Python Simulator User Manual

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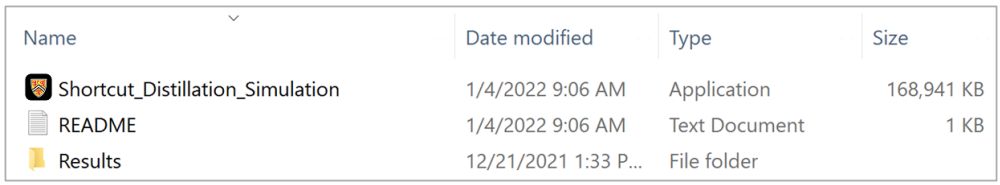
1. Instructions

1.1. Download Instructions

1.1.1.For Windows Users

1. Minimum requirements: 64-bit Windows System.
2. Select and download the simulation or design calculation or VLE calculation package onto your computer:
    - Shortcut_Distillation_Simulation.zip;
    - or Steady-state_Rigorous_Distillation_Simulation.zip;
    - or Unsteady-state_Rigorous_Distillation_Simulation.zip;
    - or Distillation_Column_Design_Calculation.zip;
    - or Vapour_Liquid_Equilibrium_Calculation.zip;
3. Unzip the downloaded file (zip file). The archive contains three files:



i. Executable file:
    - Shortcut_Distillation_Simulation.exe;
    - or Steadystate_Rigorous_Distillation_Simulation.exe;
    - or Unsteadystate_Rigorous_Distillation_Simulation.exe
    - or Distillation_Column_Design_Calculation.exe;
    - or Vapour_Liquid_Equilibrium_Calculation.exe;

ii. README.txt:

Brief instructions.

iii. "Results" Folder:

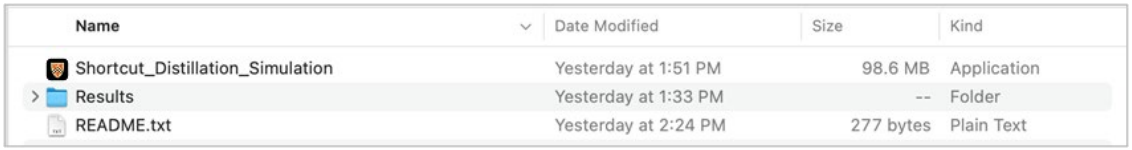
Folder to store simulation or design calculation or VLE calculation results.

4. Double-click on the executable file icon to initiate simulation or design calculation or VLE calculation.

1.1.2.For Mac Users

1. Minimum requirements: 64-bits macOS System.
2. Select and download the simulation or design calculation or VLE calculation package into the **"Downloads" folder** on your computer:
    - Shortcut_Distillation_Simulation.zip;
    - or Steady-state_Rigorous_Distillation_Simulation.zip;
    - or Unsteady-state_Rigorous_Distillation_Simulation.zip;
    - or Distillation_Column_Design_Calculation.zip;
    - or Vapour_Liquid_Equilibrium_Calculation.zip;

3. Unzip the downloaded file (zip file). The archive contains three files:



i. Application file:

- Shortcut_Distillation_Simulation.app;
- or Steadystate_Rigorous_Distillation_Simulation.app;
- or Unsteadystate_Rigorous_Distillation_Simulation.app
- or Distillation_Column_Design_Calculation.app;
- or Vapour_Liquid_Equilibrium_Calculation.app;

ii. "Results" Folder:

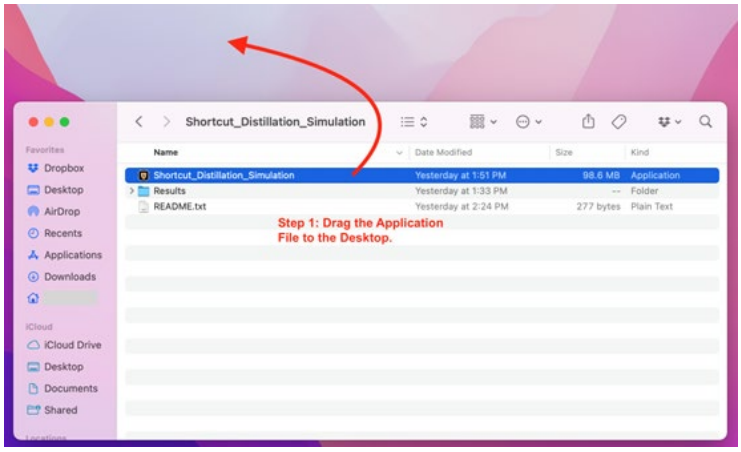
Folder to store simulation or design calculation or VLE calculation results.

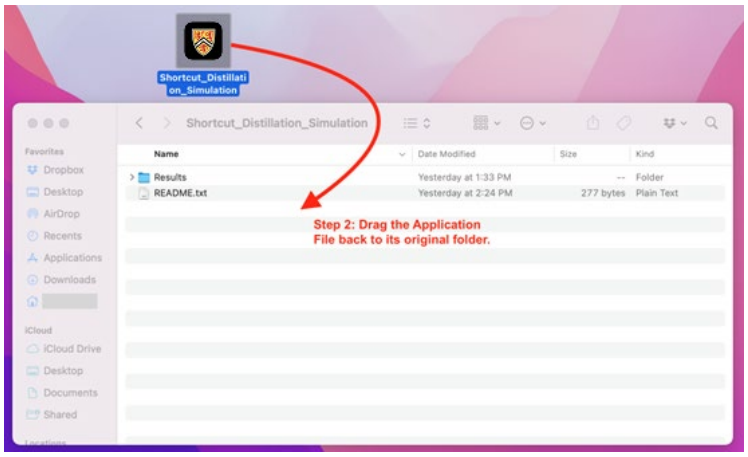
iii. README.txt:

Brief instructions.

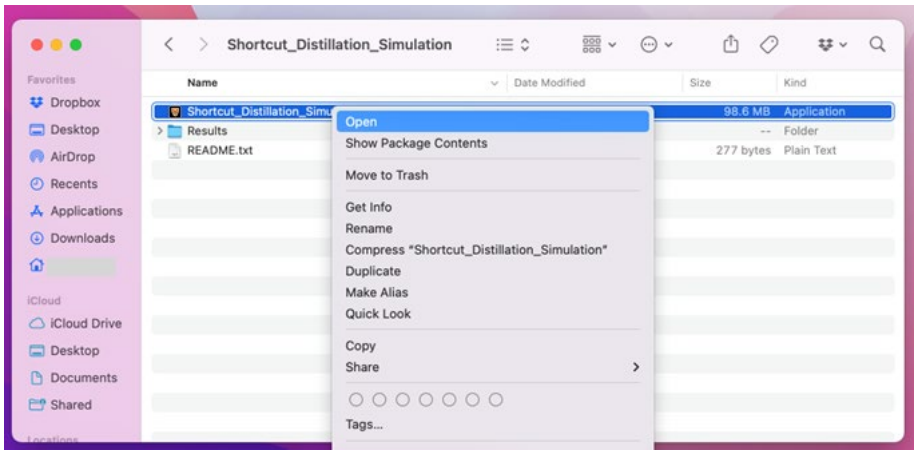
4. **Before initiating the application file for the first time, complete the following two procedures**. You **do not** need to repeat these two procedures for further use of the application file after the first initiation.

➢ Open the unzipped folder in **Finder**, drag the application file to the **Desktop**. Then, drag the application file back to the unzipped folder in **Finder**. The procedure is illustrated below.

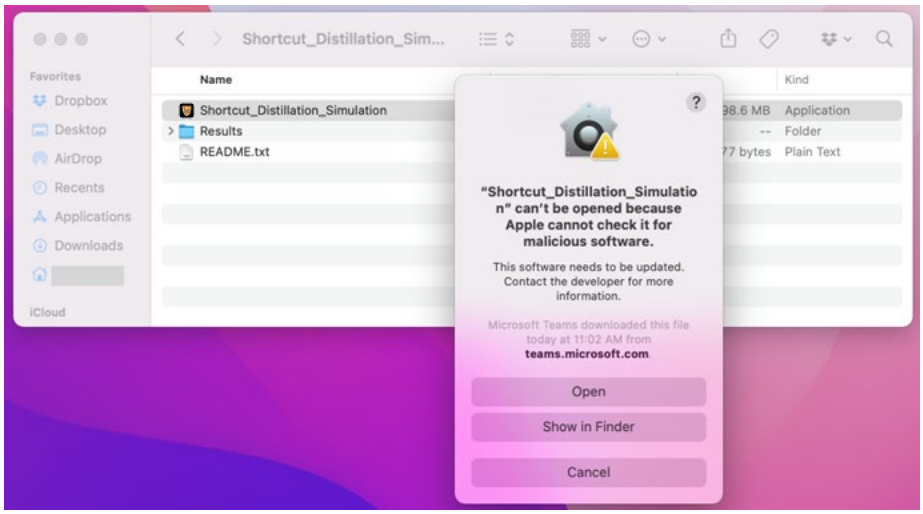




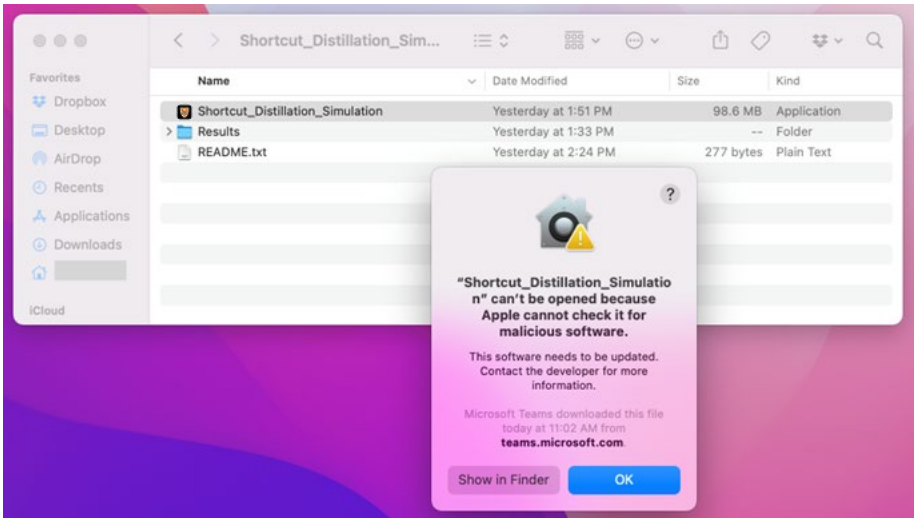
- **Control-click** (press and hold the Ctrl key down while you click the mouse) the application file icon, and then choose **Open** from the menu.



If the pop-up window indicates the application file "can't be opened because Apple cannot check it for malicious software", but there is an **Open** option (shown below), click **Open**.



If the pop-up window indicates the application file “can’t be opened because Apple cannot check it for malicious software” and the **Open** option is not available (shown below), click **OK** and redo **Control-click** again.

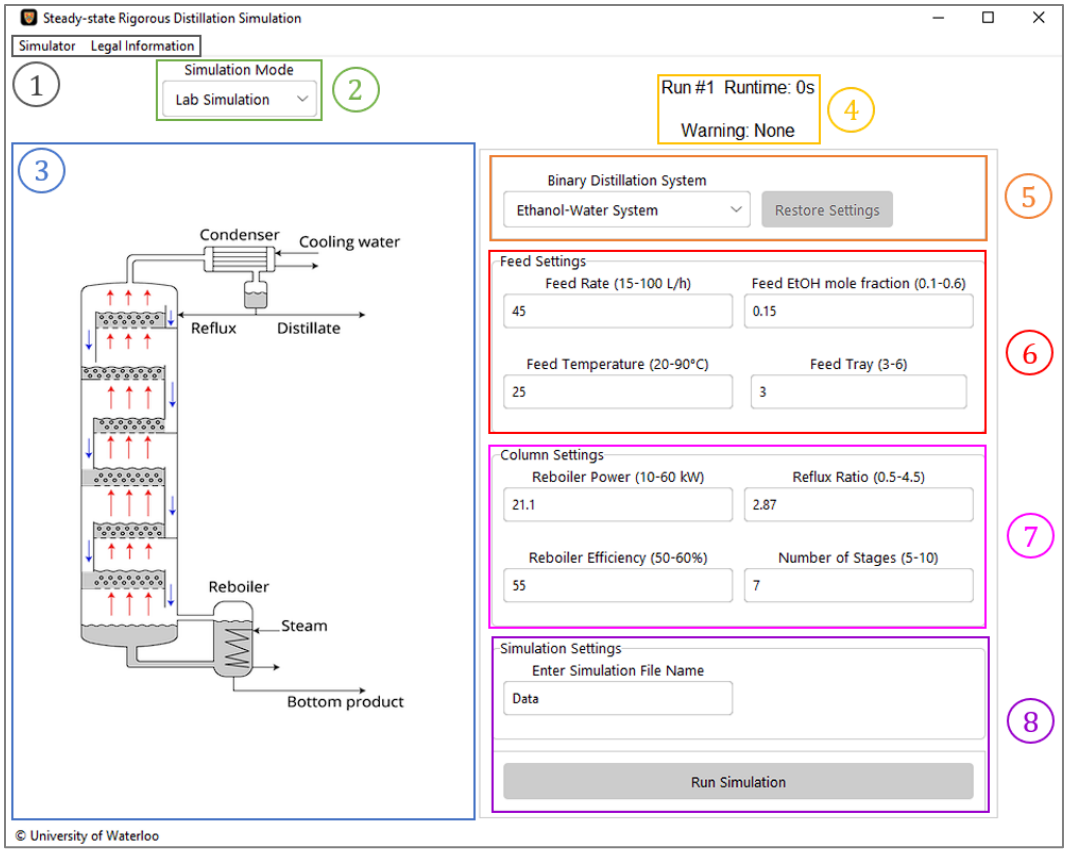


5. After the first initiation, double-click on the application file icon to initiate simulation or design calculation or VLE calculation.

*Note 1: if the results are not autosaved to the “Results” folder, repeat Step 4.
*Note 2: if the results are still not autosaved to the “Results” folder after repeating Step 4, you can download an alternative version of the simulator from.

1.2. Simulation Instructions

A typical simulation user interface is shown below:

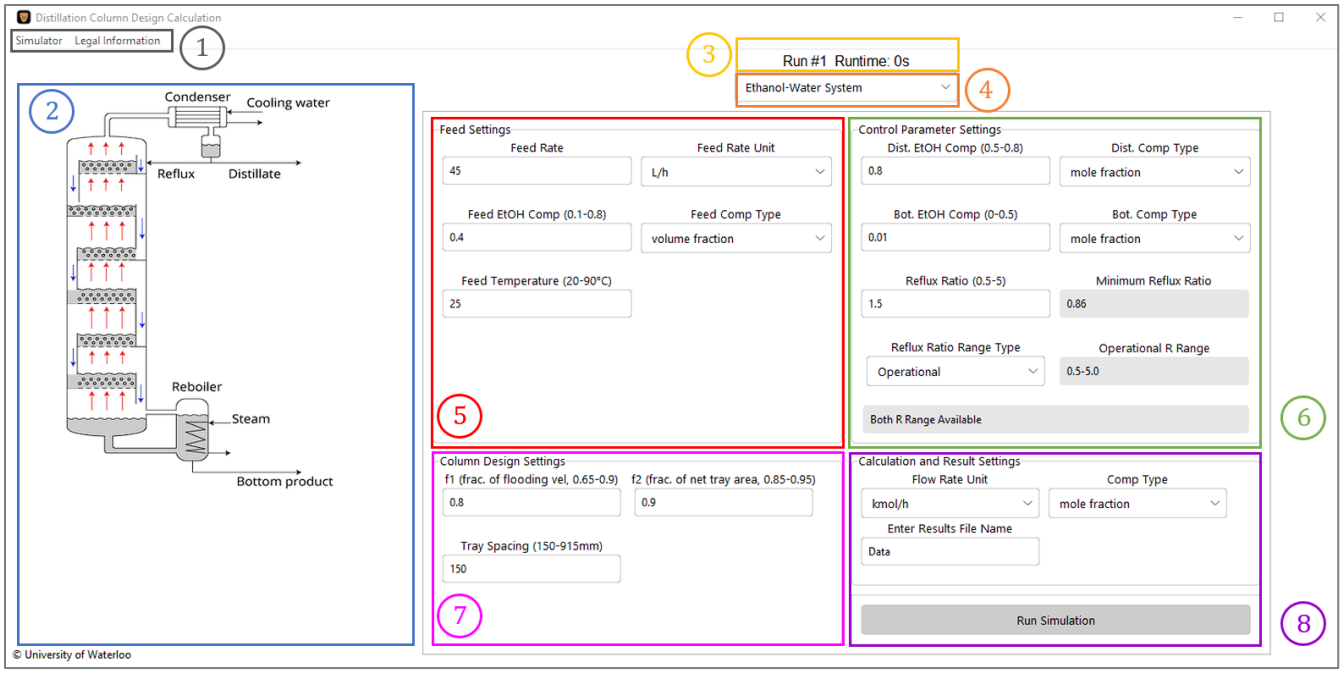


Note: for macOS system users, the menu bar is located at the top of the display window instead of the user interface.

1. Select the {2} Simulation Mode for simulation: Lab Simulation or Design Simulation.
2. Select the {5} Binary System for distillation: Ethanol-Water System or Methanol-Isopropanol System.
3. Adjust input values in {6} Feed Settings and {7} Column Settings sections.
4. Enter the simulation file name in the {8} Simulation Settings section for saving the results. **Allowed characters are: 'a-z', 'A-Z', '0-9', '_'.** If the input box is left unchanged, results will be saved with the default simulation file name "Data".
5. Click on the "Run Simulation" button in the {8} Simulation Settings section to start the simulation. **The user interface will freeze while running.** For the unsteady-state rigorous distillation simulation, it might take several minutes to run.
6. Simulation results will be automatically saved in the "Results" folder.
7. Refer to the User Guide section below for detailed instructions about running the simulation and simulation results.

1.3. Column Design Calculation Instructions

The design calculation user interface is shown below:

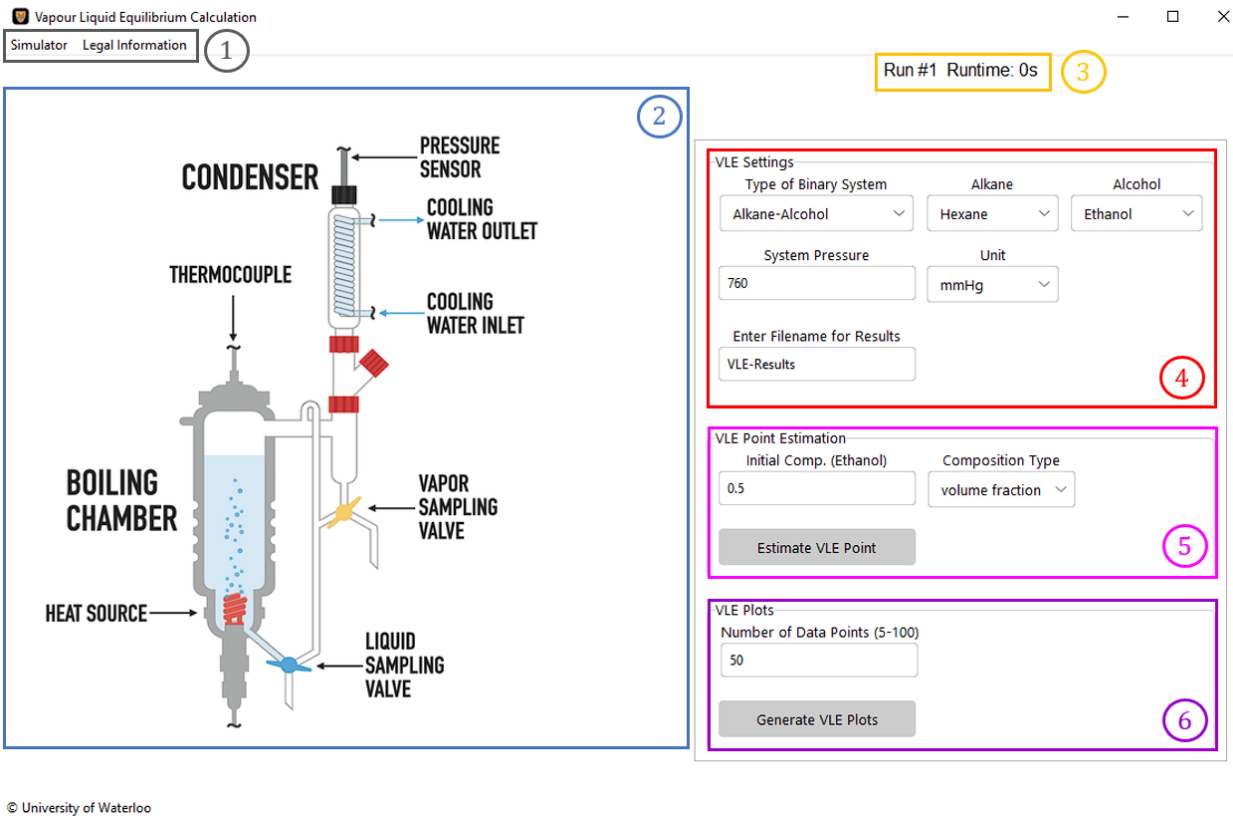


Note: for macOS system users, the menu bar is located at the top of the display window instead of the user interface.

1. Select the {4} Binary System for distillation: Ethanol-Water System or Methanol-Isopropanol System.
2. Adjust input values in {5} Feed Settings, {6} Control Parameter Settings, {7} Column Design Settings sections.
3. Enter the design calculation file name in the {8} Calculation and Result Settings section for saving the results. **Allowed characters are: 'a-z', 'A-Z', '0-9', '_'.** If the input box is left unchanged, results will be saved with the default file name "Data".
4. Click on the "Run Column Design Calculation" button in the {8} Calculation and Result Settings section to start the design calculation. **The user interface will freeze while running.**
5. Design calculation results will be automatically saved in the "Results" folder.
6. Refer to the User Guide section below for detailed instructions about running the design calculation and design calculation results.

1.4. Vapour Liquid Equilibrium Calculation Instructions

The VLE calculation user interface is shown below:



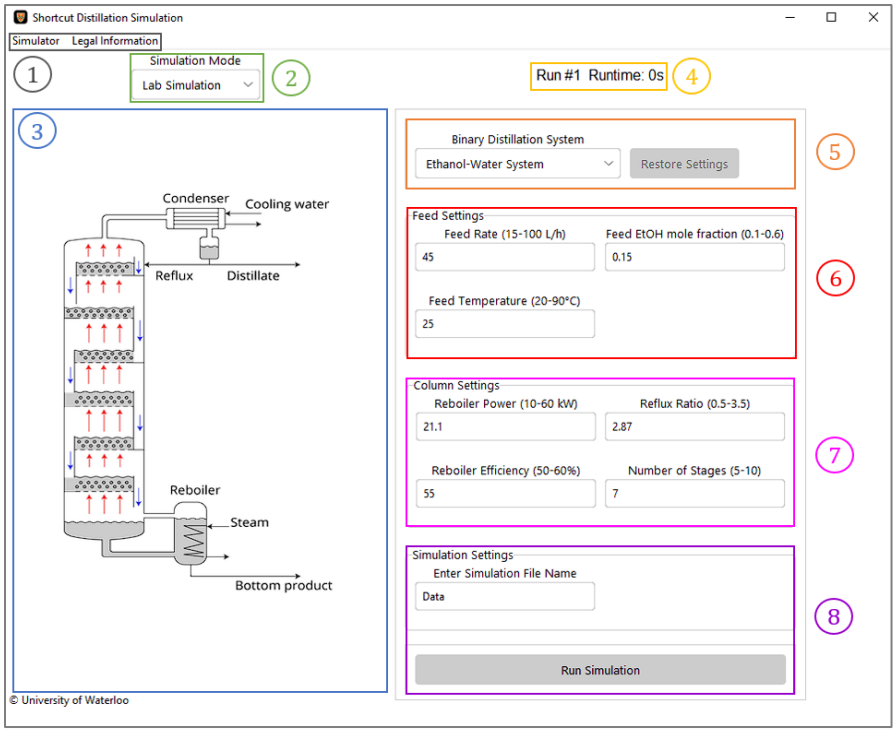
Note: for macOS system users, the menu bar is located at the top of the display window instead of the user interface.

1. In {4} VLE Settings, select the type of binary system and the two components for VLE calculation. Enter the system pressure and its unit.
2. Enter the VLE calculation file name in the {4} VLE Settings section for saving the results. **Allowed characters are: 'a-z', 'A-Z', '0-9', '_'** If the input box is left unchanged, results will be saved with the default file name "VLE-Results".
3. To estimate a VLE data point, adjust the initial composition and the composition type of the binary mixture in {5} VLE Point Estimation section and then click the "Estimate VLE Point" button. **The user interface will freeze while running.**
4. To generate T-x-y diagram and x-y diagram, adjust the number of data points used in the diagrams in {6} VLE Plots section and then click the "Generate VLE Plots" button. **The user interface will freeze while running.**
5. VLE calculation results will be automatically saved in the "Results" folder.

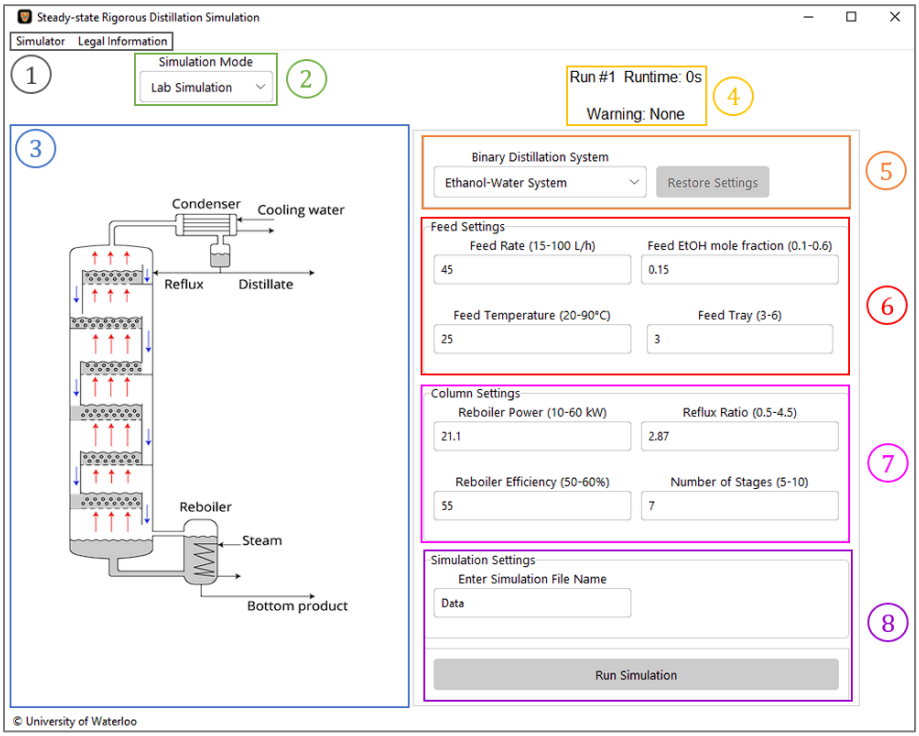
2. User Guide – Distillation Simulation Interface

2.1. Interface

2.1.1.Shortcut Distillation Simulation

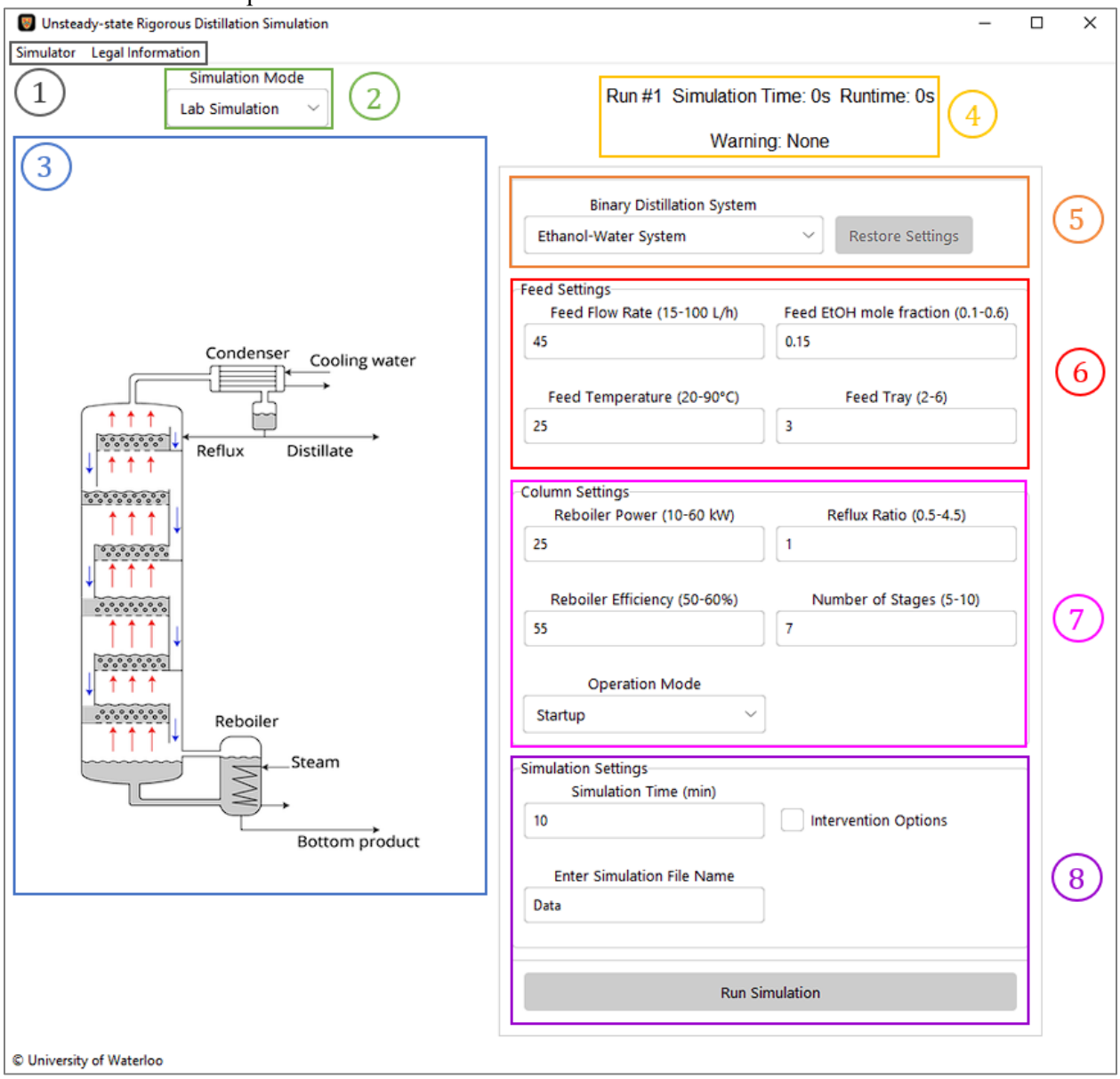


2.1.2.Steady-state Rigorous Distillation Simulation

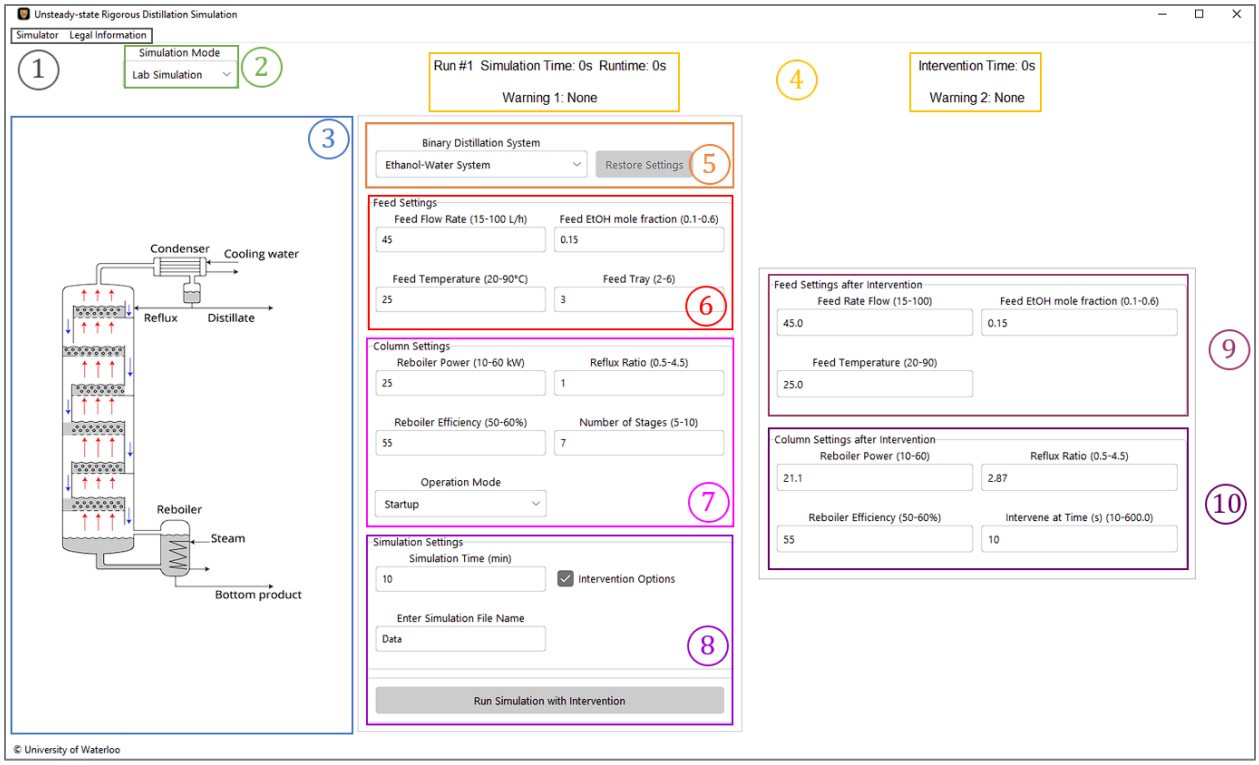


2.1.3.Unsteady-state Rigorous Distillation Simulation

Without Intervention Option:



With Intervention Option:



2.2. Major Sections on the Interfaces

{1} Dark Grey: This is the menu bar to switch between the Simulator page and the Legal Information page. The Simulator page can be accessed by pressing the 'F1' key, while the Legal Information page can be accessed by pressing the 'F2' key. **Note: for macOS system users, the menu bar is located at the top of the display window instead of the user interface.**

{2} Green: This is the Simulation Mode dropdown menu. In different simulation modes, the slider ranges in settings sections are different. There are two simulation modes available:

- Lab Simulation:

  The input ranges are narrower, closer to experimental settings in the lab. Please refer to Table 1 for input ranges under lab simulation mode.

- Design Simulation:

  The input ranges are wider, for distillation column design purposes. Usually used with Distillation Column Design Calculation. Please refer to Table 1 for input ranges under design simulation mode.

Note: The higher the number of stages used, the longer the simulation time.

{3} Blue: This is the experimental schematic of the distillation column. Some inputs and outputs are displayed on this schematic after each run. The tray number is counted from the top of the distillation column, starting from "Tray 1". The last tray is always the reboiler.

{4} Gold: This is the area with run information and warnings.

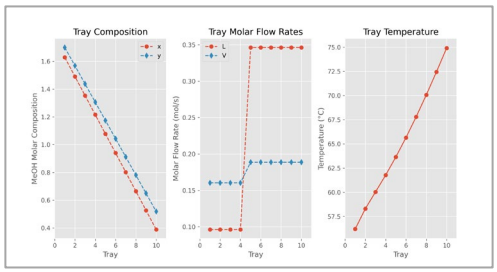
- Runtime: the time that the executable file takes to run the simulation and obtain results.

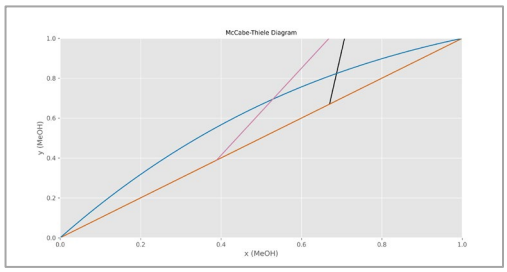
- Warning:

Warning messages include:

- Type 1: Results might be invalid due to unreasonable input settings or simulation calculation error or bad initial condition mode (for Unsteady-state Rigorous Distillation Simulation).
  - "Possible Invalid Results" (for Steady-state Rigorous Distillation Simulation)
  - "Possible Error at the End of the Simulation Time" (for Unsteady-state Rigorous Distillation Simulation)

  Note: Please cross-check numerical results with graphical results if you see this type of warnings. Examples of invalid graphical results are shown below:





- Type 2: Simulation intervened with the second set of feed and column settings before reaching intervention time (for Unsteady-state Rigorous Distillation Simulation with Intervention).
  - "Process End Before Reaching Intervention Time"

- Simulation Time (for Unsteady-state Rigorous Distillation Simulation):

  The actual time simulated. Simulation might end before reaching the simulation time set in Simulation Settings due to simulation calculation error or bad initial condition mode.

- Intervention Time (for Unsteady-state Rigorous Distillation Simulation with Intervention):

  The actual time when the feed and column settings change to Feed Settings after Intervention and Column Settings after Intervention.

{5} Brown: This area contains the dropdown menu to switch between different binary systems for distillation and the button to restore settings for the previous run.

- Binary System dropdown menu:

  This dropdown menu is used to select the binary system for distillation. Two systems are available: Ethanol-Water System and Methanol-Isopropanol System. When switching between different systems, the variable name, default values, and ranges for inputs in Feed Settings section and Column Settings section will change as well. Default values and ranges for each system and simulation mode are listed in Table 1 below.

Table 1 – Default parameter values and ranges for Ethanol-Water and Methanol-Isopropanol systems.

	Ethanol-Water System		Methanol-Isopropanol System		Design Simulation Range
Variable	Default Value	Lab Simulation Range	Default Value	Lab Simulation Range	
More Volatile Component (MVC)	Ethanol		Methanol		
Feed Rate (L/h)	45	$15 - 100$	45	$28 - 83$	$40 - 1000$
MVC Feed Molar Composition	0.15	$0.10 - 0.60$	0.44	$0.20 - 0.70$	$0.10 - 0.80$
Feed Temperature (°C)	25.0	$20.0 - 90.0$	25.0	$10.0 - 50.0$	$10.0 - 70.0$
Reflux Ratio	2.87	$0.50 - 4.5$	1.50	$0.70 - 4.00$	$0.50 - 5.00$
Reboiler Power (kW)	21.1	$10.0 - 60.0$	23.0	$13.0 - 36.0$	$10.0 - 1000.0$
Reboiler Efficiency	55%	$50\% - 60\%$	55%	$50\% - 60\%$	$50\% - 60\%$
Number of Stages (N)	7	$5 - 10$	7	$5 - 10$	$5 - 50$
Feed Tray*	3	$2 - (N - 1)$	3	$2 - (N - 1)$	$2 - (N - 1)$

*Note: Feed Tray is for Steady-State and Unsteady-State Rigorous Distillation Simulations. The upper limit of its range is always one less than the number of stages (N) selected.

- Restore Settings button:

  This button is disabled in Run #1. For Run # 2 and subsequent ones, this button is used to restore settings for the previous run, including the Simulation Mode selected for simulation, the Binary System selected for distillation, and inputs in Feed Settings section and Column Settings section.

{6} Red (Feed Settings): This is the area with sliders that control the feed settings into the distillation column.

- Feed Rate input(in L/h)
- Feed Composition input(in mole fraction)
- Feed Temperature input (in °C)
- Feed Tray input (for Steady-state and Unsteady-state Rigorous Distillation Simulations)

Note: Set these to the desired values before clicking the Run Simulation button or the Run Simulation with Intervention button.

{7} Pink (Column Settings): This is the area with sliders and dropdown menus that control the distillation column settings.

- Reboiler Power input(in kW)
- Reboiler Efficiency input(in $\%$)
- Reflux Ratio input
- Number of Stages input
- Mode dropdown menu (for Unsteady-state Rigorous Distillation Simulation):

  This dropdown menu is used to choose different initial condition modes to run the simulation. There are 3 modes available:

  1. Startup: Initial condition for start-up, based on knowledge or shortcut distillation simulation.
  2. Transient:
     - ✧ In "Run # 1", the initial condition is the default steady-state condition obtained at default feed and column settings in Table 1. The Number of Stages inputis restricted to 7.
     - ✧ In other runs, the initial condition is the condition achieved at the end of simulation time in the previous run. The Simulation Mode dropdown menu, the Binary System dropdown menu, and the Number of Stages slider will be restricted to the simulation mode, the binary system, and the number of stages used in the previous run, respectively.
  3. Transient from Default: Use the default steady-state condition obtained at default feed and column settings in Table 1 as the initial condition. The Number of Stages input will be restricted to 7.

Note: Set these to the desired values before clicking the Run Simulation button or the Run Simulation with Intervention button.

{8} Purple (Simulation Settings): This is the area with input boxes, buttons, and checkboxes to control simulation settings.

- Simulation File Name input box:

  This input box is used to enter the simulation file name for saving the results. **Allowed characters are: 'a-z', 'A-Z', '0-9', '_', up to 25 characters.** In one simulation, the results from all runs will be saved in a folder in the "Results" folder. For example, using the default simulation file name: "Data", the folder name will be: "SC_Distillation_Data" for Shortcut Distillation Simulation; "SS_Distillation_Data" for Steady-state Rigorous Distillation Simulation; "USS_Distillation_Data" for Unsteady-state Rigorous Distillation Simulation. **This input box will be disabled after Run #1, Make Sure You Enter the Simulation File Name BEFORE Run #1.**

- Run Simulation button (for Shortcut Distillation Simulation, Steady-state Rigorous Distillation Simulation, and Unsteady-state Rigorous Distillation Simulation without Intervention) or Run

Simulation with Intervention button (for Unsteady-state Rigorous Distillation Simulation with Intervention):

This button is used to start running the simulation process.

- Simulation Time (in min) (for Unsteady-state Rigorous Distillation Simulation): to set the simulated duration.
- Intervention Option checkbox (for Unsteady-state Rigorous Distillation Simulation):

  This checkbox is used to enable/disable the intervention option. The intervention option is enabled when the checkbox is checked, and vice versa.

{9} Dark Red (Feed Settings after Intervention, for Unsteady-state Rigorous Distillation Simulation): This is the area with sliders that control feed settings into the distillation column after intervention.

- Feed Rate input (in L/h)
- Feed Composition input (in mole fraction)
- Feed Temperature input (in ℃)

Note: Set these to the desired values before clicking the Run Simulation with Intervention button.

{10} Dark Purple (Column Settings after Intervention, for Unsteady-state Rigorous Distillation Simulation): This is the area with sliders that control the distillation column settings after intervention.

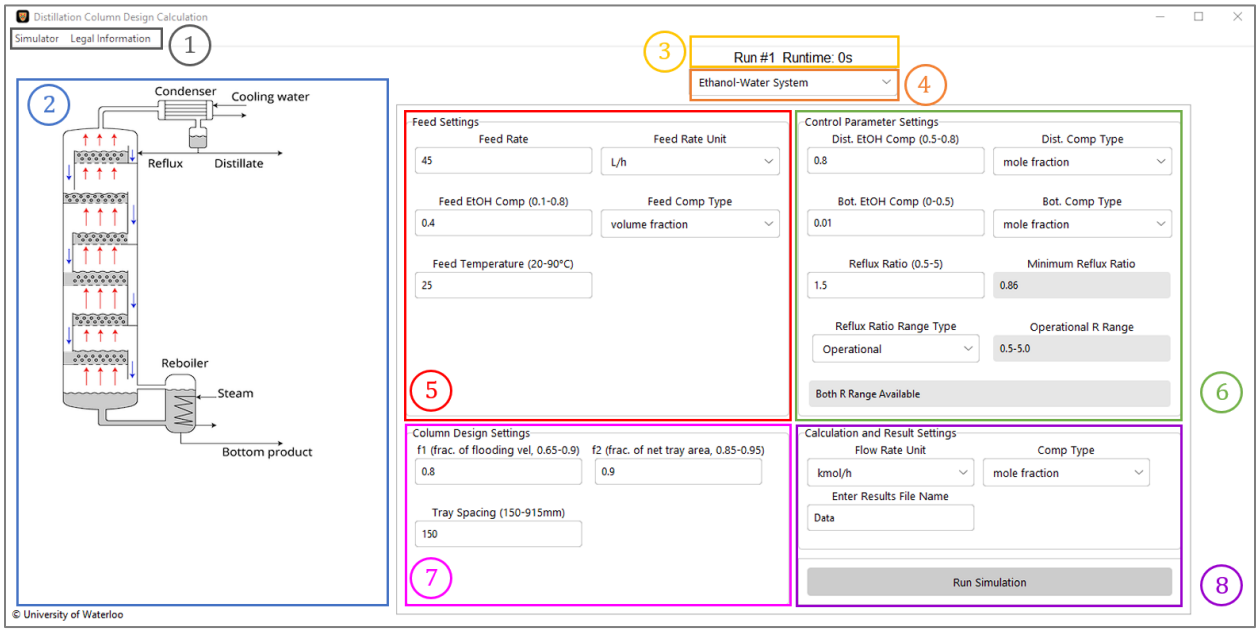
- Reboiler Power input (in kW)
- Reboiler Efficiency input (in $\%$)
- Reflux Ratio input
- Intervention at Time input(in s):

  This inputis used to set the time that the feed and column settings change to values after intervention, it will always be smaller than the value set at the Simulation Timeinput.

Note: Set these to the desired values before clicking the Run Simulation with Intervention button.

3. User Guide – Distillation Column Design Calculation Interface

3.1. Interface



3.2. Major Sections of the Interface

{1} Dark Grey: This is the menu bar to switch between the Simulator page and the Legal Information page. The Simulator page can be accessed by pressing the 'F1' key, while the Legal Information page can be accessed by pressing the 'F2' key. **Note: for macOS system users, the menu bar is located at the top of the display window instead of the user interface.**

{2} Blue: This is the experimental schematic of the distillation column. Some inputs and outputs are displayed on this schematic after each run. The tray number is counted from the top of the distillation column, starting from "Tray 1". The last tray is always the reboiler.

{3} Gold: This is the area with run information.

- Runtime: the time that the executable file takes to run the design calculation and obtain results.

{4} Brown: This area contains the dropdown menu to switch between different binary systems for design calculation.

- Binary System dropdown menu:

  This dropdown menu is used to select the binary system for distillation. Two systems are available: Ethanol-Water System and Methanol-Isopropanol System. When switching between different systems, the variable name for inputs in Feed Settings section and Control Parameter Settings section will change as well.

{5} Red (Feed Settings): This is the area with input boxes and dropdown menus that control the feed settings into the distillation column.

- Feed Rate input box:

  Positive numbers only, allowed characters are: '0-9', '.'.

- Feed Rate Unit dropdown menu:

  Four feed rate units are available: L/h, kg/h, mol/h, $kmol/h$.

- Feed Composition input

- Feed Composition Type dropdown menu:

  Three feed composition types are available: volume fraction, mass fraction, mole fraction.

- Feed Temperature input (in °C)

{6} Green (Control Parameter Settings): This is the area with inputs and dropdown menus that control the distillation control parameter settings.

- Distillate Composition input: to set desired distillate composition.
- Distillate Composition Type dropdown menu:

  This is the dropdown menu to select the desired distillate composition type. Two types are available: mass fraction, mole fraction.

- Bottom Product Composition input: to set desired bottom product composition.
- Bottom Product Composition Type dropdown menu:

  This is the dropdown menu to select the desired bottom product composition type. Two composition types are available: mass fraction, mole fraction.

- Reflux Ratio input
- Minimum Reflux Ratio label:

  This is the label that updates the real-time minimum reflux ratio based on inputs from Binary System dropdown menu, Feed Composition slider, Feed Composition Type dropdown menu, Feed Temperature slider, Distillate Composition slider, and Distillate Composition Type dropdown menu.

- Reflux Ratio Range Type dropdown menu:

  This dropdown menu is used to select the type of reflux ratio slider range. Two range types are available:

  - Normal:

    This refers to the normal operating reflux ratio range: 0.5~5.0. Under this range type, the range of the reflux ratio input is fixed between 0.5 and 5.0.

  - Recommended:

    This refers to the recommended optimum reflux ratio range based on minimum reflux ratio (R_{min}): $1.2R_{min}$~$1.5R_{min}$. Under this range type, the range of the reflux ratio input is constantly updating based on the minimum reflux ratio: between $1.2R_{min}$ and $1.5R_{min}$.

The recommended optimum reflux ratio range will NOT be available if it is outside the normal operating reflux ratio range.

- Normal R Range or Recommended R Range label:

  This is the label to notify the user which reflux ratio range type is selected and what is its reflux ratio range.

{7} Pink (Column Design Settings): This is the area with inputs that control the distillation column design settings used to determine plate diameter.

- f_1: fraction of flooding velocity (U_{NF}) slider
- f_2: fraction of column net area (A_{net}) slider
- Tray Spacing slider:

  This slider is used to set the tray spacing. The tray spacing of the PIGNAT Distillation Column is $152.4\ mm$ $(6\ inches)$.

{8} Purple (Calculation and Result Settings): This is the area with dropdown menus, input box, and button to control calculation and result settings.

- Flow Rate Unit dropdown menu:

  This dropdown menu is used to select the result (output) flow rate unit. Four flow rate units are available: L/h, kg/h, mol/h, $kmol/h$.

- Composition Type dropdown menu:

  This dropdown menu is used to select the result (output) composition type. Three composition types are available: volume fraction, mass fraction, mole fraction.

- Design Calculation File Name input box:

  This input box is used to enter the design calculation file name for saving the results. **Allowed characters are: 'a-z', 'A-Z', '0-9', '_', up to 25 characters.** In one design calculation, the results from all runs will be saved in a folder in the "Results" folder. For example, using the default file name: "Data", the folder name will be: "Distillation_Column_Design_Data". **This input box will be disabled after Run #1, Make Sure You Enter the Design Calculation File Name BEFORE Run #1.**

4. User Guide – Results

A simulation or design calculation can contain multiple runs. For one simulation or design calculation, a folder is created in the "Results" folder to store results from all runs. There can be saved results in the folder for as many runs as desired, if the executable file is not closed. The folder contains all the plots generated from each run and a single Excel file to store numerical results from all runs.

For Shortcut Distillation Simulation, the folder name will be "SC_Distillation_" + Simulation File Name; one plot is generated for each run.

For Steady-state Rigorous Distillation Simulation, the folder name will be "SS_Distillation_" + Simulation File Name; two plots are generated for each run.

For Unsteady-state Rigorous Distillation Simulation, the folder name will be "USS_Distillation_" + Simulation File Name; three plots are generated for each run.

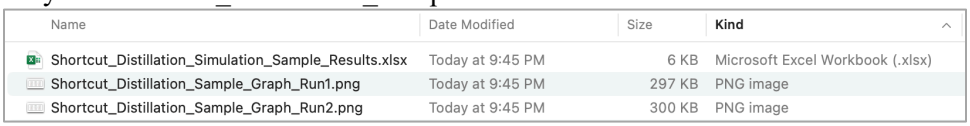
For Distillation Column Design Calculation, the folder name will be "Distillation_Column_Design_" + Design Calculation File Name; two plots are generated for each run.

4.1. Sample Results

A sample result with Simulation File Name or Design Calculation File Name "Sample" and two runs is illustrated below.

4.1.1. Shortcut Distillation Simulation

Folder Directory: "Results/SC_Distillation_Sample/"



Name	Date Modified	Size	Kind
Shortcut_Distillation_Simulation_Sample_Results.xlsx	Today at 9:45 PM	6 KB	Microsoft Excel Workbook (.xlsx)
Shortcut_Distillation_Sample_Graph_Run1.png	Today at 9:45 PM	297 KB	PNG image
Shortcut_Distillation_Sample_Graph_Run2.png	Today at 9:45 PM	300 KB	PNG image

- Numerical Results for Run #1

	x (EtOH)	y (EtOH)	T (°C)
Tray# 1	0.682	0.728	78.8
Tray# 2	0.626	0.694	79.108
Tray# 3	0.551	0.652	79.597
Tray# 4	0.443	0.597	80.453
Tray# 5	0.29	0.516	82.011
Tray# 6	0.159	0.403	84.136
Tray# 7 (Reboiler)	0.076	0.293	87.279

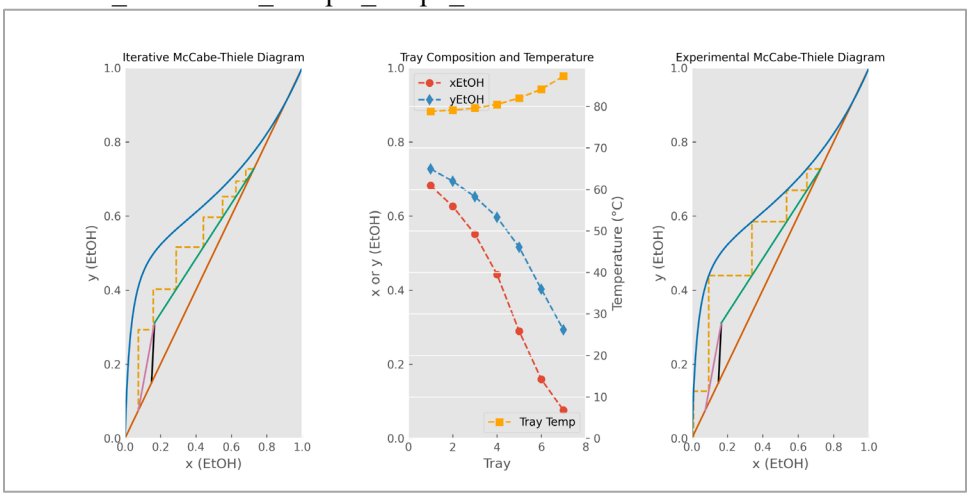
	Run Info
Simulation Mode	Lab Simulation
System	Ethanol-Water System
Run #	1
Runtime (s)	0.408

	Column Settings
R	2.87
RP (kW)	21.1
RP_eff (%)	55
F (L/h)	45
zF (EtOH)	0.15
TF (°C)	25
NS	7

	Enriching Section
xD	0.728
D (mol/s)	0.06
L (mol/s)	0.171
V (mol/s)	0.231
	Stripping Section
xB	0.076
B (mol/s)	0.464
Lb (mol/s)	0.754
Vb (mol/s)	0.29
	Column Design
Condenser Duty (kW)	9.211
Reboiler Duty (kW)	11.605
Optimum Feed Location	5

- Graphical Results for Run #1

File Name: “Shortcut_Distillation_Sample_Graph_Run1.PNG”



4.1.2.Steady-state Rigorous Distillation Simulation

- Folder Directory: “Results/SS_Distillation_Sample/”

Name	Date Modified	Size	Kind
SS_Distillation_Simulation_Sample_Results.xlsx	Today at 9:44 PM	6 KB	Microsoft Excel Workbook (.xlsx)
SS_Distillation_Sample_Run1_F1.png	Today at 8:33 PM	241 KB	PNG image
SS_Distillation_Sample_Run1_F2.png	Today at 8:33 PM	169 KB	PNG image
SS_Distillation_Sample_Run2_F1.png	Today at 9:44 PM	250 KB	PNG image
SS_Distillation_Sample_Run2_F2.png	Today at 9:44 PM	174 KB	PNG image

- Numerical Results for Run #1

	x (EtOH)	y (EtOH)	T (°C)	P (mmHg)	L (mol/s)	V (mol/s)	EmV	hcl (mm)	hFe (mm)	phiE
Tray# 1	0.598	0.668	79.285	760.003	0.166	0.224	0.623	11.191	15.812	0.708
Tray# 2	0.505	0.616	79.948	760.272	0.165	0.223	0.632	11.112	15.553	0.714
Tray# 3	0.259	0.548	82.417	760.522	0.164	0.222	0.638	10.893	14.97	0.728
Tray# 4	0.254	0.542	82.505	760.984	0.751	0.286	0.685	12.592	18.766	0.671
Tray# 5	0.242	0.528	82.691	761.442	0.751	0.286	0.684	12.559	18.66	0.673
Tray# 6	0.215	0.497	83.125	761.888	0.751	0.285	0.683	12.485	18.42	0.678
Tray# 7 (Reboiler)	0.086	0.426	86.78	762.303	0.75	0.284	1			

Run Info	
Simulation Mode	Lab Simulation
System	Ethanol-Water System
Run #	1
Runtime (s)	0.473
Warning	None

(2)

Column Settings	
R	2.87
RP (kW)	21.1
RP_eff (%)	55
F (L/h)	45
zF (EtOH)	0.15
nF	3
TF (°C)	25
NS	7

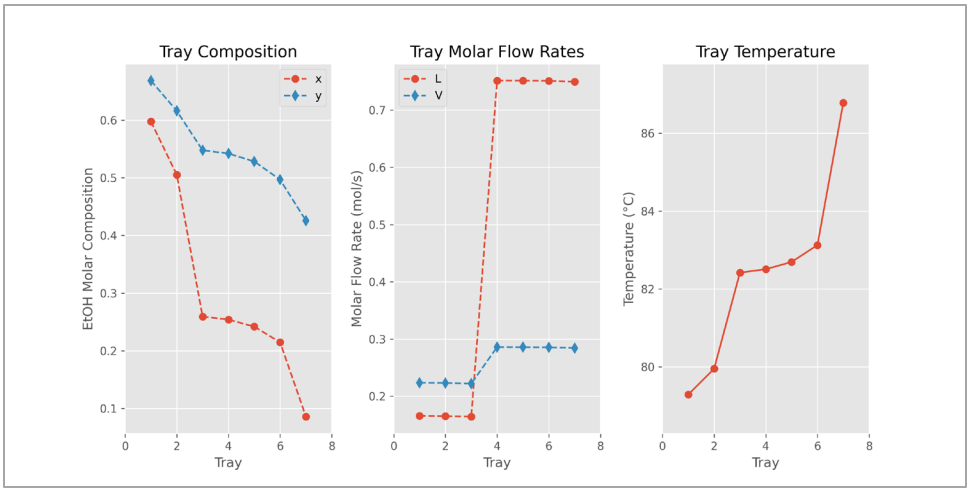
(3)

xD	D (mol/s)
0.668	0.058
xB	B (mol/s)
0.086	0.466

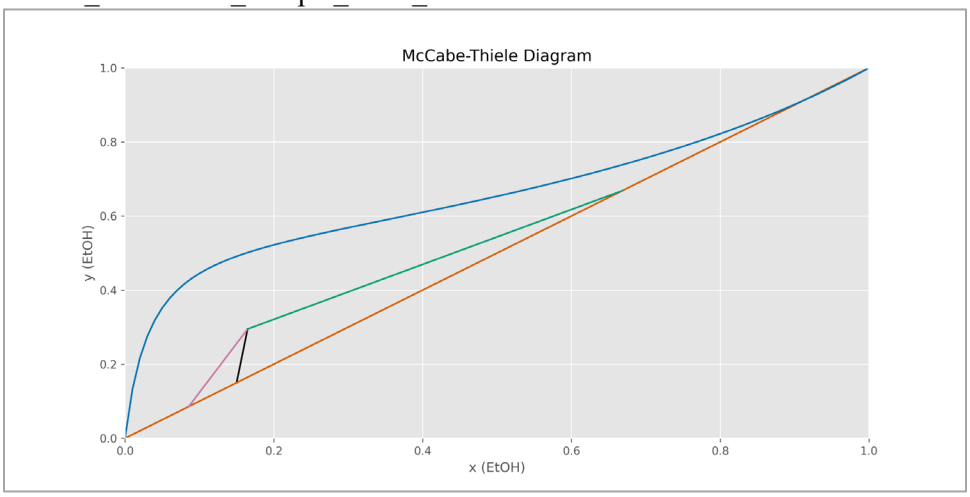
(1)

- Graphical Results for Run #1

Run #1 Plot 1: “SS_Distillation_Sample_Run1_F1.PNG”



Run #1 Plot 2: “SS_Distillation_Sample_Run1_F2.PNG”



4.1.3. Unsteady-state Rigorous Distillation Simulation

- Folder Directory: “Results/USS_Distillation_Sample/”

Name	Date Modified	Size	Kind
USS_Distillation_Simulation_Sample_Results.xlsx	Today, 6:15 PM	12 KB	Microsoft Excel Workbook (.xlsx)
USS_Distillation_Sample_Run1_Startup_F1.PNG	Today, 3:43 PM	421 KB	PNG image
USS_Distillation_Sample_Run1_Startup_F2.PNG	Today, 3:43 PM	357 KB	PNG image
USS_Distillation_Sample_Run1_Startup_F3.PNG	Today, 3:44 PM	183 KB	PNG image
USS_Distillation_Sample_Run2_Startup_F1.PNG	Today, 4:01 PM	420 KB	PNG image
USS_Distillation_Sample_Run2_Startup_F2.PNG	Today, 4:01 PM	352 KB	PNG image
USS_Distillation_Sample_Run2_Startup_F3.PNG	Today, 4:01 PM	185 KB	PNG image

- Numerical Results

Run #1: without Intervention

	x (EtOH)	y (EtOH)	T (°C)	P (mmHg)	L (mol/s)	V (mol/s)	EmV	M (mol)	hcl (mm)	hFe (mm)	phiE
Tray# 1	0.596	0.665	79.297	760	0.166	0.223	0.601	2.506	8.272	11.682	0.708
Tray# 2	0.507	0.614	79.952	760.932	0.165	0.223	0.607	2.742	8.267	11.566	0.715
Tray# 3	0.259	0.548	82.449	761.846	0.164	0.222	0.682	4.423	9.81	13.479	0.728
Tray# 4	0.254	0.542	82.548	762.855	0.753	0.286	0.675	4.162	9.159	13.645	0.671
Tray# 5	0.242	0.528	82.744	764.085	0.75	0.286	0.674	4.238	9.162	13.607	0.673
Tray# 6	0.215	0.496	83.178	765.308	0.754	0.286	0.671	4.408	9.151	13.497	0.678
Tray# 7 (Reboiler)	0.087	0.428	86.788	766.513	0.755	0.284	1				

	Run Info
Simulation Mode	Lab Simulation
System	Ethanol-Water System
Run #	1
Mode	Startup
Intervention	None
Simulation Time (min)	10
Actual Simulation Time (s)	600
Runtime (s)	204.673
Warning	None

(2)

	Column Settings
R	2.87
RP (kW)	21.1
RP_eff (%)	55
F (L/h)	45
zF (EtOH)	0.15
nF	3
TF (°C)	25
NS	7

(3)

xD	D (mol/s)
0.665	0.058
xB	B (mol/s)
0.087	0.471

(1)

Run #2: with Intervention

	x (MeOH)	y (MeOH)	T (°C)	P (mmHg)	L (mol/s)	V (mol/s)	EmV	M (mol)	hcl (mm)	hFe (mm)	phiE
Tray# 1	0.507	0.607	72.795	760	0.191	0.318	0.471	1.633	7.477	12.559	0.595
Tray# 2	0.431	0.547	74.189	761.53	0.188	0.315	0.461	1.558	7.476	12.633	0.592
Tray# 3	0.387	0.502	75.043	763.095	0.186	0.313	0.568	1.737	8.559	14.525	0.589
Tray# 4	0.333	0.438	76.063	764.745	0.407	0.333	0.556	1.64	8.334	14.722	0.566
Tray# 5	0.281	0.374	77.088	766.598	0.404	0.33	0.552	1.594	8.34	14.826	0.563
Tray# 6	0.231	0.31	78.077	768.496	0.403	0.328	0.548	1.548	8.325	14.889	0.559
Tray# 7 (Reboiler)	0.153	0.249	79.612	770.435	0.397	0.325	1				

	Run Info
Simulation Mode	Design Simulation
System	Methanol-Isopropanol System
Run #	2
Mode	Startup
Intervention	Yes
Intervention Time (s)	160
Actual Intervention Time (s)	160
Simulation Time (min)	10
Actual Simulation Time (s)	600
Runtime (s)	194.048

(2)

	Column Settings	Column Settings
Type	Before Intervention	After Intervention
R	1.5	1.5
RP (kW)	23	23
RP_eff (%)	55	55
F (L/h)	45	45
zF (MeOH)	0.44	0.44
nF	3	3
TF (°C)	25	44.1
NS	7	7
Warning	None	None

(3)

xD	D (mol/s)
0.607	0.127
xB	B (mol/s)
0.153	0.072

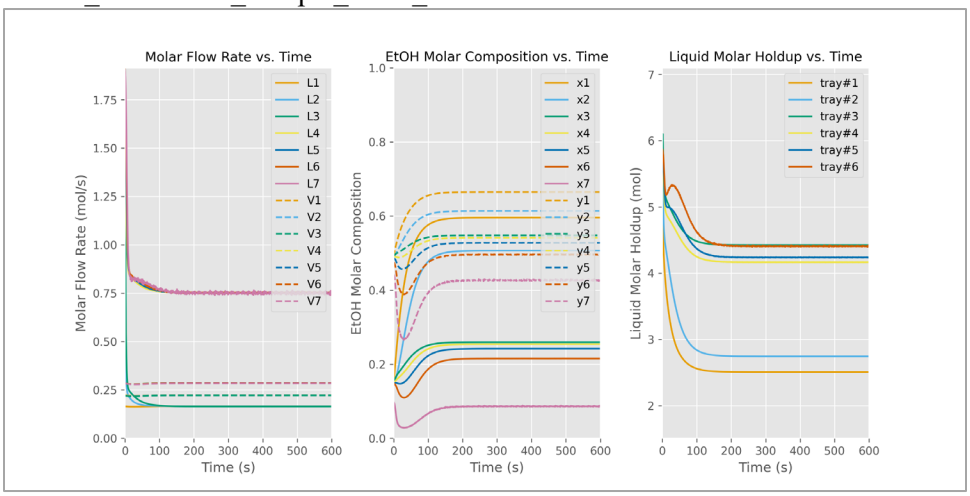
(1)

(4)

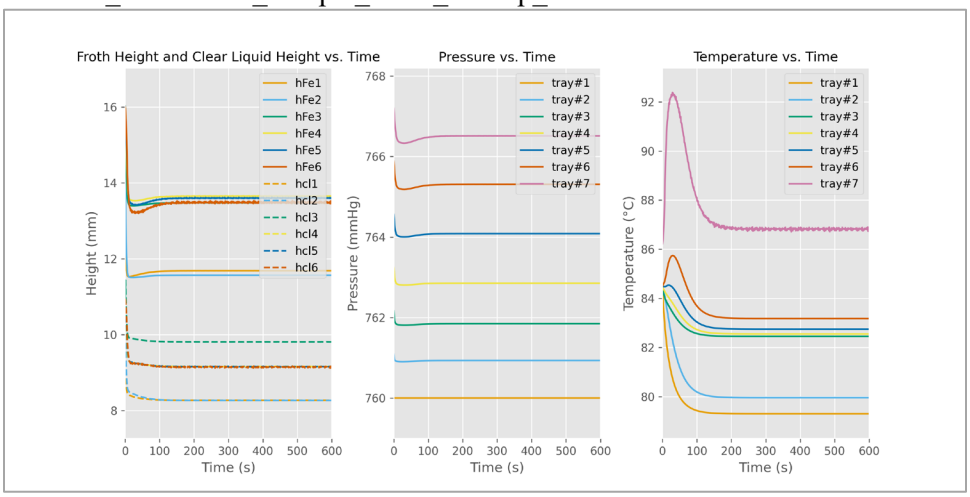
	x (MeOH)	y (MeOH)	T (°C)	P (mmHg)	L (mol/s)	V (mol/s)	EmV	M (mol)	hcl (mm)	hFe (mm)	phiE
Tray# 1	0.534	0.633	72.314	760	0.183	0.304	0.475	1.683	7.576	12.419	0.61
Tray# 2	0.457	0.573	73.696	761.42	0.18	0.302	0.465	1.604	7.575	12.492	0.606
Tray# 3	0.406	0.528	74.645	762.872	0.179	0.3	0.577	1.798	8.756	14.505	0.604
Tray# 4	0.356	0.467	75.587	764.414	0.419	0.334	0.56	1.67	8.379	14.769	0.567
Tray# 5	0.304	0.403	76.553	766.254	0.416	0.331	0.557	1.624	8.387	14.879	0.564
Tray# 6	0.254	0.339	77.514	768.138	0.416	0.329	0.553	1.575	8.37	14.944	0.56
Tray# 7 (Reboiler)	0.17	0.275	79.095	770.065	0.41	0.326	1				

- Graphical Results for Run #1:

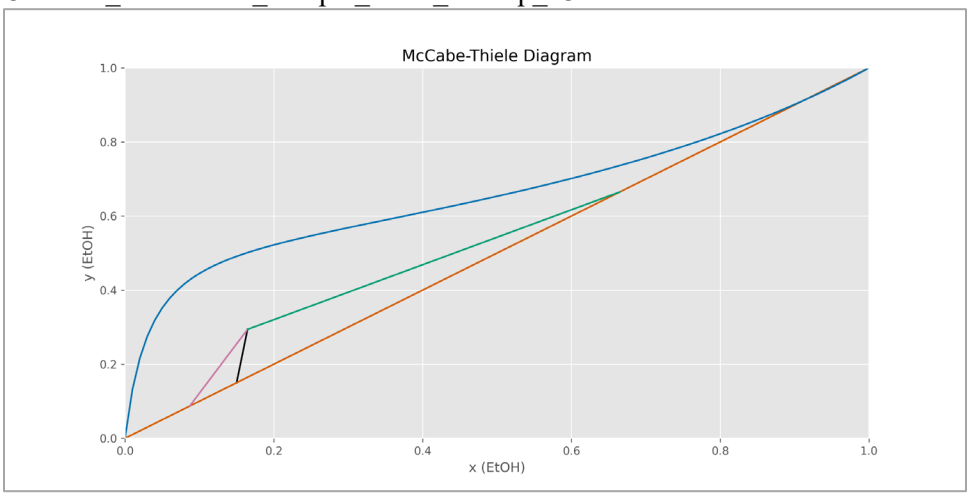
Run #1 Plot 1: "SS_Distillation_Sample_Run1_F1.PNG"



Run #1 Plot 2: “USS_Distillation_Sample_Run1_Startup_F2.PNG”

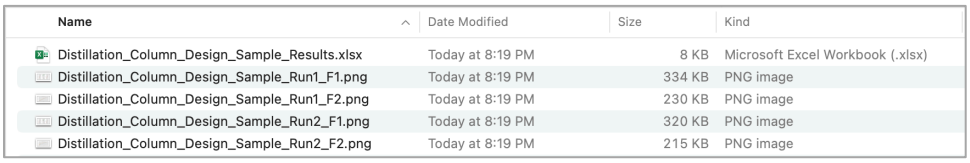


Run #1 Plot 3: “USS_Distillation_Sample_Run1_Startup_F3.PNG”



4.1.4.Distillation Column Design Calculation

- Folder Directory: “Results/Distillation_Column_Design_Sample/”



Name	Date Modified	Size	Kind
Distillation_Column_Design_Sample_Results.xlsx	Today at 8:19 PM	8 KB	Microsoft Excel Workbook (.xlsx)
Distillation_Column_Design_Sample_Run1_F1.png	Today at 8:19 PM	334 KB	PNG image
Distillation_Column_Design_Sample_Run1_F2.png	Today at 8:19 PM	230 KB	PNG image
Distillation_Column_Design_Sample_Run2_F1.png	Today at 8:19 PM	320 KB	PNG image
Distillation_Column_Design_Sample_Run2_F2.png	Today at 8:19 PM	215 KB	PNG image

- Numerical Results for Run #1

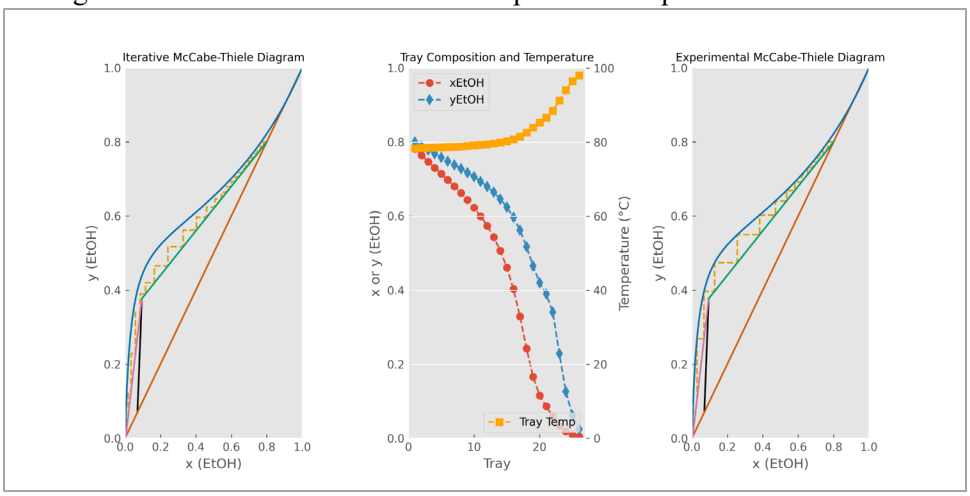
Tray# 1	0.781	0.8	78.39	0.266	0.443	Dist. Comp (EtOH mole fraction)	0.8
Tray# 2	0.764	0.789	78.45	0.266	0.443	Dist. Flow (kmol/h)	0.177
Tray# 3	0.747	0.778	78.51	0.266	0.443	xD	0.8
Tray# 4	0.73	0.768	78.58	0.266	0.443	D (mol/s)	0.049
Tray# 5	0.714	0.758	78.65	0.266	0.443	L (mol/s)	0.074
Tray# 6	0.697	0.748	78.73	0.266	0.443	V (mol/s)	0.123
Tray# 7	0.68	0.738	78.81	0.266	0.443		
Tray# 8	0.662	0.728	78.9	0.266	0.443		Stripping Section
Tray# 9	0.643	0.717	79.01	0.266	0.443	Bot. Comp (EtOH mole fraction)	0.005
Tray# 10	0.623	0.706	79.13	0.266	0.443	Bot. Flow (kmol/h)	1.974
Tray# 11	0.6	0.694	79.27	0.266	0.443	xB	0.005
Tray# 12	0.574	0.68	79.44	0.266	0.443	B (mol/s)	0.548
Tray# 13	0.543	0.664	79.66	0.266	0.443	Lb (mol/s)	0.724
Tray# 14	0.507	0.646	79.93	0.266	0.443	Vb (mol/s)	0.176
Tray# 15	0.461	0.624	80.29	0.266	0.443		
Tray# 16	0.403	0.597	80.81	0.266	0.443		Feed Information
Tray# 17	0.329	0.562	81.56	0.266	0.443	Feed. Comp (EtOH mole fraction)	0.07
Tray# 18	0.243	0.517	82.63	0.266	0.443	Feed. Flow (kmol/h)	2.152
Tray# 19	0.166	0.466	83.98	0.266	0.443	zF	0.07
Tray# 20	0.115	0.42	85.4	0.266	0.443	F (mol/s)	0.598
Tray# 21	0.086	0.389	86.67	2.606	0.632		
Tray# 22	0.059	0.341	88.5	2.606	0.632		Column Design
Tray# 23	0.034	0.228	91.26	2.606	0.632	Minimum Reflux Ratio	1.027
Tray# 24	0.018	0.126	94.13	2.606	0.632	Condenser Duty (kW)	4.901
Tray# 25	0.01	0.061	96.47	2.606	0.632	Reboiler Duty (kW)	7.059
Tray# 26 (Reboiler)	0.005	0.025	98.11	2.606	0.632	Overall Column Efficiency (%)	58.5
						Number of Equilibrium Stages	15
						Actual Number of Stages	26
						Optimum Feed Location	20
						Plate Diameter (mm)	26.985

	Run Info
System	Ethanol-Water System
Run #	1
Runtime (s)	0.463

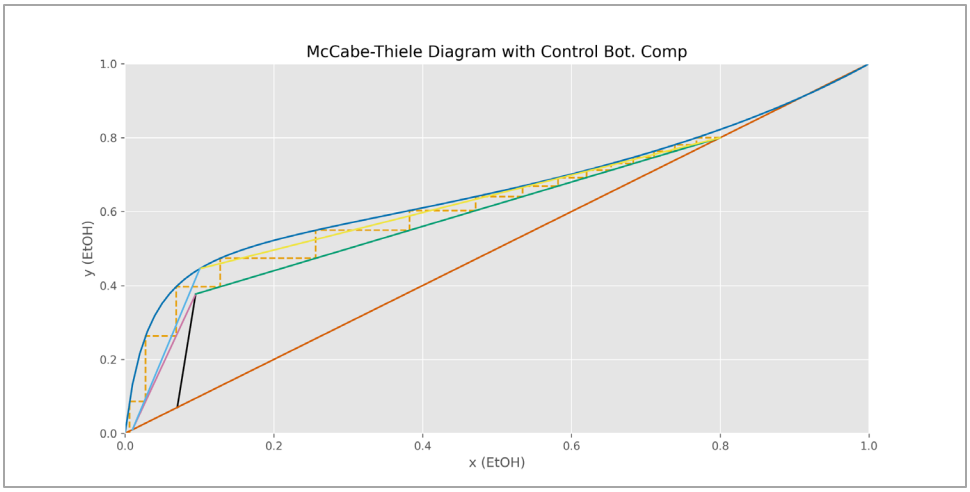
	Column Settings
Feed Rate (L/h)	45
Feed Comp (EtOH volume fraction)	0.2
TF (°C)	40.5
Dist. Comp Control (EtOH mole fraction)	0.8
Bot. Comp Control (EtOH mole fraction)	0.01
R	1.5
f1 (frac. of UNF)	0.8
f2 (frac. of Anet)	0.9

- Graphical Results for Run #1

Run #1 Plot 1: "Distillation_Column_Design_Sample_Run1_F1.PNG"
Note: This plot is generated with the calculated bottom product composition.



Run #1 Plot 2: "Distillation_Column_Design_Sample_Run1_F2.PNG"
Note: This plot is generated with the desired bottom product composition set in the Control Parameter Settings section. The number of equilibrium stages is counted from this plot.



4.2. About Numerical Results

4.2.1. Major Sections

{1} Red (for Distillation Column Design Calculation, Shortcut Distillation Simulation, and Steady-state Rigorous Distillation Simulation):
Variable values at steady-state and column design variables.

- Tray #1 ~ Tray #NS – 1: trays in the distillation column.
- Tray #NS: partial reboiler.

{1} Red (for Unsteady-state Rigorous Distillation Simulation):
Variable values at the end of actual simulation time.

- Tray #1 ~ Tray #NS – 1: trays in the distillation column.
- Tray #NS: partial reboiler.

{2} Orange: run information.
{3} Blue: column settings.
{4} Dark Purple (for Unsteady-state Rigorous Distillation Simulation with Intervention):
Variable values at the actual intervention time.

- Tray #1 ~ Tray #NS – 1: trays in the distillation column
- Tray #NS: partial reboiler.

4.2.2. Variables

Refer to the Nomenclature for details.

5. Nomenclature

A_{net}: column net area $[m^2]$
B: bottom molar flow rate $[mol/s]$
D: distillate molar flow rate $[mol/s]$
D_p: plate diameter $[mm]$
E_{MV}: tray efficiency
E_o: overall column efficiency
$EtOH$: ethanol
F: feed volumetric flow rate $[L/h]$ or feed molar flow rate $[mol/s]$
f_1: fraction of flooding velocity (U_{NF})
f_2: fraction of column net area (A_{net})
h_{cl}: clear liquid height $[mm]$
h_{Fe}: froth height $[mm]$
L: tray or enriching section liquid molar flow rate $[mol/s]$
$\bar{L}\ or\ L_b$: stripping section liquid molar flow rate $[mol/s]$
M: liquid molar holdup $[mol]$
$MtOH$: methanol
n_F: feed tray
N_{actual}: actual number of stages
N_{equil}: number of equilibrium stages
$N\ orNS$: total number of stages (including reboiler)
P: pressure $[mmHg]$
phi_E or ρ_E: froth density
R: reflux ratio
RP: reboiler power $[kW\ or\ kJ/s]$
RP_eff or RP_{eff}: reboiler efficiency [%]
T: temperature [℃]
TS: tray spacing $[mm]$
T_F: feed temperature [℃]
U_{NF}: flooding velocity $[m/s]$
V: tray or enriching section vapour molar flow rate $[mol/s]$
$\bar{V}\ or\ V_b$: stripping section vapour molar flow rate $[mol/s]$
x: liquid molar composition
x_B: bottom product molar composition
x_D: distillate molar composition
y: vapour molar composition
z_F: feed molar composition

6. Keyboard instructions

6.1. Legal Information about the Python Simulators

The following people contributed to the creation of this software:
Developers:
- Hao Wang
- Simon Rowat
- Tola Titcombe
- Evelyn Gondosiswanto
- Antonina Joukova
- Ethan Porter

Advisors:
- John Zhang
- Eric Croiset
- Stefan Pantazi

The following libraries were used:
Note: licenses listed below are POSSIBLE licenses used by the libraries. All information was found online and the sources were listed as well.

Python Standard Libraries [1] – “PSF License Agreement and the Zero-Clause BSD license” [2]
1. os library
2. math library
3. shutil library
4. timeit library
5. re library
6. tkinter library
7. tkinter.messagebox library
8. webbrowser library

Third-party Python Libraries
1. NumPy library – 'Distributed under a liberal BSD license' [3]
2. SciPy library – 'Distributed under a liberal BSD license' [4]
3. pandas library – 'BSD 3-Clause New' or 'Revised' License [5]
4. openpyxl – 'License: MIT/Expat' [6]
5. pillow (PIL fork) library – 'Like PIL, Pillow is licensed under the open source HPND License' [7]
6. matplotlib library – 'Matplotlib only uses BSD compatible code, and its license is based on the PSF license' [8]

[1] https://docs.python.org/3/library/
[2] https://docs.python.org/3/license.html
[3] https://numpy.org/
[4] https://scipy.org/
[5] https://github.com/pandas-dev/pandas/blob/master/LICENSE
[6] https://openpyxl.readthedocs.io/en/stable/
[7] https://pillow.readthedocs.io/en/stable/about.html
[8] https://matplotlib.org/stable/users/project/license.html

6.2. Windows

Action	Key
Opens Simulator (first) menu	F1
Opens Legal Information (second) menu	F2
Navigate to interactive elements	Tab - navigate forward Shift + Tab – navigate backward
Press button	Spacebar
Checkbox	Spacebar
Select (dropdown) menu	Spacebar - expand Arrow up/down - navigate between options Enter - select option and collapse
Scroll	Arrow up/down – scroll vertically

6.3. Mac

Action	Key
Opens Simulator (first) menu	F1
Opens Legal Information (second) menu	F2
Navigate to interactive elements	Tab - navigate forward Shift + Tab – navigate backward
Press button	Spacebar
Checkbox	Spacebar
Select (dropdown) menu	Spacebar - expand Arrow up/down - navigate between options Enter - select option and collapse
Scroll	Arrow up/down – scroll vertically

6.4. Unix

Action	Key
Opens Simulator (first) menu	F1
Opens Legal Information (second) menu	F2
Navigate to interactive elements	Tab - navigate forward Shift + Tab – navigate backward
Press button	Spacebar
Checkbox	Spacebar
Select (dropdown) menu	Spacebar - expand Arrow up/down - navigate between options Enter - select option and collapse
Scroll	Arrow up/down – scroll vertically