asociados, con una unidad Turboexpander.

Tabla 4: Comparación de los resultados de la simulación con la literatura

		Camacho (2021)	Este Trabajo
Sección I: Estabilización	T, °F	120,0	120,0
	P, psi	748,0	762,7
	F, MMSCFD	11,98	11,98
	CO ₂ , %vol	3,91	3,90
	H ₂ O, mg/m ³	49611,1	49542,4
	Cricon., °F	103,2	102,5
Sección II: Endulzamiento	T, °F	111,2	85,0
	P, psi	847,0	900
	F, MMSCFD	11,55	11,51
	CO ₂ , %vol	0,41	0,28
	H ₂ O, mg/m ³	49000,7	49189,8
	Cricon., °F	105,4	104,6
Sección III: Deshidratación	T, °F	22,1	28,55
	P, psi	590,0	597,8
	F, MMSCFD	11,53	10,58
	CO ₂ , %vol	0,41	0,29
	H ₂ O, mg/m ³	65,5	53,8
	Cricon., °F	11,2	6,7
Sección IV: Gas de Salida	T, °F	-13,5	-11,66
	P, psi	445,0	442,0
	F, MMSCFD	10,36	9,40
	CO ₂ , %vol	0,45	0,33
	H ₂ O, mg/m ³	73,9	46,3
	Cricon., °F	-80,8	-112,2

b) Simulaciones con los otros casos

La convergencia en las simulaciones con los demás casos fue conseguida por aumento en el flujo de solución acuosa de MEA en un 17%. Este aumento no afecta el diámetro de la torre de endulzamiento; el diámetro se encuentra en función del flujo de gas y la presión de la torre (Elbashir et al., 2019; Kolmetz, 2020; Mitra, 2015). Además, Kolmetz (2020) sugiere que, la relación entre el flujo de gas a flujo de MEA sea fijada entre 0,3 y 0,4 mol/mol, relación cumplida en todos los casos. Las otras secciones de deshidratación y criogenización no reportaron inconvenientes de convergencia con lo especificado para el caso base.

Por otra parte, pruebas en la simulación especificando gases asociados con concentraciones superiores de 11,4% mol de CO₂ reportaron fallas de convergencia en las torres de la sección de endulzamiento. Lo anterior sugiere modificaciones en los diseños de las torres en esta sección, en unidades convencionales, para el tratamiento de gases ácidos con contenidos molares de CO₂ superiores a 11,4%.

c) Perfiles en las torres

La Figura 2 expone los perfiles de temperatura de la torre de absorción, sección de endulzamiento, obtenidos por la simulación para los gases con diferentes contenidos de CO₂. Según esta figura, para los gases con contenidos de 3,91% mol y 5,79% mol, los perfiles de temperatura presentan un máximo en el plato número dos (numeración desde el plato de fondo; el gas ingresa por el fondo, mientras la solución de MEA ingresa por la cima), con valores de 225°F y 223°F,

respectivamente. Este máximo se debe al comportamiento exotérmico de la absorción de CO₂ en MEA. Posteriormente, los perfiles muestran una disminución monotonía de la temperatura de los platos superiores, hasta el valor de 112°F (plato 10), debido a la evaporación de agua (Bilyok et al., 2012; Mores et al., 2012; Rashid et al., 2014) y a la temperatura de entrada de la solución de MEA. El comportamiento de estos perfiles de temperatura es consistente con el estudio de Giri et al. (2011) y con las mediciones experimentales de Rashid et al. (2014).

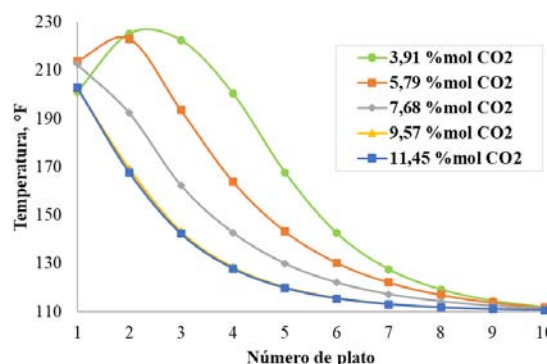


Figura 2: Perfiles de temperatura en la torre de absorción con MEA (20%) para diferentes concentraciones de CO₂

Asimismo, la Figura 2 manifiesta que, a mayores concentraciones de CO₂ en el gas de entrada

(i.e. 7,68%, 9,57% y 11,54%), el perfil de temperatura presenta un decrecimiento monótonico desde el primer plato. Esta tendencia se debe a la variación del calor de absorción con la carga de CO₂. Reportes experimentales de Kim *et al.* (2014) y Kothandaraman (2010) indican que el calor de absorción disminuye drásticamente en soluciones con cargas superiores a 0,4 mol CO₂/mol MEA. Precisamente, la operación de la torre con gases de contenido 7,68%, 9,57% y 11,54% exhibe una relación mol CO₂/mol MEA superior a 0,4 en la solución de fondo (bajo calor de absorción). De otro lado, la simulación reporta que, en la operación de la torre con gases de contenido 3,91% y 5,79%, la solución acuosa en los platos de fondo muestra una relación mol CO₂/mol MEA inferior a 0,4 (elevado calor de absorción). Con lo anterior, el calor de absorción liberado es menor en la operación con mayores contenidos de CO₂, conduciendo al perfil de temperatura sin punto máximo en los platos de fondo.

Por su parte, la Figura 3 presenta los perfiles de temperatura en la torre deshidratadora; la numeración inicia en el plato de cima. Según esta figura, la temperatura del gas experimenta un aumento en su recorrido, desde el fondo a la cima de la torre, debido a la disminución en su contenido de humedad. El flujo de TEG pobre ingresa en contracorriente a 120°F al plato 1, mientras el flujo de gas ingresa al plato 20, en promedio a 90°F. La condensación del agua contenida en el gas envuelve un enfriamiento en el respectivo plato de contacto, por lo cual, el TEG disminuye su temperatura en su recorrido (de arriba hacia abajo), mientras el gas aumenta su temperatura (de abajo hacia arriba). El incremento de temperatura del plato 19 al plato 2 es de tipo lineal, a razón de 1°F/plato. Del plato 2 al plato de cima, el gas experimenta un calentamiento brusco, con un incremento de 4°F debido a la temperatura del flujo de TEG pobre. Este perfil es característico para las diferentes concentraciones de CO₂. Según la Figura 3, el perfil presenta un desplazamiento vertical hacia abajo (menores valores de temperatura) con el aumento en la concentración de CO₂. Este desplazamiento se debe a la disminución en la capacidad calorífica del gas, con el aumento en el contenido de CO₂ ($C_{p_{CO_2}}=0,19$ BTU/lb/°F a 35°F; $C_{p_{CH_4}}=0,52$ BTU/lb/°F a 35°F). Los perfiles de la Figura 3 coinciden con lo reportado por Garmendia (2019), con base en una simulación en PROII/PROVISION de una planta de deshidratación con TEG.

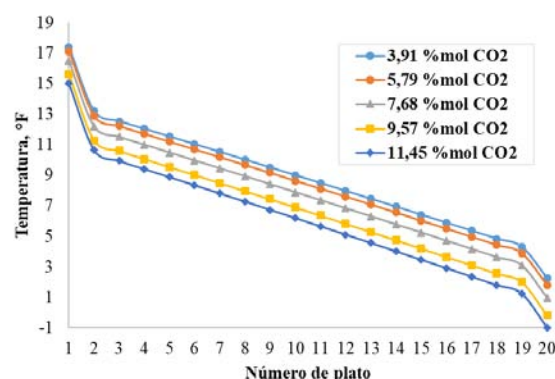


Figura 3: Perfil de temperatura torre deshidratadora con TEG

Por su parte, los perfiles de las Figuras 4 y 5 corresponden a las variaciones en las temperaturas en las torres demetanizadora (Figura 1, T100) y desetanizadora (Figura 1, T101), respectivamente. La numeración en estas torres inicia en el plato de cima; el plato de alimentación en la demetanizadora corresponde al 17, mientras en la desetanizadora, el flujo es alimentado al plato 14. Según las Figuras 4 y 5, la temperatura de cima, como se esperaba, resulta menor en la demetanizadora debido a su mayor presión de operación (450 psia, comparado con 200 psia en la desetanizadora). Asimismo, es posible apreciar que, en cada figura, los perfiles varían en los platos de cima, debido al cambio en el contenido de CO₂ del gas

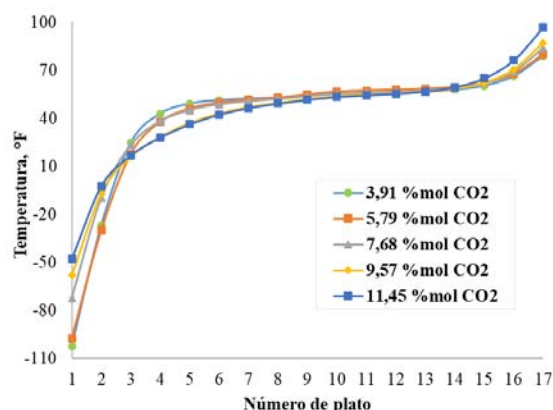


Figura 4: Perfil de temperatura torre demetanizadora

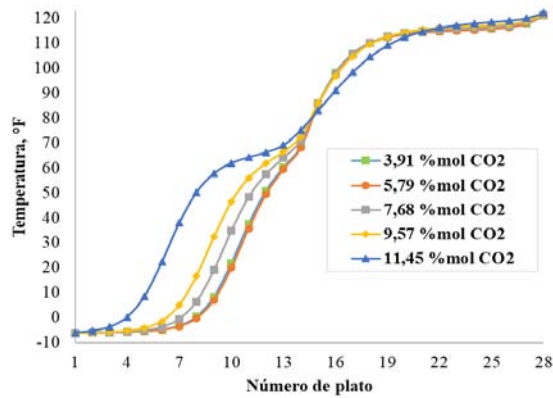


Figura 5: Perfil de temperatura torre desetanizadora

de alimentación. Los perfiles en estas zonas presentan menores temperaturas para menores contenidos de CO₂ (mayores contenidos de CH₄); lo anterior se debe a la diferencia entre las capacidades caloríficas del CO₂ (0,18 BTU/lb/°F a -55°F) y el CH₄ (0,50 BTU/lb/°F a -55°F); a mayor contenido de CO₂ menor requerimiento de flujo calórico para el aumento en las temperaturas de cima. Las tendencias de los perfiles mostrados en la Figura 4 coinciden con lo mostrado por ZareNezhad & Eggeman (2006), autores que analizaron los resultados de la aplicación de la ecuación de estado Peng-

Robinson en procesos de recuperación de NGL de mezcla de hidrocarburos. De igual manera, los perfiles presentados en la Figura 5 coinciden con lo obtenido por Binous & Bellagi (2013).

d) Consumos energéticos

Según los resultados de las simulaciones, un aumento en la concentración de CO₂ del gas asociado conduce a una disminución en la potencia generada por el Turboexpander, debido a la respectiva disminución en el flujo de metano (Tabla 3); un menor flujo disminuye la energía disponible en la expansión del gas de entrada. La Figura 6 muestra que la potencia obtenida en la etapa de expansión del Turboexpander es inversamente proporcional con respecto al incremento en la concentración de CO₂. Según esta figura, un aumento en el 1% en el contenido de CO₂ conduce a una disminución de 0,1 hp de potencia generada en el Turboexpander.

Asimismo, y en contraste, la Figura 6 expone también un aumento en el requerimiento calórico del proceso, con el aumento en el contenido de CO₂. Este aumento se debe principalmente a la etapa de regeneración de la MEA, lo cual es consistente con lo reportado por Feng *et al.* (2010).

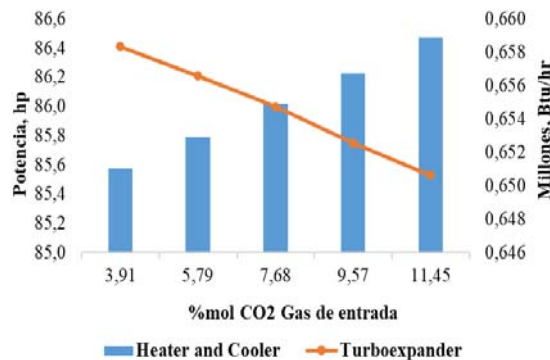


Figura 6: Variación en el requerimiento calórico y de potencia

e) Flujos de salida del proceso

Los flujos de salida del proceso comprenden: hidrocarburos condensables (GLP), el etano, el agua de la sección de endulzamiento, el CO₂ de la sección de el gas asociado acondicionado (Gas Natural), los Endulzamiento y el agua de la

Tabla 5: Calidad del Gas natural obtenido a diferentes concentraciones de CO₂

Componente	% mol CO ₂ gas asociado de entrada					RUT*
	3,91	5,79	7,68	9,57	11,45	
H ₂ O, mg/m ³	46,27	44,62	40,73	36,40	33,68	<97
O ₂ % vol	0,04	0,04	0,04	0,04	0,04	<0,1
N ₂ % vol	2,10	2,12	2,09	2,07	2,05	<3
Inertes % vol	2,47	3,90	6,09	8,77	10,77	<5
CO ₂ % vol	0,33	1,74	3,96	6,66	8,68	<2
H ₂ S, mg/m ³	0,00	0,00	0,00	0,00	0,00	<6
Poder calorífico bruto, MJ/m ³	38,2	37,6	41,6	41,8	40,2	35,4 – 42,8
Cricodentherm, °F	-112,2	-175,0	-98,3	-89,1	-79,5	<45

* Valores límites según el RUT (Resolución CREG-071 de 1999 y su modificación posterior del año 2019).

sección de Deshidratación. La Tabla 5 compara los parámetros de calidad del Gas Natural predicho por simulación, según el contenido de CO₂ del gas asociado de entrada. De esta tabla es posible mencionar que, el contenido de agua (humedad) disminuye en el Gas Natural, con el aumento en el contenido de CO₂ del gas asociado de entrada. Es decir, un aumento en el CO₂ desplaza favorablemente el equilibrio termodinámico en el proceso de deshidratación del gas asociado. Azmi *et al.* (2011) también reportan un desplazamiento favorable en el equilibrio termodinámico, en su estudio sobre la formación de hidratos en gases con diferentes concentraciones de CO₂. De igual manera, el desplazamiento del equilibrio afecta la propiedad *Cricondentherm* (punto de rocío), aumentando su valor por un incremento en el contenido de CO₂ del gas asociado. El aumento en el contenido de CO₂ desplaza el equilibrio, aumentando los niveles de etano en el Gas Natural, con el consecuente aumento en el *Cricondentherm*. El aumento de etano en el gas natural sintético con contenidos de CO₂ ha sido también reportado por Davalos *et al.* (1976) y Mørch *et al.* (2006); por su parte, el incremento en el *Cricondentherm* ha sido reportado por Brown *et al.* (2009), El-Maghraby *et al.* (2022), Louli *et al.* (2012) y Mørch *et al.* (2006), entre otros.

Asimismo, de la Tabla 5 es posible mencionar que, la disminución en la humedad del Gas Natural corresponde con un aumento en su poder calorífico bruto. Por otro lado, el contenido de O₂ en el Gas Natural resultó constante con la variación de CO₂ en el gas asociado de entrada.

Según la Tabla 5, las propiedades del Gas Natural resultante del tratamiento con la unidad Turboexpander, simulada en Aspen Hysys, cumple con los requisitos del RUT, cuando el gas asociado de entrada presenta concentraciones de CO₂ inferiores del 6% mol. Para contenidos superiores, el Gas Natural resultante se encuentra fuera de especificaciones de contenido de Inertes y contenido de CO₂. Según la Sección 3.3., los perfiles de temperatura en la torre de absorción con MEA (Figura 2) presentan diferencias, según el contenido de CO₂ del gas de entrada. Específicamente, si el contenido supera el valor del 6% mol, el perfil muestra valores bajos de temperatura, lo cual resulta como consecuencia de una relación mol CO₂/mol MEA superior a 0,4 en los platos de fondo. Según esto y la Tabla 5, la relación mol CO₂/mol MEA define el cumplimiento en las especificaciones del Gas Natural tratado.

Con lo anterior, las etapas diseñadas para la unidad Turboexpander estándar (con los parámetros definidos en la Sección 2) permiten el tratamiento de gases asociados con contenidos de CO₂ por debajo del 6% mol, obteniendo un gas con calidad adecuada para su transporte y comercialización. Para contenidos

superiores, las limitaciones en el calor de absorción (relación mol CO₂/mol MEA superior a 0,4) restringen la obtención de un gas con cumplimiento del RUT. Un rediseño de la torre y de sus condiciones operativas o un aumento en la concentración de MEA podría conllevar al cumplimiento de una relación mol CO₂/mol MEA inferior a 0,4 para un tratamiento adecuado de gases con contenidos de CO₂ superiores del 6% mol. Asimismo, los avances en el área de captura de CO₂ podrían conllevar a la proposición de un absorbente más eficiente para el endulzamiento, por ejemplo, los fluidos iónicos (Hasib-ur-Rahman *et al.*, 2010).

Por otra parte, los resultados obtenidos con el diseño propuesto en este documento son superiores a los presentados por Tristancho (2017), quien reporta un acondicionamiento adecuado para gases con concentraciones de CO₂ de hasta 4% mol. Por otro lado, las propiedades del flujo de Etano no presentan cambios significativos con la composición de CO₂ en el gas asociado. Según la Tabla 6, para todos los casos, el flujo de Etano cumple las especificaciones de calidad dispuestos por DOF (2016). Sin embargo, el aumento en la concentración de CO₂ en el gas asociado impacta en la producción de Etano, según lo mostrado en la Figura 7. La disminución del flujo se deduce del desplazamiento del equilibrio en la torre demetanizadora. Este resultado coincide con lo documentado por Fernandez *et al.* (1991).

Tabla 6: Condiciones de salida del flujo de Etano, según simulación

Etano	% mol CO ₂ en el Gas de entrada				
	3,91	5,79	7,68	9,57	11,45
Temperatura, °F	-6,2	-6,2	-6,2	-6,2	-6,1
Presión, psia	200	200	200	200	200
Flujo, MMSCFD	0,64	0,63	0,51	0,43	0,31
Etano, % mol	100	100	99,99	99,99	99,95
CO ₂ , % mol	0,00	0,00	0,01	0,01	0,01
Propano, % mol	0,00	0,00	0,00	0,00	0,04

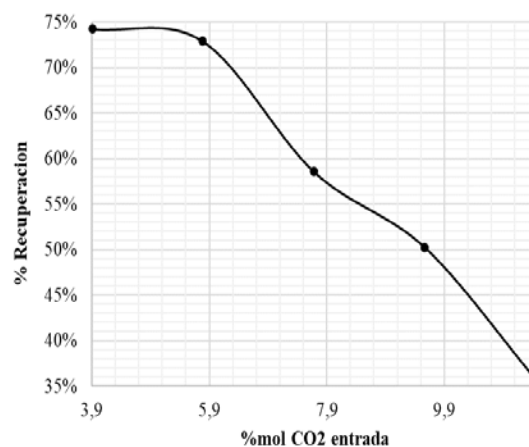


Figura 7: Recuperación de etano en el proceso para diferentes concentraciones de CO₂

Otro subproducto resultante del proceso Turboexpander es el gas licuado del petróleo (GLP). En su mayor proporción, el GLP se compone de propano y butano. La norma técnica colombiana (Ministerio de minas y energía, 2015), establece que las fracciones pesadas (C₅₊) del GLP presenten un contenido máximo

de 2% mol; lo anterior conlleva a un almacenamiento eficiente a altas presiones (UPME, 2013). La Tabla 7 presenta las propiedades para el flujo de GLP resultante del tratamiento del gas asociado, con la unidad Turboexpander.

Tabla 7: Condiciones de salida del GLP obtenido en las cinco simulaciones

GLP	% mol CO ₂ en el Gas de entrada				
	3,91	5,79	7,68	9,57	11,45
Temperatura, °F	129,5	129,3	129,0	128,7	128,4
Presión, psia	210	210	210	210	210
Flujo, MMSCFD	0,539	0,528	0,515	0,500	0,487
Etano % mol	0,00	0,00	0,00	0,00	0,03
Propano % mol	69,88	70,16	70,48	70,84	71,14
n-Butano % mol	12,81	12,69	12,54	12,36	12,21
i-Butano % mol	14,13	14,06	13,95	13,83	13,73
n-C5 % mol	0,98	0,96	0,94	0,92	0,9
i-C5 % mol	1,65	1,6	1,57	1,55	1,51
2,2-MC3 % mol	0,16	0,15	0,15	0,15	0,14
n-C6 % mol	0,36	0,35	0,34	0,33	0,32
n-C7 % mol	0,02	0,02	0,02	0,02	0,02

Según esta tabla, el contenido de hidrocarburos pesados (C₅₊) supera el límite de 2% mol, en los cinco casos de simulación. Lo anterior sugiere un tratamiento posterior de la corriente de GLP en una torre de destilación para la síntesis de gasolina natural (Abdel-Aal *et al.*, 2003; Ahmad *et al.*, 2011). El diseño y el análisis del desempeño de esta torre de purificación de gasolina natural son recomendados para trabajos futuros en el tema.

f) Formación de Hidratos

Para finalizar, unos comentarios finales sobre la formación de hidratos, tema de importancia en el aseguramiento de flujo. La Figura 8 presenta los resultados de la herramienta de detección de formación de hidratos, disponible en Aspen Hysys (Abdulmutalib & Abdulmalik, 2022; Alnaimi *et al.*, 2020); la herramienta detalla en rojo aquellas corrientes con un potencial elevado de formación de hidratos. Según esta figura, la formación de hidratos resulta probable en las corrientes del tope de la torre demetanizadora; esto acontece en los cinco escenarios de evaluación de contenido de CO₂. El tipo de hidratos que potencialmente puede ser formado corresponde al tipo II, el cual envuelve el encapsulamiento de nitrógeno y CO₂ a las condiciones de salida del gas (Abdulmutalib & Abdulmalik, 2022; Carroll, 2003).

A pesar de esta detección de hidratos, por parte de Aspen Hysys (Figura 8), las concentraciones de agua son bajas en todos los casos, con lo cual, la formación de hidratos sería indetectable a nivel industrial, sin consecuencias importantes para el proceso. Abdulmutalib & Abdulmalik (2022) reportan una regla heurística de alrededor de 35 mg de agua por m³ de gas, como contenido ideal para el transporte de

gas. La Tabla 5 muestra que la mayoría de los Gases Naturales generados cumplen esta regla heurística. Para el caso de gases con concentraciones un poco más elevadas de 35 mg de agua por m³ de gas, el contenido bajo de CO₂ evitaría la formación apreciable y detectable de hidratos (Van-Denderen *et al.*, 2009). Por otra parte, en caso de una formación importante de hidratos, esta puede ser inhibida por diferente tipo de compuestos como metanol, etanol y glicol (Abdulmutalib & Abdulmalik, 2022; Bharathi *et al.*, 2021; Koh *et al.*, 2011).

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Adsorption Kinetics and Mass Balance Mathematical Model of Monoethanolamine Surface-Modified Palm Shell Activated Carbon for Carbon Dioxide Dynamic Adsorption in Fixed Bed Column

By Saad Hashim Khalil

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Keywords: adsorption kinetics, activated carbon, impregnation, MEA, fixed bed column.

GJRE-C Classification: LCC: TP156.A3



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I. INTRODUCTION

The removal of carbon dioxide (CO₂) is significant for oil and gas industry due to its harmful acidic effects on oil and gas pipelines with no added energy value to natural gas [1]. Because of the increasing indications of CO₂ implication in global warming [2], capturing CO₂ from its emitting sources is becoming a vital topic. Adsorption is offering an effective alternative for CO₂ capturing comparing to other capture technologies [3]. There are many types of gas adsorbents; conventional, like, activated carbons, silica gel, ion-exchange resins, zeolites, and mesoporous silicates, activated alumina, metal oxides, and new like, carbon fibers and metal-organic frameworks. [4]. Adsorbent most important feature is adsorbing capacity [5], besides, good adsorbent should be selective and chemically and mechanically durable [6]. AC is cost-effective and adaptable microporous adsorbent [7] and is considered a superb adsorbent due to its high specific surface area, appropriate pore size distribution, diversity of surface chemistry [8]. It's mostly micropore structure were used extensively in

liquids and gases systems. The micropores and mesopores of the AC particles were utilized to accommodate the impregnating molecules, which can be attached chemically (grafting) or physically (impregnation) to the AC particles [9]. Impregnation of AC particles with chemicals improves their natural adsorption capability to adsorb gases [10]. Alkanolamines, such as, monoethanolamine (MEA), diethanolamine (DEA), and methyldiethanolamine (MDEA) are very important absorbents for acidic gases in the field of natural gas sweetening and for mitigation the adversity of these gases on environment [11] and they are extensively used in CO₂ absorption from different gas sources [12]. MEA, which is a primary amine, has been used intensively to capture CO₂ from gas streams and from many various sources due to its fast reaction kinetics with CO₂, low coast and thermal stability, as it is more favorable than other alkanolamines [13] [14]. Because of the effectiveness of liquid amine absorption process researchers were encouraged to utilize amines in their solid state for CO₂ capture [15]. Adsorption kinetics is essential tool used to evaluate the performance of an adsorbent and to understand the mechanism of adsorption [16] and many researches had included kinetics of batch CO₂ adsorption on different adsorbents in their works [17]. They found that the restriction step is the intraparticle diffusion (pore diffusion). On contrary to the findings of this paper where the restrictive step to CO₂ adsorption was the film diffusion. In this research, dynamic adsorption experiments were conducted to investigate the adsorption kinetics of MEA-impregnated AC particles packed in adsorption column to adsorb CO₂ from gas mixture.

II. MATERIALS AND METHODOLOGY

a) Materials

1. Certified analytical reagent monoethanolamine (MEA), C₂H₇NO, molecular weight 61.

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2. Commercial palm shell AC was purchased from Bravo Green SDN BHD (Sarawak, Malaysia).
3. Gases
 - a. Mixture of 15% CO₂ with 85% N₂.
 - b. Pure N₂.

b) *Methodology*

i. *AC Particles Characterization*

Granulated palm shell AC particles were physically activated by steam. The mostly micropore particles have total Bet surface area of 838 cm²/g, while the micropore surface area of that total area is 675 cm²/g and micropore volume is 0.32 cm³/g.

ii. *AC Beds Perpetration*

A household coffee grinder crushed the AC particles. 710 and 500 μm sieves were employed to characterize the AC particles to the required particle size of 500 μm (particles passing 710 and stopping on 500 μm sieve).

iii. *Impregnation of AC Samples*

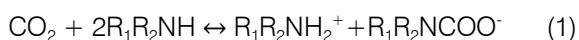
Impregnation was carried out by placing 5 g of granular AC in a beaker, 2 g of MEA added to the beaker with 10 g of deionized water as an environmentally friendly medium and to facilitate the impregnation process. The beaker contents were stirred at 500 rpm for 1 hour at room temperature. The final slurry then dried completely in Heraeus Instrument Vacuthermo oven at 70°C under 0.1 bar vacuum pressure (absolute) for 6 hours. Samples of AC particles prepared for CO₂ adsorption separation experiments are, non-impregnated AC particles and MEA-impregnated AC particles.

iv. *Working Breakthrough Time*

Working breakthrough time was utilized as a method to evaluate the performance of AC beds.



The overall reaction is as in equation 1:



vi. *Rate and Mechanism of Adsorption*

To investigate the rate of adsorption two equations were explored namely, pseudo first order (SFO) and pseudo second order (PSO) equations. The mechanism of adsorption and the adsorption controlling step was determined by Weber-Morris intraparticle diffusion model.

III. RESULTS AND DISCUSSIONS

a) *Impacts of MEA Surface-Modification on AC Particles*

MEA molecules occupied the pores of the mostly micropore AC particles and blocked them, reducing significantly the micropore surface area from 675 to 36m²/g (96%) and micropore volume from 0.32 to 0.02cm³/g (94%). MEA-blocked AC particles adsorb selectively more CO₂ comparing to non-impregnated AC

Breakthrough time can be defined as the time spanning from the beginning of the adsorption experiment to the point when CO₂ molecules start to break through out of the adsorption column, which was monitored by Guardian Plus CO₂ monitor. Data Acquisition Logger was connected to the CO₂ monitor to measure the breakthrough time in minutes.

Experimental setup is presented in another work [18].

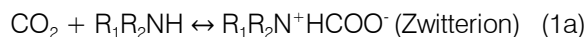
v. *Amine-CO₂ Reactions*

Amines remove CO₂ in a two-step process:

1. The gas absorbs by the liquid forming a weak acid.
2. The weak acid reacts with amines as a weak base [19].

The suggested [20] reaction path of primary and secondary unhindered amines with CO₂ is known as the carbamate formation reaction proceeds through the formation of zwitterion, which was recognized as the reaction mechanism [21].

The first step of the reaction is the formation of amine-CO₂ zwitterion as shown in Equation 1a:



The second step is the deprotonation of the zwitterion. For liquid amine reaction, the water would act as a base acquiring the proton released by the zwitterions. In the case of solid amine reaction, another amine molecule would acquire the released proton as the maximum theoretical amount of CO₂ reacting with amine would be 0.5 mol CO₂/1 mol N₂ as shown in equation 1. In this step, the zwitterion would be stabilized by producing carbamate as in equation 1b.

particles by 172%, as the adsorption capacity increased from 49 to 18 mg/g, respectively.

b) *Adsorption Kinetics*

i. *Adsorption Rate*

Pseudo first and second order models were investigated to find out which model is predicting the adsorption rate appropriately.

a. *Pseudo First Order Model (SFO)*

Lagergren [22] published his SFO model to describe homogenous adsorption on solid phase as in equation 2. The equation depends on the adsorption capacity of an adsorption bed rather than concentration of adsorbate as in the case of first order model equation and the adsorption rate is related to the availability of adsorption sites [23]. It had been reported that SFO model can be applied adequately for the adsorption kinetics of CO₂ on AC [24].

$$\frac{dq_t}{dt} = k_1(q_e - q_t) \quad (2)$$

The linear form of equation 1 is as in equation 3:

$$\ln(q_e - q_t) = \ln q_e - \frac{k_1}{2.303} t \quad (3)$$

Where,

q_e : Adsorption capacity at equilibrium, mg/g.

q_t : Adsorption capacity at any time t , mg/g.

k_1 : Pseudo-first order rate constant, 1/min.

t : Time, min.

Figure 1 is a plot of $\ln(q_e - q_t)$ against t for the whole adsorption experiment showing that the straight line fitting the experimental results has good value of R^2 equal to 0.9967, which is suggesting that the SFO kinetic model is applicable for this research. The slope of the straight line from equation 3 is $(\frac{k_1}{2.303})$, where the value of the SFO rate (k_1) was found to be 0.00552721/min.

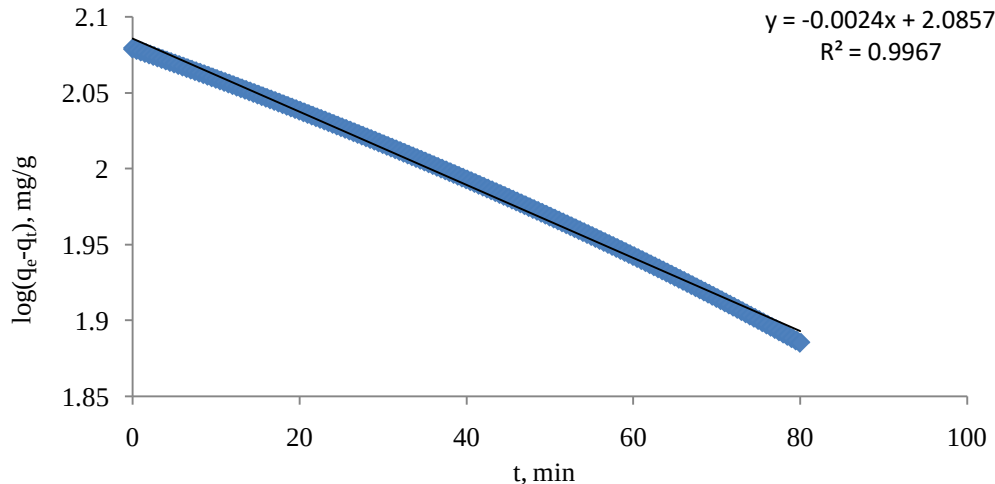


Figure 1: Plot of $\ln(q_e - q_t)$ against time

b. Pseudo Second Order Model (PSO)

PSO model is usually applied for chemisorption kinetics sorption of liquid solutions [25], the model is in equation 4 and its linear form is as in equation 5:

$$\frac{dq_t}{dt} = k(q_e - q_t)^2 \quad (4)$$

$$\frac{t}{q} = \frac{1}{k^2 q_e^2} + \frac{1}{q_e} t \quad (5)$$

The plot of t/q against t for PSO model as in equation 5, didn't yield straight line for the whole experimental data or even for any of its portions on contrary to the straight line of plot $\ln(q_e - q_t)$ against t for PFO model, which covers the whole experimental data and suggesting that the adsorption rate here is following PFO model which would be applied to calculate adsorption rate constant (k_1).

ii. Verification the Rate-Determining Step of the MEA- Impregnated AC Adsorption Bed

Equation 6 is the intraparticle diffusion equation [26],

$$q_t = k_p t^{1/2} + c \quad (6)$$

Where:

q_t : Amount of adsorbate absorbed at any time, mg g⁻¹.

k_p : Intraparticle diffusion rate constant, mg g⁻¹ min^{-1/2}.

t : Time, min.

c : Intercept, mg g⁻¹

The multilinearity displayed in Figure 2, the plot of the amount of CO₂ adsorbed (q_t) against the square root of time ($t^{1/2}$) is suggesting that more than one step is taking place. The straight line fitting the curve is not passing through the origin, indicating that the intraparticle diffusion is not the adsorption rate restrictive step [27]. The curve is divided into three zones where the slope of the linear part indicating the rate of adsorption and the rate controlling step is represented by the linear section with lowest slope value [28]. The first zone is the initial zone where the external diffusion of CO₂ molecules through the bulk gas phase is taking place and the slope which is representing the adsorption rate is low. The second zone is the film diffusion where the mass transfer of CO₂ molecules is continuing through the CO₂ film surrounding the AC particles. The slope of the straight line of the second zone is higher than that of the initial zone but lower than that of the third zone due to the resistance exerted by CO₂ gas film, which is indicating that this step combining with the initial zone step are slow and the overall adsorption rate is controlled by mass transfer and film resistances respectively. In the third zone, where the amount of CO₂ molecules adsorbed (q_t)

versus $t^{1/2}$ is displaying a straight line with high slope value indicating that CO_2 molecules intraparticle diffusion step is fast, where CO_2 molecules adsorption is enhanced by the fast CO_2 -MEA reaction. The intercept (c) is an indicator of the thickness of the boundary layer surrounding the MEA-impregnated AC particles. Higher values of intercept suggest that the boundary layer is

building up as the value of the c in the initial zone is less than that of zone 1, which is in turn less than that of zone 2 deducing that diffusion through the gas film may be considered as the controlling step [29]. CO_2 adsorption in zone 2 is approaching its final stage and the active sites on MEA-impregnated AC particles are not able to adsorb more CO_2 molecules.

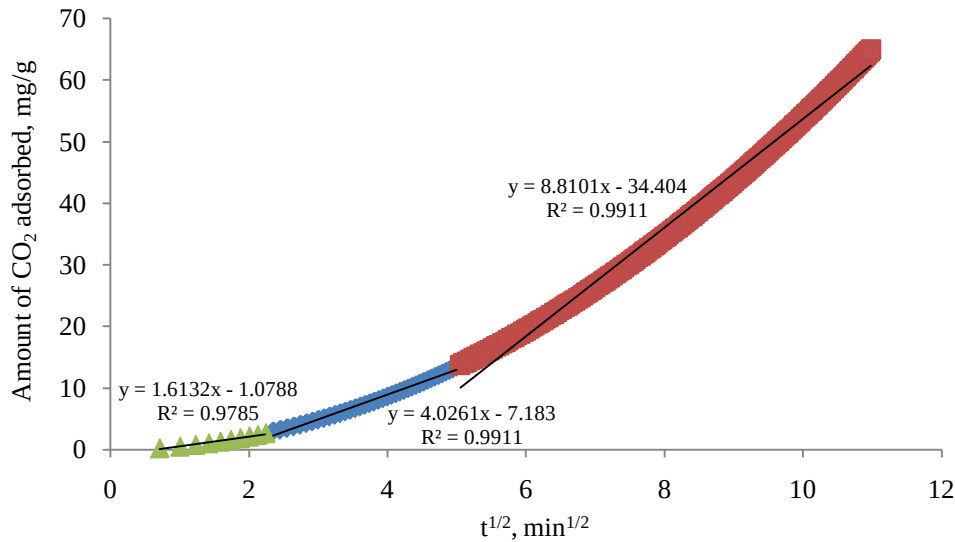


Figure 2: CO_2 Amount adsorbed, mg/g against square root of time, $\text{min}^{1/2}$

iii. Gas Film Diffusion Model

The transportation of CO_2 molecules from the gas stream bulk to the surface of the AC particles is playing a major role as the analysis of the intraparticle model showed that the mass transfer of CO_2 molecules through the gas film is the limiting step of CO_2 adsorption. To further inspect that gas film is the limiting step in CO_2 molecules adsorption, gas film diffusion model was applied [30], [31] and [32]:

$$\frac{q_t}{q_e} = 1 - e^{-k_{fd}t} \quad (7)$$

The linearized form of equation 7 is as in equation 8:

$$\ln(1 - F) = -k_{fd}t \quad (8)$$

Where,

F: Fractional adsorption equilibrium ($F = q_t/q_e$).

k_{fd} : Film diffusion coefficient, min^{-1} .

A plot as in Figure 3 of $-\ln(1 - F)$ vs t with intercept equal to zero and R^2 equal to 0.99 is suggesting that adsorption kinetics is controlled by diffusion through the CO_2 gas film surrounding the AC particles.

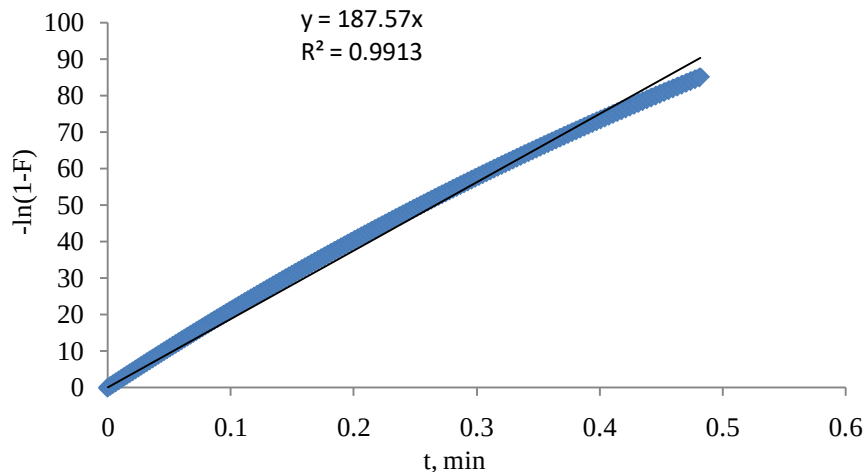


Figure 3: Plot of $-\ln(F-1)$ against time

iv. *Avrami (JMAK) Model*

Johnson-Mehl-Avrami-Kolmogorov (JMKA) model, which is called Avrami model too, is expressed in equation 9, [33] and [34]. Avrami equation describes the growth of crystallites with respect to time. In this work Avrami equation is describing the increasing numbers of CO₂ molecules by adsorption inside the AC pores.

$$\alpha = 1 - \exp(-k_{Av}(t)^n) \quad (9)$$

Where, α is adsorption fraction at time t , k_{Av} is the Avrami kinetic constant, and n is a constant which represents the mechanism of particles adsorption (growth).

The linearized form is as in equation 10:

$$\ln(-\ln(1-\alpha)) = n \ln k_{Av} + n \ln t \quad (10)$$

Plotting $\ln(-\ln(1-\alpha))$ against $\ln t$ as in Figure 4 producing straight line ($R^2=0.9991$) with intercept equal to $n \ln k_{Av}$ and slope equal to n . If Avrami constant n equal to 1. Furthermore the value of Avrami exponent n , which is $1 \leq n \leq 2$ suggesting one dimensional growth of crystallites and that the growth is homogenous [35], which is agreeing with exponent n in micropore filling method of Dubinin-Astakhov (D-A), equation 11 and its linearized form equation 13. D-A equation is applicable for homogeneous carbonaceous adsorbents with micropore structures [36]. It was found in other study [37] that the value of D-A exponent n for MEA-impregnated beds is showing less heterogeneity and more homogeneity with their exponent n value equal to 2, where the value of exponent n in AC is 3 - 1.5. Moving from 3 to 1.5 the microporous system would be getting more heterogeneous [38] and [39].

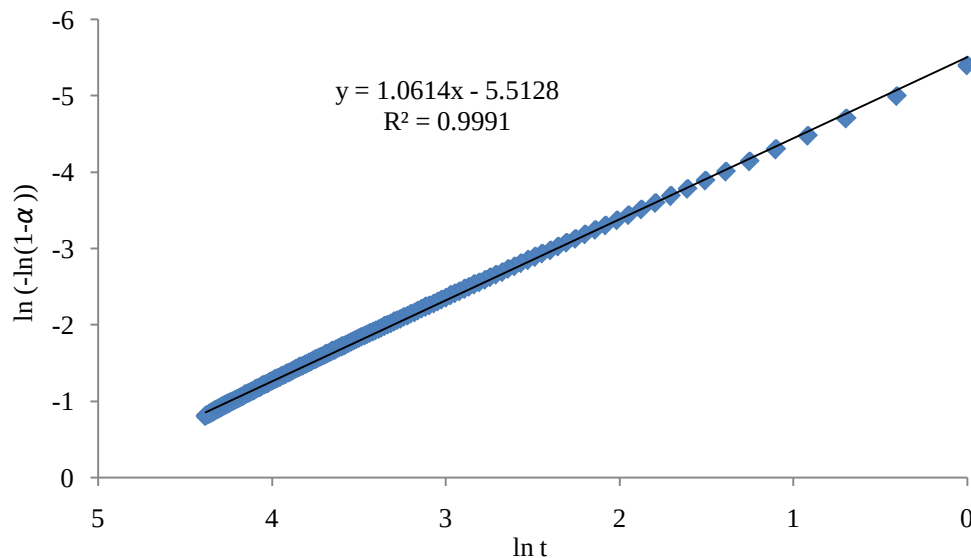


Figure 4: Plot of $\ln(-\ln(1-\alpha))$ against $\ln(t)$

c) *Mass Balance Mathematical Modeling*

Adsorption of CO₂ molecules from feed gas stream containing 15% CO₂ and 85% N₂ was performed in fixed bed packed column of non-impregnated and MEA-impregnated AC beds. Breakthrough time was employed as real time tool to evaluate the efficiency of the adsorption beds. CO₂ monitor was used to display the concentration (%) of the gas stream exiting the adsorption column. Graphs of CO₂ molecules concentration leaving the adsorption column plotted against time were obtained from the data acquisition logger connected to the outlet of the adsorption column.

i. *Mathematical Modeling of MEA-Impregnated 500 μ m Adsorption Bed*

To formulate a general mathematical model corresponding to the mainly micropore adsorption mechanism and to cover the two stages mentioned earlier, the following assumptions were made:

1. The system operates under isothermal, isobaric and diabatic conditions.
2. The porosity of the adsorption bed was uniform and constant.
3. The equilibrium of adsorption is a nonlinear isotherm.
4. The velocity distribution is constant across the column diameter.
5. The volumetric flow rate is constant along the column.

Summarizes of the experimental parameters and simulation boundary conditions for the mathematical model validation are in Table 1:

Table 1: Experimental data and simulation boundary conditions

Operating conditions		
Pressure	1 atm	
Temperature	25°C	
Inlet concentration	6.05118E10 ⁻⁶ mol/ml	
Inlet volumetric flow rate	10 ml/min	
Adsorption column		
Material	Glass	
Inside diameter	1 cm	
Bed height	9 cm	
Bed weight	5 g	
Bed Volume	7.23 cm ³	
Adsorbent properties		
Bed type	Non-impregnated AC	MEA-impregnated AC
Particles size	500 μm	500 μm
Micropore surface area	675 m ² /g	65 m ² /g
Micropore particle porosity	0.0956 cm ³ /g	0.020 cm ³ /g
Porosity	0.684	0.620
Bulk density	1.6387 cm ³ /g	1.6228 cm ³ /g
Bed Volume	7.2285 cm ³	6.2857 cm ³
Pseudo 1 st order reaction constant (k)	-	0.004836 1/min

ii. Mathematical Model of MEA-Impregnated AC Bed

The mathematical model was based on the CO₂ molecules breaking through the adsorption bed.

The adsorption of CO₂ molecules was declining and more CO₂ molecules were exiting the bed.

The general equation of mass balance with first order chemical reaction for CO₂ in the feed gas:

$$\text{Accumulation} = \text{Input} - \text{Output} + \text{Generation}$$

As the mass balance would be conducted on CO₂ molecules exiting the adsorption bed, the mass balance equation would be:

$$\text{Output} = \text{Input} - \text{Accumulation} + \text{Generation}$$

$$v \frac{dc_o}{dt} = qc_i - qc_{acc} + vk_1c \quad (14)$$

Where:

K₁: Pseudo first order reaction constant, 1/min.

C_i: Concentration of CO₂ entering the AC bed, mol/ml.

C_o: Concentration of CO₂ exiting the AC bed, mol/ml.

C_{acc}: Concentration of CO₂ accumulated in the AC bed, mol/ml.

Equation 14 is an ordinary first order linear differential equation and the final solution would be as in Equation 15.

$$C = C_i + n e^{-(q/v - k_1)t} \quad (15)$$

Initial boundary condition:

$$\text{At } t = 0, C = 0$$

$$n = -C_i$$

Then equation 15 would be:

$$C = C_i - C_i e^{-(q/v - k_1)t} \quad (16)$$

Rearranging equation 16:

$$C = C_i \left(\frac{q/v}{(q/v) - k_1} \right) (1 - e^{-(q/v - k_1)t}) \quad (17)$$

The simulated results were validated by using the experimental results of the MEA-impregnated activated carbon bed. The simulated results were compared with the experimental data. The simulated data demonstrated a reasonable agreement with the experimental data, as the root mean square error (RMSE) calculated was 6.75915E-06. The simulated and experimental data of MEA-impregnated AC beds were plotted in Figure 5.

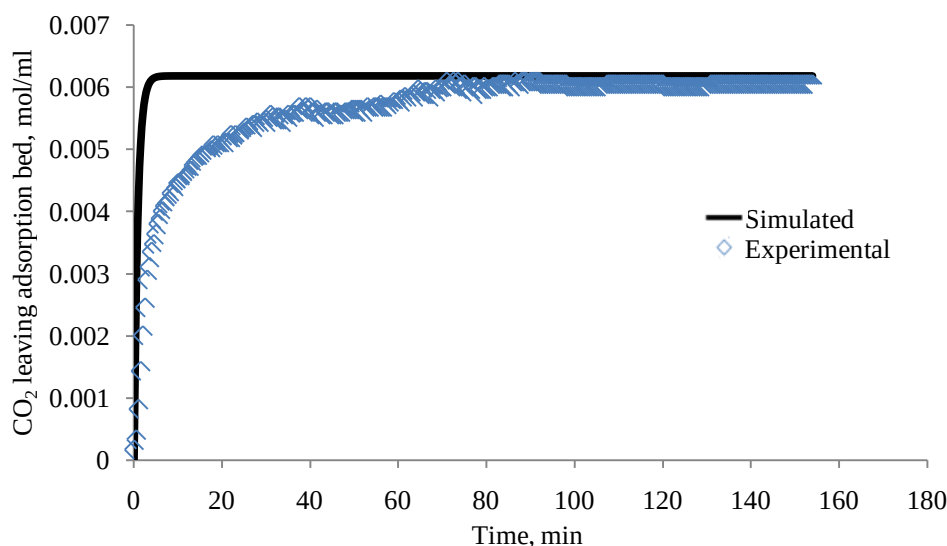


Figure 5: Comparison of CO₂ experimental and simulated breakthrough curves for MEA-impregnated AC bed (Sampled at column outlet)

IV. CONCLUSIONS

MEA-impregnated AC particles were used to adsorb CO₂ from gas mixture. Results are showing that AC particles impregnated with MEA adsorb CO₂ molecules in a pseudo first order reaction manner and that the controlling step in this reaction is the mass transfer of CO₂ molecules from through the CO₂ gas film and not the intraparticle diffusion of CO₂ molecules inside the pores of MEA-impregnated AC particles. Due to the homogeneity of the MEA-impregnated activated carbon particles the adsorption of CO₂ molecules follows the Avrami model of homogenous crystallites growth. The mass balance mathematical model showed that the experimental and simulated breakthrough curves have good agreement, as the root mean square error (RMSE) was 5.7678E-09 and 3.8853E-09 for non-impregnated and MEA-impregnated beds respectively, which also proved that the adsorption mechanism of both beds is the same.

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Potential of Rain Water Harvesting and Ground Water Improvement at RVCE

By Pavan Bandakli B R & M Lokeshwari

R V College of Engineering

Abstract- Water is a primary resource for the development of any country. Increase of population in urban areas has resulted in failure of typical water supply system to meet the growing demand. Rainfall is the major source of fresh water. To reach the water demand, utilization of rain water by adopting decentralized rain water harvesting approach is need of the hour. The present study area is R V College of Engineering, Mysore road, Bengaluru. Annual rainfall records and the data required for estimation of potential of rain water and runoff coefficients of different catchment surfaces were collected. It was observed from the study that RVCE campus has the potential of collecting 21.49 Million liters of water annually from roof tops of different buildings and 32.72 Million liters of water by runoff from major catchment areas like play grounds, pavements, parks and sites.

Keywords: rain water harvesting, ground water recharge.

GJRE-C Classification: FOR Code: 090499



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Potential of Rain Water Harvesting and Ground Water Improvement at RVCE

Pavan Bandakli B R ^α & M Lokeshwari ^σ

Abstract- Water is a primary resource for the development of any country. Increase of population in urban areas has resulted in failure of typical water supply system to meet the growing demand. Rainfall is the major source of fresh water. To reach the water demand, utilization of rain water by adopting decentralized rain water harvesting approach is need of the hour. The present study area is R V College of Engineering, Mysore road, Bengaluru. Annual rainfall records and the data required for estimation of potential of rain water and runoff coefficients of different catchment surfaces were collected. It was observed from the study that RVCE campus has the potential of collecting 21.49 Million liters of water annually from roof tops of different buildings and 32.72 Million liters of water by runoff from major catchment areas like play grounds, pavements, parks and sites. The collected water can be used for flushing, gardening purposes, further ground water recharging can be done by artificial recharging techniques. Sustainability in water management can be achieved at RVCE campus by adopting RWH technique.

Keywords: rain water harvesting, ground water recharge.

I. INTRODUCTION

2.5% of Earth's water is fresh water out of which 68.9% is of Glaciers and Ice caps, 30.8% is locked up in ground. Only 0.3% is surface water which serves most of life needs [1]. Water is a primary requirement for our daily activities, Safe and readily available water is required for public health, food production, recreational use, drinking and domestic use. Water management is directly relatable to the economic growth of the country, Water availability is one of the primary criteria for setting up of industries which are associated with local and foreign investments. Majorly many parts of North Karnataka are facing water crisis which is also an indirect reason for poor generation of employment opportunities hence many youths are heading towards metropolitan cities like Bengaluru resulted in rapid increase of population failure of typical water supply system to meet the requirement.

According to Composite Water Management Index, August 2019 released by NITI Aayog 5 out of 20 world largest cities are under water stress are in India, Indian urban population is expected to reach 600 million by 2030 with expected demand supply gap of 50Bcm [2].

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In recent years India has experienced weak monsoons resulted in drought conditions at many places. Ground water table is reducing day by day in many parts of the country, Punjab which produces 10% of India's paddy utilizes 80% ground water for paddy irrigation depleting its own ground water resource, 70% of India's thermal power faces water stress by 2030 which contributes 83% of India's energy power generation in 2016, Presently 40% of India's thermal power plants are in water scare regions, 14 of them faced shutdown in 2013-16 due to water scarcity [2].

Recently Indian government introduced ministry of jalshakthi, which launched programs like Jalshakthi abhiyan to encourage and promote water conservation, Rain water harvesting, renovation and rejuvenation of water bodies, bore well structures. Once a drought village Jakhni of Bunderkhand district, Uttar Pradesh is emerged as self-water reliable village by adopting methods like collection and storage of rain water, Restoration of ponds, Grey water usage with no external funding. Sustainable water management has to be incorporated in private and public buildings to overcome the water demand. Decentralized approach has to be adopted in order to achieve this state. Rain water harvesting by roof top water collection and ground water improvement by simple techniques are the easy, suitable and sustainable solutions for the problems associated with water requirement and its management.

II. RAIN WATER HARVESTING AND GROUND WATER RECHARGE

Rain water is the ultimate and primary source of fresh water. Lakes, ponds, Rivers, Ground water are the secondary sources. Rain water has highest potential to meet the demand of people if public are involved in conservation of rain water in their houses, public building's, Institutions. Rain water harvesting has been carried out from decades from simple harvesting techniques like collection of water through small drums by using normal cloth as a filter medium to modern techniques. Rain water harvesting is defined as collection of rain water from the surface where it falls, either it may be roof top harvesting or open space harvesting. Rain water harvesting potential depends on catchment area, intensity of rainfall. Rain water collected is stored and utilized or the water from open source can be utilized for ground water recharging.



Rain water is collected from roof tops and is filtered to remove dry leaves, waste materials, dirt present on the roof top, the water is taken to storage tank which can be overhead tank, surface tank and overhead tank by using down take pipes. The stored water can be treated and can be used as potable water or can be used for non-potable purposes like irrigation, gardening etc. The stored water can also be used for recharging of ground water by different methods such as recharging through establishment of recharge pits or trenches, constructing artificial recharge wells or by using abandoned or existing bore wells.

III. STUDY AREA

R V College of Engineering is spread over 50.97 acres located at Bengaluru south which receives an

average annual rainfall of 877.8 mm [3]. Satellite view of RVCE campus is shown in figure 1 below. The main motto of the institution to achieve sustainability in terms of water, energy and waste management, in road to achieve this the institution has setup rain water harvesting units in three phases across the campus which has collection capacity of 3.6 lakh liters in total, two bore wells are also established for the purpose of ground water recharging, Campus also has Reverse osmosis water treatment and softening plant of 22000 liters capacity and Sewage treatment plant of 50 kld output [4].

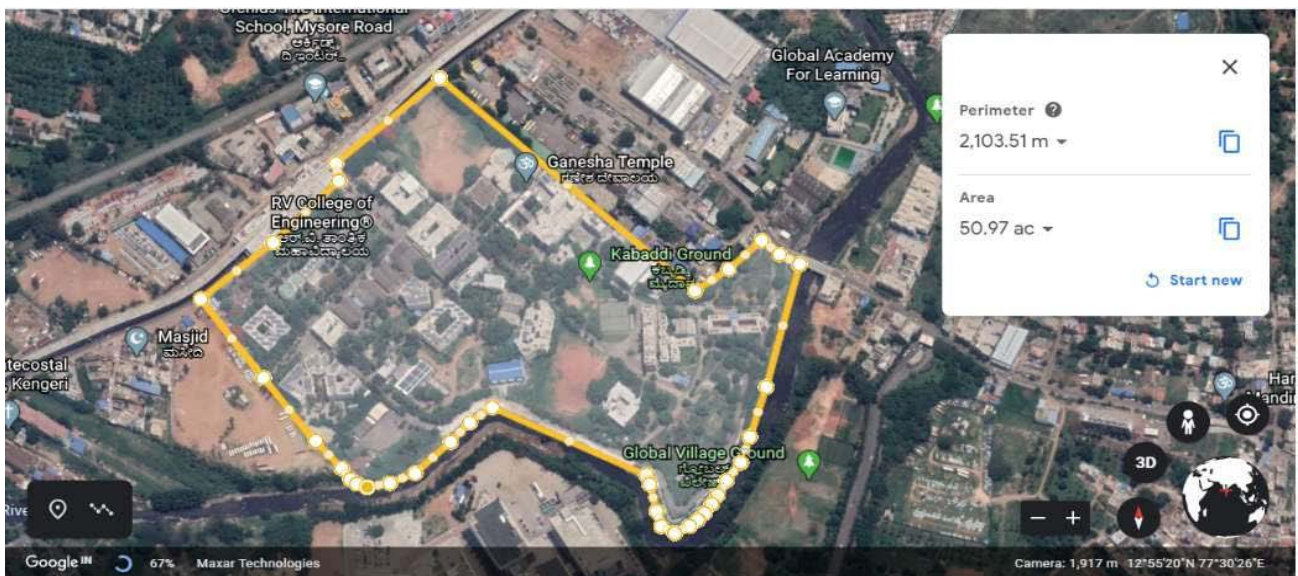


Figure 1: Satellite view of R V College of Engineering (Source: Google Earth®)

IV. OBJECTIVES

Present study aims at estimating potential of rain water and runoff which can be collected annually from different roof top area of different buildings located at RVCE.

V. METHODOLOGY

1. Obtaining roof top area of different buildings at RVCE campus using Google earth.
2. Collection of rainfall data from India Meteorological Department (IMD) website.
3. Runoff co-efficient of different materials are obtained from
4. A building is considered and the monthly/annual water demand and monthly/annual rain water yield from the roof top area is measured and the rain water harvesting tank capacity is determined according to IS 15979: 2008.
5. Similar calculations are extended to other buildings of RVCE to obtain total potential of Rain water.

VI. ESTIMATION OF RAIN WATER HARVESTING CAPACITY

New Cauvery hostel, Male residential hostel for 2nd and 3rd year students is considered to estimate rain water harvesting capacity, Satellite image of new Cauvery hostel is shown in figure 2 below.

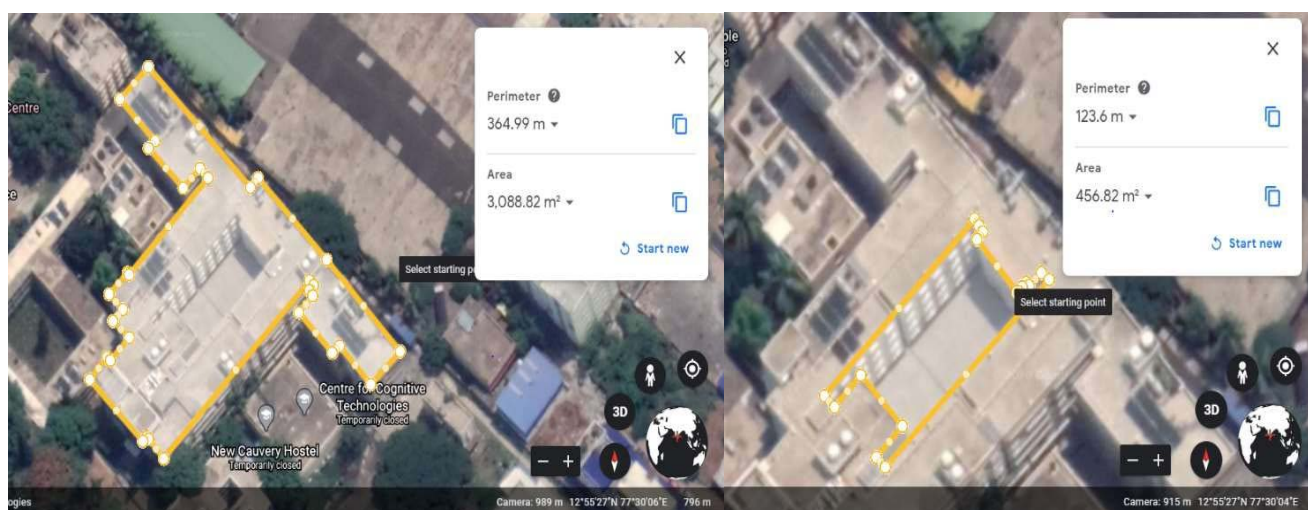


Figure 2: Satellite image of New cauvery hostel (Source: Google Earth®)

Annual rain water yield is given by the formula

$$Q = A \times R \times C \times F$$

Where Q = Annual rainwater yield

A = Catchment area in m²

R = Annual precipitation

C = Runoff coefficient of catchment material

Annual rain water yield of Cauvery hostel

Catchment area, A = 2632 m²

Annual precipitation, R = 877.8mm

Runoff coefficient of RCC roof, C = 0.8 [5]

Filter efficiency, considering F = 0.8

$$Q = A \times R \times C \times F$$

$$Q = 2632 \times 877.8 \times 0.8 \times 0.8 = 1478637$$

$$\text{liters} = 1478.637 \text{ m}^3$$

Annual water demand of Cauvery hostel for flushing purpose

Number of people residing at New Cauvery hostel = 528

Quantity of water require for flushing per person = 10 liters

$$\text{Total Quantity of water required monthly} = 528 \times 10 \times 30 = 158400 \text{ liters} = 158.4 \text{ m}^3$$

$$\text{Total Quantity of water required annually} = 528 \times 10 \times 365 = 1927200 \text{ liters} = 1927.2 \text{ m}^3$$

a) Calculation of storage tank size according to monthly demand

Table 1: Calculation of storage tank size according to monthly demand

Month	Average Rainfall (mm)	Monthly yield(l)	Cumulative yield(l)	Monthly demand(l)	Cumulative demand(l)	Volume stored(l)	Surplus(l)
May	96	161710	161710	158400	158400	3310	3310
June	85.7	144359	306069	158400	316800	0	0
July	100.3	168953	475022	158400	475200	0	10553
August	117.8	198431	673453	158400	633600	39853	40031
September	194.6	327799	1001252	158400	792000	209252	169399
October	154.5	260252	1261504	158400	950400	311104	101852
November	43.9	73948	1335452	158400	1108800	226652	0
December	15.8	26614	1362066	158400	1267200	94866	0
January	2.3	3874	1365940	158400	1425600	0	0
February	6.4	10780	1376720	158400	1584000	0	0
March	16	26951	1403671	158400	1742400	0	0
April	44.5	74959	1478630	158400	1900800	0	0
Total	877.8	1478630		1900800			

Table 1 shows the calculation of storage tank size according to monthly demand, Minimum storage required is the difference of maximum volume stored and surplus water left at the end of the year which equals to 311104 liters, Hence, Storage tank of capacity

311.1 m³ is suggested for the hostel with roof top area of 2632 m² which yields 1478637 liters annually which could meet the demand of flushing purpose with 76.72% water reliability.

VII. ANNUAL WATER YIELD OF DIFFERENT BUILDINGS AT RVCE

Similarly annual water yield from different roof tops of different buildings is calculated by obtaining roof

top areas of determined using Google earth and represented in table 2 below, figure 3 represents satellite image of civil department.

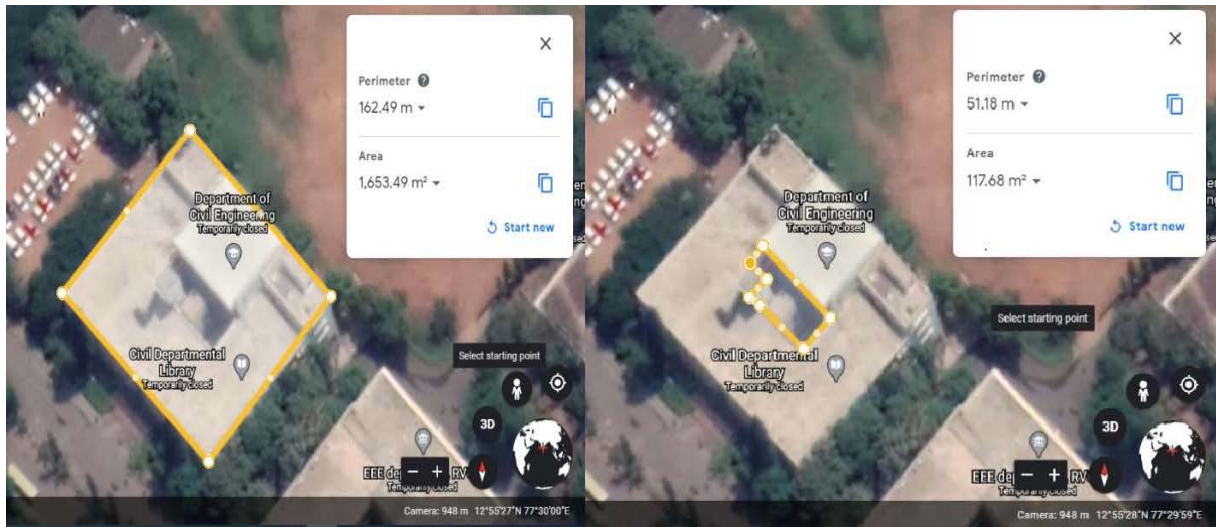


Figure 3: Satellite image of civil department building (Source: Google Earth®)

Table 2: Annual water yield from different roof tops of different buildings of RVCE

Sl. No.	Building name	Area	Annual water yield
1	Department of CV	1535.81	862805.77
2	Department of ME	1431.69	804311.98
3	Department of CSE	1063.36	597387.14
4	Department of EC	1262.1	709037.68
5	Department of EEE	1773.06	996090.92
6	Department of AS and ISE	1911.81	1074039.56
7	Department of BT and EIE	1050.23	590010.81
8	Department of MCA	1596.28	896777.33
9	Department of TE	894.95	502775.75
10	CRC Complex	803.41	451349.31
11	Department of CE	1586.42	891238.06
12	Administrative block	1330.78	747621.55
13	Mechanical PG block	486.43	273272.48
14	Department of IEM	925.75	520078.94
15	Old sports complex	547.44	345990.83
16	New sports complex & Gym center	1239.1	826638.30
17	Food Court	1354.09	855806.54
18	Bank and Post office	153.29	86117.09
19	Aero-space lab	862.21	575204.43
20	Library building	873.11	490506.21
21	Hospital Building	301.61	169442.08
22	Cognitive and Research Block	863.28	484983.78
23	Workshops	3213.01	2143488.935
24	Old cauvery hostel	1251.64	703161.33
25	New cauvery hostel	2632	1478636.54
26	Sir m v hostel	2041.95	1147151.17
27	Chamundi hostel	1159.33	651302.31

28	Dj hostel	1061.77	596493.89
29	Employee's residence	393.74	221199.98
30	Miscellaneous	1265.24	799651.92
	Total annual yield		21492572.62

By harvesting rain water from different buildings of RVCE we can collect 21492572 liters of water annually making RVCE campus self-reliable and self-sustainable in water usage. Collected water can be utilized for flushing, gardening purposes, since the daily requirement of the institution is high adopting RWH techniques is found to be simple and sustainable technique which can be implanted in the campus.

VIII. ESTIMATION OF RUNOFF POTENTIAL

Runoff is defined as the ratio of precipitation that makes its way towards rivers or oceans as surface or subsurface flow to the precipitation received. After undergoing infiltration and other losses from the rainfall, to determine potential runoff water that can be collected from different catchment surfaces like playgrounds, parks, pavements etc. present at RVCE campus, figure

4 and figure 5 shown below gives satellite image of cricket ground and site respectively. area of the catchment surfaces are determined using Google earth and represented in table 3, runoff coefficients of different surfaces were collected and annual water yield from runoff is obtained by knowing area and average annual rainfall of the catchment.

Annual water yield, Q is obtained by using the formula

$$Q = R \times A \times C$$

Where, R is the average annual precipitation

A is the catchment area

C is the runoff coefficient

Runoff coefficient of pavements = 0.7-0.95,

parks = 0.1-0.25,

unimproved areas = 0.1-0.3,

tiles = 0.8-0.9, playgrounds = 0.2-0.35 [5].

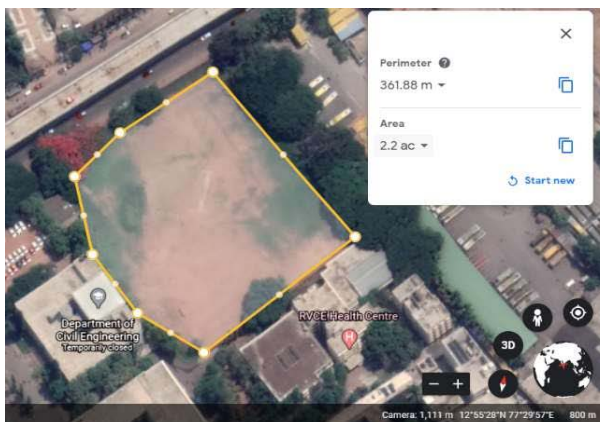


Figure 4: Satellite image of cricket ground
(Source: Google Earth®)

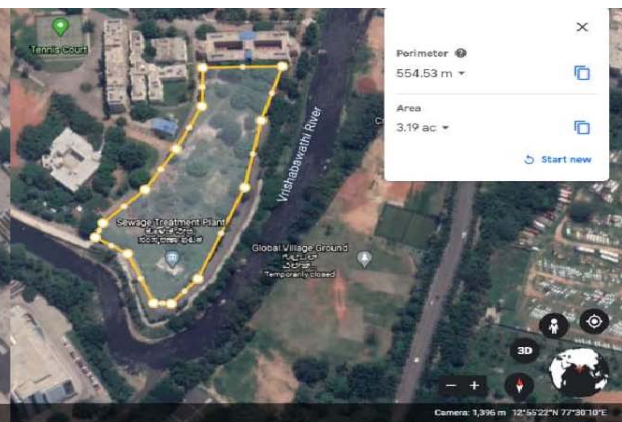


Figure 5: Satellite image of Site behind DJ block
(Source: Google Earth®)

Table 3: Estimation of annual runoff potential of RVCE

Sl. No.	Type of catchment	Area (m ²)	Annual water yield(l)
1	Pavements	27913.06	11760975.1
2	Play grounds	20507.54	4950417.62
3	Unimproved areas/ sites	37633.28	8258623.3
4	Parks/greenery	24187.23	4246310.1
5	Brick/tiles/concrete	4996.95	3509058.17
	Total runoff		32725384.29

The runoff water which can be collected from different surfaces such as pavements, parks, sites, playgrounds located at RVCE campus is 32725384.29 liters which can be utilized for recharging of ground water by adopting recharge structures.

IX. CONCLUSIONS

The present study concludes that by adopting RWH facility to collect the water from roof tops of all the buildings of RVCE campus, 21.49 Million liters of water

can be collected. It is evident that adopting RWH and artificial ground water recharge techniques in all the public buildings can be a solution to water availability and management problems at urban areas.

X. RECOMMENDATIONS

1. Sustainability in water management can be achieved at RVCE by adopting decentralized RWH and Ground water recharge structures.

2. Presently RVCE is collecting 3.6 Million liters of water annually from RWH, by adopting RWH technique to all the roof tops RVCE campus has potential of collecting 21.49 Million liters of water annually from roof tops of different buildings.
3. RVCE has the potential of collecting 32.72 Million liters of water by runoff from major catchment areas like play grounds, pavements, parks and sites, the run-off water collected can be used for improving ground water resources.
4. Open wells can be established near Bus parking, near temple, near DJ hostel and near food court in addition to the existing recharge structures for ground water recharge purpose.
5. Monitoring of existing RWH structures and Recharge structures needs to be done.

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Design and Economic Analysis of a Small Scale Formaldehyde Plant from Flared Gas

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Keywords: *design, height, diameter, volume, composition, formaldehyde.*

GJRE-C Classification: FOR Code: 090499



Strictly as per the compliance and regulations of:



Design and Economic Analysis of a Small Scale Formaldehyde Plant from Flared Gas

Muesi Zornata Noble ^α, Emmanuel O. Ehirim ^σ, Wordu Animia ^ρ & Jaja Zina ^ω

Abstract- The Simulation of a 10,000 ton/yr capacity Formaldehyde plant from flared gases was performed using Aspen Hysys version 8.8, and the Hysys model of the plant was developed using data from literature. A material and energy balance for the various components of the plant was performed manually and with Hysys for comparison. The design/equipment sizing, Mechanical design, costing and economic evaluation, process control of the functional parameters of the various equipments and finally the full Hysys process flow diagram of the model was performed. The Formaldehyde reactors was simulated to study the effect of process functional parameters such as reactor dimensions, temperature, pressure, The effect of reactor size and number on Formaldehyde output was studied by simulating the plant with a compressor, mixer, conversion reactor, cooler, CSTR, heat exchanger, and storage tank. The results of the material and energy balance of the various components of the plant performed manually and with Hysys showed a maximum deviation of 0.8%. The design and sizing results of various functional parameters of the reactor in terms of Volume, Diameter, Height, Spacetime, SpaceVelocity, and Volume flowrate respectively were: 45m³, 3.368m, 5.052m, 1.8892hr, 0.5293/hr, 23.82m³/hr. The design and sizing results of the heat exchanger in terms of Heat load, Heat transfer area, log mean temperature difference (LMTD), Overall heat transfer coefficient, tube length, number of tubes, pitch were: 69.94KW, 60.32m², 49.79°C, 23.29W/m²K, 4.83m, 160, 50mm. The effect of reactor size and number showed that At 90% conversion the following output results were obtained for formaldehyde product in terms of mass flow rate, molar flow rate, composition (mole fraction), and yield: 479.53kg/hr, 0.79kgmole/hr, 0.0541, and 0.8988 respectively.

Keywords: design, height, diameter, volume, composition, formaldehyde.

1. INTRODUCTION

Formaldehyde is produced in industrial scale from methanol. It uses atmospheric pressure to perform the production. There are steps in formaldehyde production. The first step involves the liquid methanol which vapourized into an air stream while steam was added to the resulting gaseous mixture. Also, the other step involves the gaseous mixture lead over a catalyst bed. The methanol was finally converted to formaldehyde through partial dehydrogenation and partial oxidation. (Alfaree & Adnan, 2016).

Besides, the report by Welch shows that 10 million of formaldehyde was produced annually and met the demand of the industries as at then, but as population increases, the demand of formaldehyde was increased and the production rate was not able to met industrial scale based on its wide application. (Alzein & Nath, 2018), the process industry would need more of formaldehyde production rate to met world production annually. This increase in population that occurs result to more production of formaldehyde at a later year. In the 2012, the production of formaldehyde amount to 32.5 million tons per year. According to (Sukunya *et al.*, 2014), this increase in demand was due to the applications of formaldehyde in chemical synthesis such as resin products. These resins are used for polywood production. Also, formaldehyde solution can destroy bacteria and fungi.

However, the 32.5 million tons per year was a report as at 2012, but we are now in 2019. This has resulted to increase in population of the world as well as the demand for formaldehyde base on its usage in process industries. (Cameroon *et al.*, 2019).

Today, many researchers are looking for new areas in which formaldehyde can be applied, technology has increase and new methods are been discovered. (Chauvel & Lefebvre, 2015), The production based on report cannot met the demand today and so more researchers are to go into designing of units operations for the production of formaldehyde to met world demand which as a results of the current population density. Also, more processes for the production of formaldehyde can be added to the existing two processes and hence these calls for more future research to be carried out with a view of which production process gives the most yield with the least cost of production. (Chouldhary *et al.*, 2017).

The study of formaldehyde plant calls for new design of reactor that would produce formaldehyde in excess in other to take care of the world's population that requires the uses and applications of formaldehyde. The production of formaldehyde using the silver contact process amounts to 80% of total formaldehyde process. The type of reactor determines the desired productions which depend on feed quality (Antonio *et al.*, 2010; Geoffrey *et al.*, 2004) and the reactor temperature (Geoffrey *et al.*, 2004). The work focus on the type of reactor design would produce formaldehyde in excess as to met the current demand of society today. This is

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base on the wide application of formaldehyde. The study require the development of design parameters or sizes of continuous stirred tank, plug flow and batch reactor for the two routes used in producing formaldehyde. The reactor types would be tested in its design to compute and simulate to ascertain which reactor type would be suitable to produce formaldehyde in the required quantity to supply to the needs of the process industry for various applications.

Besides, the various reactor models would be tested with the reaction mechanisms and kinetics for simulations of variables which would be used to ascertain the reactor that best give the highest production. The products from the reactors are fed into absorber to form formaldehyde 37% by mass called formalin or more (Andre *et al.*, 2002).

However, the formalin formed at room temperature was not stable and formed paraformaldehyde. The paraformaldehyde formed was high concentration of formaldehyde. But formalin has methanol of 1.14% by mass for more stability in solution and its temperature was more than 313k (Geoffrey *et al.*, 2004), the study focuses on the design of reactor types for the production of formaldehyde. This formaldehyde has the formula HCHO and the first series of aliphatic aldehyde which was discovered in 1859. The production of formaldehyde which started during the twentieth century had continued even till date. The study becomes more imperative for industries, engineers and producers who wants to exploits the opportunity to design reactor types for the production of formaldehyde.

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The production and optimization of formaldehyde can include the streams for air, methanol and water in a suitable composition in a plug flow reactor under certain conditions of temperatures and pressure (Andreasen *et al.*, 2003). The purpose of using a plug flow reactor is to get desired product which can be optimized to get best yield of formaldehyde (Antonio *et al.*, 2010; Geoffrey *et al.*, 2004).

(Lauks *et al.*, 2015), on the other hand, when the production of formaldehyde involves the use of silver catalyst, the operation is carried out adiabatically by lagging the system which helps to obtain a selectivity of 90%. (Marton *et al.*, 2017), the life of the catalyst is short depending on the impurities in the methanol and the gases at exist that contain considerable amount of hydrogen and water. However, the silver being a metal would have low catalytic activity for the decomposition of methanol even at a very high temperature. (Mazanec *et al.*, 2019), the chemisorption of the monoatomic oxygen in the metal brings its activation.

(Meisong, 2015), thermal decomposition of formaldehyde depends on the gas stream, the gas stream is cooled when it passes through the catalyst. The formaldehyde produced is then absorbed in an absorber by water to get pure formaldehyde. Since the gaseous form of formaldehyde is unstable, it is better absorbed in water. (Mohamad, 2016), the products of reaction contains the formaldehyde diluted in water other gases which mainly contains nitrogen. Finally, the commercial and final product is obtain from the absorber of about 55% weight of formaldehyde in water or formalin.

(Mohsenzadeh, 2019), the design and optimization of the reactor for the production of formaldehyde which uses two different routes and each would be considered during the design of the reactor because we want to know which of the route would be best in the production of formaldehyde. Also, the reactors would be batch, continuous stirred tank and plug flow reactor. Each reactor would follow both routes

required for the production of formaldehyde and the optimization of each routes of production and in each of the reactor types. Finally, the physical properties would be presented in tabular form below (Reuss *et al.*, 2003). Jaja *et al.*, (2020), Methane is a major component of flared gas as well as natural gas and its composition varies from 70 to 90% in both cases.

II. MATERIALS AND METHODS

a) Materials

The Materials used in this Research includes:

- i. Plant data of flared gas composition obtained from the Port Harcourt Refining Company
- ii. Aspen Hysys software version 8.8
- iii. Matlab software
- iv. Microsoft excel
- v. Computer

b) Methods

The methods that will be adopted in this Research includes:

- (a) Material Balance
- (b) Energy Balance
- (c) Equipment Sizing

(d) Mechanical Design

(e) Costing

(a) Material Balance

Material balance are the basics of process design. A material balance taken over the complete process will determine the quantities of raw materials required and products produced. Balances over individual process unit set the process stream flows and compositions. A good understanding of material balance calculations is essential in process design.

Material balances are also useful tools for the study of plant operation and trouble shooting. They can be used to check performance against design; to extend the often limited data from the plant instrumentation; to check instrument calibrations and to locate source of material loss.

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

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

$$[Material\ out] = [Material\ in] + [Generation] - [Consumption] - [Accumulation] \quad (1)$$

For steady state process the accumulation term will be zero except in nuclear process, mass is neither generated nor consumed; but if a chemical reaction take place a particular chemical species may be formed or consumed in the process. If there is no chemical reaction the steady state balance reduces to:

$$[Materials\ in] = [Materials\ Out] \quad (2)$$

(b) Energy Balance

A general energy balance equation can be written as:

$$\left[\begin{matrix} \text{Rate of Outflow} \\ \text{of Energy} \end{matrix} \right] = \left[\begin{matrix} \text{Rate of Inflow} \\ \text{of Energy} \end{matrix} \right] + \left[\begin{matrix} \text{Rate of Generation} \\ \text{of Energy} \end{matrix} \right] - \left[\begin{matrix} \text{Rate of Consumption} \\ \text{of Energy} \end{matrix} \right] - \left[\begin{matrix} \text{Rate of Accumulation} \\ \text{of Energy} \end{matrix} \right] \quad (3)$$

If no chemical reaction occurs

$$\left[\begin{matrix} \text{Rate of Consumption} \\ \text{of Energy} \end{matrix} \right] = \left[\begin{matrix} \text{Rate of Generation} \\ \text{of Energy} \end{matrix} \right] = 0 \quad (4)$$

Equation (3) becomes

$$\left[\begin{matrix} \text{Rate of Outflow} \\ \text{of Energy} \end{matrix} \right] = \left[\begin{matrix} \text{Rate of Inflow} \\ \text{of Energy} \end{matrix} \right] - \left[\begin{matrix} \text{Rate of Accumulation} \\ \text{of Energy} \end{matrix} \right] \quad (5)$$

If the system is a steady state process

$$\left[\begin{matrix} \text{Rate of Accumulation} \\ \text{of Energy} \end{matrix} \right] = 0 \quad (6)$$

Equation (5) becomes

$$\left[\begin{matrix} \text{Rate of Inflow} \\ \text{of Energy} \end{matrix} \right] = \left[\begin{matrix} \text{Rate of Outflow} \\ \text{of Energy} \end{matrix} \right] \quad (7)$$

Energy flow for each stream shall be computed in terms of Heat Flow using the formula

$$\dot{Q} = \dot{m}C_{p_{mean}}(T - T_{ref}) \quad (8)$$

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

$\dot{m}$ = mass flow rate in kg/hr

$$C_{p_{mean}} = \text{Mean Specific Heat Capacity in KJ/kg } ^\circ\text{C}$$

T = Temperature of the stream in $^\circ\text{C}$

T_{ref} = Reference Temperature of stream
sometimes assumed to be zero

(c) Equipment Sizing

The different categories of equipment to be sized in this project includes:

- i. Conversion Reactor Unit
- ii. Continuous Stirred Tank Reactor (CSTR) Unit
- iii. Heat Exchange Unit
- iv. Storage Tank Unit

(d) Mechanical Design

A vessel must be designed to withstand the maximum pressure to which it is likely to be subjected in operation. For vessels under internal pressure, the design pressure is normally taken as the pressure at which the relief device is set. This will normally be 5 to 10 per cent above the normal working pressure, to avoid spurious operation during minor process upsets. When deciding the design pressure, the hydrostatic pressure in the base of the column should be added to the operating pressure if significant.

Vessels subject to external pressure should be designed to resist the maximum differential pressure that is likely to occur in service. Vessels likely to be subjected to vacuum should be designed for a full

negative pressure of 1 bar unless felt with an effective and reliable vacuum breaker.

(e) Cost Estimation and Economic Evaluation

Economic evaluation is very important for the proposed plant. We have to be able to estimate and decide between either native design and for project evaluation. Chemical plants are built to make profit and estimate of the investment is required and the cost of production are needed before the profitability for a project is the sum of the fixed and working capital.

Fixed capital is the total cost of the plant ready to start up. It is the cost paid to the contractors. **Working capital** is the additional investment needed, over and above the fixed capital to start up the plant and operate it to the point when income is earned. Most of the working capital is recovered from at the end of the project. The full detail of the costing is given in the appendix.

III. DESIGN SIMULATION (HYSYS)

This section represents a process simulation of plant design for the production of Formaldehyde from flared gas. The simulation covers the following equipments/units:

U001	-	Compression unit
U002	-	Mixing unit
U003	-	Conversion Reactor unit
U004	-	Cooling unit
U005	-	CSTR unit
U006	-	Heat Exchanger unit
U007	-	Storage tank unit
S ₁ (Stream 1)	-	Flared Gas
S ₂ (Stream 2)	-	Compressed Flared Gas
S ₃ (Stream 3)	-	Air
S ₄ (Stream 4)	-	Mixed Product
S ₅ (Stream 5)	-	Vapour product
S ₆ (Stream 6)	-	Cooled Vapour
S ₇ (Stream 7)	-	Formaldehyde Liquid
S ₈ (Stream 8)	-	Vapour Out
S ₉ (Stream 9)	-	Formaldehyde Liquid Out
S ₁₀ (Stream 10)	-	Hot Water Inlet
S ₁₁ (Stream 11)	-	Cooled Water Outlet
S ₁₂ (Stream 12)	-	Tank Product

Figure 1 shows the full PFD of the Hysys design Simulation Where formaldehyde from flared gas using the reaction between absorbed methane gas from flared gas and oxygen. The procedure begins with compressing of flared gasses using a compressor. The component of interest being methane is being compressed and mixed with air stream inside a mixer and then sent to a conversion reactor where reaction of

methane and oxygen occurs to Formaldehyde, Carbon [iv] oxide and water as products. The overhead products from the conversion reactor is being cooled and sent to a Continuous Stirred Tank Reactor [CSTR] for further reaction and more yield of the formaldehyde.

The product from the CSTR is being sent to the heat exchanger for further hitting to the desired temperature and subsequently sent to the storage tank

for storage. The process was able to convert about 90% of methane and the yield of Formaldehyde is up to 45% making the process very economical to set up a plant for the production process using flared gas and trapping methane as base component of reaction. This is a new innovation in the technology of the production of formaldehyde and a scale up of the plant should be executed in the future.

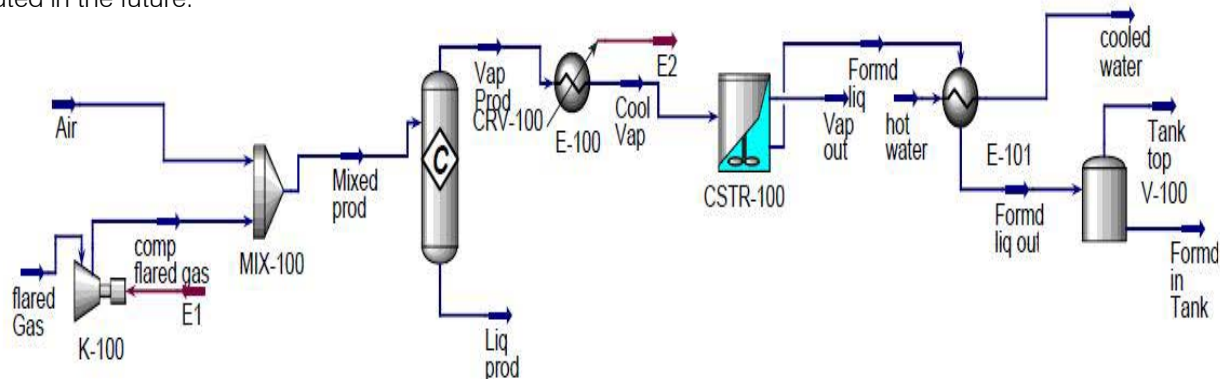


Figure 1: Hysys Simulation PFD

IV. RESULTS AND DISCUSSION

a) Material Balance Results

The following results of material balance with manual calculation compared with Hysys simulation is presented in tables below for each unit.

Table 4.1: Comparison of Material Balance Result of Hysys Simulation with Manual Calculation for Compression Unit

Streams	Manual calc.	Hysys Simulation	% Deviation
Flared Gas (S_1)			
Mass Flow (kg/hr)	1.23×10^4	1.20×10^4	2.5
Molar Flow (kgmole/hr)	600.50	600.10	0.7
Compressed Flared Gas (S_2)			
Mass Flow (kg/hr)	1.23×10^4	1.20×10^4	2.5
Molar Flow (kgmole/hr)	600.50	600.10	0.7

In Table 4.1 above the mass flow rate of Flared Gas Stream (S_1) for Hysys simulation is 1.2×10^4 kg/hr while that for the manual calculation is 1.23×10^4 kg/hr with a deviation of 2.5%. the molar flow rate for Hysys simulation was found to be 600.10 kgmole/hr while that of manual calculation is 600.50 kgmole/hr with a deviation of 0.7% we also observe that since this unit is

a single input, single output stream and applying the principles of conservation of mass, input mass equals output mass, hence the output been Compressed Flared Gas has the same mass and molar flow rates of the input stream which is Flared Gas as well as the same deviation.

Table 4.2: Comparison of Material Balance Result of Hysys Simulation with Manual Calculation for Mixing Unit

Streams	Manual calc.	Hysys Simulation	% Deviation
Air (S_3)			
Mass Flow (kg/hr)	1.1×10^4	1×10^4	10
Molar Flow (kgmole/hr)	346.60	346.30	0.9
Flared Gas (S_2)			
Mass Flow (kg/hr)	1.23×10^4	1.20×10^4	2.5
Molar Flow (kgmole/hr)	600.50	600.10	0.7
Mixed Product (S_4)			
Mass Flow (kg/hr)	2.10×10^4	2.20×10^4	4.5
Molar Flow (kgmole/hr)	947.40	947.10	3.0

In Table 4.2 above the mass flow rate of the Air Stream is 1×10^4 kg/hr for Hysys simulation while for manual calculation is found to be 1.1×10^4 kg/hr having a deviation of 10%. The molar flow rate for the Hysys simulation is 343.3 kgmole/hr while that of the manual calculation is 343.3 kgmole/hr having a deviation of 0.9%. This Flared Gas stream has been stated in the discussion of Table 4.1, however we are to note that Air stream (S_3) and Flared Gas Stream (S_2) are both input streams respectively which are mixed inside a mixer to produce an outlit stream Mixed Product (S_4) having a

mass flow rate of 2.20×10^4 kg/hr for Hysys simulation and 2.10×10^4 kg/hr for manual calculation with a 4.5%. the molar flow rate of this stream is 947.10 kgmole/hr for Hysys simulation and 947.40 for manual calculation with a deviation of 3%. Applying the principles of conservation of mass to this unit shows that if mass flow rates of the inlet streams are added together the results equals the mass flow rate of the outlet stream which makes our results to be valid for inflow of mass is equal to outflow of mass.

Table 4.3: Comparison of Material Balance Result of Hysys Simulation with Manual Calculation for Conversion Reactor Unit

Streams	Manual calc.	Hysys Simulation	% Deviation
Mixed Product (S_4)			
Mass Flow (kg/hr)	2.10×10^4	2.20×10^4	4.5
Molar Flow (kgmole/hr)	947.40	947.10	3.0
Vapour Product (S_5)			
Mass Flow (kg/hr)	2.10×10^4	2.20×10^4	4.5
Molar Flow (kgmole/hr)	947.40	947.10	3.0
Reaction Extent		24.25	
Fractional Conversion		0.1102	

In Table 4.3 the mass flow rate of the Mixed Product Stream (S_4) for Hysys simulation is 2.20×10^4 kg/hr while the manual calculation is 2.10×10^4 kg/hr with deviation of 4.5%. The molar flow rate of the Mixed Product Stream (S_4) is 947.10 kgmole/hr for Hysys simulation and 947.40 kgmole/hr for manual calculation with a deviation of 3.0%. We also observe that since this unit is a single input, single Output Stream and applying

the principles of conversation of mass, input mass equals output mass, hence the output been Vapour Product (S_5) has same mass and molar flow rates of the Input Stream as well as the same % Deviation. Also the Extent of Reaction for this unit for Hysys simulation is 24.27. The fractional conversion for Hysys simulation is 0.1102 while for manual calculation is 0.1105.

Table 4.4: Comparison of Material Balance Result of Hysys Simulation with Manual Calculation for Cooling Unit

Streams	Manual calc.	Hysys Simulation	% Deviation
Vapour Product (S_5)			
Mass Flow (kg/hr)	2.10×10^4	2.20×10^4	4.5
Molar Flow (kgmole/hr)	947.40	947.10	3.0
Cooled Vapour (S_6)			
Mass Flow (kg/hr)	2.10×10^4	2.20×10^4	4.5
Molar Flow (kgmole/hr)	947.40	947.10	3.0

In Table 4.4 the mass flow rate of the input stream Vapour Product has been stated in the discussion of Table 4.3, this unit contains a single input, single output streams. Hence, the same mass and molar flow rate of the Vapour Product Stream (S_5) is the

same for the cooled Vapour Stream (S_6) which is 2.2×10^4 kg/hr for Hysys simulation and 2.10×10^4 kg/hr for manual calculation. Also the molar flow is 947.10 for Hysys simulation and 947.40 for manual calculation.

Table 4.5: Comparison of Material Balance Result of Hysys Simulation with Manual Calculation for CSTR Unit

Streams	Manual calc.	Hysys Simulation	% Deviation
Cooled Vapour (S_6)			
Mass Flow (kg/hr)	2.10×10^4	2.20×10^4	4.5
Molar Flow (kgmole/hr)	947.40	947.10	3.0
Formaldehyde Liquid (S_7)			
Mass Flow (kg/hr)	888.5	888.7	0.2
Molar Flow (kgmole/hr)	45.04	45.03	0.3

Vapour Out (S_8)			
Mass Flow (kg/hr)	2.12×10^4	2.111×10^4	0.4
Molar Flow (kgmole/hr)	903.2	902.1	0.1

In Table 4.5 the mass flow rate of cooled vapour stream (S_8) is 2.20×10^4 kg/hr for Hysys simulation and 2.10×10^4 kg/hr for manual calculation with a deviation of 4.5%. The molar flow rate for Hysys simulation is 947.10 kgmole/hr and for manual calculation 947.40 kgmole/hr with a deviation of 3.0%. The mass flow rate of Formaldehyde Liquid stream for Hysys simulation and manual calculation are 888.7 kg/hr and 888.5 kg/hr

respectively having a deviation of 0.2%. While the molar flow rate are 45.03 kgmole/hr and 45.04 kgmole/hr having a deviation of 0.3%. The mass and molar flow rate of the Vapour Out Stream for Hysys simulation and manual calculation are 2.111×10^4 kg/hr and 2.12×10^4 kg/hr having a deviation of 0.4% while molar flow rate are 902.1 kgmole/hr and 903.12 kgmole/hr having deviation of 0.1%.

Table 4.6: Comparison of Material Balance Result of Hysys Simulation with Manual Calculation for Heat Exchanger Unit

Streams	Manual calc.	Hysys Simulation	% Deviation
Formaldehyde Liquid (S_7)			
Mass Flow (kg/hr)	888.5	888.7	0.2
Molar Flow (kgmole/hr)	45.04	45.03	0.3
Formaldehyde Liquid Out (S_9)			
Mass Flow (kg/hr)	888.5	888.7	0.2
Molar Flow (kgmole/hr)	45.04	45.03	0.3
Hot Water Inlet (S_{10})			
Mass Flow (kg/hr)	900.20	900	0.2
Molar Flow (kgmole/hr)	50.00	49.96	0.1
Cooled Water Outlet (S_{11})			
Mass Flow (kg/hr)	900.20	900	0.2
Molar Flow (kgmole/hr)	50.00	49.96	0.1

In Table 4.6 Formaldehyde Liquid Stream has the same mass and molar flow rate as Formaldehyde Liquid Out. While Hot Water Inlet Stream has the same mass and molar flow rate as Cooled Water Out. This is expected for the design of the Heat Exchanger.

b) Energy Balance Results

The following results of energy balance with manual calculation compared with Hysys simulation is presented in tables below for each unit.

Table 4.7: Comparison of Energy Balance Result of Hysys Simulation with Manual Calculation for Compression Unit

Streams	Manual calc.	Hysys Simulation	% Deviation
Flared Gas (S_1)			
Temperature ($^{\circ}\text{C}$)	25	25	0.0
Pressure (kpa)	101.3	101.3	0.0
Heat Flow (kJ/hr)	-4.682e7	-4.686e7	4.7
(E1)			
Temperature ($^{\circ}\text{C}$)	-	-	
Pressure (kpa)	-	-	
Heat Flow (kJ/hr)	3.421e5	3.427e5	1.4
Compressed Gas (S_2)			
Temperature ($^{\circ}\text{C}$)	38.84	38.84	0.0
Pressure (kpa)	120	120	0.0
Heat Flow (kJ/hr)	-4.6479e7	-4.6478e7	1.3

In Table 4.7 above the heat flow of Stream (S_1) and Stream (E1) when added equals the heat flow of stream (S_2) and this is in line with the principles of

Conservation of Energy for a steady state process with chemical reaction occurring.

Table 4.8: Comparison of Energy Balance Result of Hysys Simulation with Manual Calculation for Mixing Unit

Streams	Manual calc.	Hysys Simulation	% Deviation
Compressed Gas (S_2)			
Temperature ($^{\circ}\text{C}$)	38.84	38.84	0.0

Pressure (kpa)	120	120	0.0
Heat Flow (kJ/hr)	-4.6478e7	-4.6474e7	5.4
Air (S ₁)			
Temperature (°C)	25	25	0.0
Pressure (kpa)	101.3	101.3	0.0
Heat Flow (kJ/hr)	0	0	0.0
Mixed Product (S ₄)			
Temperature (°C)	34.84	34.84	0.0
Pressure (kpa)	101.3	101.3	0.0
Heat Flow (kJ/hr)	-4.6478e7	-4.6474e7	5.4

In Table 4.8 it is observed that the heat flow of the air stream is zero because the temperature of this stream equals its reference temperature hence no heat flow. Also the heat flow of Compressed Gas Stream (S₂) and Mixed Stream (S₄) are equal.

Table 4.9: Comparison of Energy Balance Result of Hysys Simulation with Manual Calculation for Conversion Reactor Unit

Streams	Manual calc.	Hysys Simulation	% Deviation
Mixed Product (S ₄)			
Temperature (°C)	34.84	34.84	0.0
Pressure (kpa)	101.3	101.3	0.0
Heat Flow (kJ/hr)	-4.6478e7	-4.6474e7	5.4
Vapour Product (S ₅)			
Temperature (°C)	34.84	34.84	0.0
Pressure (kpa)	101.3	101.3	0.0
Heat Flow (kJ/hr)	-4.6478e7	-4.6474e7	5.4

In Table 4.9 above the flow of Mixed Stream (S₄) and Vapour Product Stream (S₅) are equal since it is a Single Input, Single Output Stream and also in with the principles of conservation of energy.

Table 4.10: Comparison of Energy Balance Result of Hysys Simulation with Manual Calculation for Cooling Unit

Streams	Manual calc.	Hysys Simulation	% Deviation
Vapour Product (S ₅)			
Temperature (°C)	34.84	34.84	0.0
Pressure (kpa)	101.3	101.3	0.0
Heat Flow (kJ/hr)	-4.6478e7	-4.6478e7	5.4
(E ₂)			
Temperature (°C)	-	-	
Pressure (kpa)	-	-	
Heat Flow (kJ/hr)	2.636e7	2.636e7	0.0
Cooled Vapour (S ₆)			
Temperature (°C)	800	800	0.0
Pressure (kpa)	101.3	101.3	0.0
Heat Flow (kJ/hr)	-7.283e7	-7.285e7	2.4

In table 4.10 the sum of the Heat Flow of Stream E2 and cooled Vapour Stream equals that of Vapour Product Stream (S₅) which is line with the principles of conservation of energy.

Table 4.11: Comparison of Energy Balance Result of Hysys Simulation with Manual Calculation for CSTR Unit

Streams	Manual calc.	Hysys Simulation	% Deviation
Cooled Vapour (S ₆)			
Temperature (°C)	800	800	0.0
Pressure (kpa)	101.3	101.3	0.0
Heat Flow (kJ/hr)	-7.283e7	-7.285e7	2.4
Formaldehyde Liquid (S ₇)			

Temperature (°C)	80	80	0.0
Pressure (kpa)	101.3	101.3	0.0
Heat Flow (kJ/hr)	-1.169e7	-1.167e7	3.0
Vapour Out (S ₈)			
Temperature (°C)	800	800	0.0
Pressure (kpa)	101.3	101.3	0.0
Heat Flow (kJ/hr)	-6.114e7	-6.116e7	12.5

In Table 4.11 the sum of the heat flow Formaldehyde Liquid Stream (S₇) and Hot Water Inlet Stream (S₁₀) equals to the sum of the heat flow of Formaldehyde Liquid Out Stream (S₉) and cooled Water Stream (S₁₁) which is in line with the principles of

conservation of energy which states that inflow of energy is equal to outflow of energy provided that the system is a steady state process and no chemical reaction occurs.

Table 4.12: Comparison of Energy Balance Result of Hysys Simulation with Manual Calculation for Heat Exchanger Unit

Streams	Manual calc.	Hysys Simulation	% Deviation
Formaldehyde Liquid (S ₇)			
Temperature (°C)	80	80	0.0
Pressure (kpa)	101.3	101.3	0.0
Heat Flow (kJ/hr)	-1.169e7	-1.167e7	3.0
Formaldehyde Liquid Out (S ₉)			
Temperature (°C)	120	120	0.0
Pressure (kpa)	101.3	101.3	0.0
Heat Flow (kJ/hr)	-1.154e7	-1.156e7	3.6
Hot Water Inlet (S ₁₀)			
Temperature (°C)	200	200	0.0
Pressure (kpa)	101.3	101.3	0.0
Heat Flow (kJ/hr)	-1.160e7	-1.162e7	3.2
Cooled Water Outlet (S ₁₁)			
Temperature (°C)	195	195	0.0
Pressure (kpa)	101.3	101.3	0.0
Heat Flow (kJ/hr)	-1.175e7	-1.174e7	1.4

In Table 4.12 the design parameters such as Column Height, Column Diameter, Cross-sectional Area, Volume, Space time, Space Velocity, Thickness and Corrosion Allowance was compared with Hysys simulation and Manual calculation and the maximum deviation was found to be 3.2%.

b) Design /Sizing Results

The equipment design and sizing of each equipment of the plant is presented in the table below, for manual calculation compared to Hysys Simulation.

Table 4.13: Comparison of Sizing/Design Results of Hysys Simulation with Manual Calculations for Conversion Reactor Unit

Design/Sizing Item	Hysys Simulation	Manual Calculation	% Deviation
Flow Type			
Materials of Construction	Stainless steel	Stainless steel	
Column Height	3.86	3.84	2.4
Column Diameter	2.57	2.54	5.3
Cross Sectional Area	5.18	5.17	5.6
Volume	20	21	4.8
Space Time	0.43	0.42	2.3
Space Velocity	2.32	2.34	6.3
Thickness	18.63	18.65	3.1
Corrosion allowance	2.00	2.00	0.00

In Table 4.13 the design parameters such as Column Height, Column Diameter, Cross-sectional Area, Volume, Space time, Space Velocity, Thickness and Corrosion Allowance was compared with Hysys

simulation and Manual calculation and the maximum deviation was found to be 6.3%.

Table 4.14: Comparison of Sizing/Design Results of Hysys Simulation with Manual Calculations for CSTR Unit

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)	0.74	0.75	1.33
Space Velocity(hr ⁻¹)	1.35	1.33	6.06
Thickness(mm)	21.60	21.59	1.67
Corrosion allowance(mm)	2.00	2.00	0.00

In Table 4.14 the design parameters such as Column Height, Column Diameter, Cross-sectional Area, Volume, Space time, Space Velocity, Thickness and Corrosion Allowance was compared with Hysys simulation and Manual calculation and the maximum deviation was found to be 6.06%.

Table 4.15: Comparison of Sizing/Design Results of Hysys Simulation with Manual Calculations for Heat Exchanger Unit

Design/Sizing Item	Hysys Simulation	Manual Calculation	% Deviation
Equipment Name	Shell and tube heat exchanger	Shell and tube heat exchanger	
Objective.	Cooling the reactor effluent	Cooling the reactor effluent	
Equipment Number	U-007	U-007	
Designer			
	MUESI NOBLE PG.2017/02618	MUESI NOBLE PG.2017/02618	
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)	945	947	0.0
Heat transfer Area (m²)	53.4	53.5	0.2
LMTD (°C)	32	32.1	0.2
U (W/m²K)	640	640.3	0.1
Inlet temperature (°C)	80	80	0.0
Shell Diameter (mm)	476	476	0.0
Shell coefficient W/m ² C	1516	1516.4	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

In Table 4.15 Heat Exchanger Design Parameter was compared between Hysys simulation and manual calculation and the maximum deviation was found to be 0.2%

V. SENSITIVITY ANALYSIS

The functional parameters such as length of Reactor, Diameter, Space time, Space velocity were studied to see how they change with conversion and are presented in figures – to

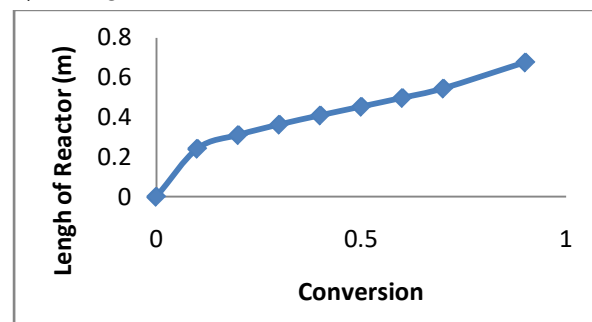
a) Length of Reactor with Conversion**Figure 1:** Profile Reactor versus Conversion

Figure 1 demonstrates the profile variation of length of the reactor varying with conversion. The results in the profile gives an increase of the length of reactors value with conversion increase. The length of reactor values increased from 0 m to 0.76m due to increase in conversion from 0 to 0.9. the increase in length resulted to increase in volume of the reactor and decrease in the rate of reaction values. The volume of the reactor is a function of length and rate of reaction.

b) *Diameter of Reactor with Conversion*

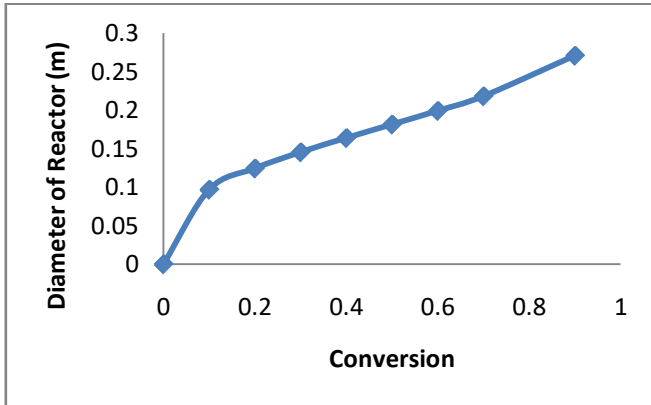


Figure 2: Plot of Diameter of Reactor versus Conversion

Similarly, figure 2 demonstrates the variation of the diameter the variation of the diameter of the reactor for the production of formaldehyde with conversion. The relationship is such that the length increases with increase in conversion and results to values such that when $D=0$, $X_A=0$ and $D=0.27\text{m}$, $X_A=0.9$. since the volume of reactor increases, the length and diameter of the reactor too increases to achieved the production of ethylene oxide and proper sizing of the reactor.

c) *Space Time with Conversion*

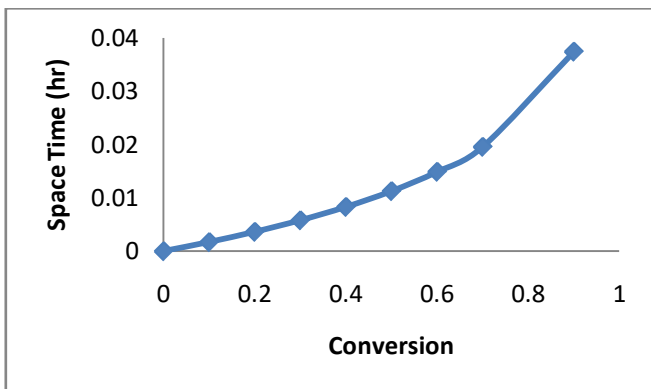


Figure 3: Profile of Space Time of the Reactor versus Conversion

Figure 3 depicts the variation of space time of reactor varying with conversion. The profile of the space time is exponentially increasing with conversion starting from 0-0.035hr when $X_A=0$ -0.9 respectively. Space time is defined as the time taken for one reactor feed volume converted to product. From the results, the

space time values are very small meaning the reaction is a fast one. Increasing the space time values, leads to increase in the value of the reactor and higher yields of the product formed.

d) *Space Velocity with Conversion*

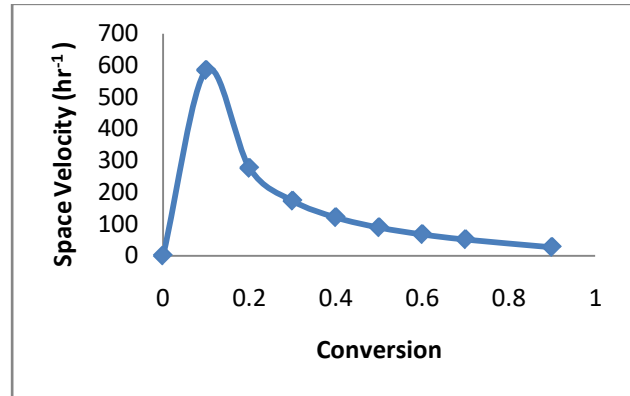


Figure 4: Graph of Space Velocity versus Conversion

Figure 4 shows the graph of space velocity varying with conversion. The universe of space time gives the space velocity's values. The space velocity's values are higher and increases from 0-600hr⁻¹ when conversion increases too from 0-0.1 and then drops exponentially from 600-10hr⁻¹ when conversion increases from 0.1-0.9. The space velocity should be reduced to achieve higher yield at lower cost as shown from the profile plot.

e) *Volume of Reactor with Conversion*

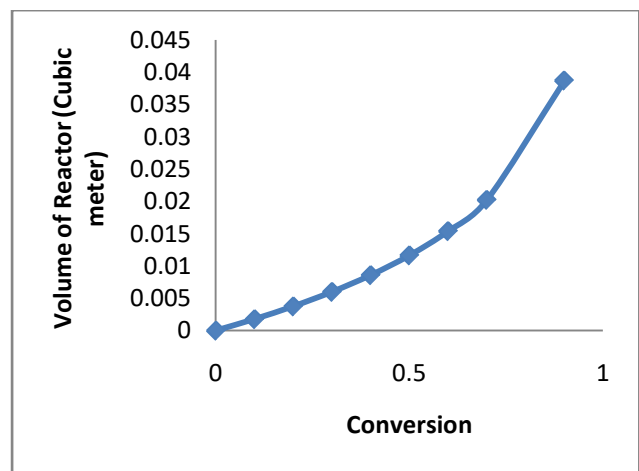


Figure 5: Variation of Volume of Plug Flow Reactor versus Conversion

Figure 5 depicts the variation of volume of plug flow reactor for formaldehyde production from methane and oxygen. The volume increases exponentially from 0m³ to 0.038m³ as conversion too increases from 0-0.9. The increase in volume is achieved as a result of decrease in the rate values.

VI. CONCLUSION

The design of a 10,000 ton/yr Formaldehyde plant has been executed. The design considered first the material balance of the plant using the principles of conservation of mass which states that for steady state process the inflow of mass equals the outflow of mass, hence the mass balance of each unit/equipment was extensively evaluated, the principles of conservation of energy which states that outflow of energy equals inflow of energy for a steady state process was applied to evaluate the flow of energy for each stream. The design also considered other aspect such as equipment sizing/design specification, mechanical design, costing and economic evaluation, instrumentation and process control, layout, safety and environmental consideration and finally Hysys design simulation. Comparison of the material balance results between manual calculation and Aspen Hysys simulation and the highest difference was 0.8% for the energy balance result the difference between the manual calculation and Aspen Hysys simulation was 0.5% for the sizing results, the highest difference between the manual calculation and Aspen Hysys simulation was 0.3%.

Mechanical design to determine the thickness of vessels to withstand pressure was also considered as we as adding corrosion allowance. A detailed cost estimation and economic evaluation was analyzed to determine the profitability of the plant before setting up and it is given in the appendix.

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APPENDIX

Unit operation

Name	Equipment Cost [USD]	Installed Cost [USD]	Equipment Weight [LBS]	Installed Weight [LBS]	Utility Cost [USD/HR]
CSTR-100	43900	174300	3200	15911	0
E-100	23500	121600	2700	11110	17.982
K-10	835600	1034500	12900	40584	8.67225
E-101	7700	48500	270	4478	0
V-100	23800	83300	7000	23244	0
CRV-100	0	0	0	0	0
MIX-100	0	0	0	0	0

Summary

Name	Summary
Total Capital Cost [USD]	4890900
Total Operating Cost [USD/Year]	1917740
Total Raw Materials Cost [USD/Year]	0
Total Product Sales [USD/Year]	0
Total Utilities Cost [USD/Year]	261300
Desired Rate of Return [Percent/Year]	20
P.O.Period [Year]	0
Equipment Cost [USD]	934500
Total Installed Cost [USD]	1462200

Utilities

Name	Fluid	Rate	Rate Units	Cost per Hour	Cost Units
Electricity		152.598	KW	11.826345	USD/H
Cooling Water	Water	0.14985	MMGAL/H	17.982	USD/H

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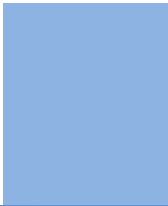
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Acknowledgments

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The following is the official style and template developed for publication of a research paper. Authors are not required to follow this style during the submission of the paper. It is just for reference purposes.



Manuscript Style Instruction (Optional)

- Microsoft Word Document Setting Instructions.
- Font type of all text should be Swis721 Lt BT.
- Page size: 8.27" x 11", left margin: 0.65, right margin: 0.65, bottom margin: 0.75.
- Paper title should be in one column of font size 24.
- Author name in font size of 11 in one column.
- Abstract: font size 9 with the word "Abstract" in bold italics.
- Main text: font size 10 with two justified columns.
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- First character must be three lines drop-capped.
- The paragraph before spacing of 1 pt and after of 0 pt.
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- The names of first main headings (Heading 1) must be in Roman font, capital letters, and font size of 10.
- The names of second main headings (Heading 2) must not include numbers and must be in italics with a font size of 10.

Structure and Format of Manuscript

The recommended size of an original research paper is under 15,000 words and review papers under 7,000 words. Research articles should be less than 10,000 words. Research papers are usually longer than review papers. Review papers are reports of significant research (typically less than 7,000 words, including tables, figures, and references)

A research paper must include:

- a) A title which should be relevant to the theme of the paper.
- b) A summary, known as an abstract (less than 150 words), containing the major results and conclusions.
- c) Up to 10 keywords that precisely identify the paper's subject, purpose, and focus.
- d) An introduction, giving fundamental background objectives.
- e) Resources and techniques with sufficient complete experimental details (wherever possible by reference) to permit repetition, sources of information must be given, and numerical methods must be specified by reference.
- f) Results which should be presented concisely by well-designed tables and figures.
- g) Suitable statistical data should also be given.
- h) All data must have been gathered with attention to numerical detail in the planning stage.

Design has been recognized to be essential to experiments for a considerable time, and the editor has decided that any paper that appears not to have adequate numerical treatments of the data will be returned unrefereed.

- i) Discussion should cover implications and consequences and not just recapitulate the results; conclusions should also be summarized.
- j) There should be brief acknowledgments.
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The full postal address of any related author(s) must be specified.

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The abstract is the foundation of the research paper. It should be clear and concise and must contain the objective of the paper and inferences drawn. It is advised to not include big mathematical equations or complicated jargon.

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A major lynchpin of research work for the writing of research papers is the keyword search, which one will employ to find both library and internet resources. Up to eleven keywords or very brief phrases have to be given to help data retrieval, mining, and indexing.

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One should start brainstorming lists of potential keywords before even beginning searching. Think about the most important concepts related to research work. Ask, "What words would a source have to include to be truly valuable in a research paper?" Then consider synonyms for the important words.

It may take the discovery of only one important paper to steer in the right keyword direction because, in most databases, the keywords under which a research paper is abstracted are listed with the paper.

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Numerical methods used should be transparent and, where appropriate, supported by references.

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Authors must list all the abbreviations used in the paper at the end of the paper or in a separate table before using them.

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Authors are advised to submit any mathematical equation using either MathJax, KaTeX, or LaTeX, or in a very high-quality image.

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1. Choosing the topic: In most cases, the topic is selected by the interests of the author, but it can also be suggested by the guides. You can have several topics, and then judge which you are most comfortable with. This may be done by asking several questions of yourself, like "Will I be able to carry out a search in this area? Will I find all necessary resources to accomplish the search? Will I be able to find all information in this field area?" If the answer to this type of question is "yes," then you ought to choose that topic. In most cases, you may have to conduct surveys and visit several places. Also, you might have to do a lot of work to find all the rises and falls of the various data on that subject. Sometimes, detailed information plays a vital role, instead of short information. Evaluators are human: The first thing to remember is that evaluators are also human beings. They are not only meant for rejecting a paper. They are here to evaluate your paper. So present your best aspect.

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3. Ask your guides: If you are having any difficulty with your research, then do not hesitate to share your difficulty with your guide (if you have one). They will surely help you out and resolve your doubts. If you can't clarify what exactly you require for your work, then ask your supervisor to help you with an alternative. He or she might also provide you with a list of essential readings.

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12. Know what you know: Always try to know what you know by making objectives, otherwise you will be confused and unable to achieve your target.

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Verbs have to be in agreement with their subjects. In a research paper, do not start sentences with conjunctions or finish them with prepositions. When writing formally, it is advisable to never split an infinitive because someone will (wrongly) complain. Avoid clichés like a disease. Always shun irritating alliteration. Use language which is simple and straightforward. Put together a neat summary.

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- Write your paper in the form which is presented in the guidelines using the template.
- Please note the criteria peer reviewers will use for grading the final paper.

Final points:

One purpose of organizing a research paper is to let people interpret your efforts selectively. The journal requires the following sections, submitted in the order listed, with each section starting on a new page:

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This will provide understanding of the data and projections as to the implications of the results. The use of good quality references throughout the paper will give the effort trustworthiness by representing an alertness to prior workings.

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- Use paragraphs to split each significant point (excluding the abstract).
- Align the primary line of each section.
- Present your points in sound order.
- Use present tense to report well-accepted matters.
- Use past tense to describe specific results.
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Write your summary when your paper is completed because how can you write the summary of anything which is not yet written? Wealth of terminology is very essential in abstract. Use comprehensive sentences, and do not sacrifice readability for brevity; you can maintain it succinctly by phrasing sentences so that they provide more than a lone rationale. The author can at this moment go straight to shortening the outcome. Sum up the study with the subsequent elements in any summary. Try to limit the initial two items to no more than one line each.

Reason for writing the article—theory, overall issue, purpose.

- Fundamental goal.
- To-the-point depiction of the research.
- Consequences, including definite statistics—if the consequences are quantitative in nature, account for this; results of any numerical analysis should be reported. Significant conclusions or questions that emerge from the research.

Approach:

- Single section and succinct.
- An outline of the job done is always written in past tense.
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The introduction should "introduce" the manuscript. The reviewer should be presented with sufficient background information to be capable of comprehending and calculating the purpose of your study without having to refer to other works. The basis for the study should be offered. Give the most important references, but avoid making a comprehensive appraisal of the topic. Describe the problem visibly. If the problem is not acknowledged in a logical, reasonable way, the reviewer will give no attention to your results. Speak in common terms about techniques used to explain the problem, if needed, but do not present any particulars about the protocols here.

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Use past tense except for when referring to recognized facts. After all, the manuscript will be submitted after the entire job is done. Sort out your thoughts; manufacture one key point for every section. If you make the four points listed above, you will need at least four paragraphs. Present surrounding information only when it is necessary to support a situation. The reviewer does not desire to read everything you know about a topic. Shape the theory specifically—do not take a broad view.

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This part is supposed to be the easiest to carve if you have good skills. A soundly written procedures segment allows a capable scientist to replicate your results. Present precise information about your supplies. The suppliers and clarity of reagents can be helpful bits of information. Present methods in sequential order, but linked methodologies can be grouped as a segment. Be concise when relating the protocols. Attempt to give the least amount of information that would permit another capable scientist to replicate your outcome, but be cautious that vital information is integrated. The use of subheadings is suggested and ought to be synchronized with the results section.

When a technique is used that has been well-described in another section, mention the specific item describing the way, but draw the basic principle while stating the situation. The purpose is to show all particular resources and broad procedures so that another person may use some or all of the methods in one more study or referee the scientific value of your work. It is not to be a step-by-step report of the whole thing you did, nor is a methods section a set of orders.

Materials:

Materials may be reported in part of a section or else they may be recognized along with your measures.

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- Describe the method entirely.
- To be succinct, present methods under headings dedicated to specific dealings or groups of measures.
- Simplify—detail how procedures were completed, not how they were performed on a particular day.
- If well-known procedures were used, account for the procedure by name, possibly with a reference, and that's all.

Approach:

It is embarrassing to use vigorous voice when documenting methods without using first person, which would focus the reviewer's interest on the researcher rather than the job. As a result, when writing up the methods, most authors use third person passive voice.

Use standard style in this and every other part of the paper—avoid familiar lists, and use full sentences.

What to keep away from:

- Resources and methods are not a set of information.
- Skip all descriptive information and surroundings—save it for the argument.
- Leave out information that is immaterial to a third party.

Results:

The principle of a results segment is to present and demonstrate your conclusion. Create this part as entirely objective details of the outcome, and save all understanding for the discussion.

The page length of this segment is set by the sum and types of data to be reported. Use statistics and tables, if suitable, to present consequences most efficiently.

You must clearly differentiate material which would usually be incorporated in a study editorial from any unprocessed data or additional appendix matter that would not be available. In fact, such matters should not be submitted at all except if requested by the instructor.



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- o Sum up your conclusions in text and demonstrate them, if suitable, with figures and tables.
- o In the manuscript, explain each of your consequences, and point the reader to remarks that are most appropriate.
- o Present a background, such as by describing the question that was addressed by creation of an exacting study.
- o Explain results of control experiments and give remarks that are not accessible in a prescribed figure or table, if appropriate.
- o Examine your data, then prepare the analyzed (transformed) data in the form of a figure (graph), table, or manuscript.

What to stay away from:

- o Do not discuss or infer your outcome, report surrounding information, or try to explain anything.
- o Do not include raw data or intermediate calculations in a research manuscript.
- o Do not present similar data more than once.
- o A manuscript should complement any figures or tables, not duplicate information.
- o Never confuse figures with tables—there is a difference.

Approach:

As always, use past tense when you submit your results, and put the whole thing in a reasonable order.

Put figures and tables, appropriately numbered, in order at the end of the report.

If you desire, you may place your figures and tables properly within the text of your results section.

Figures and tables:

If you put figures and tables at the end of some details, make certain that they are visibly distinguished from any attached appendix materials, such as raw facts. Whatever the position, each table must be titled, numbered one after the other, and include a heading. All figures and tables must be divided from the text.

Discussion:

The discussion is expected to be the trickiest segment to write. A lot of papers submitted to the journal are discarded based on problems with the discussion. There is no rule for how long an argument should be.

Position your understanding of the outcome visibly to lead the reviewer through your conclusions, and then finish the paper with a summing up of the implications of the study. The purpose here is to offer an understanding of your results and support all of your conclusions, using facts from your research and generally accepted information, if suitable. The implication of results should be fully described.

Infer your data in the conversation in suitable depth. This means that when you clarify an observable fact, you must explain mechanisms that may account for the observation. If your results vary from your prospect, make clear why that may have happened. If your results agree, then explain the theory that the proof supported. It is never suitable to just state that the data approved the prospect, and let it drop at that. Make a decision as to whether each premise is supported or discarded or if you cannot make a conclusion with assurance. Do not just dismiss a study or part of a study as "uncertain."

Research papers are not acknowledged if the work is imperfect. Draw what conclusions you can based upon the results that you have, and take care of the study as a finished work.

- o You may propose future guidelines, such as how an experiment might be personalized to accomplish a new idea.
- o Give details of all of your remarks as much as possible, focusing on mechanisms.
- o Make a decision as to whether the tentative design sufficiently addressed the theory and whether or not it was correctly restricted. Try to present substitute explanations if they are sensible alternatives.
- o One piece of research will not counter an overall question, so maintain the large picture in mind. Where do you go next? The best studies unlock new avenues of study. What questions remain?
- o Recommendations for detailed papers will offer supplementary suggestions.



Approach:

When you refer to information, differentiate data generated by your own studies from other available information. Present work done by specific persons (including you) in past tense.

Describe generally acknowledged facts and main beliefs in present tense.

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	A-B	C-D	E-F
Abstract	Clear and concise with appropriate content, Correct format. 200 words or below	Unclear summary and no specific data, Incorrect form Above 200 words	No specific data with ambiguous information Above 250 words
Introduction	Containing all background details with clear goal and appropriate details, flow specification, no grammar and spelling mistake, well organized sentence and paragraph, reference cited	Unclear and confusing data, appropriate format, grammar and spelling errors with unorganized matter	Out of place depth and content, hazy format
Methods and Procedures	Clear and to the point with well arranged paragraph, precision and accuracy of facts and figures, well organized subheads	Difficult to comprehend with embarrassed text, too much explanation but completed	Incorrect and unorganized structure with hazy meaning
Result	Well organized, Clear and specific, Correct units with precision, correct data, well structuring of paragraph, no grammar and spelling mistake	Complete and embarrassed text, difficult to comprehend	Irregular format with wrong facts and figures
Discussion	Well organized, meaningful specification, sound conclusion, logical and concise explanation, highly structured paragraph reference cited	Wordy, unclear conclusion, spurious	Conclusion is not cited, unorganized, difficult to comprehend
References	Complete and correct format, well organized	Beside the point, Incomplete	Wrong format and structuring



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