Report on Screening task for Autumn Internship under AI/ML Surrogate Modelling for Binary Distillation

**Task**: Build and compare ML surrogates for distillate purity & energy

Flowsheet and Simulation setup details

1. **Simulation Environment and Thermodynamic Model**
2. **Process Simulator:** The Flowsheet was designed and simulated using DWSIM, an open-source chemical process simulator.
3. **Property package:** The **NRTL (Non-Random Two Liquid)** activity coefficient model was selected as the thermodynamic property package.
4. **Justification**: The selected Ethanol & Water system is a highly non-ideal aqeous mixture that forms a minimum boiling azeotrope at approximately 95.6% mass fraction of ethanol.
5. **Flowsheet Components**

The flowsheet consists of one primary unit operation and its associated material and energy streams:

1. **Unit Operation:** A single rigorous **Distillation Column** (DCOL-1).
2. **Material Streams**:
3. feed : An inlet stream representing the Ethanol Water mixture fed to the column
4. 3: The top outlet stream, representing the high-purity **Distillate** product.
5. 4: The bottom outlet stream, representing **Bottoms** product.
6. **Energy Streams**:
   1. E1: The energy removed from the system by the condenser, representing the **Condenser Duty.**
   2. E2: The energy supplied to the system by the reboiler, representing the **Reboiler Duty (QR).** This was a key target variable for the surrogate model.
7. Distillation Column

FlowSheet Description: DWSIM Software has been used to simulate the Binary Distillation process choosing the binary system of Ethanol and Water at 1 atm