# REPORT-

## *Topic- Advances in supercritical carbon dioxide technologies*


## Team Members-(Group 2)

1. Butle Vedika Ashirwad [230008012]
2. Mannan Milind Mahajan [230008020]
3. Mohak Dadhich [230008023]


## INTRODUCTION

The increasing demand for ultrapure bioactive compounds in the pharmaceutical, nutraceutical, and food industries has led to the exploration of advanced separation techniques. Traditional solvent-based extraction methods often result in product contamination, high energy consumption, and environmental concerns. Supercritical fluid extraction **(SFE)** using supercritical carbon dioxide **(SC-$CO_2$)** presents a sustainable alternative, offering high selectivity, faster mass transfer, and solvent-free product recovery

## KEY EQUATIONS

**1. Equation of State (EOS) for Supercritical Fluids-**

Peng-Robinson EOS- P=(R*T/(V−b))-(a/(V^2+2bV-b^2))
Where: P = pressure; T = temperature; V = molar volume; a,b = substance-specific parameters

**2. Solubility of Solutes in Supercritical $CO_2$-**

Chrastil's Solubility Correlation-
S=k · ρ ^m exp(-c/T)
Where: S = solubility; ρ = fluid density; k,m,c = empirical constants

**3. Mass Transfer in Supercritical Extraction-**
Fick's Law of Diffusion-

$J = -D * dc/dx$
Where: J = diffusive  flux; D = diffusion coefficient; C = concentration; x = distance

**4. Reynolds & Sherwood Number for Mass Transfer Coefficients-**

Reynold's No.-  $Re = (\rho v d)/\mu$

Sherwood's No.-  $Sh = Kd/D$
Where: K = mass transfer coefficient; d = particle diameter; D = diffusion coefficient

# PROCESS SIMULATION

The process includes two primary stages: **extraction and separation**.
The simulation section involves implementing and analyzing a separation process using Python in Google Colab. (reference)
It primarily focuses on **liquid-liquid extraction using supercritical CO2 as a solvent** and utilizes **the Kremser equation** to determine stage-wise solute transfer and efficiency.

**Objectives**

- To simulate a counter-current liquid-liquid extraction system.
- To analyze the number of ideal stages required for a specified separation.
- To explore the effect of parameters like distribution coefficient, flow rates, and extraction efficiency

**Kremser Equation-Based Approach**:

- The Kremser equation is used to calculate the number of theoretical stages required.

**Conclusions from the Simulation**

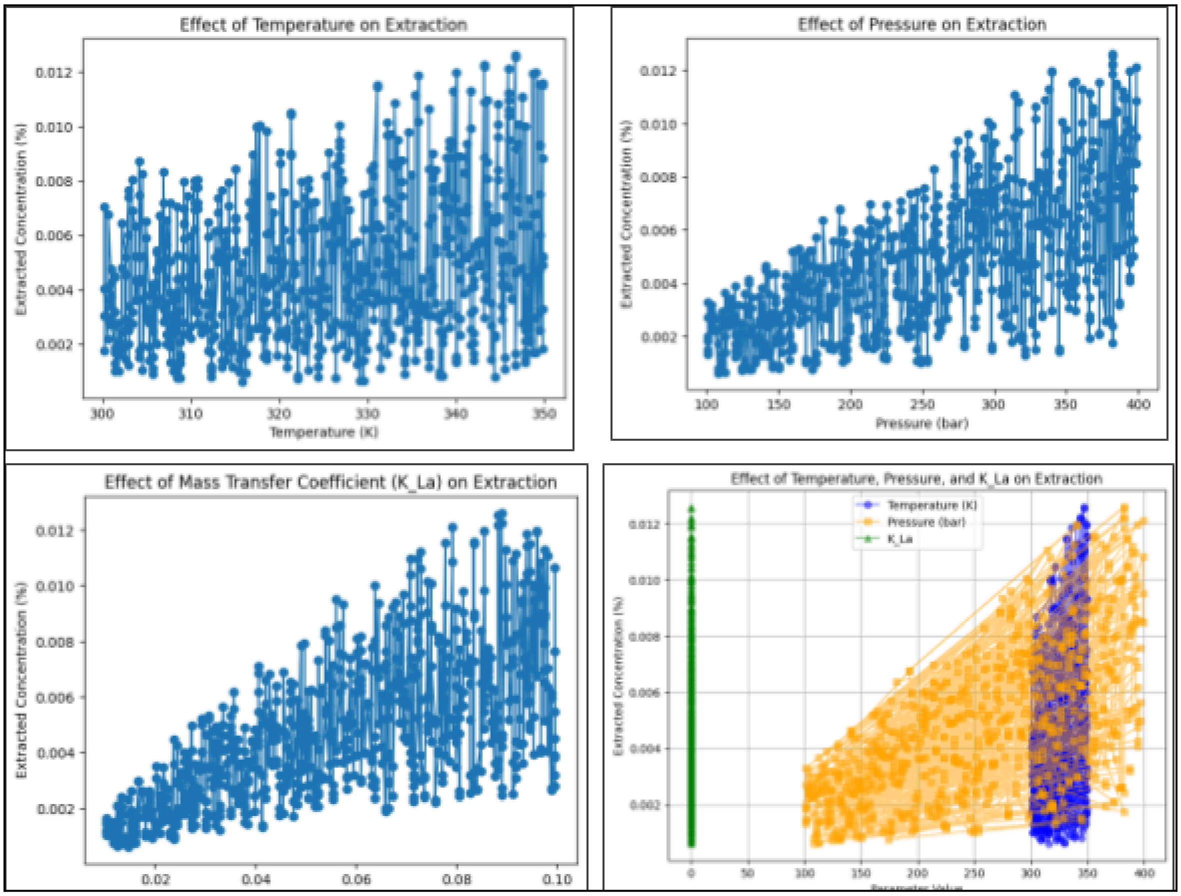
- **Impact of Stripping Factor and Tray Efficiency:** The simulation demonstrates how the stripping factor (A) and tray efficiency (E) influence the performance of the separation process.
- **A higher stripping factor improves separation**, allowing for **fewer stages** or **better separation** at constant stages.
- **Higher tray efficiency improves separation** and allows for a **reduction in the number of actual trays** required.

# SENSITIVITY ANALYSIS

The sensitivity analysis evaluates how changes in key operational parameters influence the performance of a counter-current liquid-liquid extraction system. **The focus is on how these variations affect:**

- Number of ideal and real stages
- Solute removal efficiency
- System design considerations [T, P]

| Sr No. | Parameters Analyzed | Effect |
|---|---|---|
| 1. | **Distribution Coefficient** | As KD increases, solute prefers the extract phase, and fewer stages are needed. The curve flattens at high KD, showing diminishing returns. |
| 2. | **Solvent-to-Feed Ratio (S/F)** | Higher S/F significantly improves separation, reducing stage requirements; however, the effect levels off due to solvent saturation. |
| 3. | **Stage Efficiency**: | As efficiency decreases, more actual stages are required. Shows the importance of good equipment design and mixing. |
| 4. | **Temperature (T)**: | Temperature slightly affects solubility and mass transfer. Within typical operating ranges, it causes moderate changes in stage count. Its influence is secondary compared to pressure. |
| 5. | **Pressure (P)** | Pressure **significantly impacts** phase behaviour and solvent stability, especially with volatile or compressible components. Deviations from optimal pressure lead to phase instability and increased stage count. |




## Animation of $CO_2$-Based Coffee Decaffeination-

### Objective

To visually represent the process of supercritical $CO_2$ decaffeination of coffee, highlighting mass transfer, solvent interaction, and operational parameters.

### Process Overview

The animation depicts the removal of caffeine from coffee beans using supercritical carbon dioxide ($scCO_2$)—a selective, non-toxic, and environmentally friendly solvent.

### Extraction with Supercritical $CO_2$:

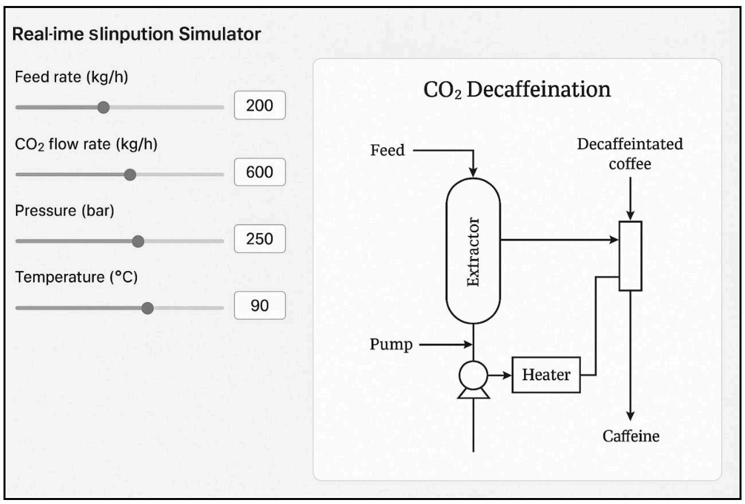
- $CO_2$ is pressurized (~100–300 bar) and heated (~31–80°C) to reach its supercritical state.
- In this state, $CO_2$ exhibits gas-like diffusivity and liquid-like solvating power, selectively dissolving caffeine.

**Caffeine Solubilization and Transport**:

- Caffeine diffuses out of the beans and into the flowing supercritical $CO_2$ stream.
- The animation shows mass transfer gradients and the role of operating conditions (T, P) in extraction efficiency.

**Caffeine Recovery (Separation Unit)**:

- $CO_2$–caffeine mixture is depressurized or cooled in a separator.
- Caffeine precipitates and is collected; $CO_2$ is often recycled.




## Overall Conclusion-

- **Pressure (P)** has the **strongest direct effect** on extraction yield. Because solubility is directly proportional to pressure, increasing P significantly boosts $CO_2$'s ability to dissolve solutes.
- **(Mass Transfer Coefficient)** has a **moderate impact**. Influences the rate at which equilibrium is approached, affecting yield.
- **Temperature (T)** has the **least direct influence**. Though it affects solubility, its effect is weaker in a selected range.
- A well-controlled pressure environment ensures optimal extraction with minimal stage requirements.

## REFERENCES

1. Advances in supercritical carbon dioxide technologies
2. Decaffeination Process Using CO2

3. Colab Link for simulation and sensitivity analysis
4. Colab Link for decaffeination animation.