# EOR Normal

# Extractive Distillation Setup for CO2 and Ethane Separation in DWSIM

This guide outlines the configuration of a two-column extractive distillation process in DWSIM to separate CO2 and ethane from a feed mixture containing CO2, ethane (C2), propane (C3), n-butane (nC4), isobutane (i-C4), n-pentane (nC5), and isopentane (i-C5), using a solvent stream of similar composition (rich in C3+ hydrocarbons) for enhanced oil recovery (EOR) processes. The first column produces CO2 as the distillate, and the second column produces ethane as the distillate, with the bottoms of the first column feeding the second.

## 1. Simulation Setup

### General Settings

* **Software**: DWSIM (Classic UI, latest version recommended, e.g., 8.3 or higher).
* **Thermodynamic Model**: Use the **Peng-Robinson (PR)** or **Soave-Redlich-Kwong (SRK)** model, as these are suitable for hydrocarbon-CO2 systems with azeotropic behavior. Peng-Robinson is preferred for EOR processes due to its accuracy with non-polar mixtures and CO2.
* **Units**: SI units (kg/s for mass flow, bar for pressure, °C for temperature).
* **Flash Algorithm**: Default (Nested Loops or Inside-Out).

### Components

Add the following components from the DWSIM database:

* Carbon Dioxide (CO2)
* Ethane (C2H6)
* Propane (C3H8)
* n-Butane (nC4)
* Isobutane (i-C4)
* n-Pentane (nC5)
* Isopentane (i-C5)

## 2. Process Flowsheet

### Streams

1. **Feed Stream**:
   * **Composition**: Example molar composition (adjust based on your EOR process data):
     + CO2: 70 mol%
     + Ethane (C2): 20 mol%
     + Propane (C3): 5 mol%
     + n-Butane (nC4): 2 mol%
     + Isobutane (i-C4): 1 mol%
     + n-Pentane (nC5): 1 mol%
     + Isopentane (i-C5): 1 mol%
   * **Flowrate**: 100 kmol/h (or adjust based on process scale).
   * **Conditions**: Saturated liquid at 20 bar and 20°C (typical for demethanizer bottoms in EOR processes).
   * **Name**: "Feed"
2. **Solvent Stream**:
   * **Composition**: NGL mixture, rich in C3+ hydrocarbons to break the CO2-ethane azeotrope:
     + CO2: 5 mol%
     + Ethane (C2): 10 mol%
     + Propane (C3): 30 mol%
     + n-Butane (nC4): 30 mol%
     + Isobutane (i-C4): 10 mol%
     + n-Pentane (nC5): 10 mol%
     + Isopentane (i-C5): 5 mol%
   * **Flowrate**: 50–100 kmol/h (optimize to meet minimum solvent requirement, typically 0.5–1.5 times feed flow).
   * **Conditions**: Liquid at 20 bar and 20°C.
   * **Name**: "Solvent"
3. **Output Streams**:
   * **CO2 Product**: Distillate from Column 1 (target: 95 mol% CO2).
   * **Ethane Product**: Distillate from Column 2 (target: 90–95 mol% ethane).
   * **Bottoms (NGL)**: Bottoms from Column 2 (C3+ hydrocarbons, low CO2 and ethane).
   * **Energy Streams**:
     + Condenser duties: "C1-Duty" (Column 1), "C2-Duty" (Column 2).
     + Reboiler duties: "R1-Duty" (Column 1), "R2-Duty" (Column 2).

### Unit Operations

1. **Column 1 (CO2 Recovery Column)**:
   * **Type**: DWSIM Rigorous Distillation Column.
   * **Name**: "CO2\_Column".
   * **Purpose**: Separate CO2 as distillate, with ethane and heavier hydrocarbons (plus solvent) in bottoms.
   * **Configuration**:
     + **Stages**: 30 (including condenser and reboiler).
     + **Feed Stage**: Feed at stage 15, solvent at stage 5 (near top to maximize CO2 entrainment).
     + **Condenser**: Total condenser, pressure 19.5 bar (0.5 bar pressure drop).
     + **Reboiler**: Kettle reboiler, pressure 20 bar.
     + **Specifications**:
       - Distillate CO2 purity: 95 mol%.
       - Bottoms CO2 content: ≤40 ppm.
       - Reflux ratio: 2–5 (adjust to meet specs).
       - Distillate flowrate: Estimate based on CO2 in feed (~70 kmol/h).
     + **Solver**: Wang-Henke (Bubble Point) for better convergence.
     + **Connections**:
       - Inlet: "Feed" to stage 15, "Solvent" to stage 5.
       - Outlet: Distillate ("CO2\_Product"), bottoms ("Bottoms\_C1"), condenser duty ("C1-Duty"), reboiler duty ("R1-Duty").
2. **Column 2 (Solvent Recovery/Ethane Column)**:
   * **Type**: DWSIM Rigorous Distillation Column.
   * **Name**: "Ethane\_Column".
   * **Purpose**: Separate ethane as distillate, recover C3+ hydrocarbons (NGL) in bottoms.
   * **Configuration**:
     + **Stages**: 20 (including condenser and reboiler).
     + **Feed Stage**: Bottoms from Column 1 ("Bottoms\_C1") at stage 10.
     + **Condenser**: Total condenser, pressure 19.5 bar.
     + **Reboiler**: Kettle reboiler, pressure 20 bar.
     + **Specifications**:
       - Distillate ethane purity: 90–95 mol%.
       - Bottoms ethane content: ≤0.1 mol%.
       - Reflux ratio: 2–4 (adjust to meet specs).
       - Distillate flowrate: Estimate based on ethane in feed (~20 kmol/h).
     + **Solver**: Wang-Henke (Bubble Point).
     + **Connections**:
       - Inlet: "Bottoms\_C1" to stage 10.
       - Outlet: Distillate ("Ethane\_Product"), bottoms ("NGL"), condenser duty ("C2-Duty"), reboiler duty ("R2-Duty").
3. **Recycle Stream** (Optional):
   * Recycle a portion of the "NGL" stream from Column 2 back to the solvent inlet of Column 1 to reduce external solvent needs. Use a **Splitter** unit to split "NGL" into "NGL\_Product" and "Solvent\_Recycle".
   * **Split Ratio**: Adjust to maintain solvent flow (e.g., 50% recycle).
   * **Pump/Valve**: Add a pump or valve to adjust "Solvent\_Recycle" pressure to 20 bar if needed.

## 3. Simulation Steps

1. **Create Simulation**:
   * Open DWSIM, start a new steady-state simulation.
   * Select Peng-Robinson thermodynamic package.
   * Add components listed above.
2. **Add Streams and Unit Operations**:
   * Add "Feed" and "Solvent" streams with specified conditions and compositions.
   * Add two Rigorous Distillation Columns ("CO2\_Column" and "Ethane\_Column").
   * Add output streams ("CO2\_Product", "Ethane\_Product", "NGL") and energy streams ("C1-Duty", "R1-Duty", "C2-Duty", "R2-Duty").
   * (Optional) Add splitter and recycle stream for solvent recycle.
3. **Configure Columns**:
   * Set up Column 1 and Column 2 as described above.
   * Ensure feed and solvent streams are properly connected to the correct stages.
   * Specify column pressures, reflux ratios, and product specifications.
4. **Run Simulation**:
   * Press "Solve Flowsheet" (F5).
   * Check for convergence errors. If errors occur:
     + Reduce tolerance in solver settings (e.g., 0.001).
     + Adjust initial estimates for reflux ratio or distillate flow.
     + Switch to a different solver (e.g., Russell Inside-Out) if Wang-Henke fails, but note potential convergence issues.
   * Verify results in the "Master Property Table" or column profiles.
5. **Analyze Results**:
   * Check "CO2\_Product" for ≥95 mol% CO2.
   * Check "Ethane\_Product" for 90–95 mol% ethane.
   * Check "NGL" for low CO2 (≤40 ppm) and ethane (≤0.1 mol%).
   * Review energy duties (C1-Duty, R1-Duty, C2-Duty, R2-Duty) for process efficiency.

## 4. Optimization and Troubleshooting

* **Solvent Flowrate**: Perform sensitivity analysis on solvent flowrate (50–150 kmol/h) to find the minimum solvent amount that achieves CO2 specifications without excessive energy use.
* **Feed Stage Location**: Adjust feed and solvent stage locations (e.g., ±5 stages) to optimize separation efficiency.
* **Reflux Ratio**: Increase reflux ratio if purity specs are not met, but balance with energy consumption.
* **Convergence Issues**:
  + Use Peng-Robinson with tuned binary interaction parameters for CO2-ethane if available.
  + Initialize column with shortcut distillation results to improve convergence.
  + Check for CO2 freezing (sublimation) in Column 1; ensure operating temperatures are above CO2 triple point (-56.6°C at 5.18 bar).
* **Energy Optimization**: Consider heat integration (e.g., use Column 1 condenser heat to preheat Column 2 feed) to reduce energy costs.

## 5. Expected Outcomes

* **Column 1**:
  + Distillate ("CO2\_Product"): ~95 mol% CO2, suitable for reinjection in EOR.
  + Bottoms ("Bottoms\_C1"): Ethane, C3+ hydrocarbons, and solvent with ≤40 ppm CO2.
* **Column 2**:
  + Distillate ("Ethane\_Product"): 90–95 mol% ethane, suitable for petrochemical use.
  + Bottoms ("NGL"): C3+ hydrocarbons (propane, butanes, pentanes) with ≤0.1 mol% ethane, recyclable as solvent or product.
* **Energy Consumption**: Expect reboiler duties to dominate energy use. Typical values: 5–10 MW for Column 1, 3–7 MW for Column 2 (scale with feed flowrate).

## 6. Notes

* **Azeotrope Handling**: The NGL solvent (C3+ rich) breaks the CO2-ethane azeotrope by altering relative volatilities, allowing CO2 to be distilled in Column 1.
* **DWSIM Limitations**: Native DWSIM columns may struggle with azeotropic systems. If convergence fails repeatedly, consider using ChemSep columns via CAPE-OPEN for better thermodynamic modeling, though this is outside the scope of this setup.
* **Validation**: Compare results with literature (e.g., HYSYS simulations for CO2-ethane separation) to ensure accuracy.
* **Safety**: Ensure operating conditions avoid CO2 solidification. Monitor column temperatures and pressures closely.

This setup provides a robust starting point for simulating CO2 and ethane separation in DWSIM for EOR processes. Adjust parameters based on specific feed compositions and process requirements.