

DSTWU – A Shortcut Distillation Model in Aspen Plus® V8.0

1. Lesson Objectives

- Learn how to use DSTWU to start distillation column design.
- Learn the strengths and limitations of shortcut methods

2. Prerequisites

- Aspen Plus V8.0

3. Background

DSTWU implements the following methods:

- Winn method to estimate minimum number of stages
- Underwood to calculate minimum reflux ratio
- Gilliland to relate actual number of stages and RR

DSTWU provides a very good starting point for distillation column design. Of course, we must be fully aware of the two assumptions on which the above three methods are based:

- Constant relative volatilities
- Constant molar overflow

DSTWU should not be used for systems that significantly deviate from these two assumptions. For systems with strongly non-ideal mixtures (e.g., ethanol-water), these shortcut methods won't work because those two assumptions just cannot represent those systems well.

If we need to design a column to separate a mixture of n-butane and cis-2-butene, DSTWU can be very helpful. In this case we would like to design a column to recover 99% of n-butane and 1% of butene in the distillate stream.

The examples presented are solely intended to illustrate specific concepts and principles. They may not reflect an industrial application or real situation.

4. Aspen Plus Solution

If you are unfamiliar with how to start Aspen Plus, select components, define methods, or construct a flowsheet, consult **Get Started Guide for New Users of Aspen Plus.pdf** for instructions.

First we will create a simulation for the separation of n-butane and cis-2-butene using the DSTWU model.

- 4.01. Start a new simulation using the **Blank Simulation** template in Aspen Plus.
- 4.02. The **Components | Specifications | Selection** sheet is displayed. Enter **N-BUTANE** in the **Component ID** column. Note that **Component name** and **Alias** are automatically filled for this component. Enter **BUTENE** as **Component ID** for the second component. Since **BUTENE** cannot uniquely identify a component, enter **CIS-2-BUTENE** as the **Component name** for the second component. Its **Alias** is automatically filled in.

The screenshot shows the 'Selection' sheet in Aspen Plus. The 'Selection' tab is active, and the 'Petroleum' sub-tab is selected. The 'Select components:' section contains a table with the following data:

	Component ID	Type	Component name	Alias
▶	N-BUTANE	<i>Conventional</i>	N-BUTANE	C4H10-1
▶	BUTENE	<i>Conventional</i>	CIS-2-BUTENE	C4H8-2
▶				

Below the table are five buttons: Find, Elec Wizard, User Defined, Reorder, and Review.

- 4.03. Define methods. Go to the **Methods | Specifications | Global** sheet. Select **PENG-ROB** for **Base method**.

The screenshot shows the 'Global' tab of a software interface. The 'Method name' is set to 'PENG-ROB'. The 'Base method' is also 'PENG-ROB'. The 'Method filter' is 'COMMON'. The 'Free-water method' is 'STEAM-TA' and 'Water solubility' is '3'. The 'EOS' is 'ESPRSTD', 'Data set' is '1', 'Liquid molar enthalpy' is 'HLMX106', and 'Liquid molar volume' is 'VLMX20'. The 'Modify' section has 'Heat of mixing', 'Poynting correction', and 'Use liquid reference state enthalpy' unchecked.

Property methods & options	Value
Method filter:	COMMON
Base method:	PENG-ROB
Henry components:	

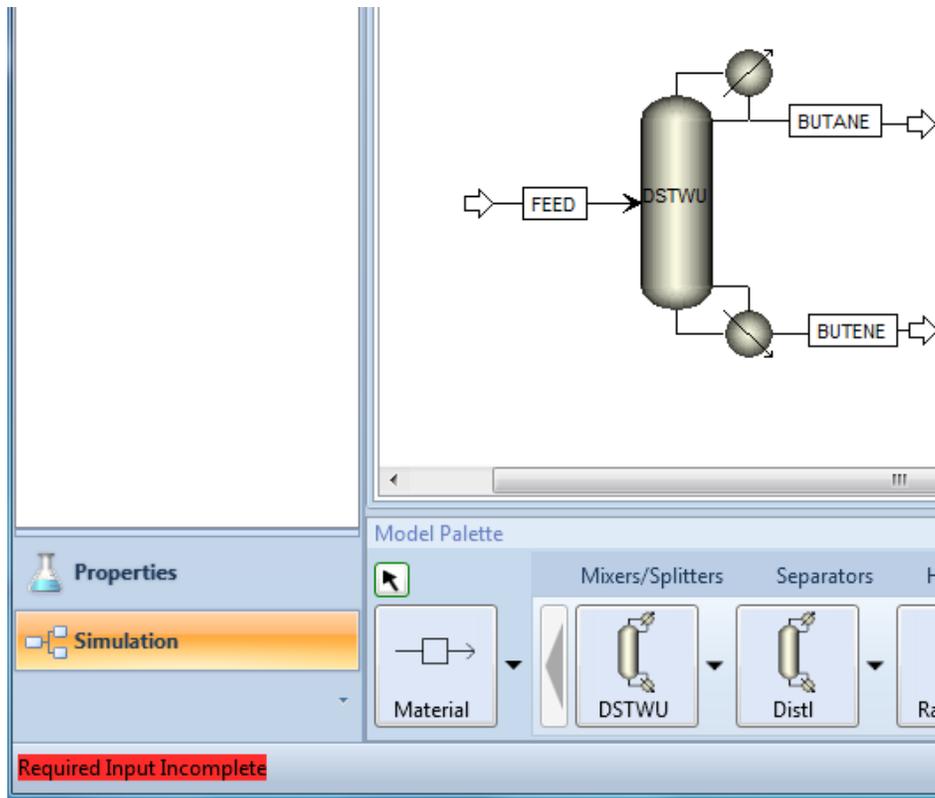
Petroleum calculation options	Value
Free-water method:	STEAM-TA
Water solubility:	3

Electrolyte calculation options	Value
Chemistry ID:	
<input checked="" type="checkbox"/> Use true components	

Method name:	Value
Method name:	PENG-ROB

Modify	Value
<input type="checkbox"/> Modify	
EOS:	ESPRSTD
Data set:	1
Liquid gamma:	
Data set:	
Liquid molar enthalpy:	HLMX106
Liquid molar volume:	VLMX20
<input type="checkbox"/> Heat of mixing	
<input type="checkbox"/> Poynting correction	
<input type="checkbox"/> Use liquid reference state enthalpy	

- 4.04. Go to the simulation environment and place a **DSTWU** block onto the **Main Flowsheet**. The **DSTWU** model is located under the **Columns** tab in the **Model Palette**. Connect the inlet and outlet ports with **Material** streams and rename them accordingly.



- 4.05. Specify feed streams. Double click on stream **FEED** or go to the **Streams | FEED | Input | Mixed** sheet. Select **Vapor Fraction** and **Pressure** for **Flash Type**. Enter **1** for **Pressure** and **0.5** for **Vapor fraction**. In the **Composition** frame, enter **50** for both **N-BUTANE** and **BUTENE**.

Mixed | CI Solid | NC Solid | Flash Options | EO Options | Costing | Information

Specifications

Flash Type: Vapor Fraction | Pressure

State variables

Temperature: [] C

Pressure: 1 | bar

Vapor fraction: 0.5

Total flow basis: Mole

Total flow rate: [] kmol/hr

Solvent: []

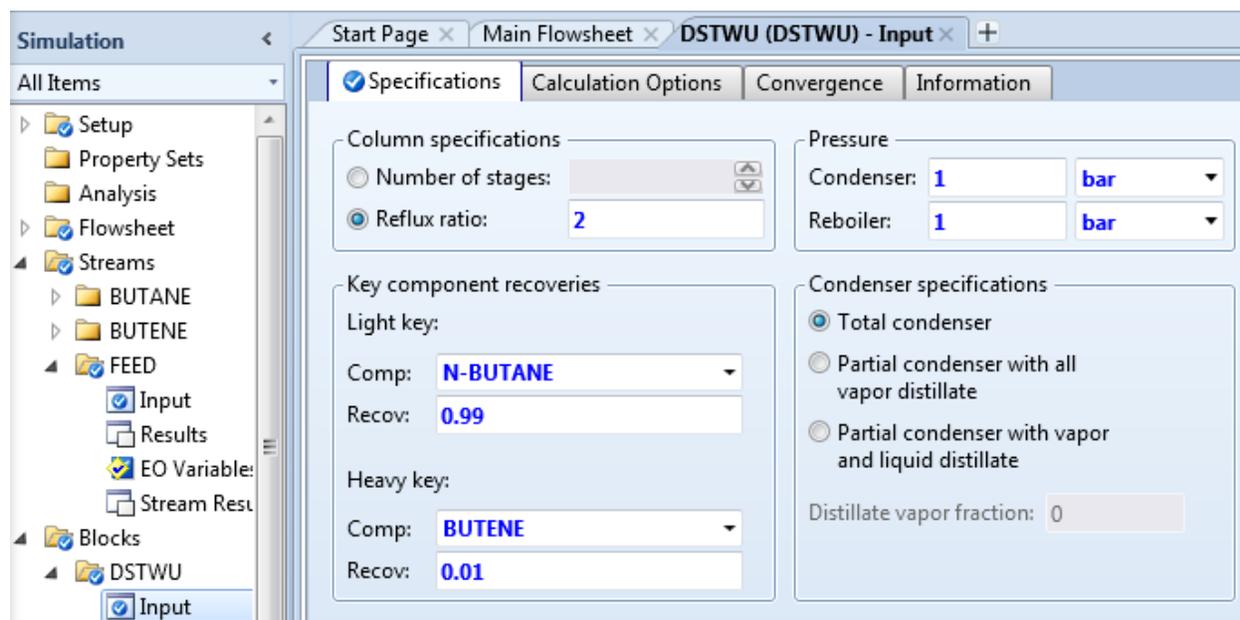
Composition

Mole-Flow | kmol/hr

Component	Value
N-BUTANE	50
BUTENE	50

Total: 100

- 4.06. Specify column operating conditions. Double click the column block on the **Main Flowsheet** or go to the **Blocks | DSTWU | Input | Specifications** sheet. In the **Column specifications** frame, select the **Reflux ratio** option and enter **2** for **Reflux ratio**. In the **Pressure** frame, enter **1** for both **Condenser** and **Reboiler**. In the **Key component recoveries** frame, select **N-BUTANE** for **Comp** and enter **0.99** for **Recov** for **Light key**. Select **BUTENE** for **Comp** and enter **0.01** for **Recov** for **Heavy key**.



- 4.07. Run the simulation by pressing the **F5** key. After running the simulation, you should receive an error for the **DSTWU** block stating that the specified reflux ratio is less than the minimum reflux ratio. **DSTWU** also took corrective action and calculated the actual reflux ratio based on the minimum reflux ratio. Therefore, the results are valid despite the error message. Go to the **Blocks | DSTWU | Results | Summary** sheet.

The screenshot shows the Aspen Plus simulation window with the 'Simulation' title bar. The 'DSTWU (DSTWU)' block is selected in the tree view, and the 'Results' sub-tab is active. The 'Results' table displays the following data:

Parameter	Value	Units
Minimum reflux ratio:	13.0904	
Actual reflux ratio:	26.1807	
Minimum number of stages:	64.4159	
Number of actual stages:	82.2863	
Feed stage:	45.9282	
Number of actual stages above feed:	44.9282	
Reboiler heating required:	1.95119e+06	cal/sec
Condenser cooling required:	2.02693e+06	cal/sec
Distillate temperature:	-0.733187	C
Bottom temperature:	3.12904	C
Distillate to feed fraction:	0.5	
HETP:		

- 4.08. This table provides very useful design information including **Minimum reflux ratio**, **Minimum number of stages**, and estimated duties. This table also provides an **Actual reflux ratio** and an **Actual number of stages**. These values will serve as good design estimates for this separation.
- 4.09. Now, save the simulation. On the ribbon, click **File** and then click **Save As** to save the simulation as **Dist-006_DSTWU-C4-C4.bkp**. Close the Aspen Plus simulation window.

- 4.10. We will now create a simulation for the separation of ethanol and water using the **DSTWU** model. Start another new simulation using the **Blank Simulation** template in Aspen Plus.
- 4.11. The **Components | Specifications | Selection** sheet is displayed. Enter **WATER** and **ETHANOL** in the **Component ID** column.

The screenshot shows the 'Selection' sheet in Aspen Plus. The 'Component ID' column contains 'WATER' and 'ETHANOL'. The 'Type' column shows 'Conventional' for both. The 'Component name' column shows 'WATER' and 'ETHANOL'. The 'Alias' column shows 'H2O' and 'C2H6O-2'. Below the table are buttons for 'Find', 'Elec Wizard', 'User Defined', 'Reorder', and 'Review'.

Component ID	Type	Component name	Alias
WATER	Conventional	WATER	H2O
ETHANOL	Conventional	ETHANOL	C2H6O-2

- 4.12. Define methods. Go to the **Methods | Specifications | Global** sheet. Select **ALL** for **Method filter**. Select **UNIQ-RK** for **Base method**.

The screenshot shows the 'Global' sheet in Aspen Plus. The 'Method filter' is set to 'ALL' and the 'Base method' is set to 'UNIQ-RK'. The 'Method name' is also 'UNIQ-RK'. The 'Modify' section is expanded, showing various options for the method, including 'Vapor EOS' (ESRK), 'Data set' (1), 'Liquid gamma' (GMUQUAC), 'Liquid molar enthalpy' (HLMX31), and 'Liquid molar volume' (VLMX01). The 'Heat of mixing' and 'Poynting correction' checkboxes are checked, while 'Use liquid reference state enthalpy' is unchecked.

Property methods & options

Method filter: ALL

Base method: UNIQ-RK

Henry components:

Petroleum calculation options

Free-water method: STEAM-TA

Water solubility: 3

Electrolyte calculation options

Chemistry ID:

Use true components

Method name: UNIQ-RK

Modify

Vapor EOS: ESRK

Data set: 1

Liquid gamma: GMUQUAC

Data set: 1

Liquid molar enthalpy: HLMX31

Liquid molar volume: VLMX01

Heat of mixing

Poynting correction

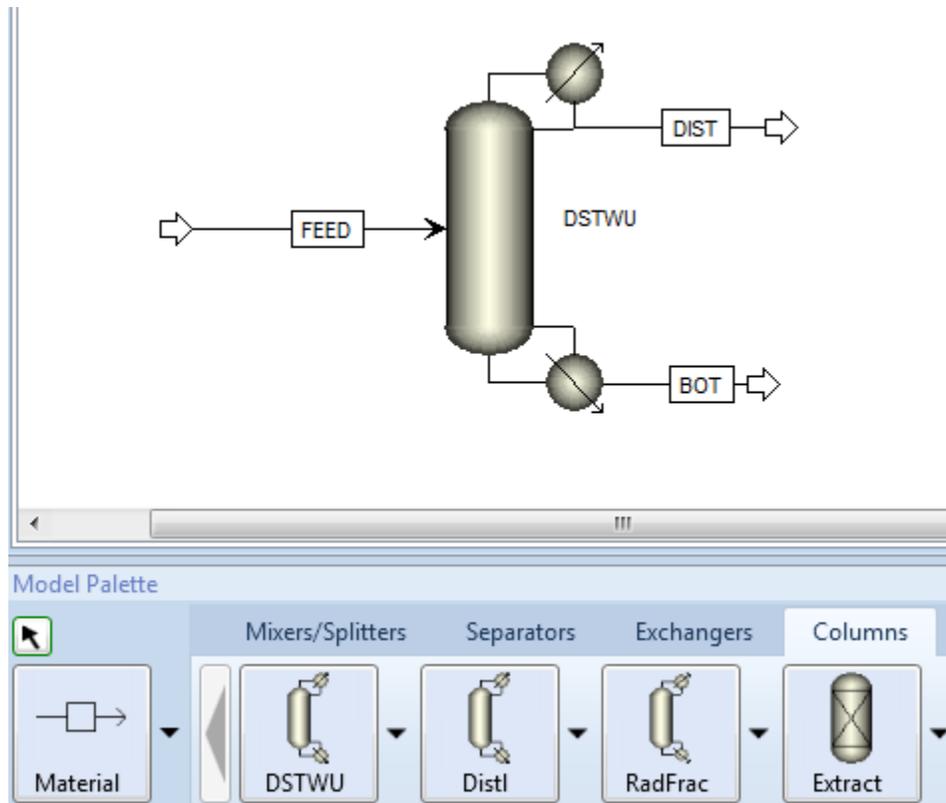
Use liquid reference state enthalpy

- 4.13. Press the **Next Input** button on the **Quick Access Toolbar** (or press the **F4** key on your keyboard). Binary parameters are automatically populated on the **Methods | Parameters | Binary Interaction | UNIQ-1 | Input** sheet.

The screenshot shows the Aspen Plus software interface. On the left is the 'Properties' tree with 'Binary Interaction | UNIQ-1' selected. The main window is titled 'Binary Interaction - UNIQ-1 (T-DEPENDENT)' and has the 'Input' tab selected. At the top, 'Parameter: UNIQ' and 'Data set: 1' are displayed. Below is a table of 'Temperature-dependent binary parameters'.

Parameter	Value	Units
Component i	WATER	
Component j	ETHANOL	
Temperature units	C	
Source	VLE-RK	
Property units		
AIJ	-2.371	
AII	1.8217	
BIJ	712.638	
BII	-664.537	
CIJ	0	
CJI	0	
DIJ	0	
DJI	0	
TLOWER	24.99	

- 4.14. Go to the **Simulation** environment and place a **DSTWU** block onto the **Main Flowsheet**. The **DSTWU** model is located under the **Columns** tab in the **Model Palette**. Connect the inlet and outlet ports with **Material** streams and name them accordingly.



- 4.15. Specify the feed stream. Go to the **Streams | FEED | Input | Mixed** sheet. Select **Vapor Fraction** and **Pressure** for **Flash Type**. Enter **1** for **Pressure** and **0.5** for **Vapor fraction**. In the **Composition** frame, enter **50** for both **WATER** and **ETHANOL**.

Mixed | CI Solid | NC Solid | Flash Options | EO Options | Costing | Information

Flash Type: **Vapor Fraction** | **Pressure**

State variables

Temperature: [] C

Pressure: **1** bar

Vapor fraction: **0.5**

Total flow basis: **Mole**

Total flow rate: [] kmol/hr

Solvent: []

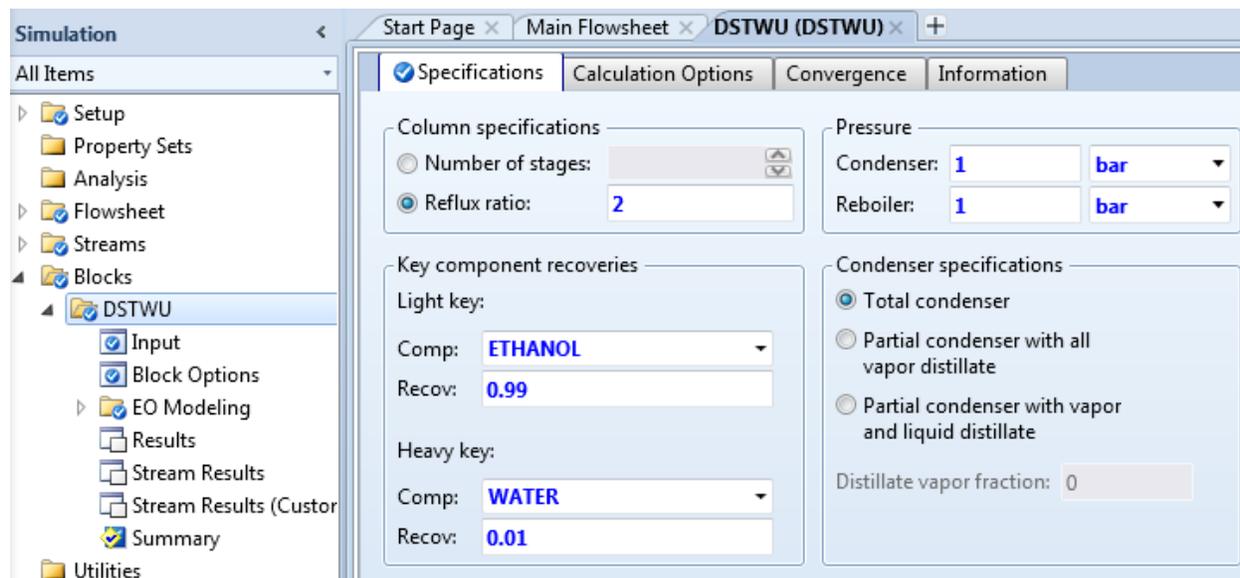
Composition

Mole-Flow | **kmol/hr**

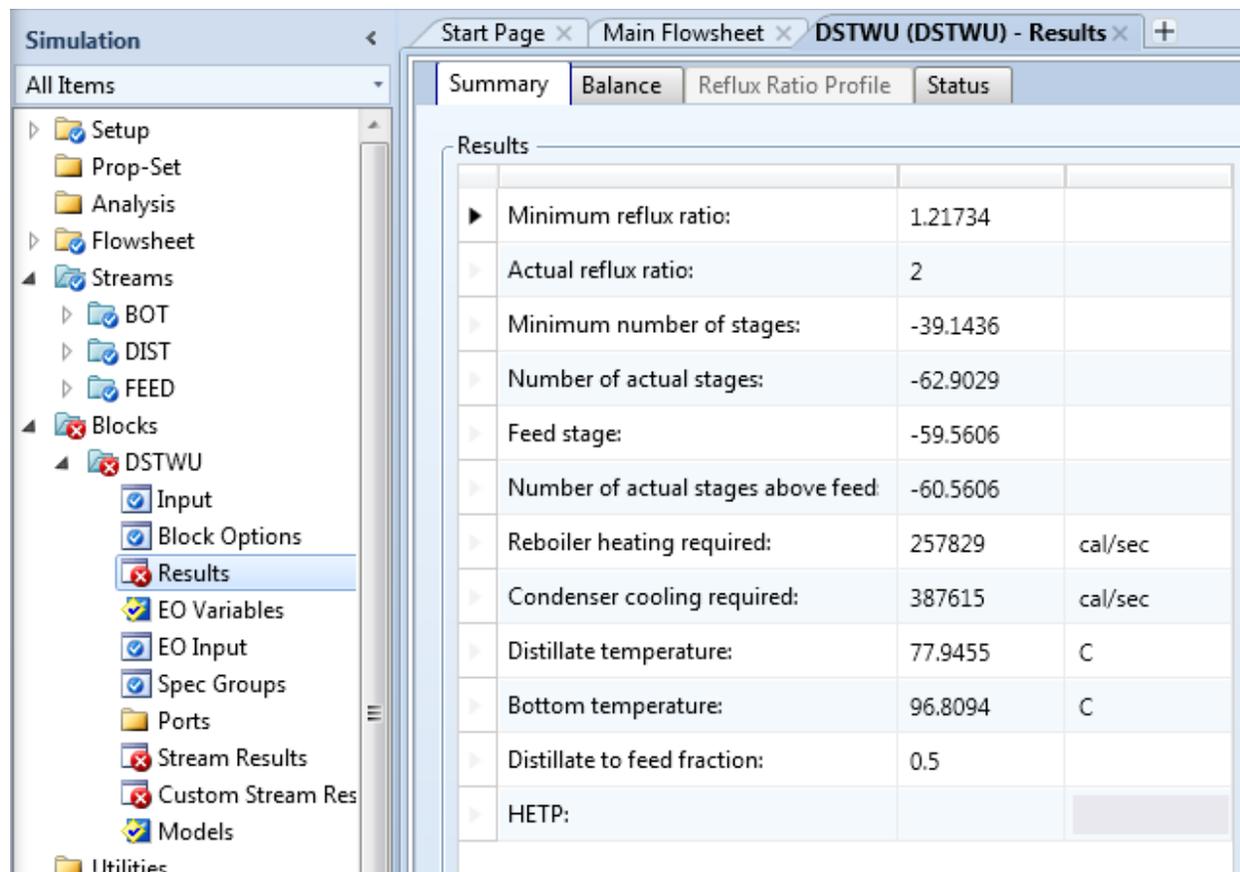
Component	Value
WATER	50
ETHANOL	50

Total: 100

- 4.16. Specify column operating conditions. Go to the **Blocks | DSTWU | Input | Specifications** sheet. In the **Column specifications** frame, select the **Reflux ratio** option and enter **2** for **Reflux ratio**. In the **Pressure** frame, enter **1** for both **Condenser** and **Reboiler**. In the **Key component recoveries** frame, select **ETHANOL** for **Comp** and enter **0.99** for **Recov** for **Light key**. Select **WATER** for **Comp** and enter **0.01** for **Recov** for **Heavy key**. Select **WATER** for **Comp** and enter **0.01** for **Recov** for **Heavy key**.



- 4.17. Run the simulation by pressing the **F5** key. There are error messages during simulation and the calculated minimum number of stages is a negative number. Therefore, the results cannot be used. We know that water and ethanol form an azeotrope and thus the assumption of constant relative volatility is not valid for this system.



Results			
▶ Minimum reflux ratio:	1.21734		
▶ Actual reflux ratio:	2		
▶ Minimum number of stages:	-39.1436		
▶ Number of actual stages:	-62.9029		
▶ Feed stage:	-59.5606		
▶ Number of actual stages above feed:	-60.5606		
▶ Reboiler heating required:	257829	cal/sec	
▶ Condenser cooling required:	387615	cal/sec	
▶ Distillate temperature:	77.9455	C	
▶ Bottom temperature:	96.8094	C	
▶ Distillate to feed fraction:	0.5		
▶ HETP:			

5. Conclusions

For mixtures where the following two assumptions are good approximations, the shortcut methods implemented in **DSTWU** are very useful and efficient to get us started.

- Constant relative volatilities
- Constant molar overflow

For systems that significantly deviate from those two assumptions (e.g., ethanol-water), these shortcut methods are not useful and we should not rely on results from these shortcut methods. For such cases, we need to use more rigorous models (e.g., **RadFrac**).

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