



ALChemE – User Manual

v0.2.0 <WIP>

github.com/PedroSeber/ALChemE
<Read the Docs website>

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Section 1 – Introduction to ALChemE

ALChemE is a software to assist users in calculations related to the chemical engineering field. As of v0.2.0, the software can assist in the analysis of heat exchange networks (HENs), with water recycle networks (WReNs), distillation, and other relevant processes to be implemented in the future.

Section 1.1 – Installation

Currently, there are two ways of installing ALChemE: downloading Python 3 and obtaining the .py files or obtaining the pre-compiled executable. The former is the easiest if the user already has or desires to install Python, and it maximizes the software customizability. It allows the software to be operated via a GUI or regular Python methods (such as Jupyter Notebooks or IDEs). The latter is better suited to those who do not have or want to install Python and are not interested in customizing the software or operating it without a GUI. Both options are completely free.

As Python is free and open-source, there are multiple ways to install it. The official Python website has a [downloads page](#) with multiple versions; installing the newest one should be sufficient for this software. A popular alternative is [Anaconda](#), which includes Python, some commonly used packages, and a package manager. Finally, there is also [Miniconda](#), which includes Python and the same package manager. If the user is new to Python and does not know which option to choose, we recommend Anaconda.

After installing Python, the user should obtain our package. Currently, we have not yet published our package, so please contact us to obtain the software. In the future, this will occur through pip, conda, and similar methods. We will update this user guide once our package is published.

Please contact us to obtain the pre-compiled executable. After downloading and extracting it, one should run the “frontend.exe” to open the GUI.

Section 1.2 – The Home Screen

The Home Screen is the first screen shown by ALChemE to the user. It lets the user access all software modules to assist in optimization. If the user is interested in HENs, please proceed to Section 2 – Heat Exchanger Networks. If the user is interested in WReNs, please proceed to Section 3 – Water Recycle Networks.

Section 2 – Heat Exchanger Networks

ALChemE allows users to analyze HENs to maximize energy recovery and minimize costs. As of v0.2.0, users can input streams and utilities (with units of measurement), plot temperature interval diagrams and composite curves, and manually add heat exchangers. The program automatically handles unit conversions, calculates properties such as MER targets or the pinch point location, and can automatically place exchangers to minimize their number. The user can request the function to automatically place exchangers to find more solutions, but there are no guarantees that all possible solutions will be found. These functions also return the cost of the HENs generated.

Section 2.1 – User Input

Stream Input

Stream Name Inlet Temperature Outlet Temperature °C Heat Capacity J/(kg·°C) Flow Rate kg/s OR Heat Load W

Heat Exchanger Input

Exchanger Name Hot Stream Cold Stream ΔT °C Reference Stream Hot OR Heat Load W

Exchanger Type Fixed Head Cost Parameter A Cost Parameter B Gauge Pressure Pa U J/(m²·s·°C)

Utility Input

Utility Name Utility Type Hot Temperature °C Cost \$/kW

Figure 1 – The user input section

The user input section of our GUI allows users to create streams, heat exchangers, and utilities. As seen in Figure 1, it consists of text boxes for text or numerical input and drop-down menus for the units of measurement.

To add a new stream, the user must supply numerical values to the “Inlet Temperature” and “Outlet Temperature” fields. The user must also supply numerical values to one of the following combinations of text boxes: (1) “Heat Capacity” and “Flow Rate”, (2) “Heat Capacity” only, which causes the value to be treated as an FC_p , or (3) “Heat Load”. Unused boxes should be left blank.

First and foremost, we highlight that we do not recommend adding heat exchangers manually. To manually add a heat exchanger, the user must supply the stream names to the “Hot Stream” and “Cold Stream”. The user can also provide numerical values for either the ΔT and choose a reference stream from which FC_p values will be obtained or the exchanger’s heat load. If both fields are left blank, the software will automatically calculate the maximum heat that can be exchanged between the two streams. The second input row consists of parameters used to calculate the exchanger’s cost. “Cost Parameter A” and “Cost Parameter B” are parameters that depend on the exchanger’s material of construction, as defined in p. 462 of Seider *et al.* [1]. If these fields are left blank, they default to 0. “U” is the overall heat transfer coefficient. If that field is left blank, it defaults to 100.

To add a new utility, select whether it is a hot or cold utility using the drop-down menu, then input its temperature and cost per power provided. As of v0.2.0, utility temperatures are used only to calculate exchanger costs. The software assumes that the hot utility is hotter and the cold utility is colder than any other stream. Thus, only one utility of each type should be used.

Section 2.2 – Object Explorer

Object Explorer						Activate/Deactivate Stream	Delete Object
<div> <div>STREAMS</div> <div> <div>H1</div> <div>H2</div> <div>C1</div> <div>C2</div> </div> </div> <div>HEAT EXCHANGERS</div> <div> <div>UTILITIES</div> </div>	<div>Inlet Temperature</div> <div>250.0 °C</div> <div>200.0 °C</div> <div>90.0 °C</div> <div>130.0 °C</div> <div>Hot Stream</div> <div>Utility Type</div>	<div>Outlet Temperature</div> <div>130.0 °C</div> <div>100.0 °C</div> <div>150.0 °C</div> <div>190.0 °C</div> <div>Cold Stream</div> <div>Temperature</div>	<div>Heat Capacity Rate</div> <div>1000.0 J/(delta_degC*s)</div> <div>4000.0 J/(delta_degC*s)</div> <div>3000.0 J/(delta_degC*s)</div> <div>6000.0 J/(delta_degC*s)</div> <div>Heat Exchange</div> <div>Cost</div>	<div>Heat Load</div> <div>120000.0 J/s</div> <div>400000.0 J/s</div> <div>180000.0 J/s</div> <div>360000.0 J/s</div> <div>FoB Cost</div>	<div>Status</div> <div>Active</div> <div>Active</div> <div>Active</div> <div>Active</div> <div>Status</div> <div>Status</div>		

Figure 2 – The Object Explorer

The Object Explorer resides below the input section. It allows the user to browse previously added streams, heat exchangers, and utilities. As seen in Figure 2, the Object Explorer shows some relevant information on each object. Double-clicking any object prints additional information about it on the Terminal. At the top-right corner of the Object Explorer, there are two buttons: “Activate/Deactivate Stream” and “Delete Object”. To use them, the user should click on an object then click on the corresponding button. Note that only streams can be activated/deactivated, but any object can be deleted. Inactive streams will not be plotted in the diagrams or taken into account during automatic stream matching.

Section 2.3 – Diagrams

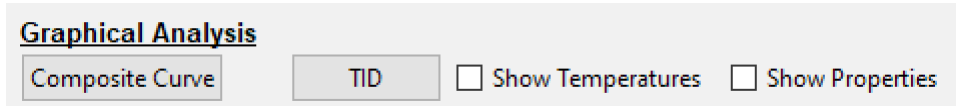


Figure 3 – The buttons used to generate plots

Based on the input provided by the user, ALChemE can automatically generate composite curves and TIDs. Composite curves also show the minimum utilities required and the maximum heat recovery possible. TIDs show the temperature of each interval, the FC_p of each stream, and the heat available for each stream in each subnetwork. The two checkboxes next to the “TID” button allow the user to show or hide that information. A sample TID with all information shown is provided in Figure 4 below.

Temperature Interval Diagram

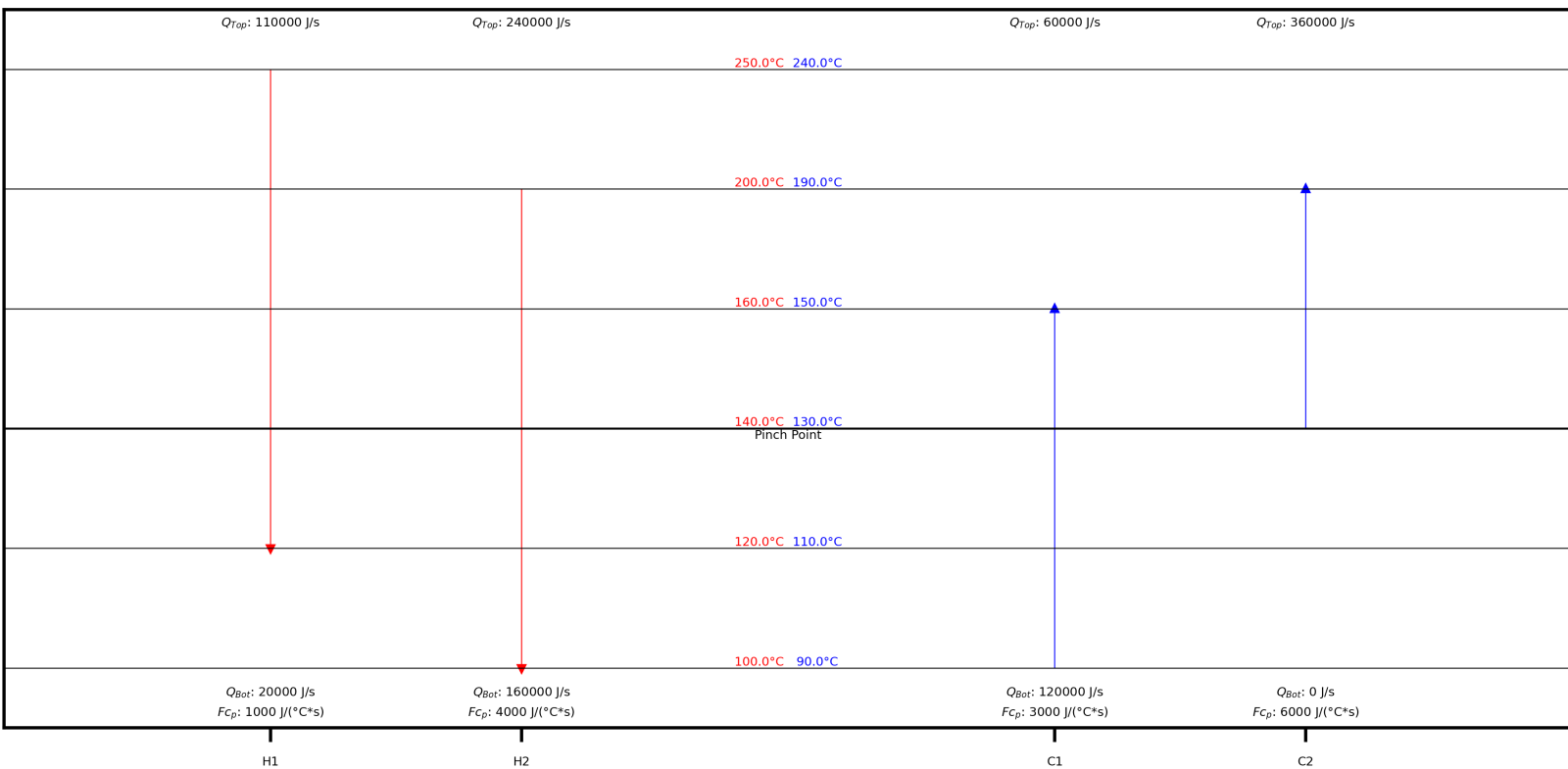


Figure 4 – A TID generated by ALChemE

Section 2.4 – Automatic HEN Optimization

Optimization Suite

☐ Above Pinch ☐ Below Pinch

Heat Transfer Constraint

Hot Stream	Cold Stream	Heat Transfer Limit	
Upper Limit ▾	<input type="text"/>	<input type="text"/>	W ▾

Add Constraint

Stream Match Constraint

Hot Stream	Cold Stream	
Forbidden ▾	<input type="text"/>	<input type="text"/>

Add Constraint

Heat Exchanger Settings

Fixed Head ▾	U	J/(°C·m ² ·s) ▾
	<input type="text"/>	

Solution Depth Setting

-	0	+
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Run HEN Optimization

Figure 5 – The automatic HEN optimization section

Using a mixed-integer linear optimization algorithm based on the streams and utilities input by the user, ALChemE can automatically place heat exchangers to minimize their number while following the MER. In its most basic form, the software calculates the maximum heat that can be exchanged between any two streams automatically and returns the location of, the heat exchanged within, and the cost of each exchanger. The user can manually set upper or lower limits on each match (for example, to prevent very small heat exchangers from being used). As of v0.2.0, if the user declares an upper limit for any match, he/she must declare upper limits for all other matches. The user can also forbid or require certain matches. No HEN may exist which simultaneously obeys the MER and the forbidden / restricted matches, which will cause the program to return an error.

Finally, the user can change the solution depth setting to have the program attempt to find novel solutions by forbidding or requiring certain matches. A depth of 0 returns only one solution, while a higher depth will attempt to find more. While there is no guarantee the software will find all possible solutions, this can provide alternative HENs, some of which may be better than the first HEN found.

Section 3 – Water Recycle Networks

<Information to be added in the future>

References

- [1]: W.D. Seider et al., PRODUCT AND PROCESS DESIGN PRINCIPLES, 4th ed., p. 462