# Minimizing Energy Consumption in Distillation Column Operations

*CL615-Optimization Term Project*


*Submitted by*

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**Nomenclature**

- F is the feed flow rate (assumed constant).
- $\Delta H_v$ is the latent heat of vaporization (assumed constant).
- $x_D$ is the distillate composition.
- $x_B$ is the bottoms composition.
- $z_F$ is the feed composition (assumed constant).
- R is the reflux ratio.
- $Q_{reb}$ is the energy required for the reboiler
- $Q_{Cond}$. is the energy required for the condenser
- $Q_{Total}$ is the total energy consumed
- $\Delta H_v$ is Latent heat of vaporization
- $D$ is distillate flow rate
- $B$ is bottoms flow rate
- LB means lower bound
- UB means upper bound

## Project Overview

Objective:

The primary objective of this project is to optimize the distillation column operation in a chemical separation process, specifically focusing on minimizing the total energy consumption while achieving the desired product purity. The distillation column is a widely used unit operation in industries like petrochemicals, pharmaceuticals, and food processing for separating mixtures based on differences in volatilities.

The key goals of this project are to minimize energy consumption, achieve the desired product purity, and optimize the design parameters of a distillation column. By reducing the energy required for both reboiler and condenser duties, which are significant components of operating costs, the project aims to lower the operational costs of distillation processes. It also seeks to ensure that the distillate and bottoms products meet specified purity levels, typically around 95% for distillate and 5% for bottoms, which is essential in many industrial applications. Through optimization, the project will determine the optimal reflux ratio, distillate flow rate, and number of stages that strike a balance between energy use and separation efficiency. The ultimate objective is to provide a cost-effective and energy-efficient design for distillation columns, leading to reduced operational costs, a lower carbon footprint, and improved sustainability in industries that rely on distillation technology.

Application:

The optimization techniques developed in this project can be applied in various industries that rely on distillation for separation processes:

1. **Petrochemical Industry:** Optimizing energy use in refinery distillation columns to reduce operational costs, improve separation efficiency, and enhance the production of high-value products like gasoline, diesel, and jet fuel.
2. **Pharmaceutical Industry:** Enhancing the production of active pharmaceutical ingredients by minimizing energy consumption while maintaining strict product purity and meeting regulatory standards.
3. **Food and Beverage Industry:** Reducing energy costs and improving the efficiency of processes such as alcohol distillation and essential oil extraction, which are essential for large-scale production.
4. **Chemical Industry:** Improving the efficiency of chemical separations by optimizing distillation column parameters to lower energy consumption and operational costs.

## Opimization Problem formulation

The objective of the optimization is to minimize the total energy consumption $Q_{Total}$, which consists of two main components: the reboiler duty $Q_{reb}$ and the condenser duty $Q_{Cond}$. These terms depend on three key variables:

- R: Reflux ratio (the ratio of the liquid returned to the column to the liquid taken off as distillate).
- xD: Distillate composition (mole fraction of the more volatile component in the distillate).
- xB: Bottoms composition (mole fraction of the more volatile component in the bottoms).

The total energy consumption:

$$Q_{Total} = Q_{reb} + Q_{Cond}$$

Where:

1. ***Reboiler duty**:*

$$Q_{Reb} = \frac{F\Delta H_v(z_F - x_B)(R+1)}{x_D - x_B}$$

2. **Condenser duty:**

$$Q_{Cond} = \frac{F\Delta H_v(z_F - x_B)R}{x_D - x_B}$$

Decision Variables:

- **Reflux ratio R** (which influences the energy consumption).
- **Distillate composition,** $x_D$ (which should be as pure as possible, but balanced with energy cost).
- **Bottoms composition,** $x_B$ (which should have a lower concentration of the volatile component).

Constraints:

The problem is subject to several constraints to ensure realistic and feasible operating conditions:

- **Distillate composition constraint**: The distillate composition must be at least 0.85 (typically, the distillate should have a higher purity of the more volatile component).
- **Bottoms composition constraint**: The bottoms composition must be less than or equal to 0.15 (this ensures the bottoms have a lower concentration of the more volatile component).

Input parameters:

- Feed flow rate, F = 100 kg/h
- Feed composition (mole fraction of more volatile component) = 0.5

- Latent heat of vaporization = 200 kJ/h

## LB and UB values and its sources

Table1:

| Variable | Lower Bound (LB) | Upper Bound (UB) |
|---|---|---|
| Reflux Ratio (R) | 2.0 | 5.0 |
| Distillate Composition (xD) | 0.9 | 1.0 |
| Bottoms Composition (xB) | 0.0 | 0.10 |

- **Reflux Ratio (R)**
    1. The **lower bound** ensures that there is enough reflux to maintain the desired separation efficiency. A value too low would result in insufficient separation, making it impractical.
    2. The **upper bound** is set to avoid excessive energy consumption. Beyond a certain point, increasing the reflux ratio yields diminishing returns and significantly increases energy costs, which is not economically viable.
- **Distillate Composition (xD)**
    1. The **lower bound** ensures a reasonable level of purity for the distillate. A value below this would be too impure for most practical applications.
    2. The **upper bound** represents the ideal scenario where the distillate is as pure as possible. However, achieving a purity of 1.0 often requires high energy input, making it less practical in real-world scenarios.
- **Bottoms Composition (xB)**
    1. The **lower bound** corresponds to the ideal situation where all the volatile components are removed from the bottoms, leading to maximum separation efficiency.
    2. The **upper bound** ensures that the bottoms composition remains low in the more volatile component while still being realistic. Higher values may indicate insufficient separation in the column, which would reduce process efficiency.

## Assumptions

The following assumptions were made in the optimization problem to simplify and make it more tractable:

- **Constant Latent Heat of Vaporization:** We assumed that the latent heat of vaporization is constant throughout the column, both in the condenser and the reboiler. This implies that the composition and temperature do not significantly change across these sections
- **Ideal Binary Mixture:** The model is based on a binary mixture, assuming ideal behavior in terms of phase equilibrium. This assumes no non-ideal interactions between the components, which can affect the actual phase behavior
- **Constant Reflux Ratio (R):** The model assumes a constant reflux ratio, meaning that the proportion of liquid returned as reflux to the distillate remains fixed throughout the column operation. In practical distillation processes, the optimal reflux ratio may vary with changes in feed composition or operating conditions.
- **Total Condenser and Reboiler:** A total condenser is assumed, where all the vapor entering the condenser is condensed. Similarly, we assume a total reboiler, where all the liquid entering the reboiler is vaporized.
- **Negligible Sensible Heat Effects:** The energy balances for the condenser and reboiler are based solely on the latent heat of vaporization, ignoring sensible heat. This means we assume that temperature changes within the liquid and vapor streams are negligible
- **Negligible Pressure Drop:** The pressure drop across the column is assumed to be negligible, which means that pressure variations across trays do not significantly affect the vapor-liquid equilibrium or energy requirements.
- **Constant Feed Composition:** The feed composition of the mixture is assumed to be constant, and there is no variation in its properties over time.
- **Purity Constraints at Extreme Points:** The purity constraints for the distillate (xD) and bottoms (xB) are set at feasible but extreme values, assuming the column can produce a nearly pure distillate or bottoms, although real systems may not always reach these limits.

These assumptions are made to simplify the problem, ensuring that the optimization process remains manageable and that the results are tractable, but they may not represent the full complexity of a real distillation column.

## Method of Implementation

We used the **SLSQP (Sequential Least Squares Quadratic Programming)** algorithm because:

1. **Nonlinear Handling:** It handles nonlinear objective and constraint functions.
2. **Constraints Support:** It can manage both equality and inequality constraints effectively.
3. **Smooth Optimization:** It works well for continuous, differentiable functions.
4. **Efficient for Medium Problems:** Suitable for small to medium-sized optimization problems with a few decision variables.

We implemented the solution using **Python**, which provides an in-built SLSQP library in the SciPy package, making it easy to apply this optimization method for our problem.
SLSQP is an optimization method that combines quadratic programming with a sequential approach. It works by approximating the objective function and constraints using quadratic terms, making the problem easier to solve iteratively. At each step, SLSQP updates the decision variables by solving a smaller quadratic problem, gradually refining the solution until it converges. The method can handle both equality and inequality constraints, ensuring the solution stays within the defined limits while minimizing the objective function. This iterative approach allows SLSQP to efficiently find the optimal solution while respecting the constraints.

## Model code

The code is available at the GitHub link: [https://github.com/uddiptta15/Minimizing-Energy-Consumption-in-Distillation-Column-Operations](https://github.com/uddiptta15/Minimizing-Energy-Consumption-in-Distillation-Column-Operations)

## Optimal Results and Verification

The optimization results suggest that a reflux ratio of 2.01, with a 97% distillate composition and 7% bottoms composition, minimizes the total energy consumption to around 47789.13 kJ/h, which is a reasonable outcome for a distillation column where the goal is to minimize energy usage while achieving the desired product purities. Distillate compositions of around 0.97 and bottoms compositions of 0.08 are typical in distillation processes requiring high purity separation.
In the process of minimizing energy, the model approaches the minimum reflux condition, where the reflux ratio is as low as possible for the desired separation. However, operating at this minimum reflux ratio is generally impractical because it would require an infinite number of stages to maintain the separation quality. This means that while our model achieves a low energy value, this condition cannot be implemented in a real column without significant trade-offs in design. Practical distillation columns operate slightly above the minimum reflux ratio, balancing energy efficiency with a feasible number of stages for construction and operation.

## Sensitivity Analysis

To perform a sensitivity analysis, we will examine how changes in input parameters and decision variables influence the optimization results. We will vary these parameters over a range of plausible values and observe the effects on the total energy consumption-

$$Q_{Total} = \frac{F\Delta H_v(z_F - x_B)(R+1)}{x_D - x_B} + \frac{F\Delta H_v(z_F - x_B)R}{x_D - x_B}$$

The total energy consumed in the distillation process is influenced by parameters like feed flow rate (F) and latent heat of vaporization (ΔHv). However, changing these values doesn't affect the optimal decision variables (reflux ratio, distillate, and bottoms compositions). These variables are optimized to minimize energy consumption for the given system, so while the total energy increases with F and ΔHv, the optimal values of reflux ratio (R), distillate composition (xD), and bottoms composition (xB) remain unchanged.

The reflux ratio (R) is directly proportional to energy consumption, meaning that as R increases, energy usage also rises. The total energy consumed is inversely correlated with the distillate composition (xD), indicating that higher energy consumption leads to greater distillate purity. However, the relationship with bottom composition (xB) is more complex, as xB appears in both the numerator and denominator, making its effect on energy consumption harder to predict directly.

Fig1:

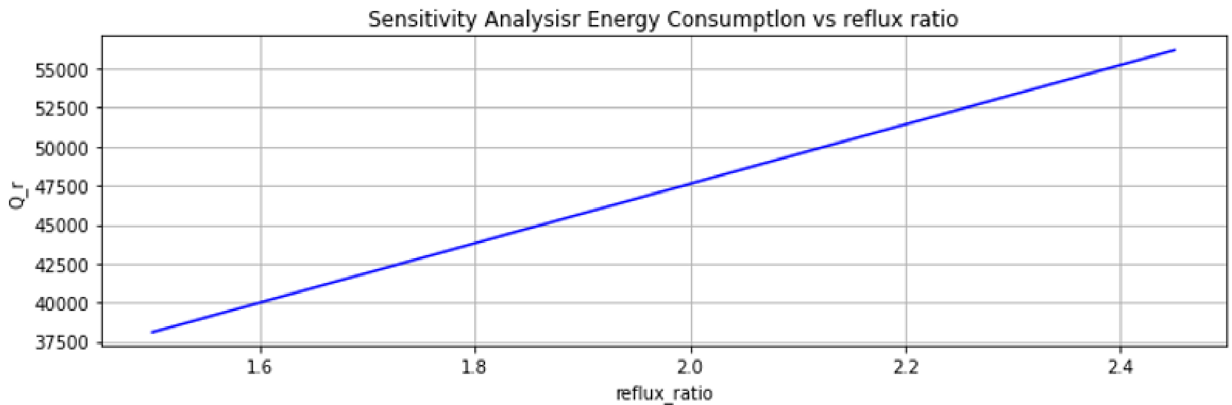



Fig2:

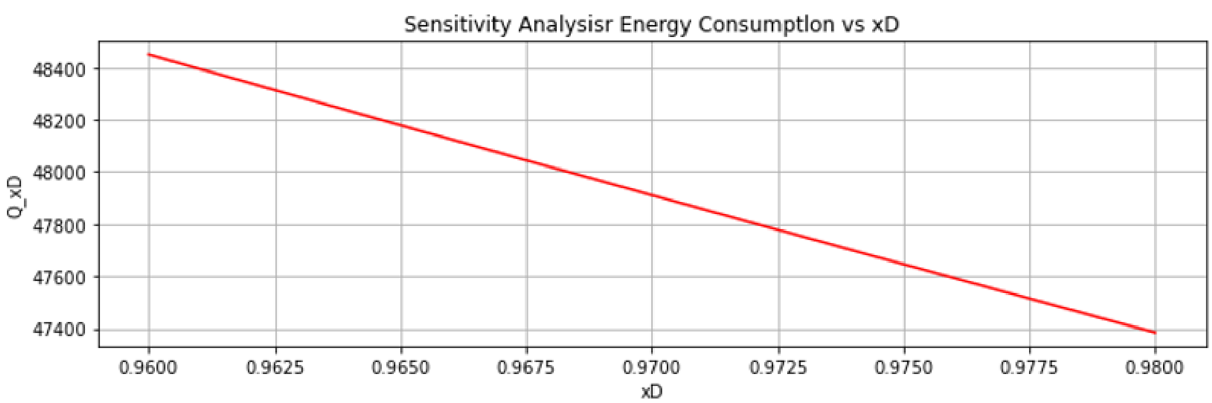
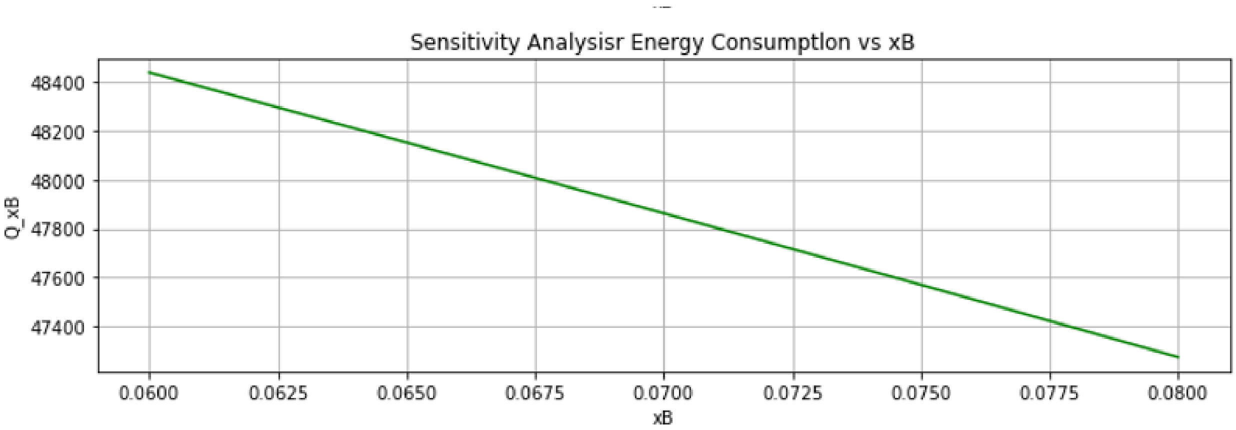


Fig3:




The graph clearly shows that energy consumption increases sharply with an increase in the reflux ratio, highlighting a direct relationship between these two variables. On the other hand, both distillate composition (xD) and bottom composition (xB) are negatively correlated with energy consumption. This suggests that less energy is required to achieve higher distillate purity, and the energy demand decreases as the composition of the distillate or the bottom product improves. These findings indicate that optimizing the reflux ratio and carefully controlling the distillate and bottom compositions can lead to more efficient energy usage in the process.

## Annexure

- **Condenser and Reboiler Heat Duty:**

  To derive the condenser and reboiler heat duties in terms of the distillate flow rate D, the reflux ratio R, and the latent heat of vaporization $\Delta H_v$, let's proceed through material and energy balances around the column-

  $$F = D + B$$

  Component Mass Balance-

  $$F \cdot z_F = D \cdot x_D + B \cdot x_B$$

  Expressing D and B-

  $$B = F - D$$

  Substitute B into the component mass balance:

  $$F \cdot z_F = D \cdot x_D + (F - D) \cdot x_B$$

  Expanding and simplifying:

  $$F \cdot z_F = D \cdot (x_D - x_B) + F \cdot x_B$$

  Solving for D:

  $$D = F \cdot \frac{z_F - x_B}{(x_D - x_B)}$$

Vapor Flow Rate at the Top (V) in Terms of D and R:

$$L = R \cdot D$$

$$V = D + L = D + R \cdot D = D(1 + R)$$

Condenser Heat Duty:

$$Q_C = V \cdot \Delta H_v$$

Substitute $V = D(1 + R)$:

$$Q_{Cond} = D(1 + R) \cdot \Delta H_v = Q_{Cond} = \frac{F\Delta H_v(z_F - x_B)R}{x_D - x_B}$$

However, if the condenser duty is defined in terms of the reflux stream only (which is often the case in simplified models), we consider only the amount of vapor required to produce the reflux. This approach assumes the following simplified form:

$$Q_C = D \cdot R \cdot \Delta H_v$$

Reboiler Heat Duty:

In the reboiler, the heat duty $Q_{Reb}$ is required to generate the vapor that goes up the column. From the material balances, the boilup rate $V_b$ at the reboiler must equal the vapor rate V at the top of the column:

$$V_b = D(1 + R)$$

So, $$Q_{Reb} = V_b \Delta H_v = D(1 + R) \cdot \Delta H_v = \frac{F\Delta H_v(z_F - x_B)(R+1)}{x_D - x_B}$$

## References


- PRINCIPLES OF MASS TRANSFER AND SEPARATION PROCESSES, Binay K. Dutta
- "Optimal Energy Utilization in Distillation Columns." Shah, P., & Agrawal, R. (2010)
- "Simulation-based optimization of distillation processes using an extended cutting plane algorithm" Juan Javaloyes-Anton, Jan Kronqvist, José A. Caballero