



Ciências
ULisboa

DWSIM SOFTWARE

**Biorefineries, Bioenergy
and Bioproducts**



April 19, 2023

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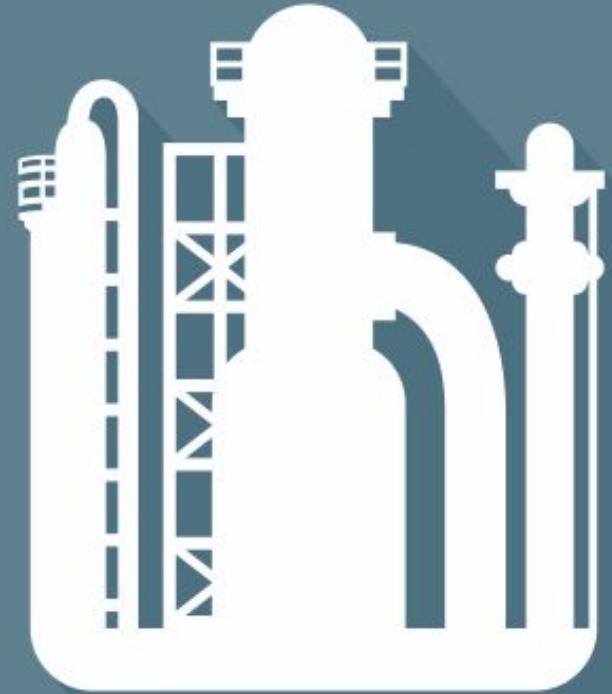
04

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FIRST SECTION 01

- *What is the DWSIM software?*
- *What is it used for?*



A graphic consisting of a teal vertical bar on the left and a white square on the right, with the text "DWSIM SIMULATOR" centered over the teal bar.

DWSIM SIMULATOR

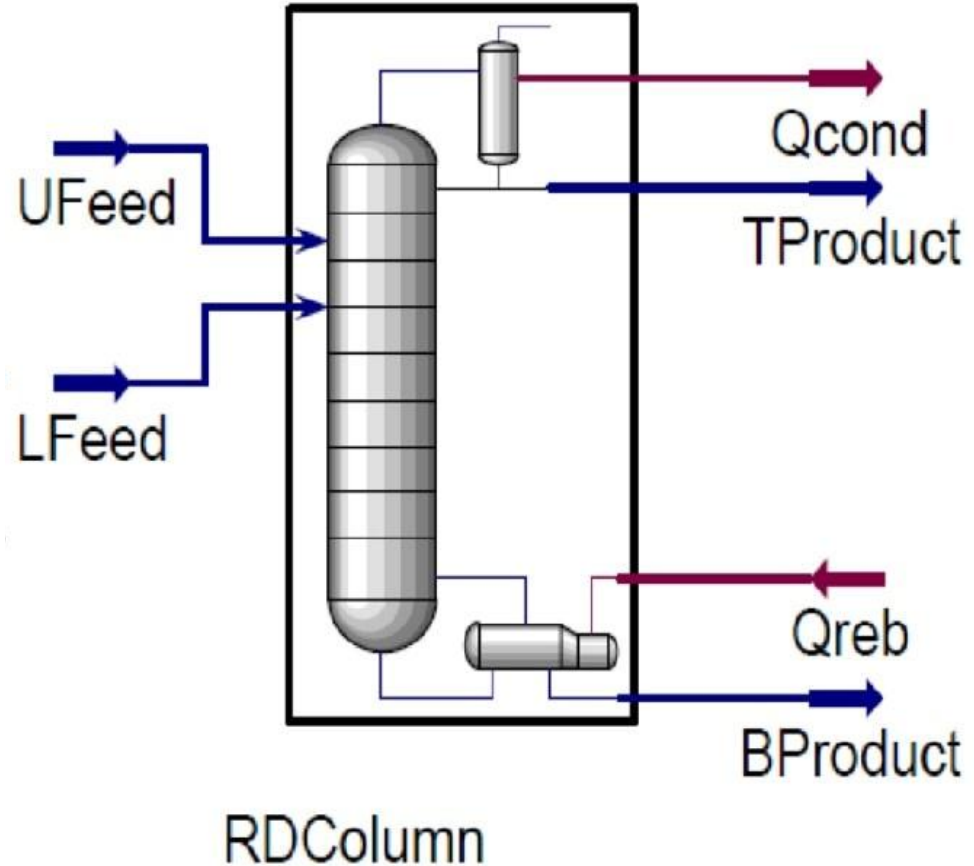
What is the DWSIM software?

- It's a free, open-source and CAPE-OPEN compliant chemical process simulator.
- It runs on all platforms, Windows, Linux, macOS, Android and iOS.

DWSIM SIMULATOR

What is DWSIM used for?

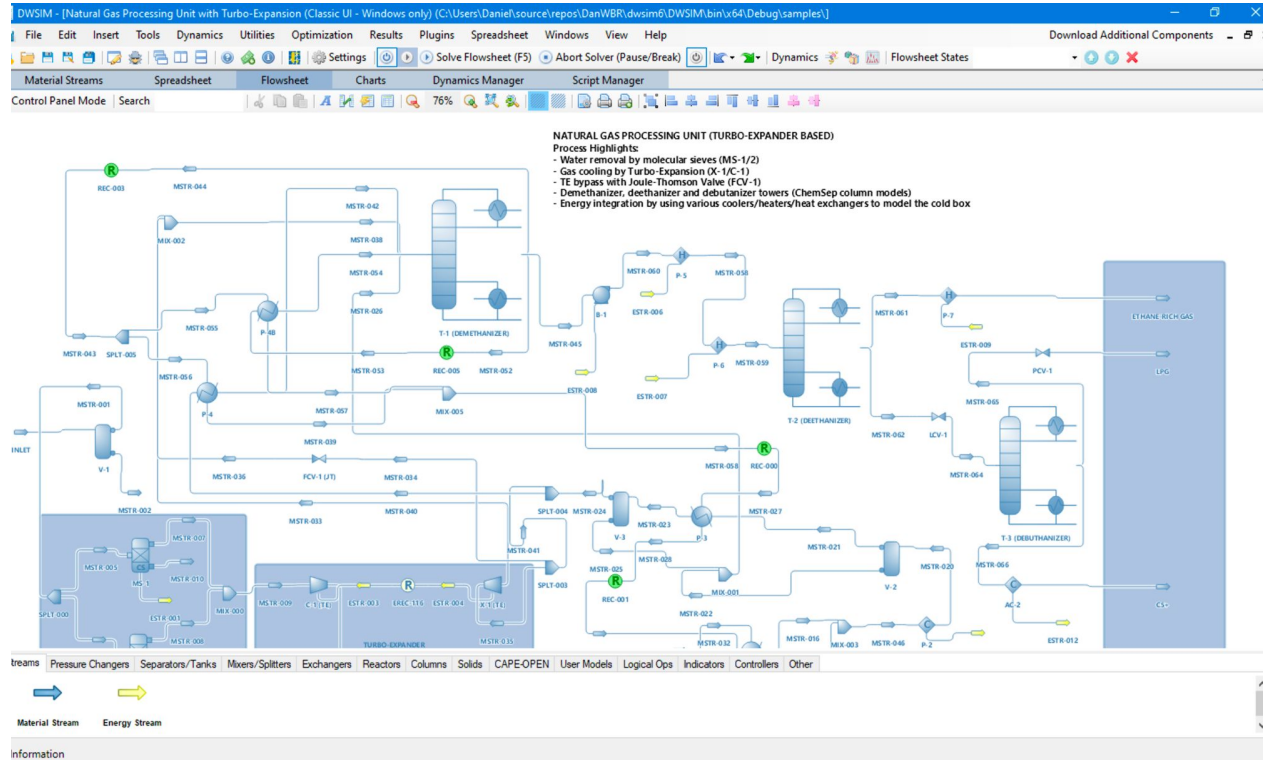
- The DWSIM simulator is used to **model processes** or the **actual plant operation** using rigorous thermodynamic and unit operations models.



EXEMPLE FROM DWSIM

What else can DWSIM do?

- Sensitivity Analysis.
- Mass and Energy balances.
- Spreadsheets and charts.
- And more.



02 SECOND SECTION

Thermodynamics

- Thermodynamics models in DWSIM
- Unit operations in steady-state and dynamic state
- Types of reactors

n_i, P_i, V_i, \dots

$W = -nRT \int_{V_1}^{V_2} \frac{dV}{V} = -nRT \ln\left(\frac{V_2}{V_1}\right)$ $H = U + pV$ $T(K) = T(^{\circ}C) + 273$

$dH = dU + d(pV)$ $dH = dU + pdV + VdP$

$U_f(n_f, P_f, V_f, \dots)$ $C_p = (\Delta H / \Delta T)_p$ $\Delta U = Q - W$

$U = dq + dw$ $C_p = \left(\frac{\partial H}{\partial T}\right)_p$ $W = P\Delta U$ $\Delta S = nRT \ln\left(\frac{V_2}{V_1}\right)$

$dH = dq - pdV + Vdp$ $dH = C_p dT$ $W = \int_{V_1}^{V_2} P dV$

$H = U + PV$ $\Delta H = q_p = C_p \times \Delta T$ $C_v = (\Delta U / \Delta T)_v$

$W = -pdV$ $\Delta S = \frac{\Delta_{\text{trn}}H}{T}$ $ds \geq \frac{dq}{T}$

$C_v = \left(\frac{\partial U}{\partial T}\right)_v$

$m(U_2 - U_1) \Delta KE$

$\frac{1}{2}m(v_2^2 - v_1^2) \Delta PE$

$mg(z_2 - z_1)$

$W_c = \frac{P_2 V_2 - P_1 V_1}{1 - \gamma}$ $\eta_{th} = \frac{W_{net}}{Q_{in}} = 1 - \frac{Q_{out}}{Q_{in}}$ $Q = \Delta U$

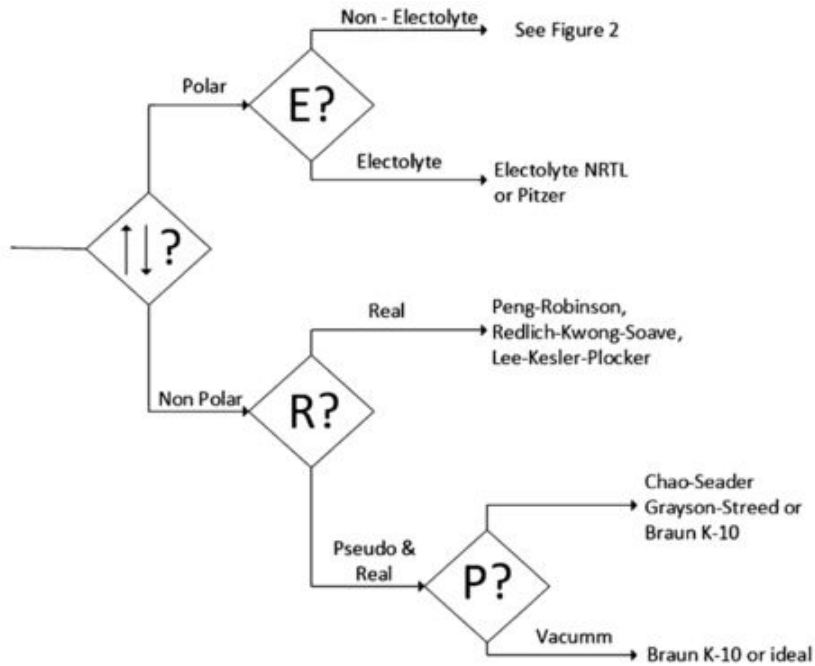
$dH = dq + Vdp$ $\Delta H = \Delta U + V\Delta p$

$T_R = \frac{T}{T_{cr}}$ $dU = C_v dT$

$\Delta U = q_v = C_v \times \Delta T$

$W_0 = P_1 V_1 \ln \frac{V_2}{V_1}$

$= P_1 V_1 \ln \frac{P_1}{P_2} = RT_1 \ln \frac{P_1}{P_2}$ $\Delta U = U_f - U_i = q(\text{heat}) + w(\text{work})$



Polarity



Electrolytes



Real or Pseudocomponents



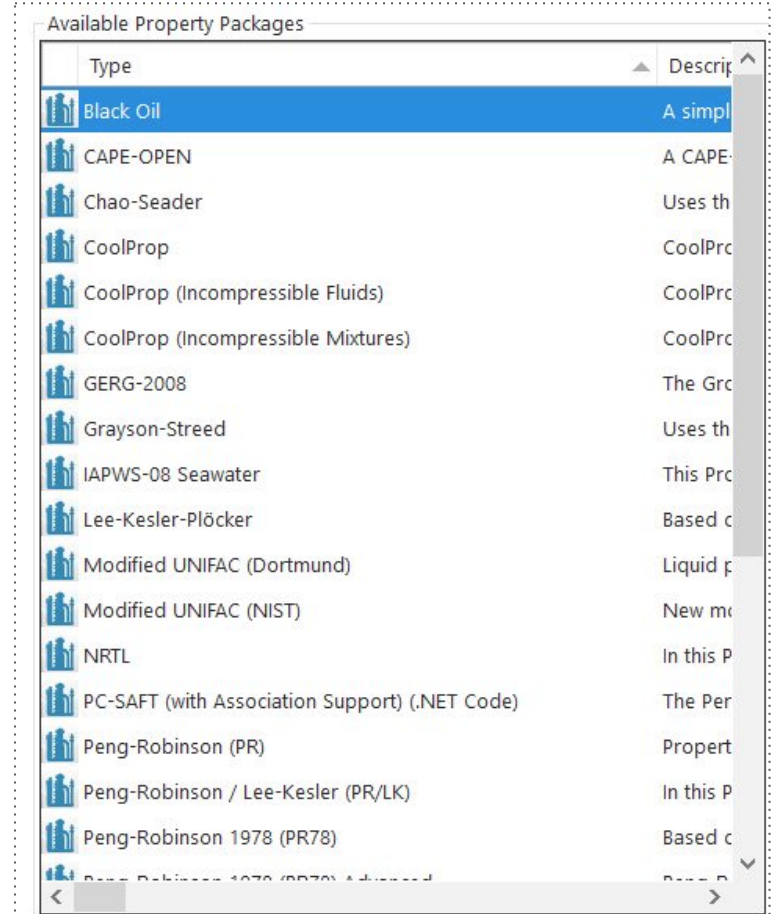
Pressure

THE PROPERTY PACKAGES

- Property packages or thermodynamics models define the mathematical equations used in a simulation.
- The selection of the property package is one of the first steps necessary in simulations, as well as one of the most important.

SOME PROPERTY PACKAGES

Name	Description
Raoult's Law	Non-polar gases at low pressures (< 10 atm)
Peng-Robinson (PR)	Non-polar gases at high pressures (> 10 atm)
Soave-Redlich-Kwong	Non-polar gases at high pressures (> 10 atm)
Peng-Robinson (PRSV2)	Polar gases at high pressures (> 10 atm); Non-polar gases at high pressures (> 10 atm)
CoolProp	Air Separation / Refrigeration systems



UNIT OPERATIONS

Some types available in DWSIM:

- **Mixers/Splitters** - Stream mixer; Stream Splitter; Energy mixer.
- **Pressure Changers** - Orifice Plate; Compressor; Pipe segment; Pump; Expander (turbine); Valve.
- **Separators/Tanks** - Compound Separator; Tank; Gas-Liquid Separator.
- **Exchangers** - Cooler; Heater; Heat exchanger; Air cooler.
- **Renewable Energies** - Hydroelectric turbines; PEM fuel cell; Solar panel; Water electrolyzer; Wind turbine.

MAIN TYPES OF REACTORS

Reactors are specialized modules that solve a particular system of reactions of the same type in sequence or in parallel.



Conversion reactor

Mass and energy
balances



Equilibrium reactor

Equilibrium
constant

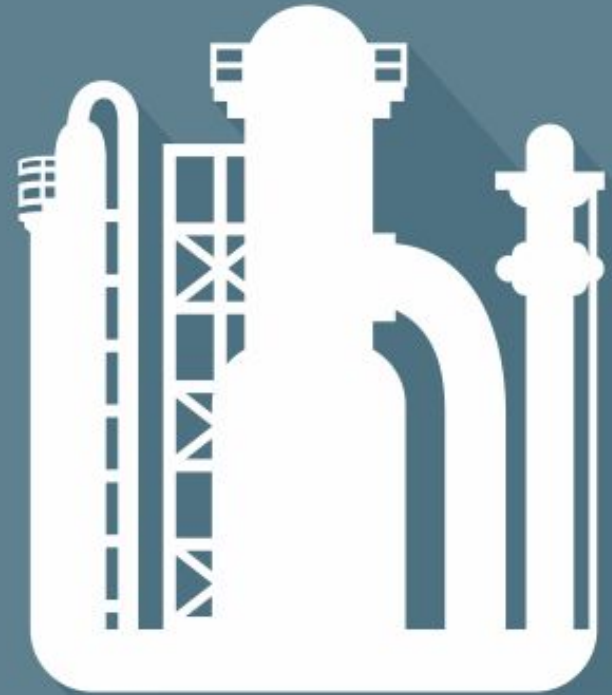


Gibbs reactor

Multiphase Gibbs
minimization
problem

FIRST SECTION 03

- *How to download and install DWSIM simulator?*



DWSIM DOWNLOAD



<https://dwsim.org/>

DWSIM

HOME DOWNLOAD ABOUT

Chemical Process Simulation for Everyone

DWSIM for Desktop is free and open-source

DOWNLOAD NOW DISCOVER DWSIM PRO SUPPORT THE PROJECT VIEW DOCUMENTATION

DWSIM is reliable and its results are comparable to commercial process simulators:



WINDOWS (64-BIT)

Installer Package
(207 MB)

DOWNLOAD

PYTHON ENVS ADD- ON

The Python Environments Add-on contains additional Python components for DWSIM. Extract the files to DWSIM's installation directory.

Portable Package
(159 MB)

DOWNLOAD

Requires Microsoft .NET 4.6.2+ /
Mono 6.8+



MACOS (64-BIT)

Disk Image File
(152 MB)

DOWNLOAD



LINUX (32/64-BIT)

64-bit Debian Installer
Package
(162 MB)

DOWNLOAD

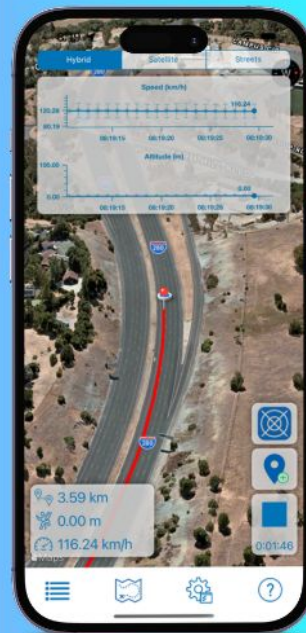
32-bit 7z-compressed
Wine Package
(383 MB)

DOWNLOAD

GeoTracker Pro

Record your position, speed, altitude and many more while you're on the move.

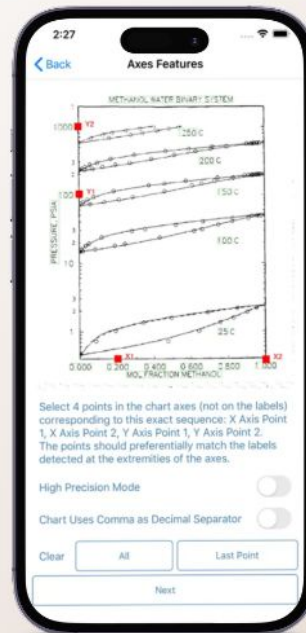
Analyze and export the recorded data with this easy-to-use app.



Download on the
App Store

Plot Digitizer

Get data from 2D XY Plots directly on your phone. Copy data to clipboard, share it, view a digital plot or fitted equations from the digitized data.



Select 4 points in the chart axes (not on the labels) corresponding to this exact point sequence: X Axis Point 1, X Axis Point 2, Y Axis Point 1, Y Axis Point 2. The points should preferentially match the labels detected at the extremities of the axes.

High Precision Mode

Chart Uses Comma as Decimal Separator

Clear

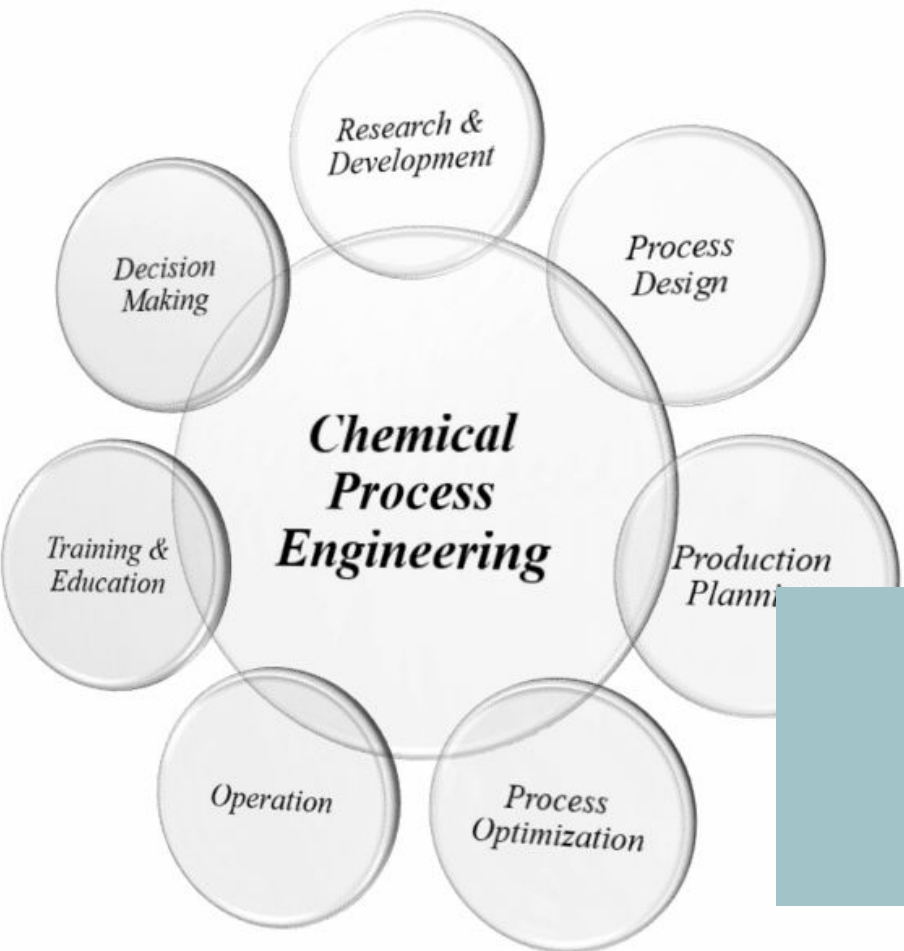
All

Last Point

Next

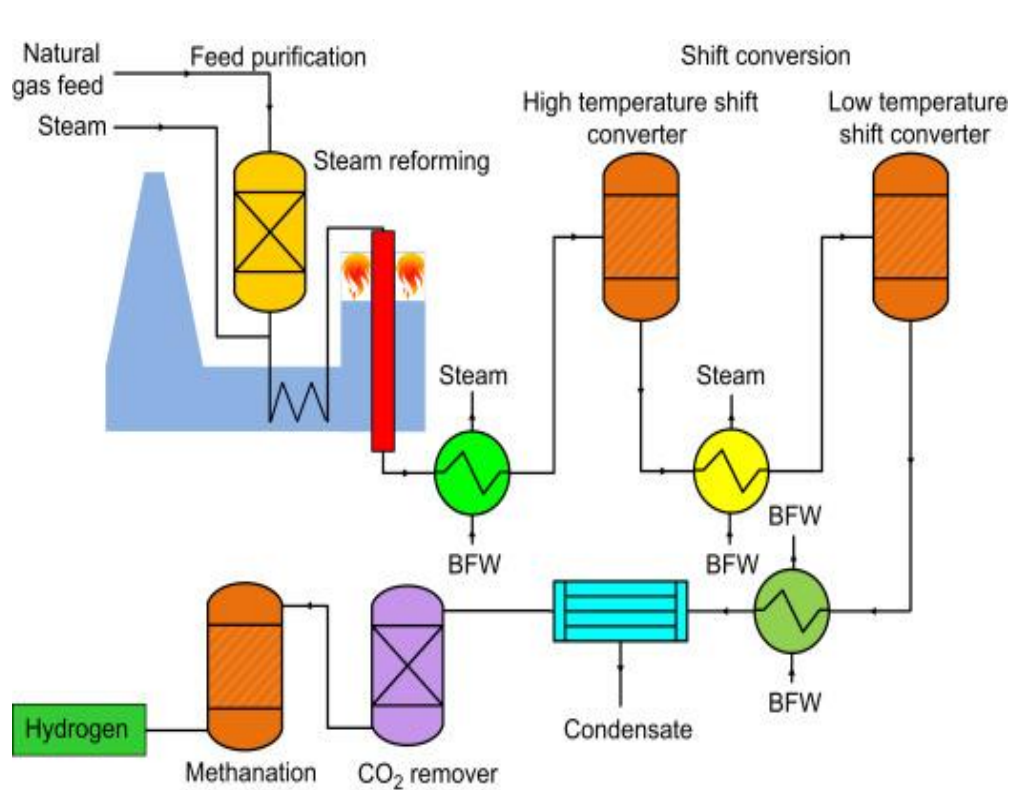
Download on the
App Store

04 SECOND SECTION



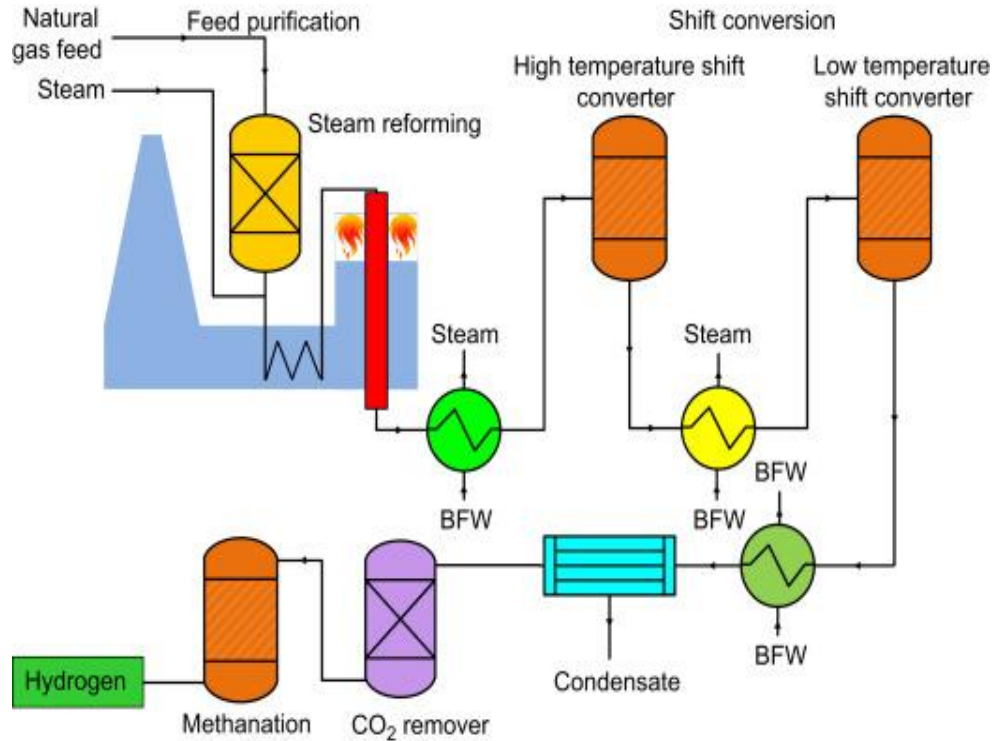
Chemical Process Engineering

- *How to create a simulation in DWSIM*
 - *Example by steps*
 - *Results Analysis*



EXERCISE FRAMEWORK

Objective: Simulation of the methane steam reforming, SMR, process to produce hydrogen, H₂.



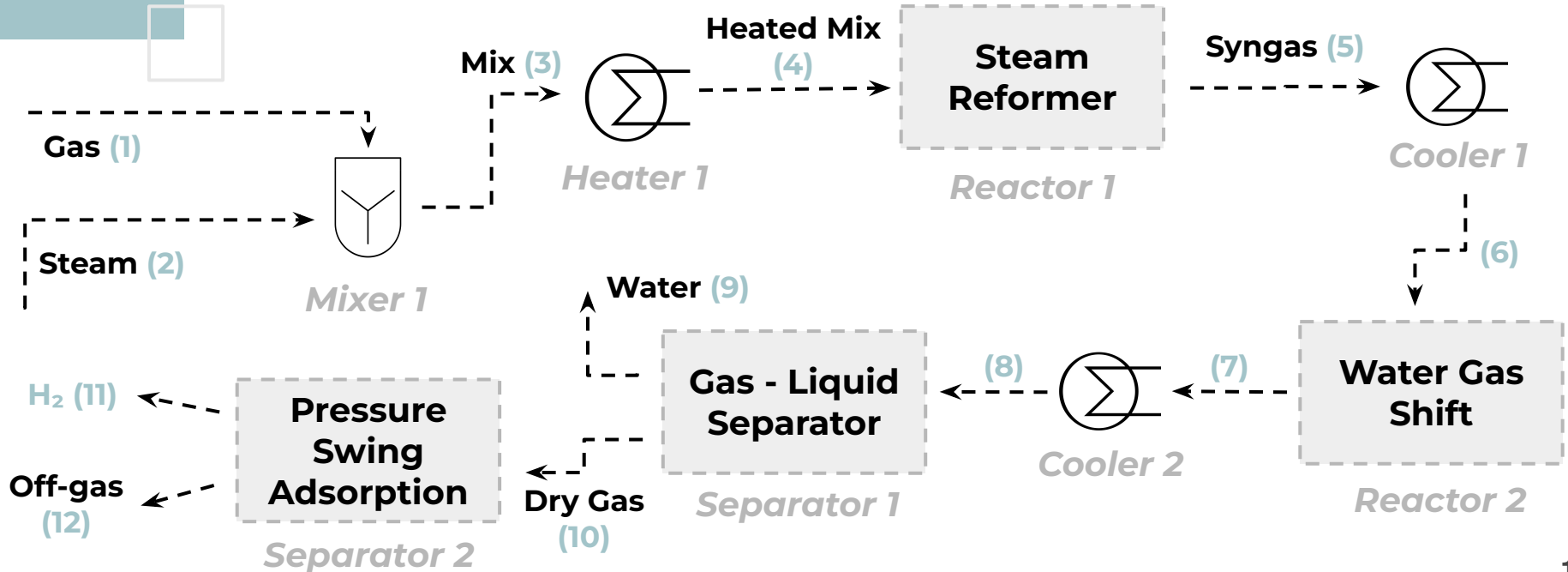
EXERCISE FRAMEWORK

Considerations:

- Shift conversion process only requires one converter instead of two. We'll consider the High Temperature Shift, HTS, reactor.
- The off-gas produced in the process will be burned to produce heat and energy.
- Hydrogen will be compressed.

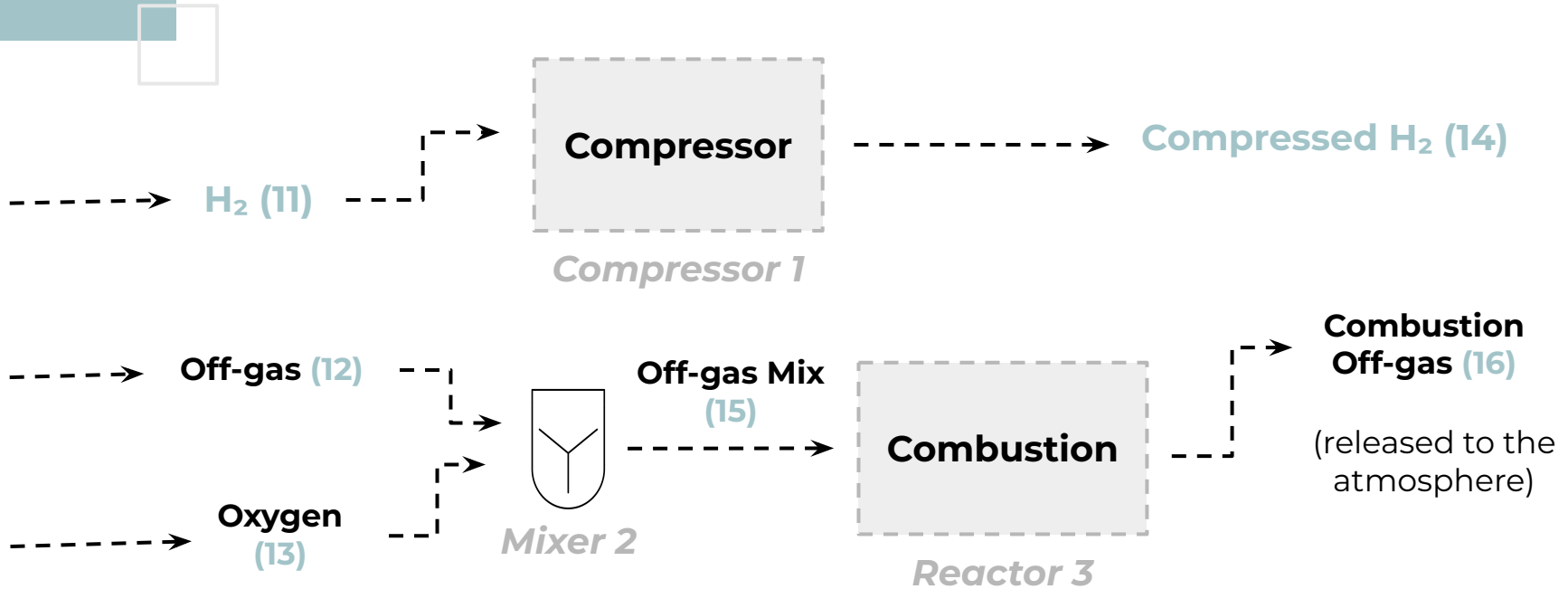
STEAM METHANE REFORMING (EXERCISE)

Scheme



STEAM METHANE REFORMING (EXERCISE)

Scheme



STEAM METHANE REFORMING (EXERCISE)

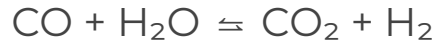
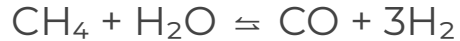
Stream
Properties

		Characteristics			Composition (% mol/mol)					
		T (°C)	P (bar)	Mass flow (kg/h)	CH_4	C_2H_6	H_2O	CO_2	N_2	H_2
(1) Feed	Natural Gas	25	1	10	86.0	11.2	0	1.5	0.8	0.5
(2)	Steam	150	1	30	0	0	100	0	0	0
(13)	Oxygen	35	15	1						

STEAM METHANE REFORMING (EXERCISE)

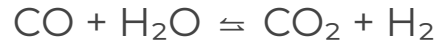
SMR REACTOR

Type: Equilibrium
Operation T: 730°C
Operation P: 30 bar
Isothermic



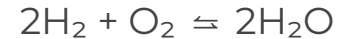
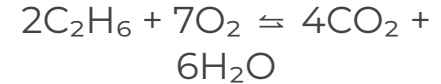
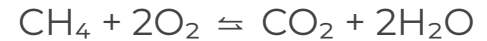
WGS REACTOR

Type: Equilibrium
Operation T: 400°C
Operation P: 29 bar
Isothermic



COMBUSTION REACTOR

Type: Conversion
Outlet T: 200°C



STEAM METHANE REFORMING (EXERCISE)

Unit
Properties

	<i>Heater 1</i>	<i>Cooler 1</i>	<i>Cooler 2</i>	<i>PSA</i>	<i>Compressor</i>
<i>Calculation Type</i>	Outlet Temperature	Outlet Temperature	Outlet Temperature	% Inlet molar flow	Outlet Pressure (Adiabatic)
<i>Outlet Temperature (°C)</i>	730	400	35	—	—
<i>Pressure (bar)</i>	30	29	15	—	200 (outlet P)
<i>Efficiency (%)</i>	100	100	100	75 (to H ₂)	75

DWSIM HOME PAGE

Create a new simulation

Open other recent files or other examples already given by the program

The screenshot displays the DWSIM software interface. The main window title is "DWSIM" and the menu bar includes "File", "Edit", "Tools", "Windows", "View", and "Help". The main content area is titled "Welcome to DWSIM!" and features several sections:

- Process Modeling:** "Create or load chemical steady-state or dynamic process models." Includes buttons for "Create New", "Load Existing", and "Load from Simulate365 Dashboard".
- Discover DWSIM Pro:** "Find out how the commercial sibling of the open-source process simulator DWSIM opens up new opportunities for you and your projects." Includes a "Get a Free Trial" button.
- Free Simulate365 Dashboard for DWSIM:** "Open and save your simulation files from DWSIM to Dashboard. Achieve greater transparency over your flowsheets with built-in version control and personalized tags." Includes a "Get Started" button.
- User Compound Creation / Data Regression:** Includes buttons for "Create New Compound", "Quick Create New Solid", "Create New (with Wizard)", "Create New Data Regression Study", and "Load Existing Study".
- DWSIM Social Responsibility Program:** "Learn more on how to help with the development of e-accessibility technologies around DWSIM while also helping people in need." Includes a "Learn More" button.
- Support/Sponsor:** "Support/Sponsor open-source DWSIM development activities." Includes buttons for "Sponsor on GitHub", "BECOME A PATRON", and "Buy me a coffee".

At the bottom, there is a footer with the text: "Support continuous development and maintenance of DWSIM for as low as 3 USD/month or with a one-time donation. One-Time Donation Monthly Donation".

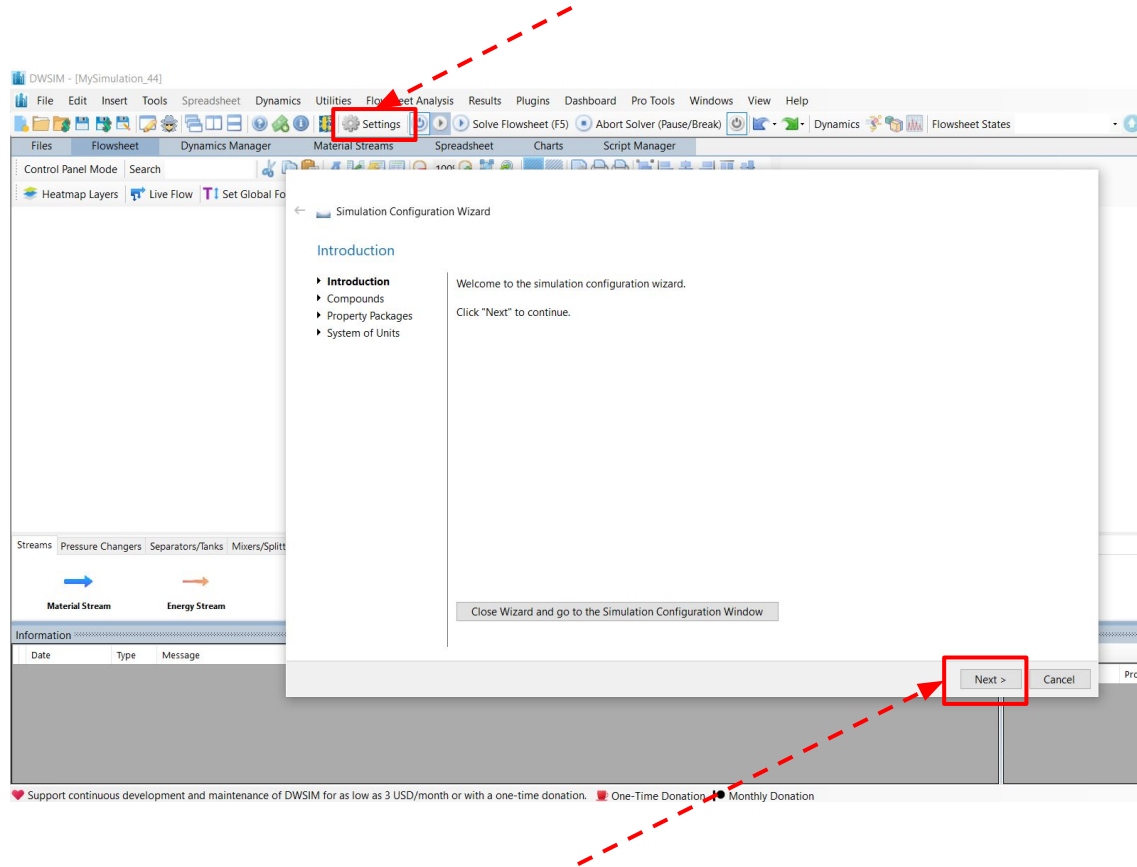
On the right side, a "Recent Files" panel is open, showing a list of files:

- 1 wgs reactor.dwxmz
- Biogas reforming (new version).dwxmz
- NG Reforming (new version).dwxmz
- Biogas off gas combustion.dwxmz
- NG off gas combustion.dwxmz
- Biogas reforming.dwxmz
- NG reforming.dwxmz
- NG reforming 1.dwxmz
- NG reforming_backup.dwxmz

Red dashed arrows point from the text "Create a new simulation" to the "Create New" button and from "Open other recent files or other examples already given by the program" to the "Recent Files" panel.

SIMULATION CONFIGURATION

- Simulation Configuration Wizard lets you pick the **compounds**, the **property package** that you want to use to solve your simulation and the **unit system**.
- These options can be **changed** anytime in the settings button.



Compounds

- ✓ Introduction
- ▶ **Compounds**
- ▶ Property Packages
- ▶ System of Units

Select the compounds that you want to add to the simulation. Use the textbox to search and select a compound in the list. Click "Next" to continue.

Added	Name	CAS Number	Formula	Source Database	CP
<input checked="" type="checkbox"/>	Air	132259-10-0	(N2)0.781 (O2)0...	ChemSep	<input type="checkbox"/>
<input type="checkbox"/>	Argon	7440-37-1	Ar	ChemSep	<input checked="" type="checkbox"/>
<input type="checkbox"/>	Bromine	7726-95-6	BrBr	ChemSep	<input type="checkbox"/>
<input type="checkbox"/>	Carbon tetrachloride	56-23-5	CCl4	ChemSep	<input type="checkbox"/>
<input type="checkbox"/>	Carbon monoxide	630-08-0	CO	ChemSep	<input checked="" type="checkbox"/>
<input type="checkbox"/>	Carbon dioxide	124-38-9	OCO	ChemSep	<input checked="" type="checkbox"/>
<input type="checkbox"/>	Carbon disulfide	75-15-0	SCS	ChemSep	<input type="checkbox"/>
<input type="checkbox"/>	Phosgene	75-44-5	COCl2	ChemSep	<input type="checkbox"/>
<input type="checkbox"/>	Trichloroacetyl chloride	76-02-8	CCl3COCl	ChemSep	<input type="checkbox"/>
<input type="checkbox"/>	Hydrogen chloride	7647-01-0	HCl	ChemSep	<input checked="" type="checkbox"/>
<input type="checkbox"/>	Chlorine	7782-50-5	Cl2	ChemSep	<input type="checkbox"/>

Search

Added Compounds

**Search
compound**

**Selected compounds
are shown here**

DWSIM COMPOUNDS

- You should add every compound that is present in the system, i.e. inputs, products and the intermediate compounds.

For this example:

- Add - CH₄; C₂H₆; CO₂; N₂; H₂; H₂O; O₂; CO;

DWSIM PROPERTY PACKAGES

We'll use the Peng-Robinson (PR) model

Simulation Configuration Wizard

Property Packages

- Introduction
- Compounds
- Property Packages**
- System of Units

Select and Add the Property Packages that you want to use in your simulation. The first on the list will be used by default by all flowsheet objects. Click "Next" to continue.

Available Property Packages	
Type	
✓	GERG-2008
✓	Grayson-Streed
✓	Raoult's Law
✓	Soave-Redlich-Kwong (SRK) Advanced
✓	Peng-Robinson / Lee-Kesler (PR/LK)
✓	Peng-Robinson 1978 (PR78)
✓	Peng-Robinson (PR)
✗	Cubic-PP (incompressible mixtures)

Add

Added Property Packages	
Name	Type
Peng-Robinson...	Peng-Robinson (PR)

BETA Recommended packages are marked with a ✓, but you can use all available packages without restrictions.

Override Phase Equilibria calculation settings? Leave as default (SVLLE) VLE (faster) VLE/LLC

[Click here to get help on selecting the best Thermodynamic Model/Property Package for your system.](#)

[Click here to learn which methods and correlations are being used by the packages to calculate fluid properties.](#)

Next > Cancel

DWSIM SYSTEM OF UNITS

We'll use a custom unit system, **C5**

← Simulation Configuration Wizard

System of Units

- ✓ Introduction
- ✓ Compounds
- ✓ Property Packages
- ▶ **System of Units**

Select the desired System of Units for your simulation. You can change individual units by selecting a custom system (other than SI, CGS or ENG). Click "Finish" to exit the wizard and start designing the simulation model.

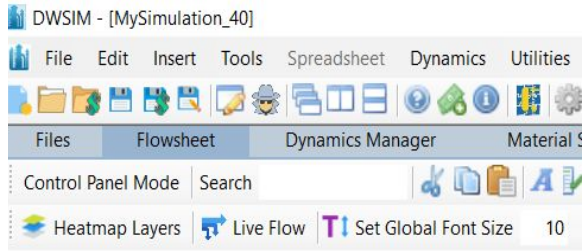
System of Units: **C5** Clone Create New

Property	Unit
Temperature	bar
Mass Flow Rate	kmol/h
Volumetric flow rate	kJ/kg
Specific Entropy	kg/kmol
Density	N/m
Heat Capacity	W/[m.K]
Kinematic Viscosity	Pa.s
Temperature Difference	bar
Length/Head	Energy Flow
Time	Volume
Molar Volume	Area
Diameter/Thickness	Force

System

Description

SI	Default
CGS	Centimeter-Gram-Seconds
ENG	English Imperial System
C(n)	Custom systems



Name change

Information Connections

General Info

Object: Natural Gas

Status: Calculated (21/03/2023 14:32:13)

Linked to:

Property Package Settings

Property Package: Peng-Robinson (PR) (1)

Input Data Results Annotations Dynamics Floating Tables

Stream Conditions Compound Amounts

Property	Value	Unit
Flash Spec	Temperature and Pressure (TP)	
Temperature	25	C
Pressure	1	bar
Mass Flow	3600	kg/h
Molar Flow	147,59	kmol/h
Volumetric Flow	2,57133	m3/h
Specific Enthalpy	-189,214	kJ/kg
Specific Entropy	1,05668	kJ/[kg.K]
Vapor Phase Mole Fraction	0	

Streams Pressure Changers Separators/Tanks

Material Stream Energy Stream



Click and drag

1

Streams Pressure Changers Separators/Tanks Mixers/Splitters Exchangers

Material Stream Energy Stream

Stream characteristics

Input Data Results Annotations Dynamics Floating Tables

Stream Conditions Compound Amounts

Basis Mole Fractions

Solvent

Compound	Amount
Air	0
Carbon monoxide	0
Carbon dioxide	1,5
Nitrogen	0,8
Hydrogen	0,5
Water	0
Methane	86,0
Ethane	11,2

Normalize

Equalize

Clear

Accept

Click **accept** when the changes are done

Total: 100

Change the **composition** accordingly

Compound	Amount
Air	0
Carbon monoxide	0
Carbon dioxide	0,015
Nitrogen	0,008
Hydrogen	0,005
Water	0
Methane	0,86
Ethane	0,112

Normalize

Equalize

Clear

Accept

Total: 1

- On the input data separator, go to *compound amounts*.
- On *basis*, 7 types of inputs for compositions are given - mole fractions; mass fractions; mole flows; mass flows; standard liquid volume flows; molarities; molalities.
- Data is given in mole fractions, so that's the one we pick.
- Change the amounts accordingly to the data and press *Accept*, otherwise the program will go back to the original compositions.

Input Data	Results	Annotations	Dynamics	Floating Tables
Stream Conditions		Compound Amounts		
Flash Spec	Temperature and Pressure (TP) ▾			
Temperature	<input type="text" value="25"/>	C	▾	
Pressure	<input type="text" value="1"/>	bar	▾	
Mass Flow	<input type="text" value="10"/>	kg/h	▾	
Molar Flow	<input type="text" value="0,553753"/>	kmol/h	▾	
Volumetric Flow	<input type="text" value="13,6916"/>	m3/h	▾	
Specific Enthalpy	<input type="text" value="-1,19117"/>	kJ/kg	▾	
Specific Entropy	<input type="text" value="0,270956"/>	kJ/[kg.K]	▾	
Vapor Phase Mole Fraction	<input type="text" value="1"/>			
Force Stream Phase	Global Definition ▾			

Change the temperature, pressure and mass flow and hit enter. The other characteristics will change automatically.

- Go back to *stream conditions*.
- *Flash Spec* allows the user to pick which of the main conditions he wants to use as base. This choice changes the conditions the program allows to change.
- From the data, we have the stream temperatures and pressures, so we pick *Temperature and Pressure (TP)*.
- Add the information given by the exercise and press Enter.

Steam (2) (Material Stream)

Information Connections

General Info

Object: Steam (2)

Status: Calculated (24/03/2023 14:16:42)

Linked to

Property Package Settings

Property Package: Peng-Robinson (PR) (1)

Input Data Results Annotations Dynamics Floating Tables

Stream Conditions Compound Amounts

Flash Spec: Temperature and Pressure (TP)

Temperature: 150 C

Pressure: 1 bar

Mass Flow: 30 kg/h

Molar Flow: 1,21105 kmol/h

Volumetric Flow: 42,5775 m3/h

Specific Enthalpy: 182,625 kJ/kg

Specific Entropy: 2,18434 kJ/[kg.K]

Files Flowsheet

Control Panel Mode S

Heatmap Layers

Streams Pressure Chan

Do the same for Steam



Input Data Results Annotations Dynamics Floating Tables

Stream Conditions Compound Amounts

Basis: Mole Fractions

Solvent

Compound	Amount	Normalize
Air	0	Equalize
Carbon monoxide	0	Clear
Carbon dioxide	0	Accept
Nitrogen	0	
Hydrogen	0	
Water	1	
Methane	0	
Ethane	0	

Total: 1

In here you can
add/remove other
connections to
the mixer



- On the units bar, go to *mixers/splitters* and drag a *stream mixer* to the flowsheet. Automatically the program will connect the material streams to the mixer.
- Change the object name and choose the calculation method - *Inlet Minimum*.

Mixer 1 (Stream Mixer)

General

Object: Mixer 1

Status: Calculated (21/03/2023 15:46:38)

Linked to:

Connections

Stream	Name	Remove	Reset
Inlet Stream 1	Steam 2	[X]	[R]
Inlet Stream 2	Natural Gas 1	[X]	[R]
Inlet Stream 3		[X]	[R]
Inlet Stream 4		[X]	[R]
Inlet Stream 5		[X]	[R]
Inlet Stream 6		[X]	[R]
Outlet Stream	Mix 3	[X]	[R]

Calculation Parameters

Pressure Calculation: Inlet Minimum

Property Package Settings

Property Package: Peng-Robinson (PR) (1)

Notes

Files Flowsheet Dynamics Manager Material S

Natural Gas 1

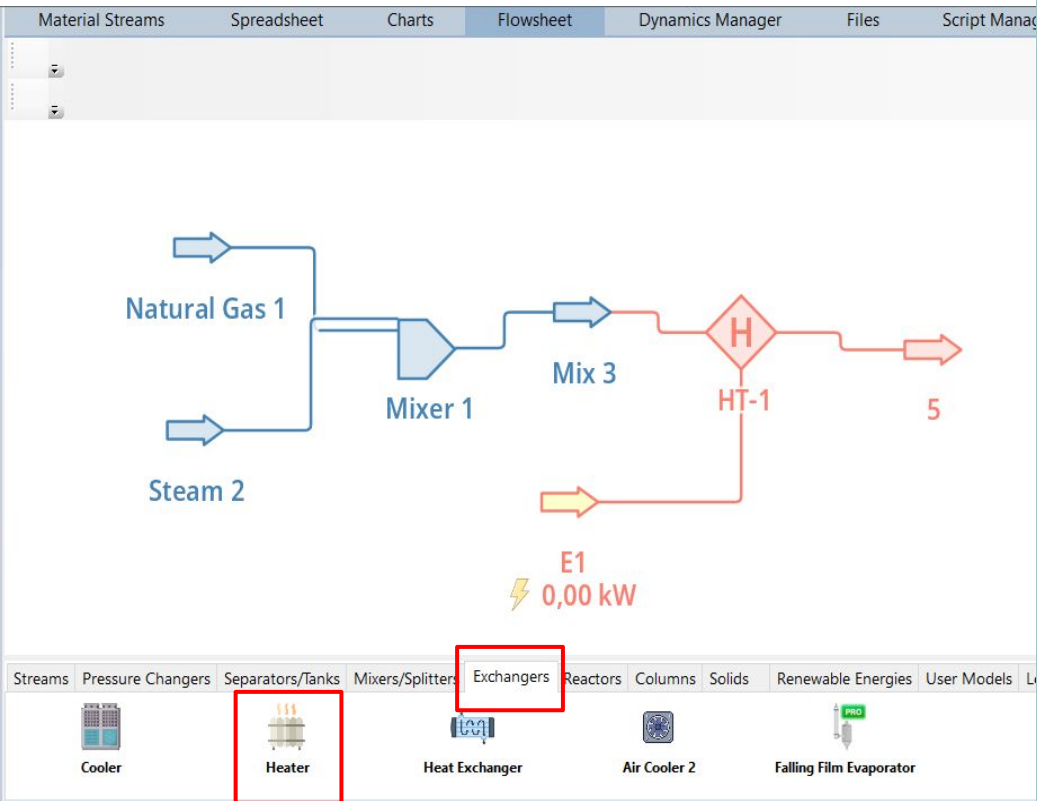
Steam 2

Mixer 1

Mix 3

Streams Pressure Changers Separators/Tanks Mixers/Splitters Exchangers

Stream Mixer Stream Splitter Energy Mixer



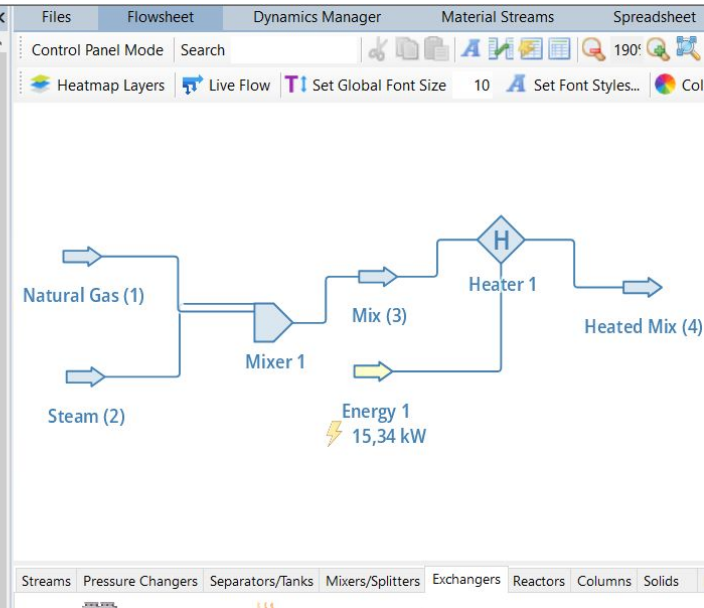
Add a Heater

- Automatically, the software will give the *mixer* output stream characteristics (mix 3).
- According to the scheme of the system, the next step is to add a heater. For that, go back to the unit operations bar, go to *Exchangers* and drag the *Heater*. The program immediately connects the last stream to the heater unit.
- It also adds another input stream, *E1*, which is an energy stream. By altering the conditions of operation of the heater, the program calculates himself the amount of energy needed for this unit to work properly.

Change conditions according to data

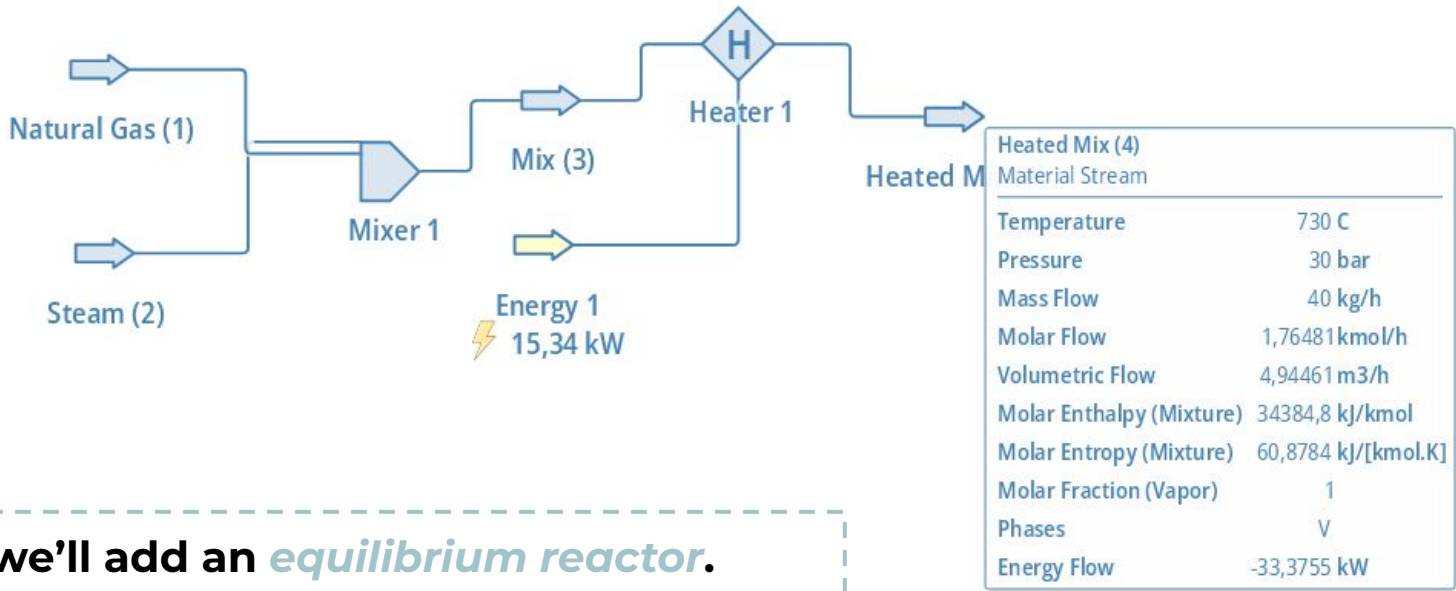
- Heaters and coolers allow for 5 types of calculation - heat added/removed; temperature change; outlet temperature; outlet vapor mole fraction; energy stream. Pick outlet temperature.
- Don't forget to press **Enter** with every change you do.

General Info		
Object	Heater 1	
Status	Calculated (24/03/2023 14:41:52)	
Linked to		
Connections		
Inlet Stream	Mix (3)	
Outlet Stream	Heated Mix (4)	
Energy Stream (Primary)	Energy 1	
Energy Stream (Secondary)		
Calculation Parameters		
Calculation Type	Outlet Temperature	
Pressure Drop	-29	bar
Efficiency (0-100%)	100	
Outlet Temperature	730	C
Temperature Change	620,85	C
Outlet Vapor Fraction	1	
Heating/Cooling	15,3377	kW

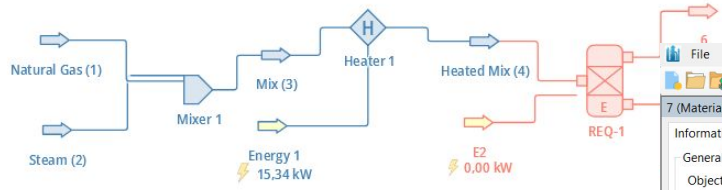


Attention to pressure - it says pressure drop, meaning how much does the pressure decreased. We want the pressure at 30 bar, and the stream is at 1 bar. Hence comes the -29.

We now have the heated mix with the correct characteristics from data and compatible with the operation conditions of the first reactor.



Now, we'll add an *equilibrium reactor*.



Now, we need to insert the reactions that are going to occur in the reactor. For that go to *settings*.

Streams Pressure Changers Separators/Tanks Mixers/Splitters Exchangers **Reactors** Columns

Conversion Reactor Continuous Stirred Tank Reactor (CSTR) **Equilibrium Reactor** Gibbs Reactor

Go to *reactors* and add an *equilibrium reactor*.

File Edit Insert Tools Spreadsheet Dynamics Utilities **Settings** Flowsheet Analysis Results Plugins Dashboard Pro Tools Windows View Help

7 (Material Stream) Information Connections

General Info Object 7 Status Not Calc Linked to

Property Package Settings Property Package Peng-R

Input Data Results Annotation Stream Conditions Compound

Flash Spec Temperature Pressure Mass Flow Molar Flow Volumetric Flow Specific Enthalpy Specific Entropy Vapor Phase Mole Fraction

Force Stream Phase Do not change this setting un

Settings

Compounds Thermodynamics Reactions Mass and Energy Balances System of Units Object Properties Number Formatting / Other

Added	Name	Tag	CAS Number	Formula	Database	CP
<input checked="" type="checkbox"/>	Carbon dioxide		124-38-9	OCO	ChemSep	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	Carbon monoxide		630-08-0	CO	ChemSep	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	Hydrogen		1333-74-0	H2	ChemSep	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	Water		7732-18-5	HOH	ChemSep	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	Oxygen		7782-44-7	O2	ChemSep	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	Nitrogen		7727-37-9	N2	ChemSep	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	Methane		74-82-8	CH4	ChemSep	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	Ethane		74-84-0	CH3CH3	ChemSep	<input checked="" type="checkbox"/>
<input type="checkbox"/>	Air		132259-10-0	(N2)0.781 (O2)0.209 (Ar)0...	ChemSep	<input type="checkbox"/>
<input type="checkbox"/>	Argon		7440-37-1	Ar	ChemSep	<input checked="" type="checkbox"/>
<input type="checkbox"/>	Bromine		7726-95-6	BrBr	ChemSep	<input type="checkbox"/>
<input type="checkbox"/>	Carbon tetrachloride		56-23-5	CCl4	ChemSep	<input type="checkbox"/>
<input type="checkbox"/>	Carbon disulfide		75-15-0	SCS	ChemSep	<input type="checkbox"/>
<input type="checkbox"/>	Phosgene		75-44-5	COCl2	ChemSep	<input type="checkbox"/>

Petroleum Fractions

Start Bulk C7+ Petroleum Characterization Utility

Start Distillation Curves Petroleum Characterization Utility

Open Assay Manager

REQ-1 (Equilibriu... E2 (Energy Strea... 6 (Material Strea... 7 (Material Strea...

Reaction Sets

Name	Description
Default Set	Default Reaction Set

Chemical Reactions

- Conversion
- Equilibrium
- Kinetic
- Heterogeneous Catalytic

How to add reactions in DWSIM:

1. Give a *name*;
2. Pick the components present in the reaction on the *include boxes*;
3. On the *BC column*, pick the base component of the reaction - CH_4 ;
4. Now we give the stoichiometric coefficients. The program considers negative numbers for reagents and positive numbers for products;
5. The equation appears in the equation box and if the stoichiometry is correct then *OK* will appear on top.
6. On *Phase* choose *Vapor*.
7. Then pick the calculation method - calculate from Gibbs Energy of Reaction;

Add New Equilibrium Reaction

Identification
Name:

Description:

Components/Stoichiometry

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	Storch. Coeff.
Carbon dioxide	44,0095	-8941,48	<input type="checkbox"/>	<input type="checkbox"/>	0
Carbon monoxide	28,0101	-3946,08	<input type="checkbox"/>	<input type="checkbox"/>	0
Hydrogen	2,01588	0	<input type="checkbox"/>	<input type="checkbox"/>	0
Water	18,0153	-13422,7	<input type="checkbox"/>	<input type="checkbox"/>	0
Oxygen	31,9988	0	<input type="checkbox"/>	<input type="checkbox"/>	0

Stoichiometry: Balance Heat of Reaction (kJ/kmol_BC) (25°C)

Equation:

Equilibrium Reaction Parameters

Basis: Fugacity Phase: **Liquid** Tmin (K) Tmax (K)

Units: Temperature Approach (K)

Equilibrium Constant (Keq)

Calculate from Gibbs Energy of Reaction $\Delta G_{G,R}$ (kJ/kmol_BC) (25°C)

T-Function: $\ln Keq [f(T)] =$ T in K

Constant Value

Use '.' as the decimal separator on math expressions.

Cancel OK



Edit Equilibrium Reaction

Identification
 Name: Methane Reforming
 Description:

Components/Stoichiometry

Name	Molar Weight	ΔHf (kJ/kg)	Include	BC	Stoich. Coeff.
Carbon dioxide	44,0095	-8941,48	<input type="checkbox"/>	<input type="checkbox"/>	0
Carbon monoxide	28,0101	-3946,08	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1
Hydrogen	2,01588	0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	3
Water	18,0153	-13422,7	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-1
Oxygen	31,9988	0	<input type="checkbox"/>	<input type="checkbox"/>	0

Stoichiometry: OK Balance Heat of Reaction (kJ/kmol_BC) (25°C): 205804

Equation: HOH + CH4 <-> CO + 3H2

Equilibrium Reaction Parameters
 Basis: Fugacity Phase: Vapor Tmin (K): 0 Tmax (K): 2000
 Units: Temperature Approach (K): 0

Equilibrium Constant (Keq)
 Calculate from Gibbs Energy of Reaction DeIG_R (kJ/kmol_BC) (25°C): 141930
 T-Function: ln Keq [f(T)] = T in K
 Constant Value: 0

Use '.' as the decimal separator on math expressions. [Cancel] [OK]



Add New Equilibrium Reaction

Identification
 Name: Water Gas Shift Reaction
 Description:

Components/Stoichiometry

Name	Molar Weight	ΔHf (kJ/kg)	Include	BC	Stoich. Coeff.
Carbon dioxide	44,0095	-8941,48	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1
Carbon monoxide	28,0101	-3946,08	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1
Hydrogen	2,01588	0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1
Water	18,0153	-13422,7	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-1
Oxygen	31,9988	0	<input type="checkbox"/>	<input type="checkbox"/>	0

Stoichiometry: OK Balance Heat of Reaction (kJ/kmol_BC) (25°C): -41166

Equation: CO + HOH <-> COO + H2

Equilibrium Reaction Parameters
 Basis: Fugacity Phase: Vapor Tmin (K): 0 Tmax (K): 2000
 Units: Temperature Approach (K): 0

Equilibrium Constant (Keq)
 Calculate from Gibbs Energy of Reaction DeIG_R (kJ/kmol_BC) (25°C): -28630
 T-Function: ln Keq [f(T)] = T in K
 Constant Value: 0

Use '.' as the decimal separator on math expressions. [Cancel] [OK]

- Still in the reactions settings, go to *reaction Sets* and *add new reaction set*.

Settings

Compounds Thermodynamics Reactions Mass and Energy Balances System of Units Object Properties Number Forma

Reaction Sets

+ Add New Reaction Set

Description
Default Reaction Set

Chemical Reactions

Name	Type
Methane Reforming	Equilibrium

- Here we can create *groups of chemical reactions* deliberately for each reactor.

DWSIM - Reaction Set Editor

Identification

Name: Steam Methane Reformer Reactions

Description:

Reactions

Reaction	Type	Equation	Active	Seq.
Methane Reforming	Equilibrium	$\text{HOH} + \text{CH}_4 \leftrightarrow \text{CO} + 3\text{H}_2$	<input checked="" type="checkbox"/>	0
Water Gas Shift	Equilibrium	$\text{CO} + \text{HOH} \leftrightarrow \text{OCO} + \text{H}_2$	<input checked="" type="checkbox"/>	0

Cancel OK

DWSIM - Reaction Set Editor

Identification

Name: Water Gas Shift Reactor

Description:

Reactions

Reaction	Type	Equation	Active	Seq.
Water Gas Shift	Equilibrium	$\text{CO} + \text{HOH} \leftrightarrow \text{OCO} + \text{H}_2$	<input checked="" type="checkbox"/>	0

Cancel OK

Steam Reformer (Equilibrium Reactor)

General Info

Object: Steam Reformer

Status: Calculated (24/03/2023 15:10:39)

Linked to:

Connections

Inlet Stream	Heated Mix (4)		
Outlet Stream 1	Syngas (5)		
Outlet Stream 2	Liquid Part 1		
Energy Stream	Energy 2		

Calculation Parameters

Parameters: Convergence

Reaction Set	Steam Methane Reformer Reactions
Calculation Mode	Isothermic
Outlet Temperature	730 C
Pressure Drop	0 bar

Reaction Set dropdown menu:

- Steam Methane Reformer Reactions
- Default Set
- Steam Methane Reformer Reactions
- Water Gas Shift Reactor

- Reactors appear with 2 output streams. *Outlet Stream 1* corresponds to the gas part of the products and the *Outlet Stream 2* represents the liquid part of the output.
- For this case study, the liquid part should have null flow. Whether or not this stream has any flow, it still needs to be connected to the reactor otherwise calculation errors will appear.
- On *reaction set*, instead of the default set, pick the set you created with the two reactions that will occur in the SR. On *calculation mode*, we'll use the isothermic mode.

Now a cooler...

The screenshot displays a process simulation software interface. The main window shows a flowsheet with the following components and streams:

- Inputs:** Natural Gas (1) and Steam (2) enter Mixer 1.
- Mixer 1:** Outputs Mix (3).
- Heater 1:** Receives Mix (3) and Energy 1 (15,34 kW). Outputs Heated Mix (4).
- Steam Reformer:** Receives Heated Mix (4) and Energy 2 (4,29 kW). Outputs Syngas (5) and Liquid Part 1.
- Cooler 1:** Receives Syngas (5) and Energy 3 (9,12 kW). Outputs Syngas (6).

The left sidebar shows the configuration for 'Cooler 1':

- General Info:** Object: Cooler 1, Status: Calculated (24/03/2023 15:36:00).
- Connections:** Inlet Stream: Syngas (5), Outlet Stream: Syngas (6), Energy Stream (Primary): E3.
- Calculation Parameters:** Calculation Type: Outlet Temperature, Pressure Drop: 1 bar, Efficiency: 100%, Outlet Temperature: 400 C, Temperature Change: -330 C, Outlet Vapor Fraction: 1, Heating/Cooling: 9,11614 kW.
- Property Package Settings:** Property Package: Peng-Robinson (PR) (1).

The bottom panel shows a message log:

Date	Type	Message	Info
24/03/2023 15:36:00	Message	Last run execution time (s): 0,006133	+ Info
24/03/2023 15:36:00	Message	The flowsheet was calculated successfully.	+ Info
24/03/2023 15:36:00	Message	The flowsheet is being calculated, please wait...	+ Info

REQ-2 (Equilibrium Reactor)

General Info
Object: REQ-2
Status: Not Calculated

Connections
Inlet Stream: Syngas (6)
Outlet Stream 1: 9
Outlet Stream 2: 10
Energy Stream: E3

Calculation Parameters
Parameters: Convergence
Reaction Set: Default Set
Calculation Mode: Adiabatic
Outlet Temperature: -273,15 C
Pressure Drop: 0 bar

WGS Reactor (Equilibrium Reactor)

General Info
Object: WGS Reactor
Status: Calculated (25/03/2023 14:06:17)

Connections
Inlet Stream: Syngas (6)
Outlet Stream 1: Syngas (7)
Outlet Stream 2: Liquid Part
Energy Stream: Energy 4

Calculation Parameters
Parameters: Convergence
Reaction Set: Water Gas Shift Reactor
Calculation Mode: Isothermic
Outlet Temperature: 400 C
Pressure Drop: 0 bar

- Add a new *equilibrium reactor*. Sometimes the program automatically connects the energy stream of the reactor to the energy stream from the former unit, presenting the energy balance between these operations.
- However, to make the reading easier we'll separate the energy balance into two different streams. On *energy stream* click on the blue button (*disconnect*) and then in the yellow (*create and connect*).
- On *Reaction Set* pick the set you created with just the water-gas shift reaction and pick *isothermic* as the *Calculation Mode*.

Add a new cooler and change the characteristics. Now, go to *Separators/Tanks* and add a *Gas-Liquid Separator*.

The screenshot displays the configuration window for a 'Gas-Liquid Separator' on the left and a flowsheet on the right. The configuration window includes the following sections:

- General:** Object: Gas-Liquid Separator; Status: Calculated (25/03/2023 14:25:50); Linked to: (empty).
- Connections:** Inlet Stream 1: Syngas 8; Inlet Stream 2-6: (empty); Vapor Stream: Dry Gas (10); Light Liquid Stream: Water (9); Heavy Liquid Stream: (empty); Energy Stream: (empty).
- Calculation Parameters:** Outlet Pressure Calculation: Inlet Minimum (highlighted with a red box); Override Sep. Temperature: 35 C.

The flowsheet on the right shows a process flow starting with 'Cooler 2' (labeled 'C'), which outputs 'Energy 5' (8,45 kW) and feeds into 'Syngas 8'. This stream then enters a 'Gas-Liquid Separator', which produces two outlet streams: 'Dry Gas (10)' and 'Water (9)'. At the bottom of the interface, the 'Separators/Tanks' tab is selected, and the 'Gas-Liquid Separator' icon is highlighted with a red box.

On *Outlet Pressure Calculation* pick *Inlet Minimum*.

PSA (Compound Separator)

General Info

Object: PSA

Status: Calculated (25/03/2023 14:42:47)

Linked to:

Connections

Inlet Stream: Dry Gas (10)

Outlet Stream 1: Hydrogen

Outlet Stream 2: Off-Gas

Energy Stream: Energy 6

Calculation Parameters

Separation Factors specified for:

Outlet Stream 1

Outlet Stream 2

Compound	Spec	Value	Units
Carbon dioxide	% Inlet Mas...	0	%
Carbon monoxi...	% Inlet Mas...	0	%
Hydrogen	% Inlet Mol...	75	%
Water	% Inlet Mas...	0	%
Oxygen	% Inlet Mas...	0	%
Nitrogen	% Inlet Mas...	0	%
Methane	% Inlet Mas...	0	%
Ethane	% Inlet Mas...	0	%

Streams Pressure Changers Separators/Tanks Mixers/Splitters Exchangers

Compound Separator Tank Gas-Liquid Separator

Information

- To simulate the Pressure Swing Adsorption, PSA, we'll use a *Compound Separator* on the Separators/Tanks.
- *Compound Separator* is a mass balance unit operation, and divides one stream into two, specified as fractions or absolute flow rates.
- We're considering that the PSA has an efficiency of 75% of splitting the hydrogen from the gas.
- On *Separation Factors* go to Hydrogen, on *spec*, choose % Inlet Molar Flow or % Inlet Mass Flow (in this case, the result will be the same) and on *value* write 75%.

Compressor (Compressor) ✕

General Info

Object: Compressor

Status: Calculated (27/03/2023 15:17:56) ✓

Linked to

Connections

Inlet Stream: Hydrogen (11)

Outlet Stream: Compressed H2 (14)

Energy Stream: Energy 7

Calculation Parameters

Calculation Type: Outlet Pressure

Thermodynamic Process: Adiabatic

Performance Curves: Edit Performance Curves

Rotation Speed: 1500 rpm

Pressure Increase: 185 bar

Outlet Pressure: 200 bar

Adiabatic Efficiency (0-100): 75 %

Polytropic Efficiency (0-100): 81,9477 %

Power Required: 1,09611 kW

Outlet Temperature: 483,82 C

Temperature Change: 448,82 C

Material Streams | Spreadsheet | Charts | Flowsheet | Dynamic

Hydrogen (11)

Compressor

Compressed H2 (14)

Energy 7
⚡ 1,10 kW

Off-Gas (12)

Now the compressor.

Streams | **Pressure Changers** | Separators/Tanks | Mixers/Splitters | Exchangers | Reactors | Columns

Orifice Plate | **Compressor** | Pipe Segment | Pump

Oxygen (13) (Material Stream)

Information Connections

General Info

Object: Oxygen (13)

Status: Calculated (27/03/2023 15:33:37)

Linked to

Property Package Settings

Property Package: Peng-Robinson (PR) (1)

Input Data Results Annotations Dynamics Floating Tables

Stream Conditions Compound Amounts

Compound	Amount
Carbon dioxide	0
Carbon monoxide	0
Hydrogen	0
Water	0
Oxygen	1
Nitrogen	0
Methane	0
Ethane	0

Material Streams Spreadsheet

Hydrogen (11) Co

Energy 7 1,10 kW

Off-Gas (12)

Input Data Results Annotations Dynamics Floating Tables

Stream Conditions Compound Amounts

Flash Spec: Temperature and Pressure (TP)

Temperature: 35 C

Pressure: 15 bar

Mass Flow: 1 kg/h

Molar Flow: 0,0312512 kmol/h

Volumetric Flow: 0,0527611 m3/h

Specific Enthalpy: 5,0631 kJ/kg

Specific Entropy: -0,680201 kJ/[kg.K]

Vapor Phase Mole Fraction: 1

Force Stream Phase: Global Definition

Do not change this setting unless you know what you're doing.

Now the combustion part:

- First we'll add a new material stream for the oxygen. Change the inputs accordingly.
- Add a new mixer that connects the off-gas stream with the new oxygen stream.
- Use the *Inlet Minimum* as the calculation parameter.
- Now, go to reactors and drag a *conversion reactor*.

Edit Conversion Reaction

Identification

Name: Methane Combustion

Description:

Components/Stoichiometry

Name	Molar Weight	ΔH_f (kJ/kg)	Include	BC	Stoich. Coeff.
Carbon dioxide	44,0095	-8941,48	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1
Carbon monoxide	28,0101	-3946,08	<input type="checkbox"/>	<input type="checkbox"/>	0
Hydrogen	2,01588	0	<input type="checkbox"/>	<input type="checkbox"/>	0
Water	18,0153	-13422,7	<input checked="" type="checkbox"/>	<input type="checkbox"/>	2
Oxygen	31,9988	0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-2

Stoichiometry: Heat of Reaction (kJ/kmol_BC) (25 °C): -802618

Equation: $2O_2 + CH_4 \rightarrow CO_2 + 2H_2O$

Conversion Reaction Parameters

Base Comp: Methane Phase: Vapor

Conversion [%, f(T)] = 100 T in K

Use '.' as the decimal separator on the conversion expression.

- First we need to add the combustion reactions, so check slide 21 and on the program go back to *Settings* → *Reactions* → *Chemical Reactions* → *Add Conversion*.
- Add all 4 reactions. Remember - negative stoichiometric coefficients mean reagents and positive stoichiometric coefficients mean products.
- On *Phase* choose Vapor.
- On *Conversion* we'll consider 100%.
- On *Reactions* go to *Reactions Sets* and create a new set with the four reactions you just added.

Reaction	Type	Equation	Active	Seq.
Methane Combustion	Conversion	$2O_2 + CH_4 \rightarrow OCO + 2HOH$	<input checked="" type="checkbox"/>	0
Ethane Combustion	Conversion	$7O_2 + 2CH_3CH_3 \rightarrow 4OCO + 6...$	<input checked="" type="checkbox"/>	0
Hydrogen Combustion	Conversion	$2H_2 + O_2 \rightarrow 2HOH$	<input checked="" type="checkbox"/>	0
Carbon Monoxide Oxidation	Conversion	$2CO + O_2 \rightarrow 2OCO$	<input checked="" type="checkbox"/>	0

Temperature Difference	0	C.
Heat Load	0	kW

Alter the parameters.

Combustion (Conversion Reactor)

General Info

Object: Combustion

Status: Calculated (27/03/2023 16:14:06)

Linked to:

Connections

Inlet Stream: Off-gas Mix (15)

Outlet Stream 1: Combustion Off-gas (16)

Outlet Stream 2: Liquid Part 3

Energy Stream: Energy 8

Calculation Parameters

Parameters

Reaction Set: Combustion Reactor

Calculation Mode: Define Outlet Temperature

Outlet Temperature: 200 C

Pressure Drop: 0 bar

Property Package: Peng-Robinson (PR) (1)

External Solver:

Material Streams | Spreadsheet | Charts | Flowsheet | Dynamics M

Off-gas Mix (15)

Combustion

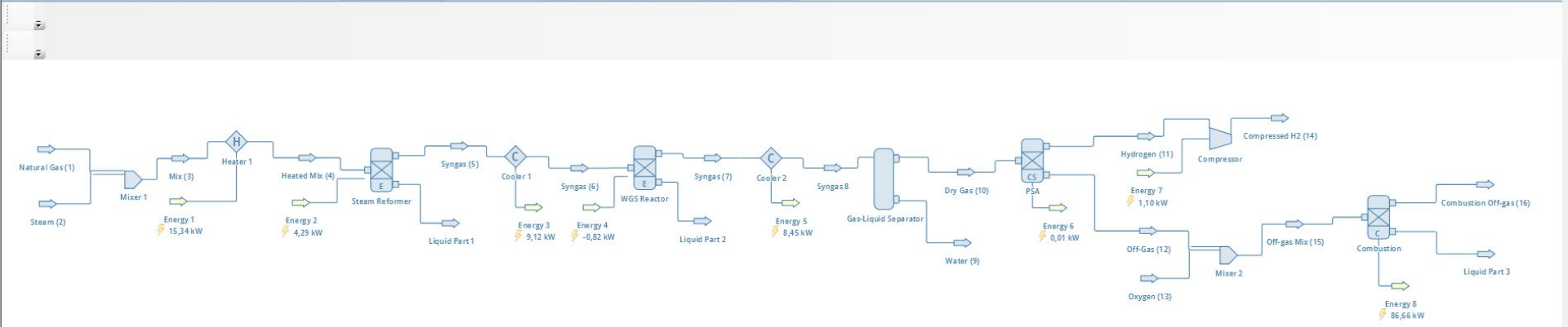
Combustion Off-gas (16)

Liquid Part 3

Energy 8
86,66 kW

Streams | Pressure Changers | Separators/Tanks | Mixers/Splitters | Exchangers | Reactors | Columns | S

Conversion Reactor | Continuous Stirred Tank Reactor (CSTR) | Equilibrium Reactor | Gibbs Reactor



We now have the full system, and can start analyzing the results.

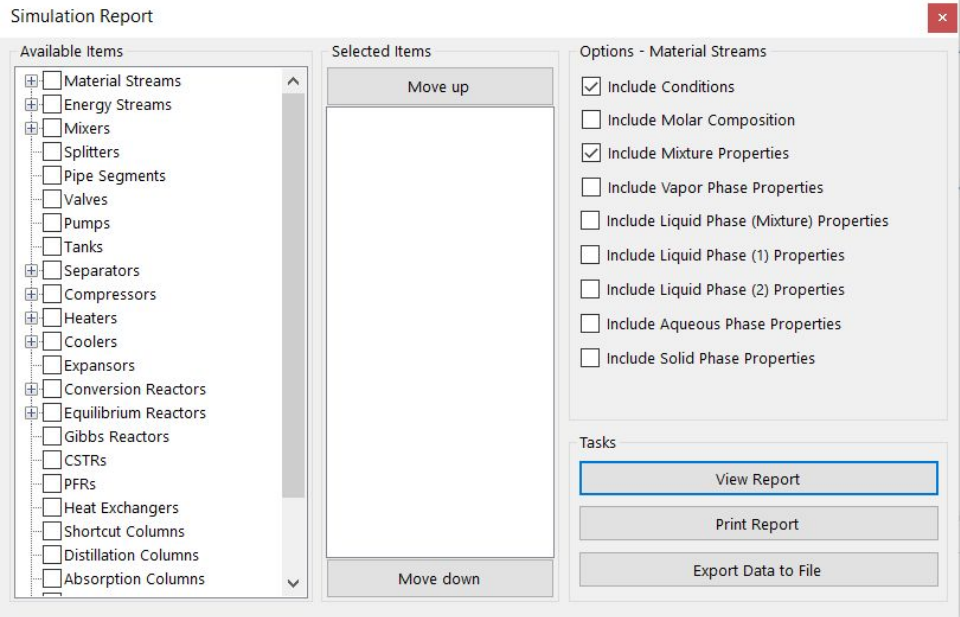
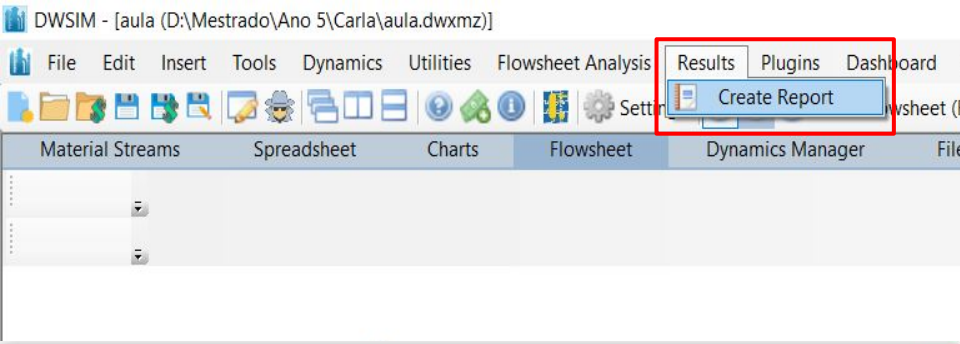
Compound Separator Tank Gas-Liquid Separator

Information

Date	Type	Message	Info
27/03/2023 16:18:32	Message	File D:\Mestrado\Ano 5\Carla\aula.dvwxm saved successfully.	+ Info
27/03/2023 16:14:07	Message	Last run execution time (s): 0,01934	+ Info
27/03/2023 16:14:07	Message	The flowsheet was calculated successfully.	+ Info
27/03/2023 16:14:07	Warning	Combustion: the energy balance did not converge within tolerance. (0,188381237831456 > 0,01)	+ Info
27/03/2023 16:14:07	Message	The flowsheet is being calculated, please wait...	+ Info

Watch Panel

Object	Property	Value



The full view of the process shown in the last slide already displays some results of the system, but not all. Here's some other ways to obtain more information about our simulation.

- Go to *Results* and *Create Report*.
- A window like the one on the left will open, where you can pick the type of data you want to analyse. For example, on *Available Items* check all boxes that have a plus sign on the side (plus sign means that those are the components with information/ components you implemented in the system).

Simulation Report

Available Items

- Material Streams
- Energy Streams
- Mixers
- Splitters
- Pipe Segments
- Valves
- Pumps
- Tanks
- Separators
- Compressors
- Heaters
- Coolers
- Expanders
- Conversion Reactors
- Equilibrium Reactors
- Gibbs Reactors
- CSTRs
- PFRs
- Heat Exchangers
- Shortcut Columns
- Distillation Columns
- Absorption Columns

Selected Items

Move up

- Liquid Part 3
- Combustion Off-gas (16)
- Off-gas Mix (15)
- Oxygen (13)
- Compressed H2 (14)
- Syngas (6)
- Syngas (5)
- Heated Mix (4)
- Liquid Part 1
- Mix (3)
- Steam (2)
- Natural Gas (1)
- Syngas (7)
- Liquid Part 2
- Syngas 8
- Dry Gas (10)
- Water (9)
- Hydrogen (11)
- Off-Gas (12)

Options - Material Streams

- Include Conditions
- Include Molar Composition
- Include Mixture Properties
- Include Vapor Phase Properties
- Include Liquid Phase (Mixture) Properties
- Include Liquid Phase (1) Properties
- Include Liquid Phase (2) Properties
- Include Aqueous Phase Properties
- Include Solid Phase Properties

Tasks

View Report

Print Report

Export Data to File

Move down

Untitled

Print Zoom % 100 Rows 1 Cols 1 Page 1 of 14

Simulation Report

DWSIM 8.2

Details

Title: MySimulation_15

Comments:

Object: Liquid Part 3

Type: Material Stream

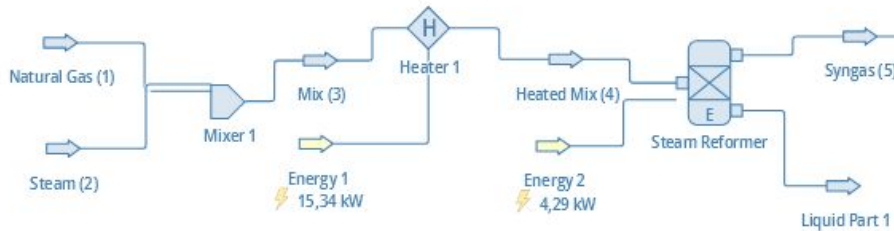
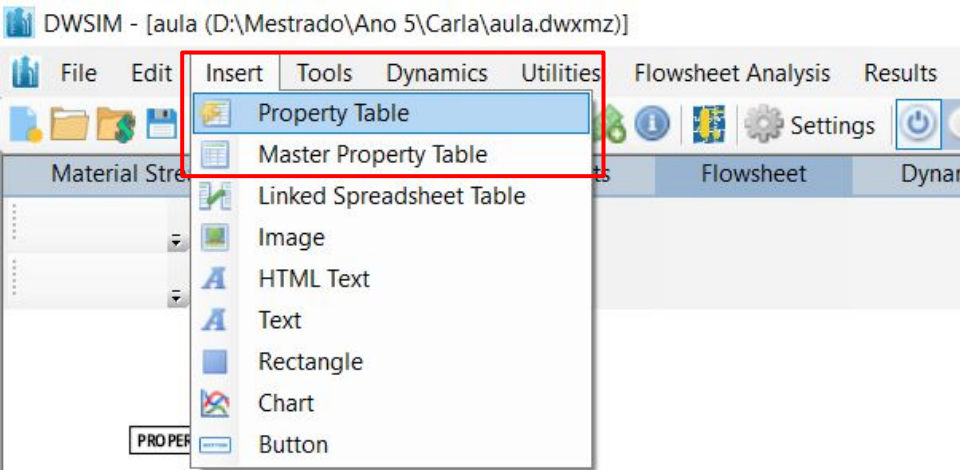
Property	Value	
Temperature	200	C
Pressure	15	bar
Mass Flow	-8.83736E-15	kg/h
Molar Flow	∞	kmol/h
Volumetric Flow	0	m3/h
Density (Mixture)	∞	kg/m3
Molecular Weight (Mixture)	0	kg/kmol
Specific Enthalpy (Mixture)	0	kJ/kg
Specific Entropy (Mixture)	0	kJ/[kg.K]
Molar Enthalpy (Mixture)	0	kJ/kmol
Molar Entropy (Mixture)	0	kJ/[kmol.K]
Thermal Conductivity (Mixture)	0	W/[m.K]

Object: Combustion Off-gas (16)

Type: Material Stream

Property	Value	
Temperature	200	C
Pressure	15	bar
Mass Flow	39,7999	kg/h
Molar Flow	1.41479	kmol/h

You'll get this document
with more detailed
information.



- Another way to see results is by adding a property table.
- Go to *Insert* and pick *Master Property Table* (for this case), or property table .
- As you can see you can also insert other components to your flowsheet, for example, *Charts*.
- Once you click on master property table, a little box will appear on the flowsheet. Double click on it.
- On this table you can add every detail you want.
- Let's create TWO tables, one for material flows and one for energy.

Configure Master Property Table

Name: Material Flows

Object type: Material Stream

Order objects by: Name | DESC

Properties to display:

- Select All Objects
- Select All Properties
- Default Properties Only
- Process Flowsheet
- Deselect Objects
- Deselect Properties

Grouping Rows: 1

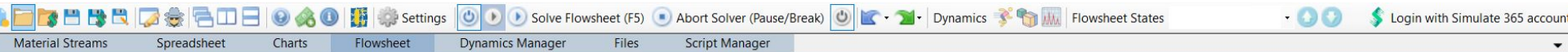
Order: ^ v

Object	Property
<input type="checkbox"/> Liquid Part 3	<input type="checkbox"/> Volumetric Fraction (Solid)
<input checked="" type="checkbox"/> Combustion Off-gas (16)	<input type="checkbox"/> Molar Fraction (Mixture) / Carbon dioxide
<input checked="" type="checkbox"/> Off-gas Mix (15)	<input checked="" type="checkbox"/> Mass Fraction (Mixture) / Carbon dioxide
<input checked="" type="checkbox"/> Oxygen (13)	<input type="checkbox"/> Molar Flow (Mixture) / Carbon dioxide
<input checked="" type="checkbox"/> Compressed H2 (14)	<input type="checkbox"/> Mass Flow (Mixture) / Carbon dioxide
<input checked="" type="checkbox"/> Syngas (6)	<input type="checkbox"/> Molar Fraction (Vapor) / Carbon dioxide
<input checked="" type="checkbox"/> Syngas (5)	<input type="checkbox"/> Molar Fraction (Overall Liquid) / Carbon dioxide
<input checked="" type="checkbox"/> Heated Mix (4)	<input type="checkbox"/> Molar Fraction (Liquid 1) / Carbon dioxide
<input type="checkbox"/> Liquid Part 1	<input type="checkbox"/> Molar Fraction (Liquid 2) / Carbon dioxide
<input checked="" type="checkbox"/> Mix (3)	<input type="checkbox"/> Molar Fraction (Aqueous) / Carbon dioxide
<input checked="" type="checkbox"/> Steam (2)	<input type="checkbox"/> Mass Fraction (Vapor) / Carbon dioxide
<input checked="" type="checkbox"/> Natural Gas (1)	<input type="checkbox"/> Mass Fraction (Overall Liquid) / Carbon dioxide
<input checked="" type="checkbox"/> Syngas (7)	<input type="checkbox"/> Mass Fraction (Liquid 1) / Carbon dioxide
<input type="checkbox"/> Liquid Part 2	<input type="checkbox"/> Mass Fraction (Liquid 2) / Carbon dioxide
<input checked="" type="checkbox"/> Syngas 8	<input type="checkbox"/> Mass Fraction (Aqueous) / Carbon dioxide
<input checked="" type="checkbox"/> Dry Gas (10)	<input type="checkbox"/> Molar Flow (Vapor) / Carbon dioxide
<input checked="" type="checkbox"/> Water (9)	<input type="checkbox"/> Molar Flow (Overall Liquid) / Carbon dioxide
<input checked="" type="checkbox"/> Hydrogen (11)	<input type="checkbox"/> Molar Flow (Liquid 1) / Carbon dioxide

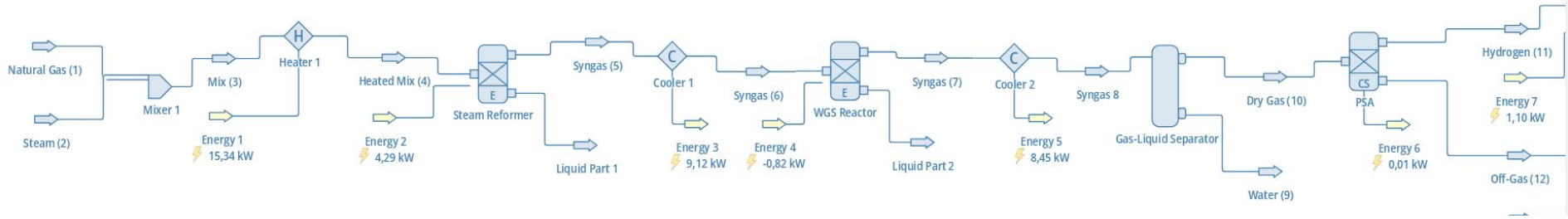
For the compositions you can also pick *Molar Fraction (Mixture) / Compound*.

- Give a *Name* to your table.
- On *Object Type* choose *Material Stream*.
- On object, you'll have every material stream that appear in your simulation. We are not interested in the liquid parts so pick all boxes except these ones.
- On Property, you can choose the information you want to the represented in your table. Let's go with: Temperature; Pressure; Mass Flow; Molar Flow. And for the compositions you have to pick, Mass Fraction (Mixture) / Compound, for every element.

■ After selection just close the window and a table will appear.



Object	Water (9)	Syngas 8	Syngas (7)	Syngas (6)	Syngas (5)	Steam (2)	Oxygen (13)	Off-gas Mix (15)	Off-Gas (12)	Natural Gas
Temperature	35	35	400	400	730	150	35	34,9901	35	
Pressure	15	15	29	29	30	1	15	15	15	
Mass Flow	0,606252	40	40	40	40	30	1	39,7999	38,7999	
Molar Flow	0,0336145	1,8923	1,8923	1,8923	1,8923	1,21105	0,0312512	1,59536	1,56411	0,553
Mass Fraction (Mixture) / Carbon dioxide	0,00188463	0,227821	0,227821	0,142514	0,142514	0,222075	0	0,228937	0,234838	0,0365
Mass Fraction (Mixture) / Carbon monoxide	3,56782E-07	0,117467	0,117467	0,171761	0,171761	0,141341	0	0,118058	0,1211	
Mass Fraction (Mixture) / Hydrogen	1,58741E-07	0,019794	0,019794	0,0158865	0,0158865	0,0101722	0	0,00497338	0,00510157	0,00055
Mass Fraction (Mixture) / Water	0,998108	0,0181324	0,0181324	0,0530528	0,0530528	0,0909062	0	0,0030196	0,00309743	
Mass Fraction (Mixture) / Oxygen	6,85612E-06	0,121101	0,121101	0,121101	0,121101	0,161468	1	0,146835	0,124846	
Mass Fraction (Mixture) / Nitrogen	3,18278E-07	0,10912	0,10912	0,10912	0,10912	0,141357	0	0,109669	0,112496	0,01
Mass Fraction (Mixture) / Methane	2,97275E-08	0,226144	0,226144	0,226144	0,226144	0,0809512	0	0,227281	0,233139	0,763
Mass Fraction (Mixture) / Ethane	5,06766E-10	0,16042	0,16042	0,16042	0,16042	0,15173	0	0,161226	0,165382	0,186



Energy Flows									
Object	Energy 8	Energy 7	Energy 6	Energy 5	Energy 4	Energy 3	Energy 2	Energy 1	
Energy Flow	86,6642	1,09611	0,0105673	8,45411	-0,816428	9,11614	4,28632	15,3377	kW

Now, let's do the same for the energy flows.

Configure Master Property Table

Name: Energy Flows

Object type: Energy Stream | Order objects by: Name | DESC

Properties to display:

- Object:
 - Energy 8
 - Energy 7
 - Energy 3
 - Energy 2
 - Energy 1
 - Energy 4
 - Energy 5
 - Energy 6
- Property:
 - Energy Flow

Buttons: Select All Objects, Select All Properties, Default Properties Only, Process Flowsheet, Deselect Objects, Deselect Properties

Grouping Rows: 1

Order: ^ v

Factors | Column

Results in the format of the property table are more useful if you're interested in doing more calculation.

- You can right click on the tables, *Copy Process Data to Clipboard*, and then paste on the spreadsheet separator.
- You can use this separator as your calculation sheet, or save it an open it on Excel.

	A	B	C	D	E	F	G	H	I	J	K
1											
2			Material Flows								
3			Object	Water (9)	Syngas 8	Syngas (7)	Syngas (6)	Syngas (5)	Steam (2)	Oxygen (13)	Off-gas Mix
4			Temperatur	35	35	400	400	730	150	35	34,9901
5			Pressure	15	15	29	29	30	1	15	15
6			Mass Flow	0,606252	40	40	40	40	30	1	39,7999
7			Molar Flow	0,0336145	1,8923	1,8923	1,8923	1,8923	2,21105	0,0312512	1,59536
8			Mass Fracti	0,00188463	0,227821	0,227821	0,142514	0,142514	0,222075	0	0,228937
9			Mass Fracti	5,6782E-07	0,117467	0,117467	0,171761	0,171761	0,141341	0	0,118058
10			Mass Fracti	5,8741E-07	0,019794	0,019794	0,0158865	0,0158865	0,0101722	0	0,004973380
11			Mass Fracti	0,998108	0,0181324	0,0181324	0,0530528	0,0530528	0,0909062	0	0,00301960
12			Mass Fracti	8,5612E-06	0,121101	0,121101	0,121101	0,121101	0,161468	1	0,146835
13			Mass Fracti	1,8278E-07	0,10912	0,10912	0,10912	0,10912	0,141357	0	0,109669
14			Mass Fracti	9,7275E-08	0,226144	0,226144	0,226144	0,226144	0,0809512	0	0,227281
15			Mass Fracti	0,06766E-10	0,16042	0,16042	0,16042	0,16042	0,15173	0	0,161226
16											
17											
18											

THANKS

Do you have any questions?

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