Screening Task 2: Python Automation of DWSIM

1. Objective

The objective of this task is to evaluate a candidate's ability to use Python to control DWSIM via its Automation API, construct flowsheets programmatically, simulate a Plug Flow Reactor (PFR) and a Distillation Column, perform parametric sweep studies, and run simulations headlessly without opening the DWSIM GUI.

2. Deliverables

1. run_screening.py – Main Python script
2. requirements.txt – Python dependencies
3. README.md – Setup and execution instructions
4. results.csv – Automatically generated output file
5. Optional plots showing parametric trends

3. Constraints

1. DWSIM must be installed
2. Must use Python + DWSIM Automation
3. No prebuilt flowsheets
4. No GUI interaction
5. Script must handle failed cases gracefully

4. Part A – PFR Reactor Simulation

Simulate a single irreversible reaction A → B using kinetic expressions. The PFR must operate isothermally with volume-based sizing. Report conversion, outlet flow of B, heat duty (if applicable), and outlet temperature.

5. Part B – Distillation Column Simulation

Simulate a binary mixture separation using a distillation column. Specify number of stages, feed stage, reflux ratio, and one additional specification. Report purities, condenser duty, and reboiler duty.

6. Part C – Parametric Sweep

PFR: Sweep at least two variables (e.g., reactor volume and temperature).
Column: Sweep at least two variables (e.g., reflux ratio and number of stages).
All cases must be logged.

7. Output Requirements

results.csv must include case metadata, sweep variables, success flag, error messages, and all required KPIs for both PFR and distillation cases.

8. Evaluation Criteria

Correctness, robustness, parametric sweep implementation, headless execution, code quality, and documentation.

9. Submission Guidelines

Keep all the necessary files (as listed in deliverables) in a folder and compress it. Upload the compressed folder in the g-drive and submit the link of g-drive in this form: https://forms.gle/WFA3Wem6nZKu414UA