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A Project Report on

Process Simulation of Distillation Column Using Aspen HYSYS

Submitted by,

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A Report submitted to MIT Academy of Engineering, Alandi(D), Pune, An Autonomous Institute Affiliated to Savitribai Phule Pune University in partial fulfillment of the requirements of

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CERTIFICATE

It is hereby certified that the work which is being presented in the B-TECH Project Report entitled "**Process Simulation of Distillation Column Using Aspen HYSYS**", in partial fulfillent of the requirements for the award of the Bachelor of Technology in Chemical engineering. And submitted to the **School of Chemical Engineering** of **MIT Academy of Engineering,Alandi(D), Pune, Affiliated to Savitribai Phule Pune University (SPPU),Pune**, is an authentic record of work carried out during Academic Year **2022– 2023**,under the supervision of **Dr. Sandeep Shewale School of Chemical Engineering.**

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DECLARATION

We the under signed so lemnly declare that the project report is based on our own work carried out during the course of our study under the super vision of Dr Sandeep Shewale

We assert the statements made and conclusions drawn are an outcome of our project work. We further certify that

1. The work contained in there port is original and has been done by us under the general supervision of our supervisor.
2. The work has not been submitted to any other Institution for any other degree /diploma/certificate in this Institute/University or any other Institute/University of India or abroad.
3. We have followed the guide lines provided by the Institute inwriting the report.
4. Whenever we have used materials (data, theoretical analysis, and text) from other sources, we have given due credit to them in the text of the report and giving their details in the references.

Om Birar **(PRN 202202050031)**

Abstract

The simulation and optimization of distillation columns are fundamental in the field of chemical engineering, particularly for the separation of chemical components in refinery and petrochemical industries. This report focuses on the steady-state simulation of a distillation column using **Aspen HYSYS** , a widely adopted process modeling software. The study involves the separation of a binary mixture, specifically propane and propylene, employing a rigorous column model configured with 94 theoretical stages, a total condenser, and a reboiler.

The primary objective of this work is to evaluate the operational parameters and performance characteristics of the column under defined conditions, including feed stage location, operating pressures, and reflux ratio. A systematic approach was adopted beginning with component and property method selection, followed by stream and equipment configuration, column internals setup, and ultimately, simulation convergence and analysis.

Key simulation parameters such as condenser pressure (19.31 bar), reboiler pressure (20.68 bar), feed at stage 47, and a high reflux ratio were used to ensure adequate separation efficiency. The results were analyzed through tray-by-tray pressure and temperature profiles, as well as net vapor and liquid flow rates across each stage. A graphical representation of pressure versus tray number demonstrated a consistent and realistic pressure gradient throughout the column, confirming the thermodynamic validity of the model.

The findings underscore the effectiveness of Aspen HYSYS as a powerful tool for simulating complex unit operations. Furthermore, the results highlight the importance of precise input parameter selection to achieve convergence and desired separation specifications. This simulation serves as a basis for further optimization studies, energy analysis, and potential scale-up for industrial applications. Ultimately, this project not only reinforces the theoretical aspects of distillation but also enhances practical modeling skills essential for process engineers.

Acknowledgment

We are taken efforts in this project. However, it would not have been possible without the kind support and help of many individuals and organizations. We would like to extend our sincere thanks to all of them. We are highly indebted to Dr Sandip Shewale and for their guidance and constant supervision as well as for providing necessary information regarding the project also for their support in completing the project. Our thanks and appreciations also go to my colleague in developing the project and people who have willingly helped me out with their abilities. We deeply express our sincere thanks to our Dean of School of Chemical Engineering for encouraging and allowing us to present the project on the topic “Process simulation of Distillation Colum using Aspen Hysys at our department premises for the partial fulfillment of the requirements. We take this opportunity to thank all our lecturers who have directly or indirectly helped our project.

Contents

Chapter1

Introduction

1. Introduction

Distillation is one of the most critical and widely used separation processes in the chemical process industry. It plays a vital role in separating components of a mixture based on their volatilities by utilizing differences in boiling points. From crude oil refining to petrochemical production, the efficiency and reliability of distillation columns are essential for the economic and technical feasibility of industrial operations. Given its complexity, the design, optimization, and control of distillation columns require precise engineering tools capable of modeling real-world behavior with high fidelity.

In this context, **Aspen HYSYS**, a process simulation software developed by AspenTech, is an industry-standard tool used for modeling steady-state and dynamic processes. It enables chemical engineers to simulate a wide variety of unit operations, analyze thermodynamic behavior, and assess the performance of process designs before actual plant implementation. The simulation of distillation columns in Aspen HYSYS provides a comprehensive view of process variables such as temperature, pressure, vapor and liquid flow rates, composition, and energy consumption, making it an invaluable resource for both design and educational purposes.

This project specifically focuses on the steady-state simulation of a **binary distillation column** used to separate **propylene and propane**, two important hydrocarbons in petrochemical manufacturing. The simulation involves a **94-stage distillation column** with a **total condenser** and a **reboiler**, with the feed introduced at the 47th stage. The thermodynamic behavior is modeled using the **Soave-Redlich-Kwong (SRK)** property package, which is well-suited for light hydrocarbon systems.

The primary purpose of this simulation is to evaluate the separation efficiency of the column, assess operational conditions such as feed temperature, pressure profile, and reflux ratio, and to determine whether the desired product specifications can be achieved. Tray-by-tray data such as temperature and pressure distributions are analyzed to verify the accuracy and feasibility of the model. The simulation also helps in understanding how various parameters influence the separation and how energy usage can be minimized while maximizing product purity.

Through this project, users gain hands-on experience in building a distillation model from scratch, modifying parameters, interpreting results, and using the insights gained to improve process performance. The ability to replicate industrial scenarios virtually helps reduce design errors, improve safety, and optimize capital and operational costs.

In summary, the use of Aspen HYSYS in this study bridges the gap between theoretical distillation concepts and their practical application, empowering engineers to make data-driven decisions in process design and optimization.

1.1 Project Idea

The central idea of this project is to simulate and analyze a **multistage distillation column** using **Aspen HYSYS** to understand the thermodynamic behavior, operational parameters, and efficiency of separation for a binary mixture. The project is designed to bridge the gap between theoretical knowledge and practical implementation in chemical process design, control, and optimization.

This simulation-based project targets one of the most vital unit operations in chemical engineering — distillation — and applies advanced process simulation tools to visualize and optimize it. The focus is not only on understanding the separation of components based on their volatilities but also on exploring how different design and operating conditions affect the performance of the column.

Why Aspen HYSYS?

Aspen HYSYS is widely recognized in academia and industry for its ability to simulate and optimize chemical processes with great accuracy. Using this tool:

- Engineers can design distillation columns with varying degrees of complexity.
- Process variables like tray temperatures, pressures, flowrates, and energy requirements can be monitored and tuned.
- Accurate thermodynamic property packages (such as **SRK**) enable realistic simulation results.
- The platform allows quick scenario analysis, design optimization, and process troubleshooting.

Scope of the Project:

- **Feed System**: Binary hydrocarbon mixture with known feed composition, pressure, and temperature.
- **Column Design**: Includes a total condenser, reboiler, and 94 equilibrium stages.
- **Simulation Analysis**: Includes convergence analysis, temperature and pressure profiling, energy consumption evaluation, and product specification validation.
- **Outputs**: Graphical plots (e.g., pressure vs. stage), tray-by-tray data, column schematic, and stream tables.

Chapter 2

Literature Review

- **Paper-1**

TITLE: Fundamental Modeling and Simulation of a Binary Continuous Distillation Column

JOURNALNAME: IEEE ICIAS Conference

AUTHOR'S NAME: H. S. Truong, I. Ismail, R. Razali

CONCLUSION:
In simpler terms, this paper developed a model to understand how a system that separates liquid mixtures into different components works, especially when there are changes in the feed. The study shows that the composition changes behave like a first-order system—meaning the response is smooth and predictable. The effect of changing the feed composition is stronger than just changing the feed flow rate.

Small changes in flow rates produce predictable changes, but larger changes deviate from the simple model. This means accurate modeling is crucial, especially for control purposes. Future work will involve testing the model in real conditions and developing better ways to control the system when more factors come into play.

- **Paper- 2**

TITLE: Rigorous Design of Complex Distillation Columns Using Process Simulators and the Particle Swarm Optimization Algorithm

JOURNALNAME: Industrial & Engineering Chemistry Research

AUTHOR'S NAME: J. Javaloyes-Antón, R. Ruiz-Femenia, J. A. Caballero

CONCLUSION:

In simpler terms, the paper proposes a new way to design complex distillation systems more efficiently by combining a commercial process simulator (Aspen Hysys) with a smart search method called Particle Swarm Optimization (PSO). This approach doesn't need detailed mathematical gradients and avoids common issues like getting stuck in bad solutions. It helps determine the best setup (like tray numbers and feed positions) to reduce energy use and cost. The method worked well on several examples and proved flexible, robust, and user-friendly for real-world chemical process design

- **Paper-3**

TITLE: Modeling and Control of Distillation Column in a Petroleum Process.

JOURNALNAME: IEEE Conference on Industrial Electronics and Applications

AUTHOR'S NAME: Vu Trieu Minh

CONCLUSION:

This paper developed and tested a simplified model of a distillation column used in petroleum processing. The aim was to maintain product purity even when the input feed changes. A special control strategy called Model Reference Adaptive Control (MRAC) was applied. Simulations showed that this controller could adjust effectively to disturbances and model mismatches. It confirms that simplified models can guide controller design, and adaptive control methods are practical for managing complex, changing chemical processes

- **Paper-4**

TITLE: Optimal Design of Extractive Distillation Columns — A Systematic Procedure Using a Process Simulator

JOURNALNAME: Chemical Engineering Research and Design

AUTHOR’S NAME: Marcella F. de Figueirêdo, Brenda P. Guedes, João M. M. de Araújo, Luís G. S. Vasconcelos, Romildo P. Brito

CONCLUSION:

This paper presents a smart and simplified method for designing extractive distillation columns using a process simulator. Instead of running many simulations and manually checking results, the authors use a systematic approach that optimizes key variables (like number of stages, feed locations, and solvent flow) in one go. The method reduces time and effort while meeting purity requirements. Using ethanol-water separation as a case study, they show it's possible to design energy-efficient and cost-effective systems more easily.

- **Paper-5**

TITLE: Modeling and Simulation of Mini Batch Distillation Column

JOURNALNAME: IEEE International Conference on Instrumentation, Communications, Information Technology, and Biomedical Engineering

AUTHOR'S NAME: Renny Maulidda, Pranoto H. Rusmin, Arief S. Rohman, Egi M. I. Hidayat, Dimitri Mahayana

CONCLUSION:

This study built a mathematical model of a small-scale batch distillation column used for separating ethanol and water. The model was based on real experimental data and included nonlinear equations that describe the system's behavior. Simulations showed good agreement with real experiments, especially for predicting ethanol purity. The results showed that controlling the reflux valve can significantly affect product quality and processing time. Future improvements could involve adding a controller to automate and enhance distillate purity.

Chapter3

Problem Definition and Scope

3.1 Problem statement

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Goals and Objectives

Objectives of the Project:

1. To model a distillation column for separating a binary mixture (e.g., propane and propylene).
2. To understand the effect of key design parameters like feed stage location, reflux ratio, number of stages, and column pressure.
3. To evaluate the pressure and temperature profiles along the column.
4. To interpret tray-by-tray composition data for assessing separation quality.
5. To use Aspen HYSYS for designing and validating column performance based on industrial standards.

Significance of the Project:

- Develops practical skills in process simulation.
- Demonstrates how energy and separation efficiency can be balanced.
- Lays a strong foundation for future work in distillation control, intensification, and optimization.
- Provides insights into how theoretical distillation concepts translate into real-world industrial applications.

Distillation: Concept and Principle

Distillation is a physical separation process that exploits differences in the **boiling points** of components in a liquid mixture. It is based on the principle that, under given pressure and temperature conditions, each component in a mixture vaporizes to a different extent. By carefully controlling these variables, the more volatile components (lower boiling points) can be separated from the less volatile ones (higher boiling points), thereby achieving purification or fractionation.

At its core, the idea of distillation revolves around **phase equilibrium**. When a liquid mixture is heated, the component with a lower boiling point vaporizes more readily, enriching the vapor phase in that component. Conversely, when this vapor is condensed, it yields a liquid richer in the more volatile component. This principle is applied iteratively in a **distillation column** through a series of vapor–liquid contacts known as **trays or stages**, which allow for continuous separation.

There are two major types of distillation:

1. **Simple (or Flash) Distillation** – A one-stage process suitable for mixtures with widely different boiling points. It is less efficient for complex separations.
2. **Fractional (or Multistage) Distillation** – Involves multiple equilibrium stages in a vertical column, where the feed is introduced, and heat is supplied to drive the separation. This is the type modeled in this simulation.

A typical distillation column consists of the following main components:

- **Condenser:** Located at the top of the column, it condenses rising vapors into liquid.
- **Reflux Drum:** Collects condensed liquid and returns part of it as reflux to maintain separation efficiency.
- **Trays or Packing:** Internals that facilitate vapor-liquid contact and promote equilibrium.
- **Reboiler:** Supplies heat at the bottom to vaporize the liquid, driving the separation upward.
- **Feed Inlet:** The stage at which the mixture to be separated is introduced.

Key operational parameters in distillation include:

- **Reflux Ratio:** The ratio of liquid returned to the column versus that taken off as distillate.
- **Number of Stages:** The number of equilibrium stages or trays required for desired separation.

- **Pressure and Temperature Profiles:** Vary along the column and directly influence separation efficiency.
- **Column Pressure:** Affects the volatility of components and energy requirements.

The **efficiency** of a distillation column depends on several factors including tray design, feed composition, energy input, and control of operating conditions. Industrial distillation columns are optimized to minimize energy consumption while maximizing product purity, often integrating advanced simulation tools like **Aspen HYSYS** for design, control, and optimization.

In this project, we simulate a multistage distillation column for a binary hydrocarbon mixture using Aspen HYSYS, demonstrating the practical application of the distillation principle in chemical process engineering.

Chapter4

Methodology

Methodology for Simulating a Distillation Column in Aspen HYSYS
To simulate the distillation column in Aspen HYSYS, follow these steps:

1. **Create a New Case:** Open Aspen HYSYS and create a new case, selecting the appropriate template (e.g., "Distillation Column").

2. **Define the Fluid Package:** Choose the SRK (Soave-Redlich-Kwong) equation of state as the fluid package, as specified in the problem.

3. **Specify the Feed Stream:** Define the feed stream with the given specifications:
   - Composition: Propane (0.4) and Propene (0.6)
   - Flow rate: 600 (units not specified, likely kg/h or lb/h)
   - Pressure: 2068 (units not specified, likely kPa or psi)

4. **Add the Distillation Column:** Add a distillation column to the simulation, specifying:
   - Number of stages: 94
   - Feed stage: 47
   - Reflux ratio: 16.4
   - Condenser pressure: 280 psi
   - Reboiler pressure: 300 psi
   - V/F (vapor-to-feed ratio): 1

5. Run the Simulation: Run the simulation, ensuring that the column converges.

6. Analyze the Results: Analyze the simulation results, including:

- Column profiles (temperature, pressure, and composition)
- Stream results (flow rates, compositions, and properties)
- Energy balances and duties

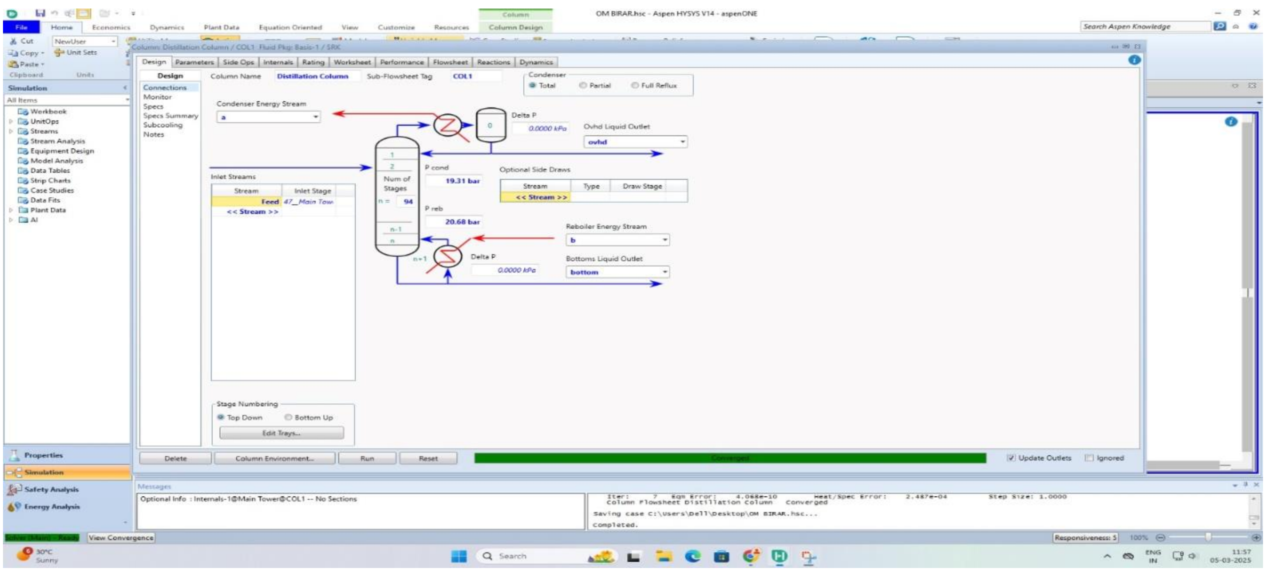
Chapter 6

Results

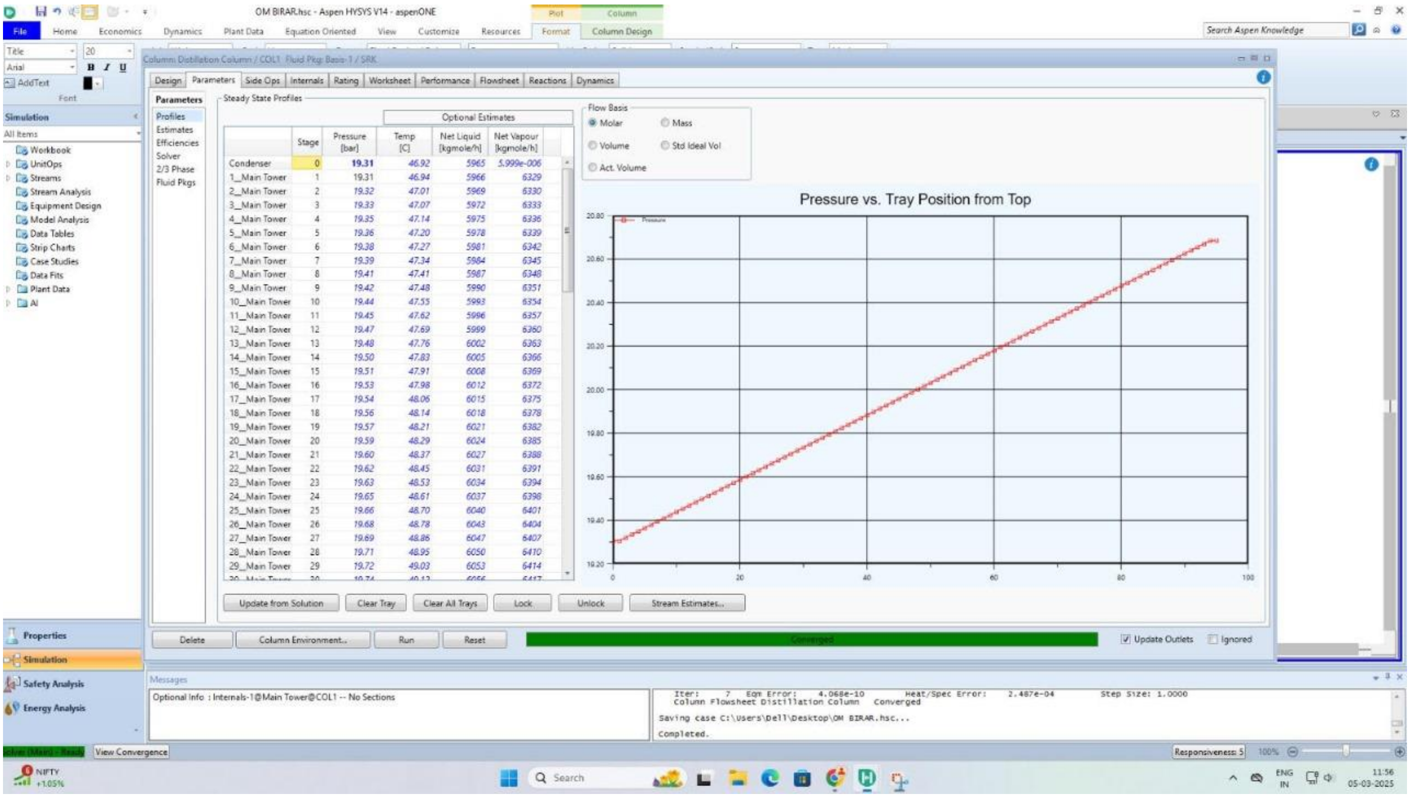
The simulation results indicate a steady-state operation, with the column achieving convergence after seven iterations. Key findings include:

- A high reflux ratio ensures product purity but increases condenser duty.
- Tray temperature profiles indicate effective separation along the column.
- Net liquid and vapor flows across the trays remain consistent, which is essential for stable mass transfer.
- Energy demands at the condenser and reboiler are within design expectations.

The feed placement at stage 47 appears optimal, coinciding with the feed tray's composition requirements for effective splitting.



Actual Simulation



Graph: Shows a linear pressure increase from top (condenser) to bottom (reboiler).

Pressure Range:

Top Tray (Condenser): 19.31 bar

Bottom Tray (Reboiler): 20.68 bar

Tray Temperatures: Gradually increase from top to bottom, typical for distillation:

Top Tray (Stage 1): 46.92°C

Bottom Tray (Stage 94): Estimated around 80+°C

Conclusion

The simulation of a distillation column in Aspen HYSYS provided valuable insights into its operation and design. The selected operating parameters and reflux conditions resulted in effective separation of propane and propylene. The visual outputs and data analysis affirm the column's stability and efficiency. Aspen HYSYS continues to be an invaluable tool for process simulation and optimization in chemical engineering.

References

- **Truong, H. S., Ismail, I., Razali, R.,** *Fundamental Modeling and Simulation of a Binary Continuous Distillation Column*, Proc. of *International Conference on Intelligent and Advanced Systems (ICIAS)*, Universiti Teknologi PETRONAS, Tronoh, MALAYSIA, IEEE, 2010.

- Javaloyes-Antón, J., Ruiz-Femenia, R., Caballero, J. A., *Rigorous Design of Complex Distillation Columns Using Process Simulators and the Particle Swarm Optimization Algorithm*, Proc. of *Industrial & Engineering Chemistry Research*, DOI: 10.1021/ie400918x, American Chemical Society, 2013.

- Vu Trieu Minh, *Modeling and Control of Distillation Column in a Petroleum Process*, Proc. of *5th IEEE Conference on Industrial Electronics and Applications (ICIEA)*, Universiti Teknologi PETRONAS, MALAYSIA, 2010, ISBN: 978-1-4244-5046-6.

- Figueirêdo, M. F., Guedes, B. P., Araújo, J. M. M., Vasconcelos, L. G. S., Brito, R. P., *Optimal Design of Extractive Distillation Columns—A Systematic Procedure Using a Process Simulator*, *Chemical Engineering Research and Design*, Vol. 89, pp. 341–346, 2011, Elsevier, DOI: 10.1016/j.cherd.2010.06.011.

- Maulidda, R., Rusmin, P. H., Rohman, A. S., Hidayat, E. M. I., Mahayana, D., *Modeling and Simulation of Mini Batch Distillation Column*, Proc. of *5th International Conference on Instrumentation, Communications, Information Technology, and Biomedical Engineering (ICICI-BME)*, Bandung, INDONESIA, NOV 6–7, 2017, IEEE, ISBN: 978-1-5386-3455-4.