A brief introduction to Aspen plus

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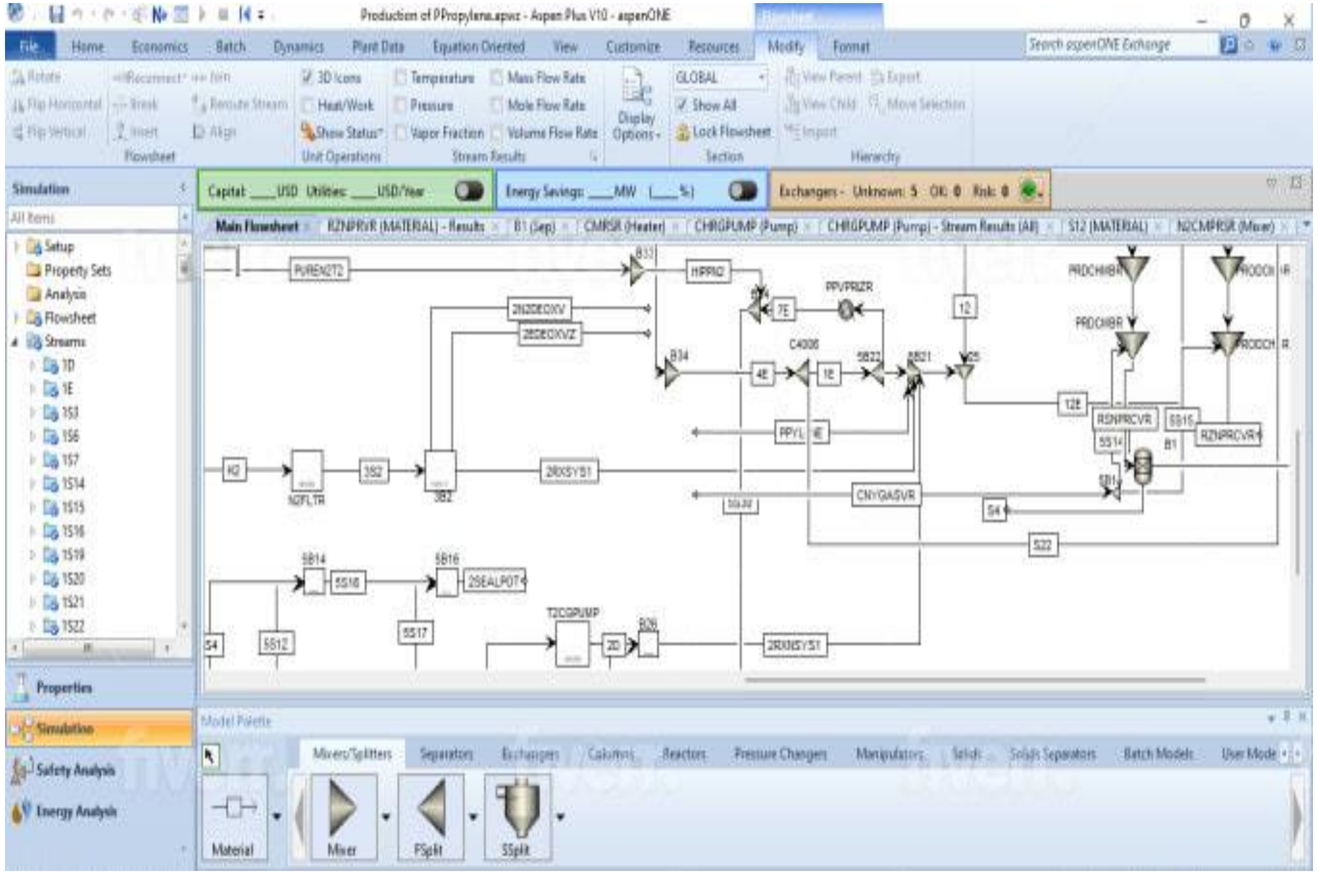
Content

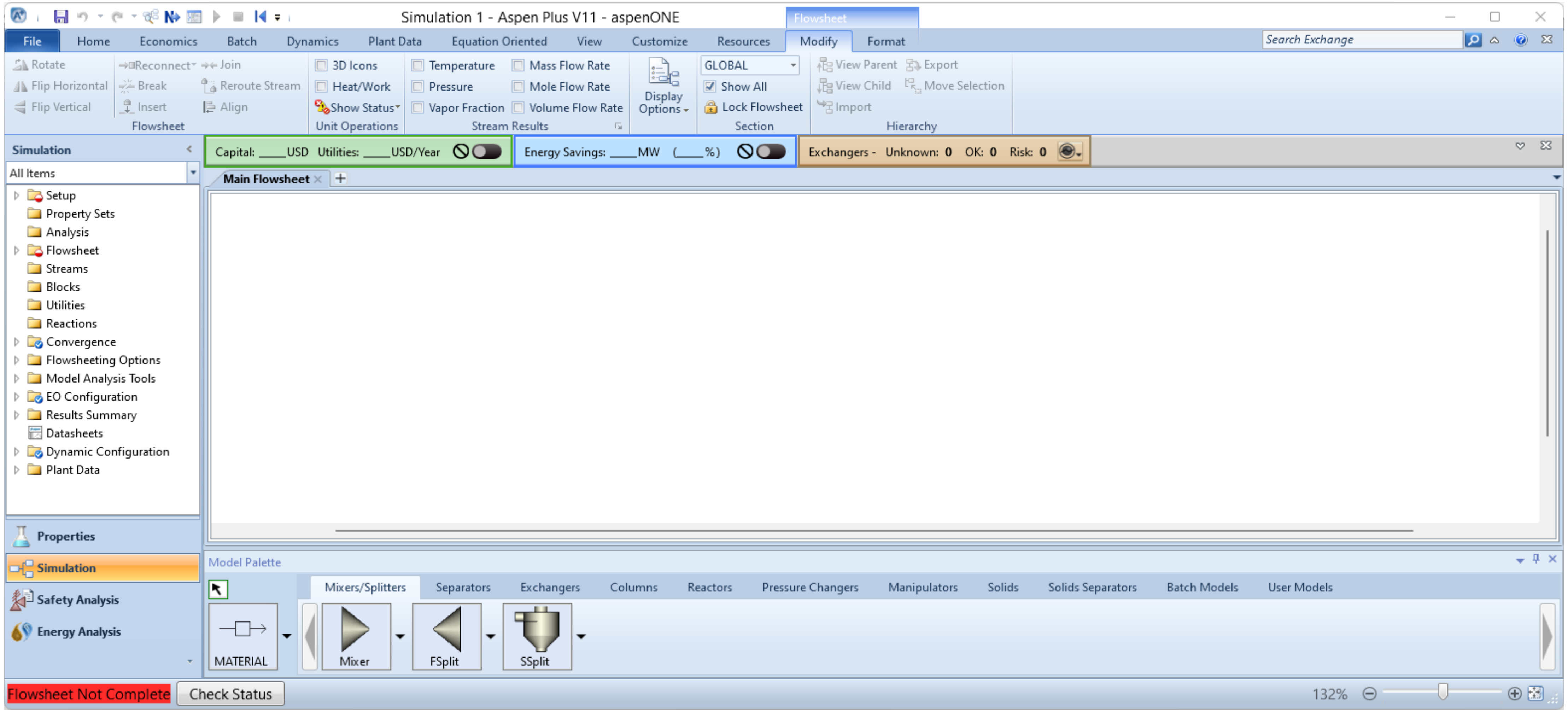
- What Aspen Plus is?
- Installing Aspen Plus
- Basic steps to simulate a process plant with Aspen Plus
- Simulation example: simple process configuration and simulation
- Rankine cycle exercise

Aspen Plus

Aspen Plus is **one** of the leading Chemical Process Simulator in the market. It is based on a database of **component properties** and different **property methods** to compute the thermodynamic and transport properties.



Graphic User Interface



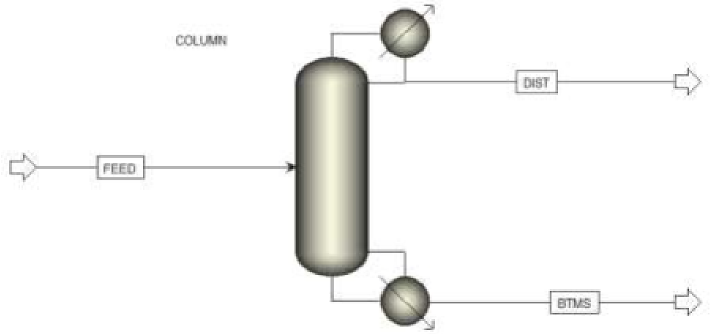
Basic steps to simulate a process plant with Aspen Plus

1. **Components definition:** in every simulation, you must define the components that will make up the simulation. In other words, you must specify which chemicals Aspen Plus should take from its large database of chemicals and use in the simulation.

2. **Property method choice:** A property method is a collection of methods and models (equation of states, advanced equation of states etc ..) that Aspen Plus uses to compute thermodynamic (Enthalpy, Entropy, Gibbs free energy..etc..) and transport properties (Viscosity, Thermal conductivity…etc).

Property method

Ooops… the results are different!



Specification:
- 30 stages
- Distillate rate 500 kmol/hr
- Reflux ratio 1.3

	Units	IDEAL FEED	IDEAL BTMS	IDEAL DIST	NRTL BTMS	NRTL DIST	PENG-ROBINSON BTMS	PENG-ROBINSON DIST
− Mole Flows	**kmol/hr**	**2328.31**	**1828.31**	**500**	**1828.31**	**500**	**1828.31**	**500**
WATER	kmol/hr	1754.07	1691.96	62.1051	1753.92	0.147487	1754.05	0.0143418
METHANOL	kmol/hr	574.243	136.349	437.895	74.3909	499.853	74.2578	499.986
− Mole Fractions								
WATER		0.753365	0.925424	0.12421	0.959312	0.000294974	0.959384	2.86836e-05
METHANOL		0.246635	0.0745763	0.87579	0.0406884	0.999705	0.0406155	0.999971

Image from https://t.ly/2D4no

Basic steps to simulate a process plant with Aspen Plus

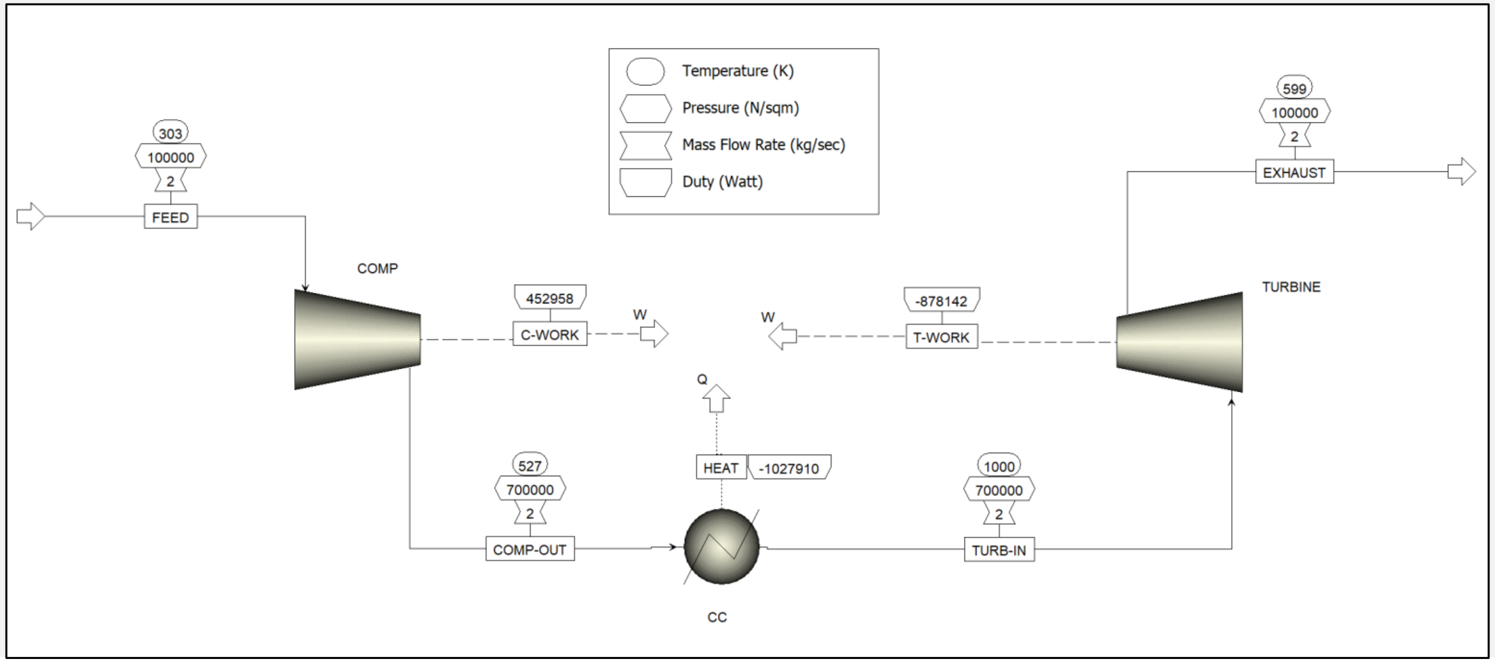
Property method choice: You must select one (or more) Property Methods to model the properties of specific systems (chemicals) in your flowsheet. Choosing the appropriate property method *is often the key decision* in determining the accuracy of your simulation results. Aspen Plus includes a large number of built-in property methods that are sufficient for most applications.

How to choose the correct property method ?

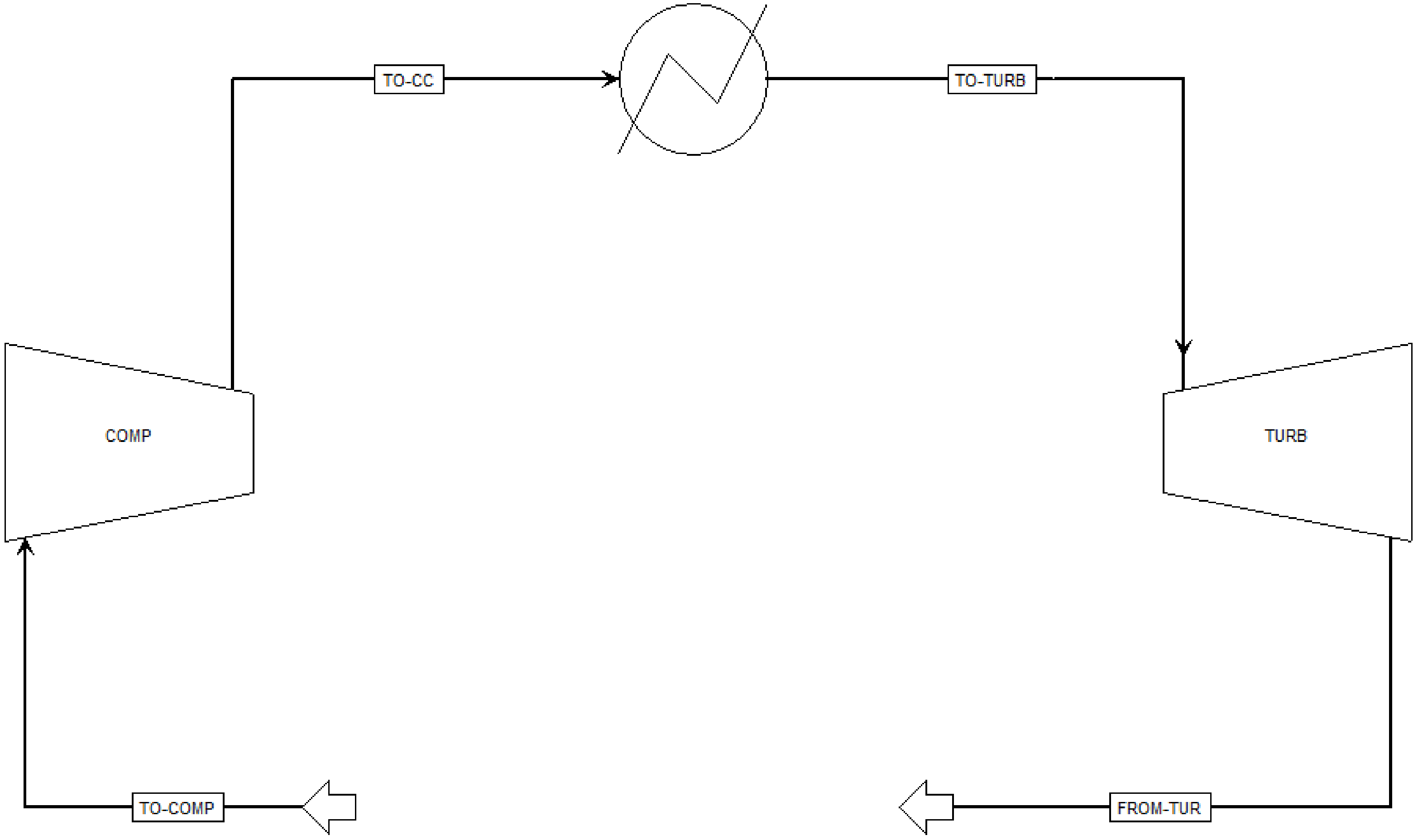
- Aspen Plus recommended methods for different plant (oil and gas production, gas processing, Petrochemicals et…)
- Literature analysis on similar works
- Experience (experimental data comparison)

Basic steps to simulate a process plant with Aspen Plus

3. **Process flowsheet definition**: "drawing" of the process plant by means of choosing the *unit operations model*, *materials* and *energy streams*.



Example



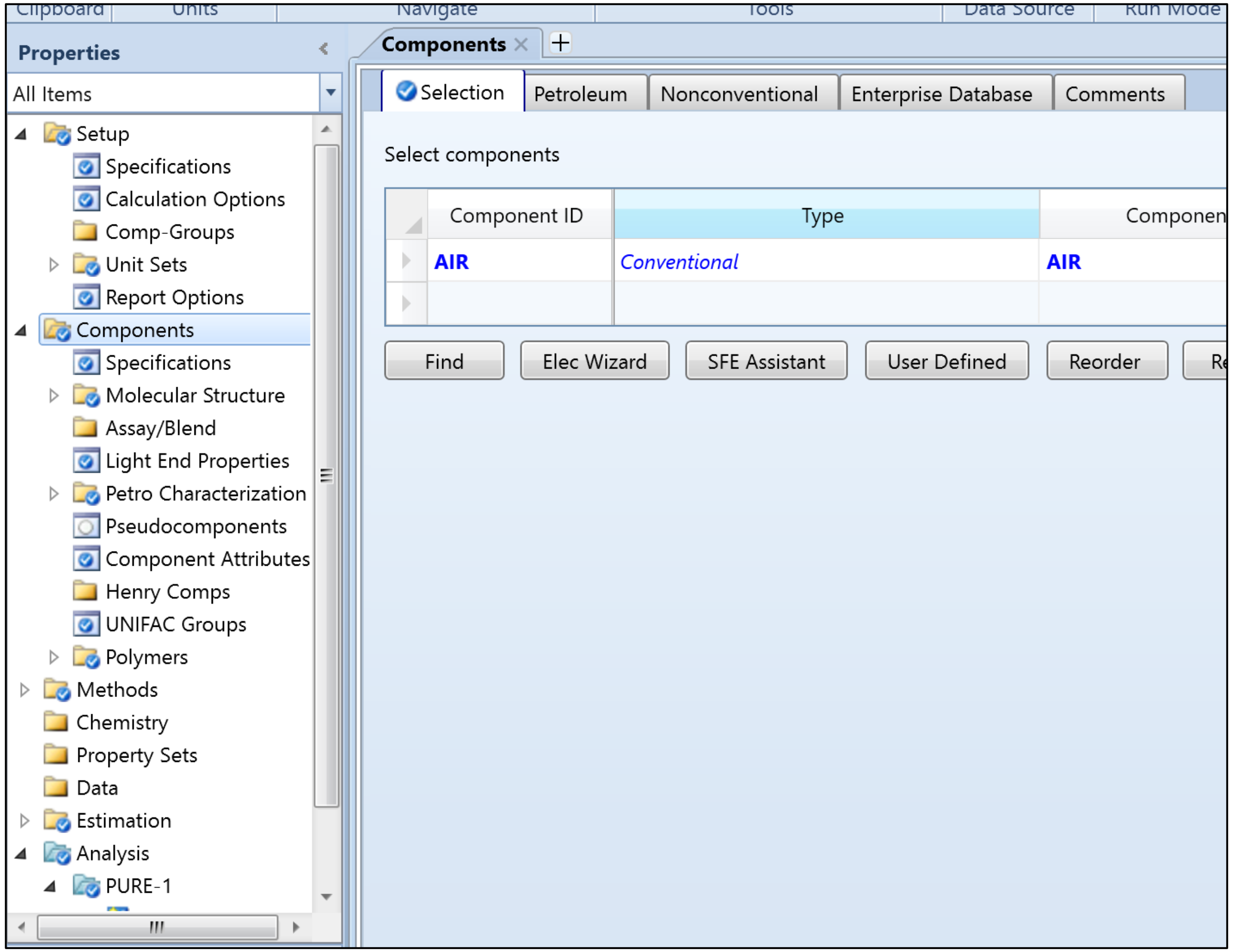
Specification

- Fluid: air
- Feed air mass flow: 500 kg/h
- Feed air pressure and temperature: 1 bar, 30° C
- Compressor pressure ratio: 10
- Turbine inlet temperature: 1.000 °C
- Turbine outlet pressure: 1 bar

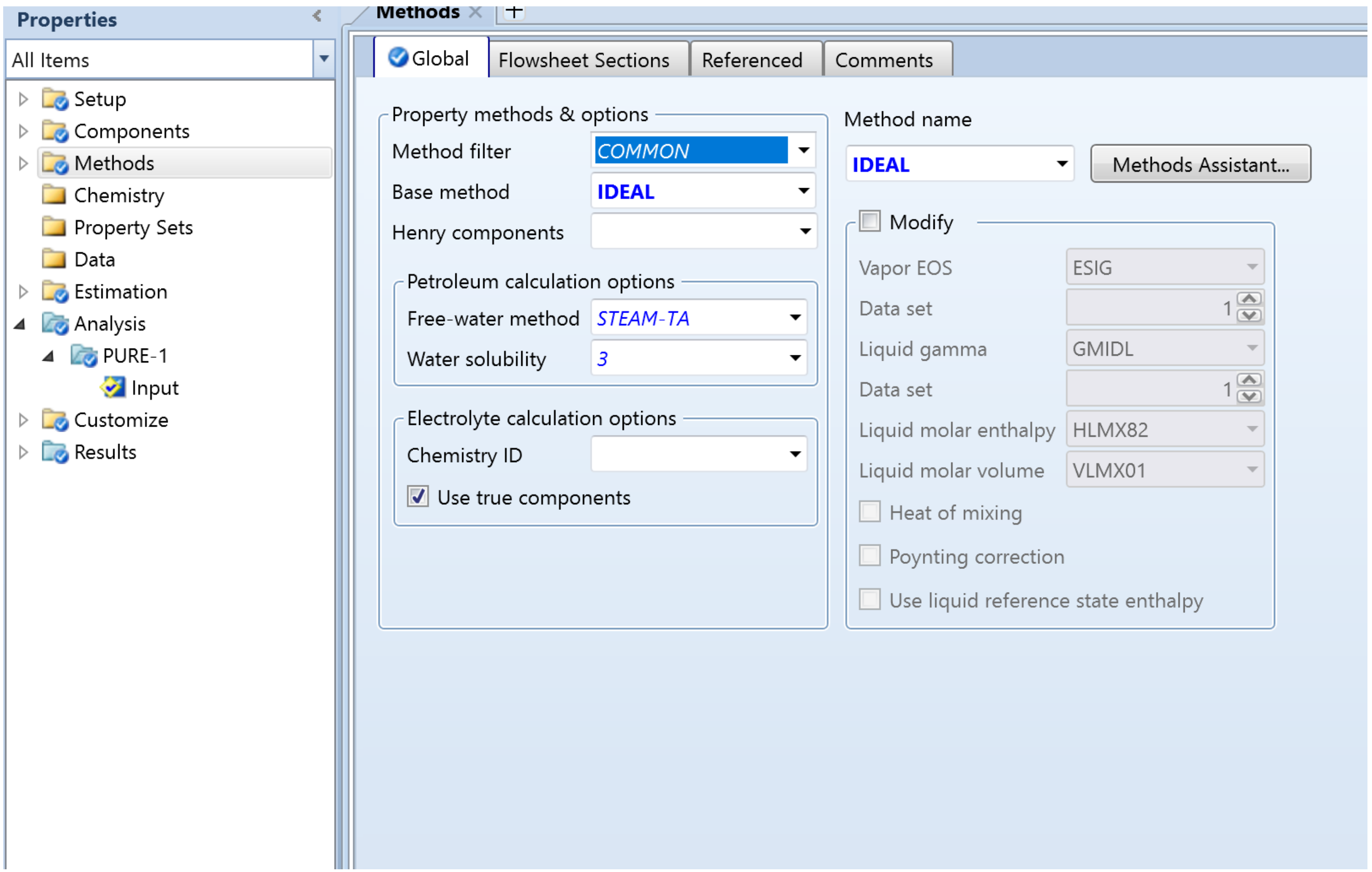
Calculate

  - Streams temperature and pressure
  - Compressor work
  - Turbine work

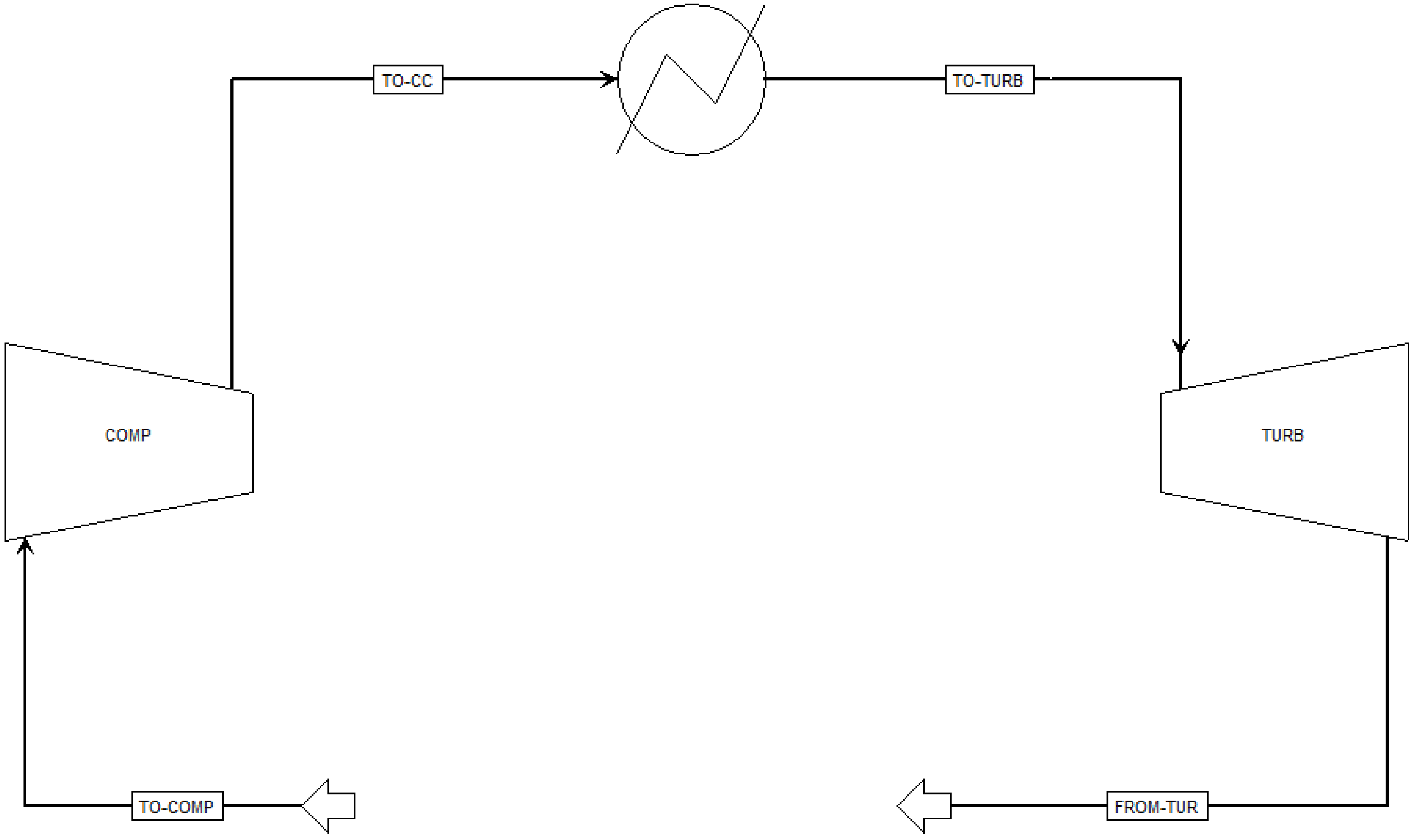
Component definition



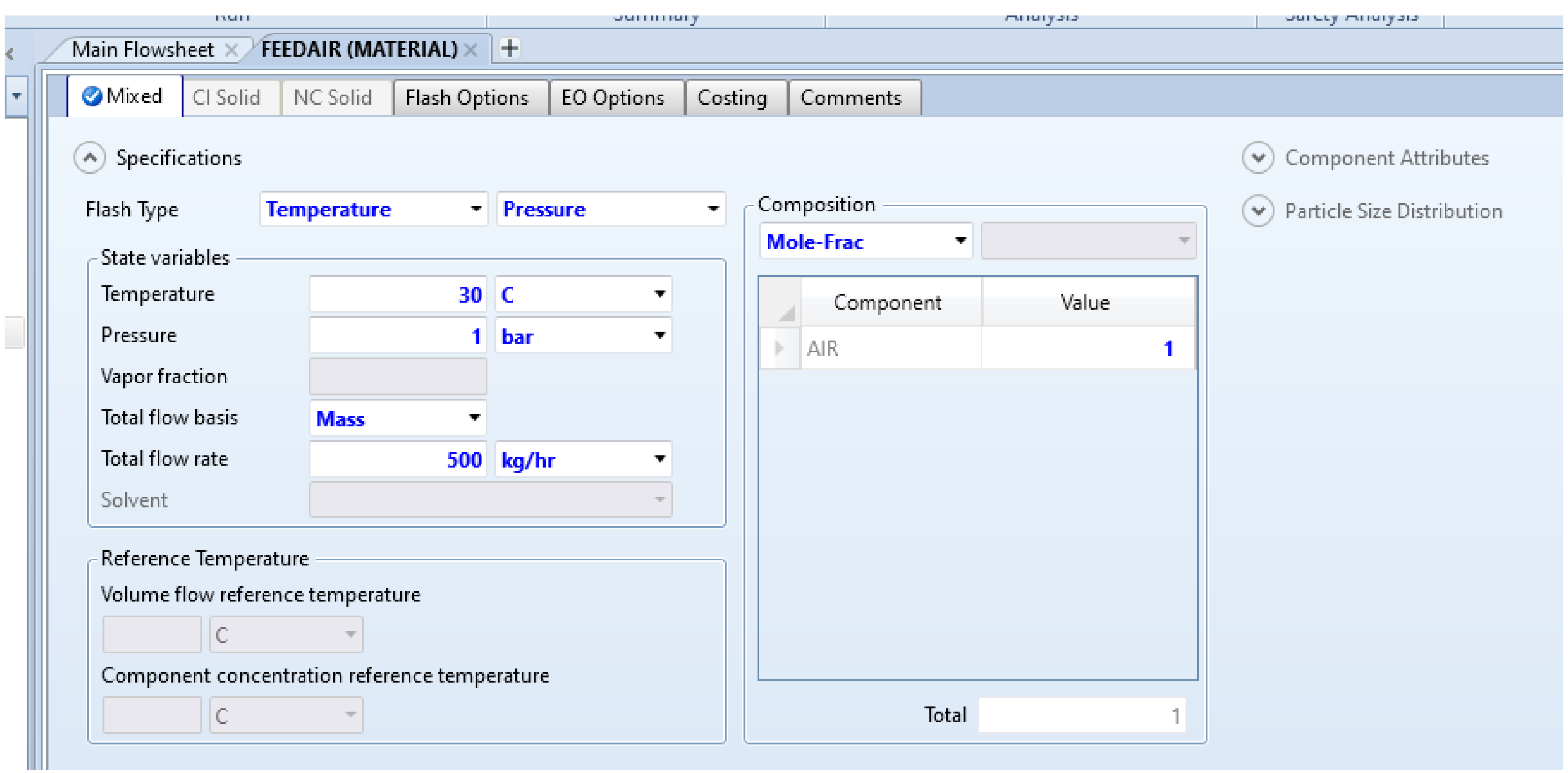
Method choice



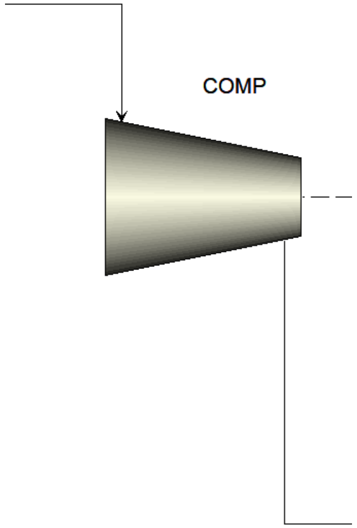
Blocks, materials and streams

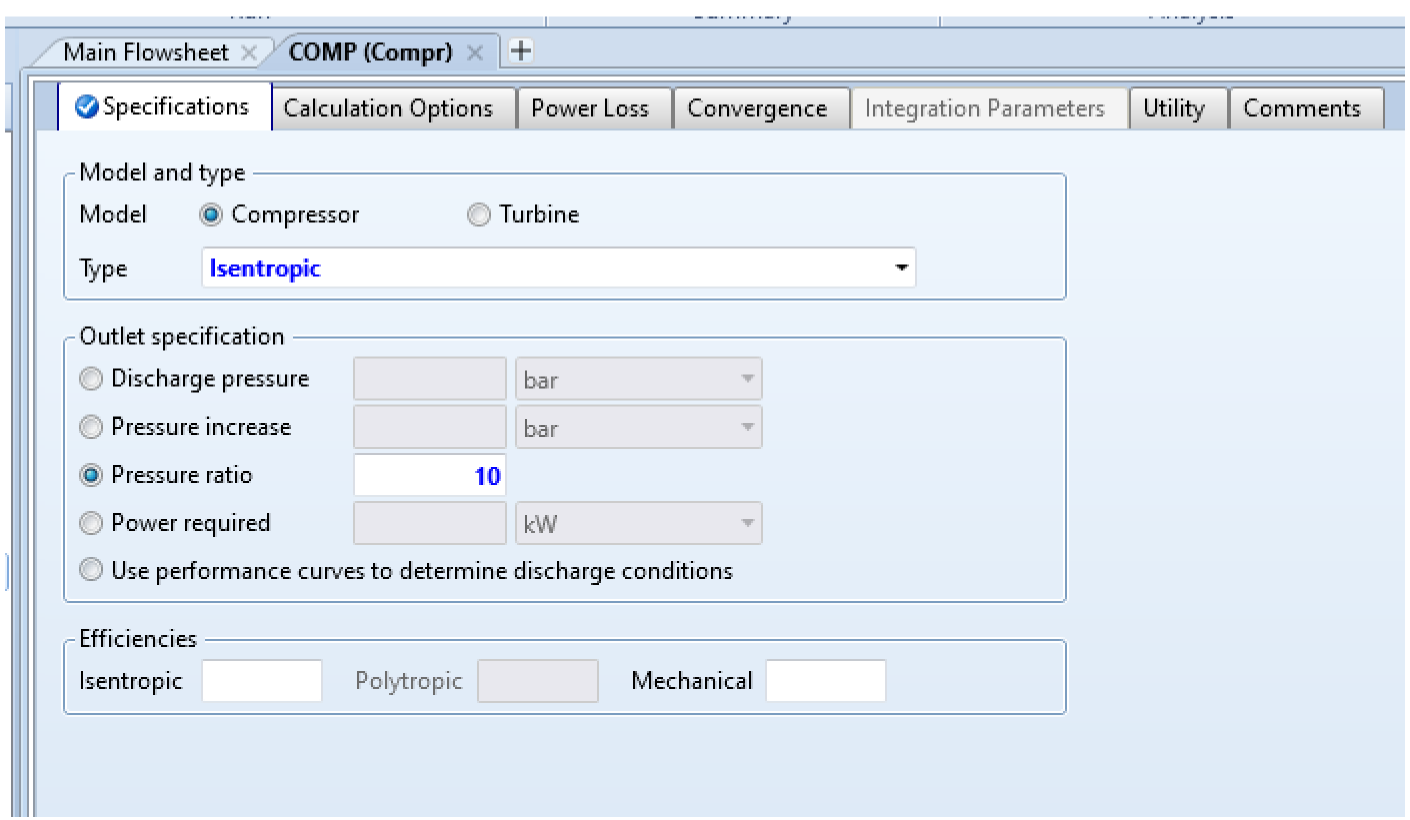


Feed flow rate and composition

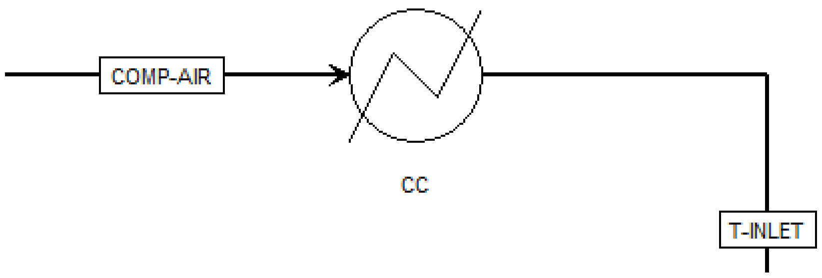


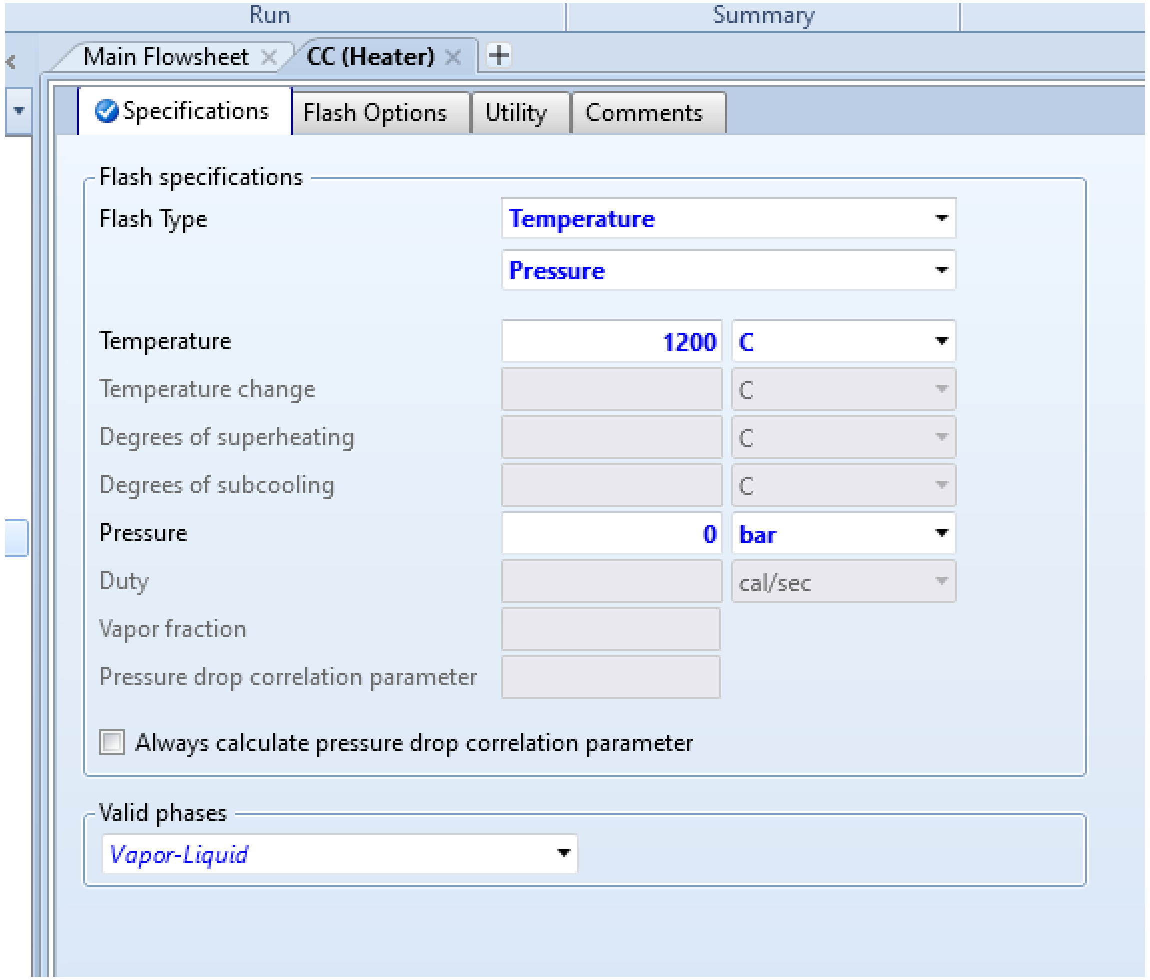
Compressor block



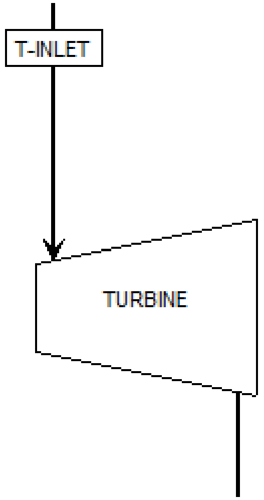


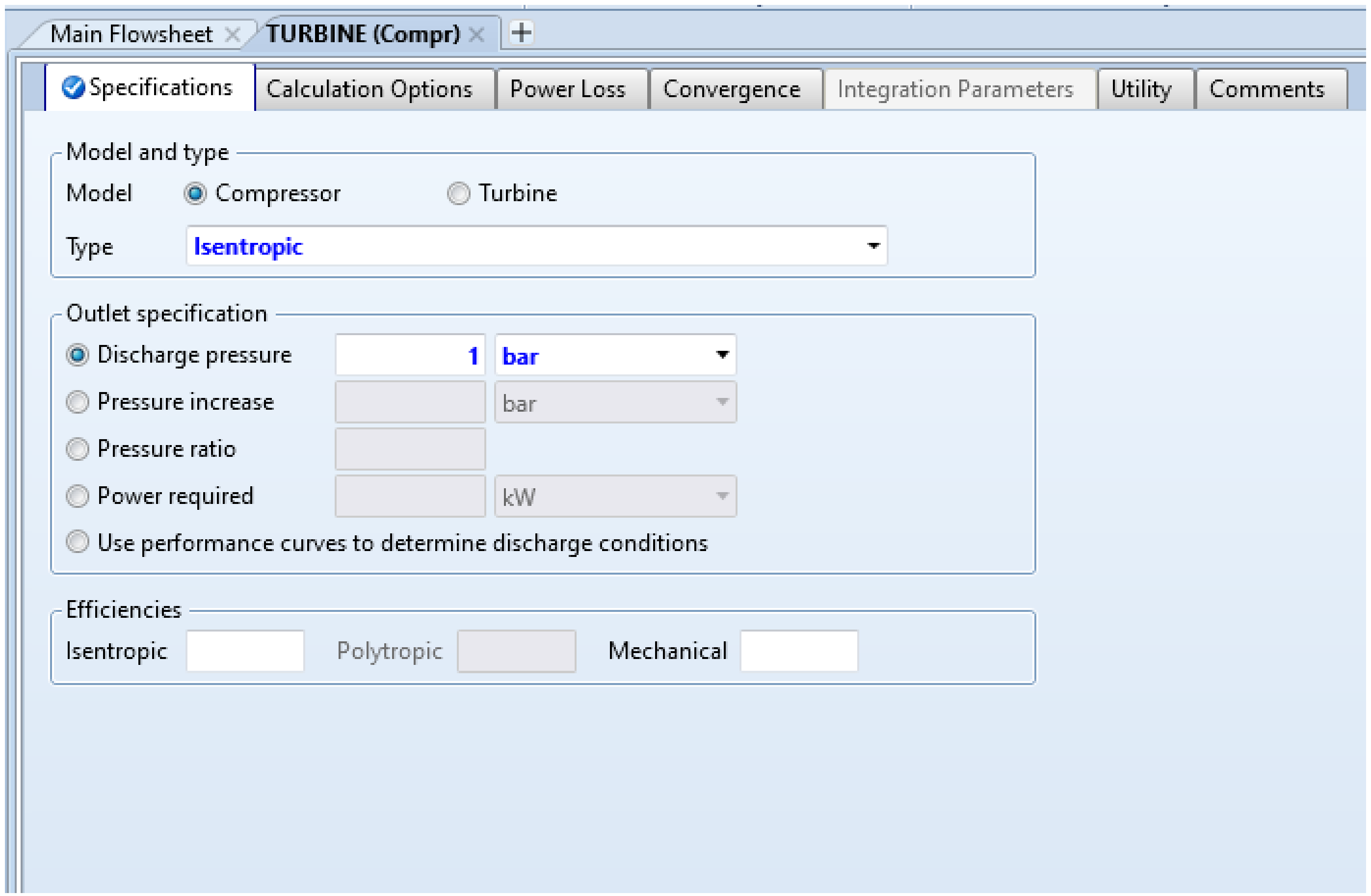
Heater block





Turbine block

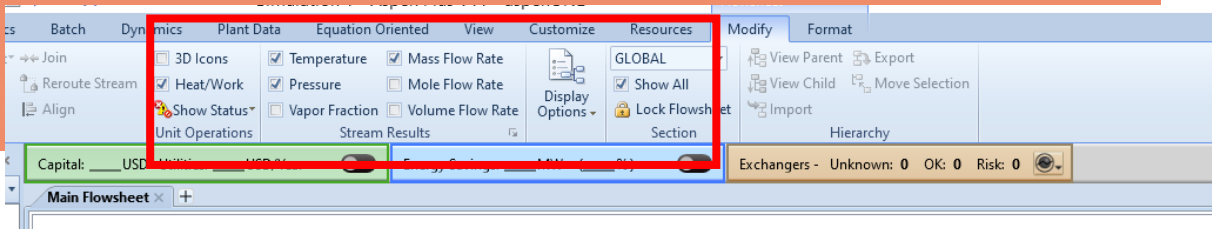


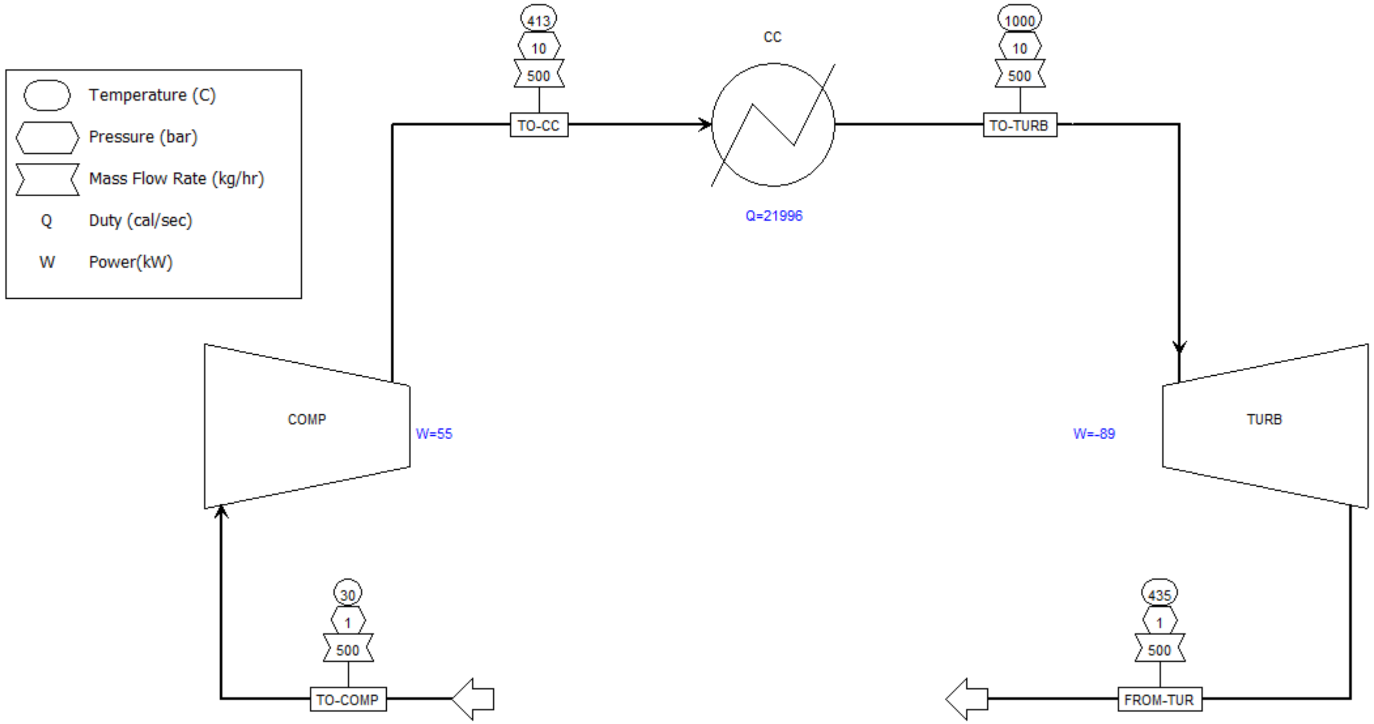


Run the simulation, showing results, change units of measure

- Streams data (temperature, pressure etc..)
- Compressor and turbine work
- Combustion chamber heat
- How to change units of measure
- How to change unit visualization

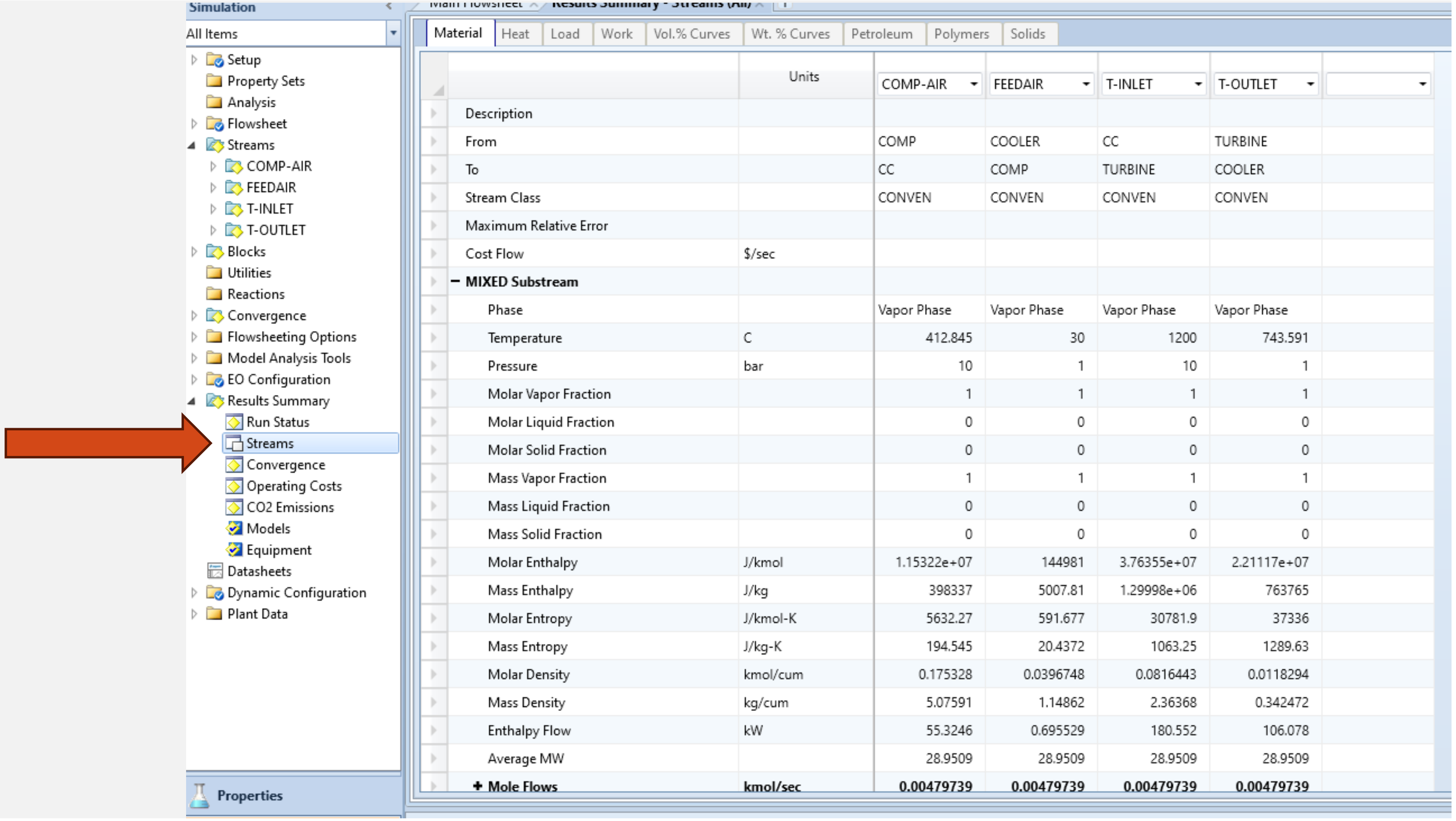
Show results





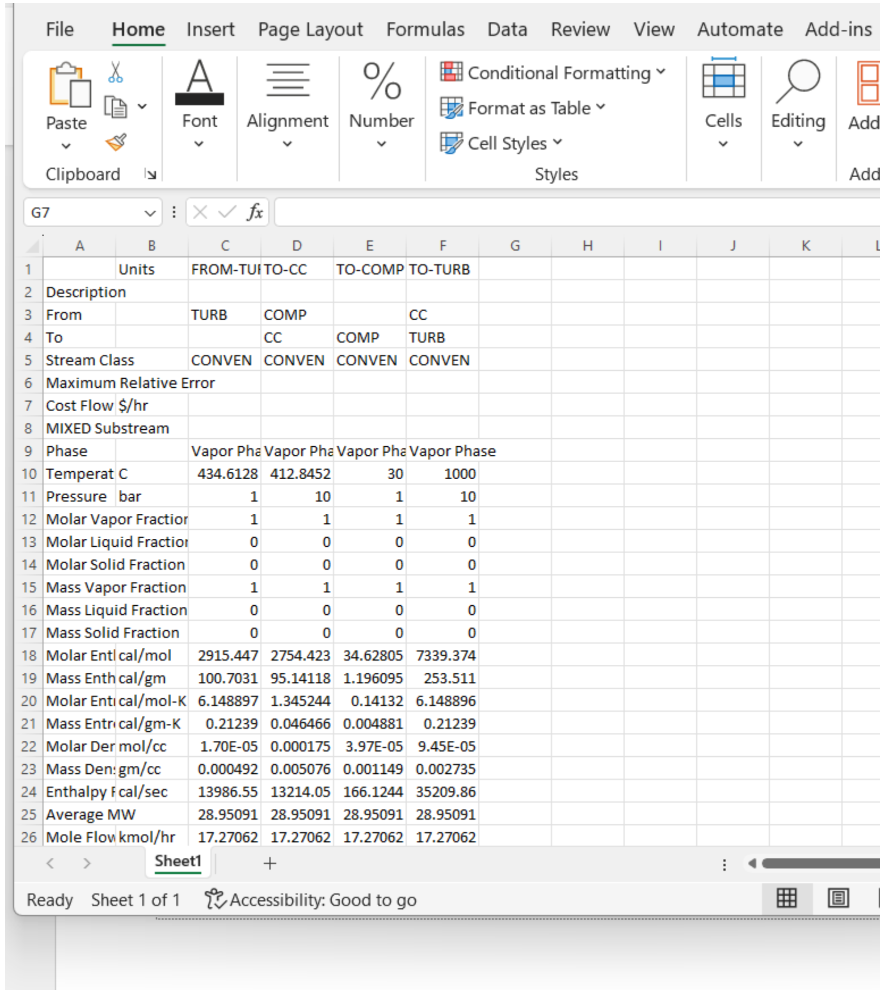
Stream stream results table

- Streams table



	Units	COMP-AIR	FEEDAIR	T-INLET	T-OUTLET
Description					
From		COMP	COOLER	CC	TURBINE
To		CC	COMP	TURBINE	COOLER
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN
Maximum Relative Error					
Cost Flow	$/sec				
− MIXED Substream					
Phase		Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase
Temperature	C	412.845	30	1200	743.591
Pressure	bar	10	1	10	1
Molar Vapor Fraction		1	1	1	1
Molar Liquid Fraction		0	0	0	0
Molar Solid Fraction		0	0	0	0
Mass Vapor Fraction		1	1	1	1
Mass Liquid Fraction		0	0	0	0
Mass Solid Fraction		0	0	0	0
Molar Enthalpy	J/kmol	1.15322e+07	144981	3.76355e+07	2.21117e+07
Mass Enthalpy	J/kg	398337	5007.81	1.29998e+06	763765
Molar Entropy	J/kmol-K	5632.27	591.677	30781.9	37336
Mass Entropy	J/kg-K	194.545	20.4372	1063.25	1289.63
Molar Density	kmol/cum	0.175328	0.0396748	0.0816443	0.0118294
Mass Density	kg/cum	5.07591	1.14862	2.36368	0.342472
Enthalpy Flow	kW	55.3246	0.695529	180.552	106.078
Average MW		28.9509	28.9509	28.9509	28.9509
+ Mole Flows	**kmol/sec**	**0.00479739**	**0.00479739**	**0.00479739**	**0.00479739**

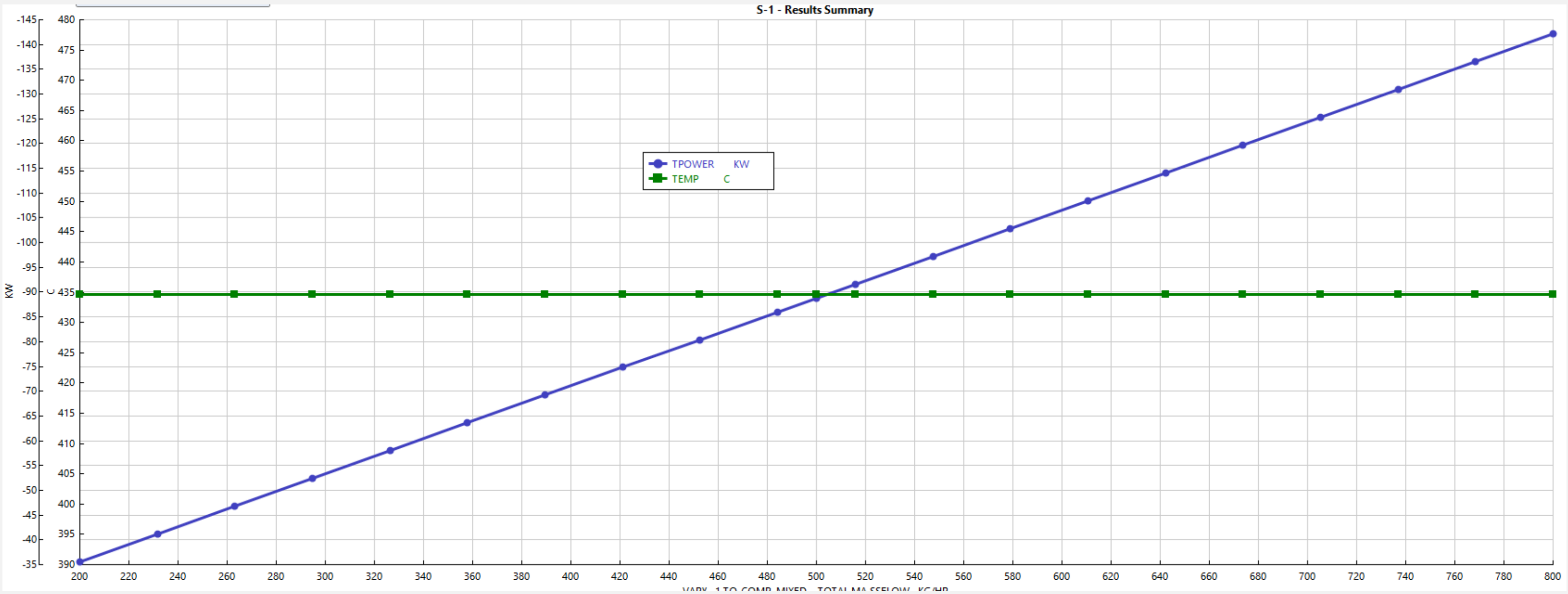
Copy paste to excel



	A	B	C	D	E	F
1		Units	FROM-TUI	TO-CC	TO-COMP	TO-TURB
2	Description					
3	From		TURB	COMP		CC
4	To			CC	COMP	TURB
5	Stream Class		CONVEN	CONVEN	CONVEN	CONVEN
6	Maximum Relative Error					
7	Cost Flow	$/hr				
8	MIXED Substream					
9	Phase		Vapor Pha	Vapor Pha	Vapor Pha	Vapor Phase
10	Temperat	C	434.6128	412.8452	30	1000
11	Pressure	bar	1	10	1	10
12	Molar Vapor Fractior		1	1	1	1
13	Molar Liquid Fractior		0	0	0	0
14	Molar Solid Fraction		0	0	0	0
15	Mass Vapor Fraction		1	1	1	1
16	Mass Liquid Fraction		0	0	0	0
17	Mass Solid Fraction		0	0	0	0
18	Molar Entl	cal/mol	2915.447	2754.423	34.62805	7339.374
19	Mass Enth	cal/gm	100.7031	95.14118	1.196095	253.511
20	Molar Enti	cal/mol-K	6.148897	1.345244	0.14132	6.148896
21	Mass Entr	cal/gm-K	0.21239	0.046466	0.004881	0.21239
22	Molar Der	mol/cc	1.70E-05	0.000175	3.97E-05	9.45E-05
23	Mass Den	gm/cc	0.000492	0.005076	0.001149	0.002735
24	Enthalpy F	cal/sec	13986.55	13214.05	166.1244	35209.86
25	Average MW		28.95091	28.95091	28.95091	28.95091
26	Mole Flow	kmol/hr	17.27062	17.27062	17.27062	17.27062

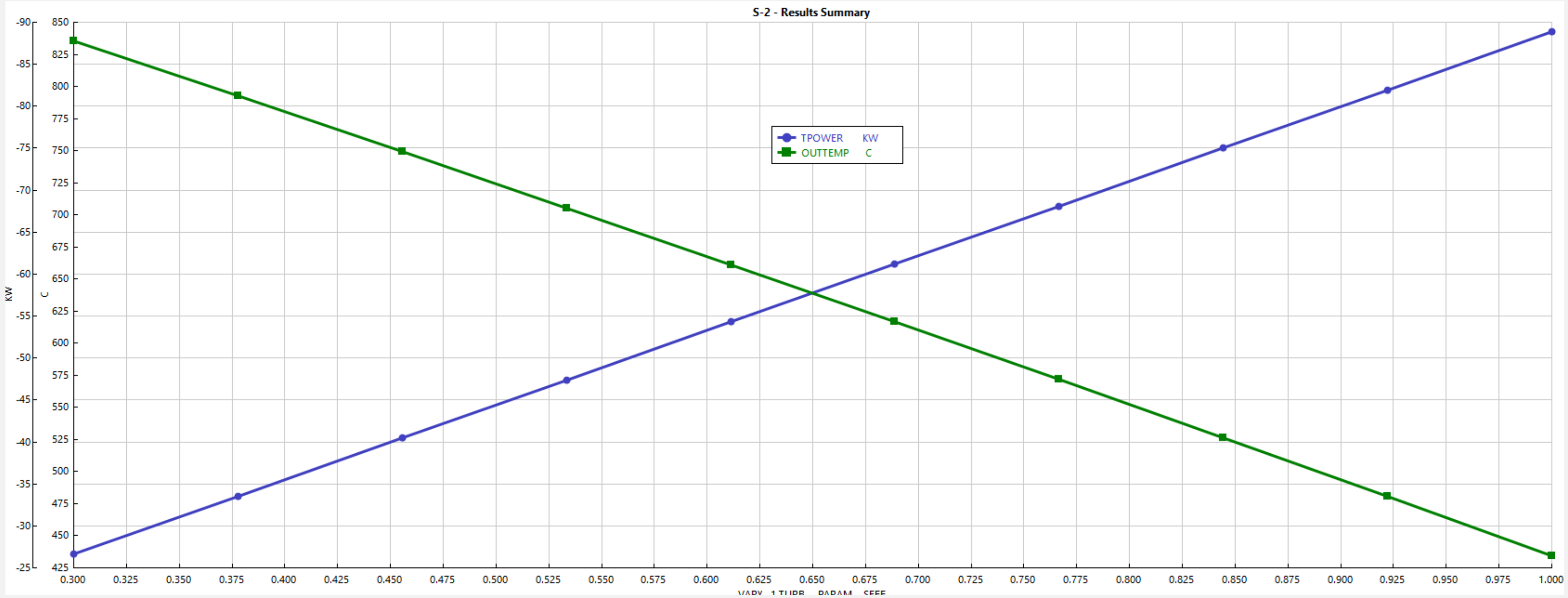
Model analysis tool: sensitivity analysis

Aim: evaluate the turbine power and output temperature change with air flow rate change

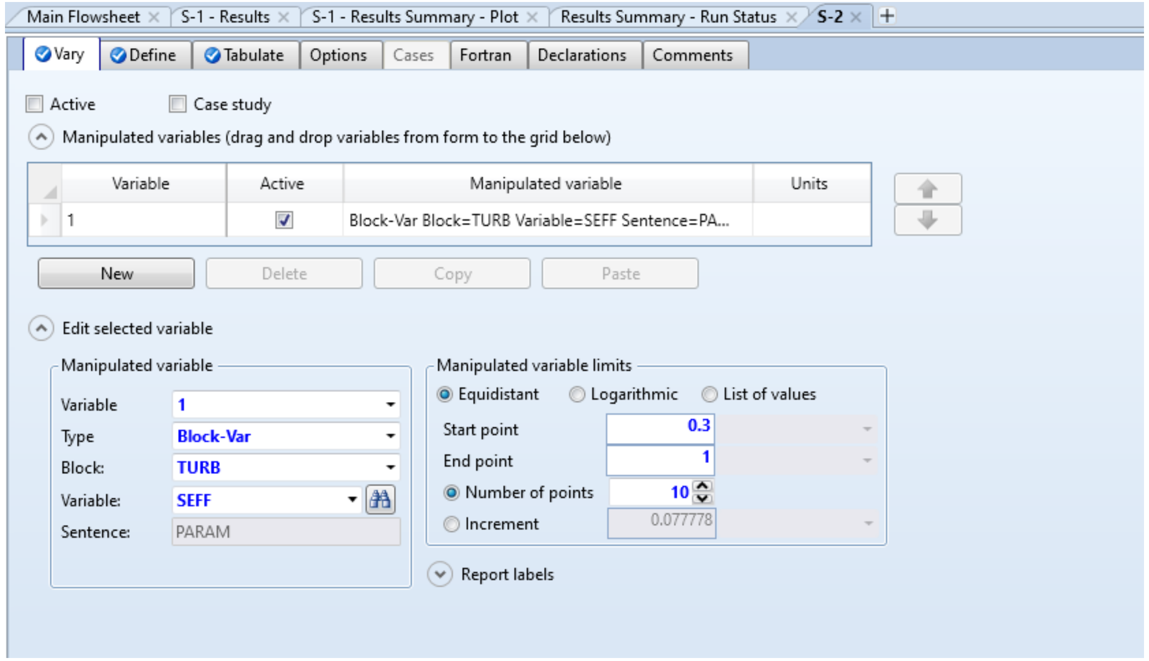


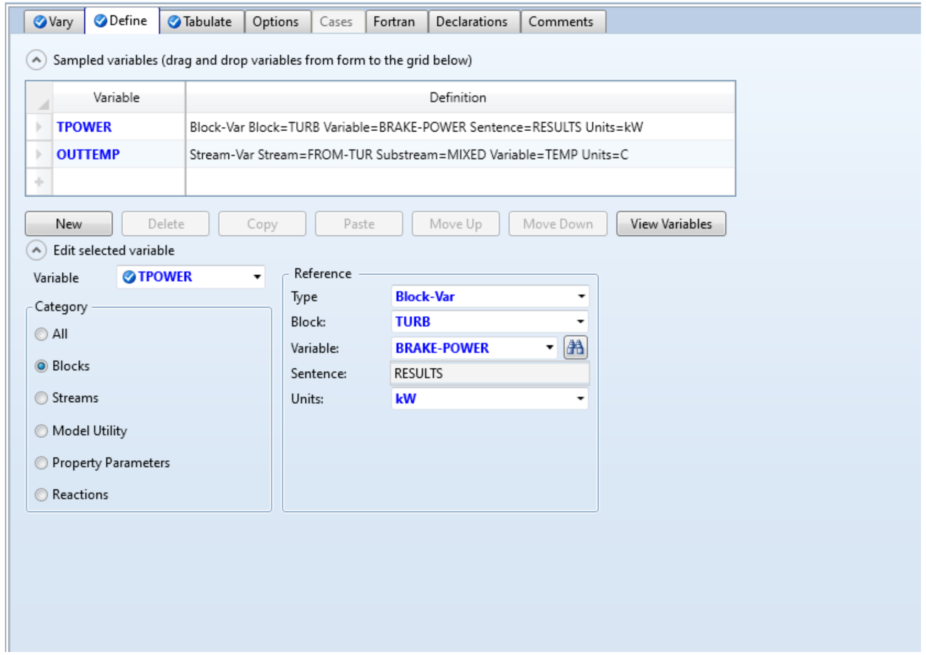
Model analysis tool: sensitivity analysis

Aim: evaluate the turbine power and output temperature change with turbine isentropic efficiency change



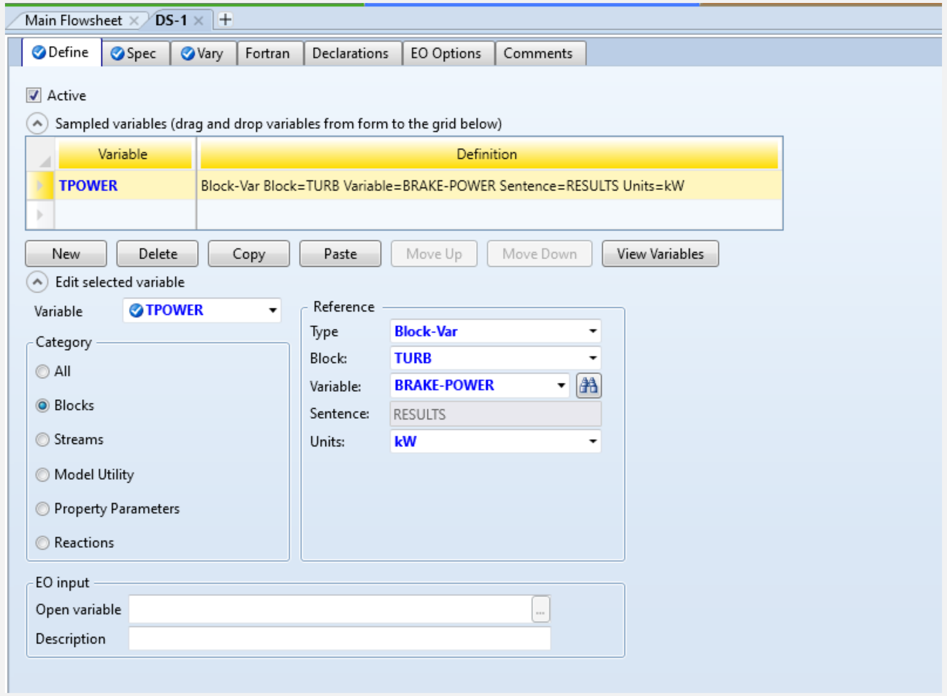
Model analysis tool: sensitivity analysis

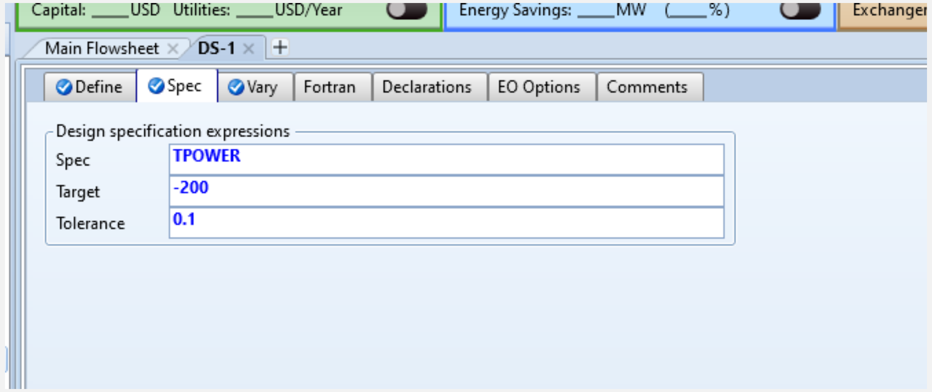




Flowsheet options: design specifications

Aim: find the air flow rate to produce 200 kW from turbine





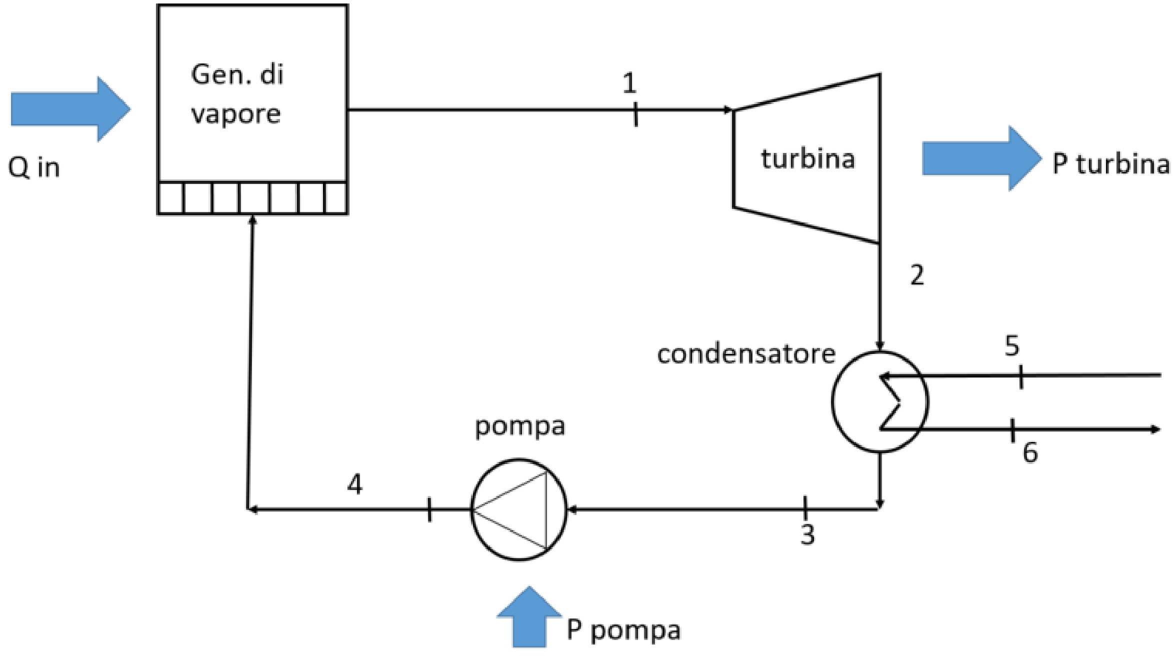
Ciclo Rankine, esercizio

Ciclo Rankine, esercizio

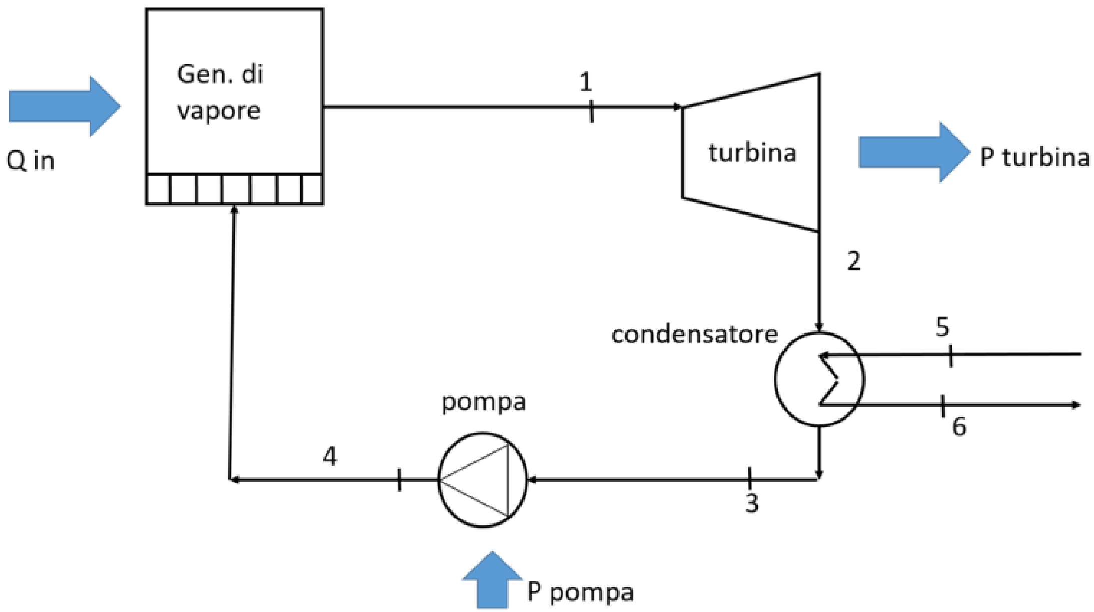
Calcolare la portata d'acqua necessaria per ottenere una potenza netta del ciclo pari a 100 MW

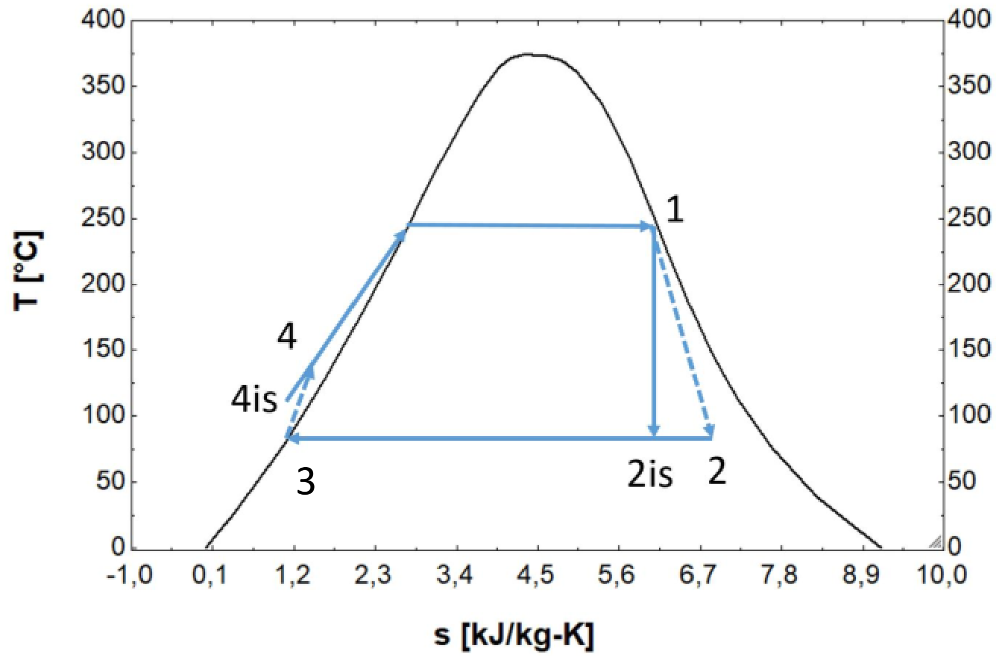
Dati

- Pressione al condensatore 0.08 bar
- Liquido saturo all'uscita del condensatore
- Pressione all'ingresso in turbina 80 bar
- Vapore saturo all'ingresso in turbina
- Rendimenti isoentropici pompa e turbina 85%
- Si trascurano le perdite di carico
- Temperature dell'acqua al condensatore ingresso e uscita: 15°C e 35°C



Ciclo Rankine



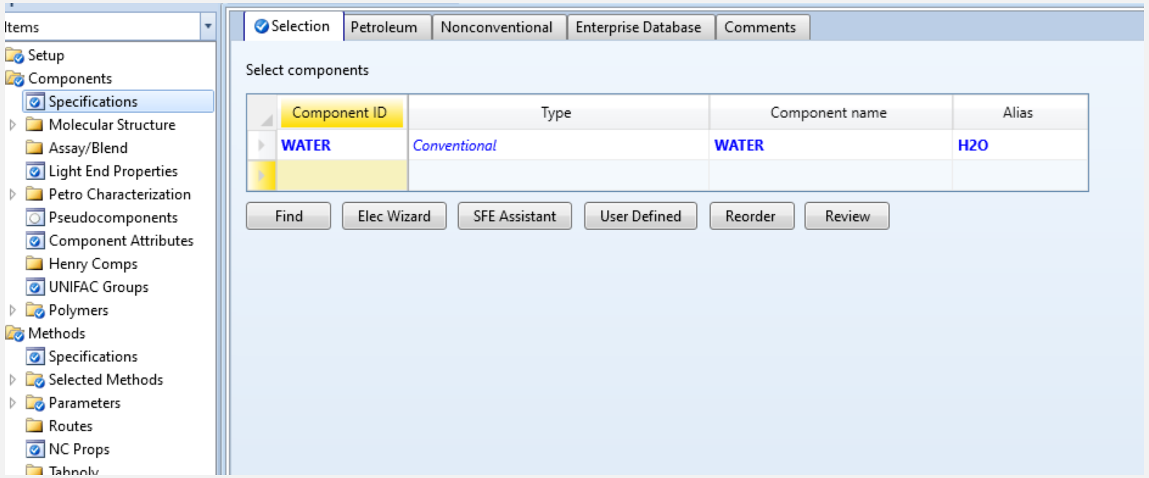


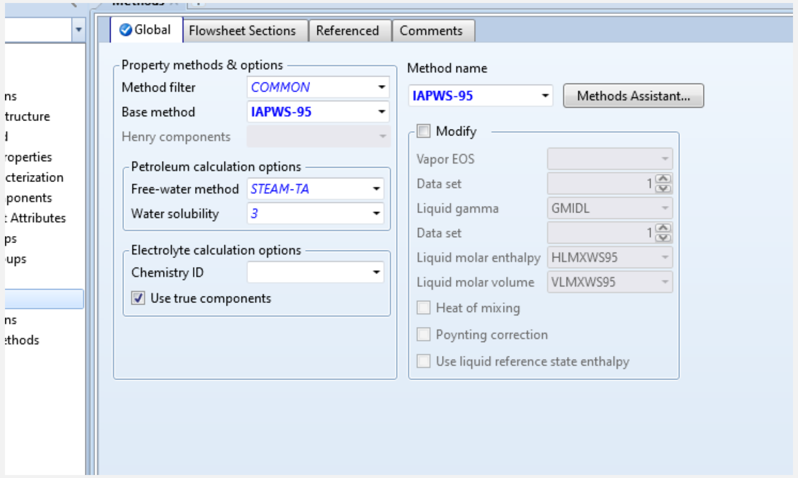
$$\eta_{th} = \frac{P_{NET}}{\dot{Q}_{in}} = \frac{P_{turbina} - P_{pompa}}{\dot{m}(h_1 - h_4)}$$

Simulazione di processo con Aspen Plus

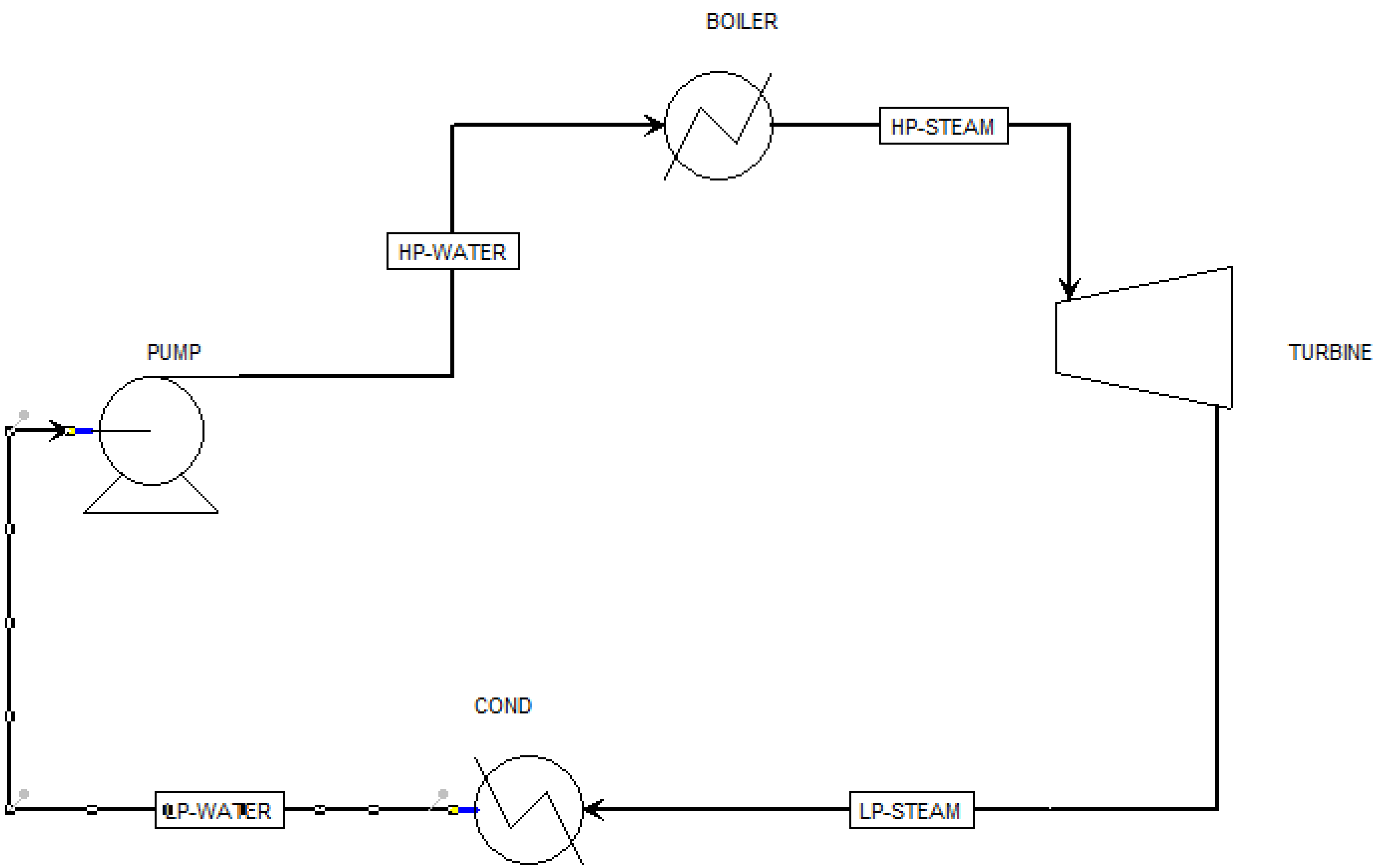
Definizione delle proprietà della simulazione

- Scelgo come componente l’acqua
- Scelgo il metodo: IAPWS-59 (International Association for the Properties of Water and Steam)

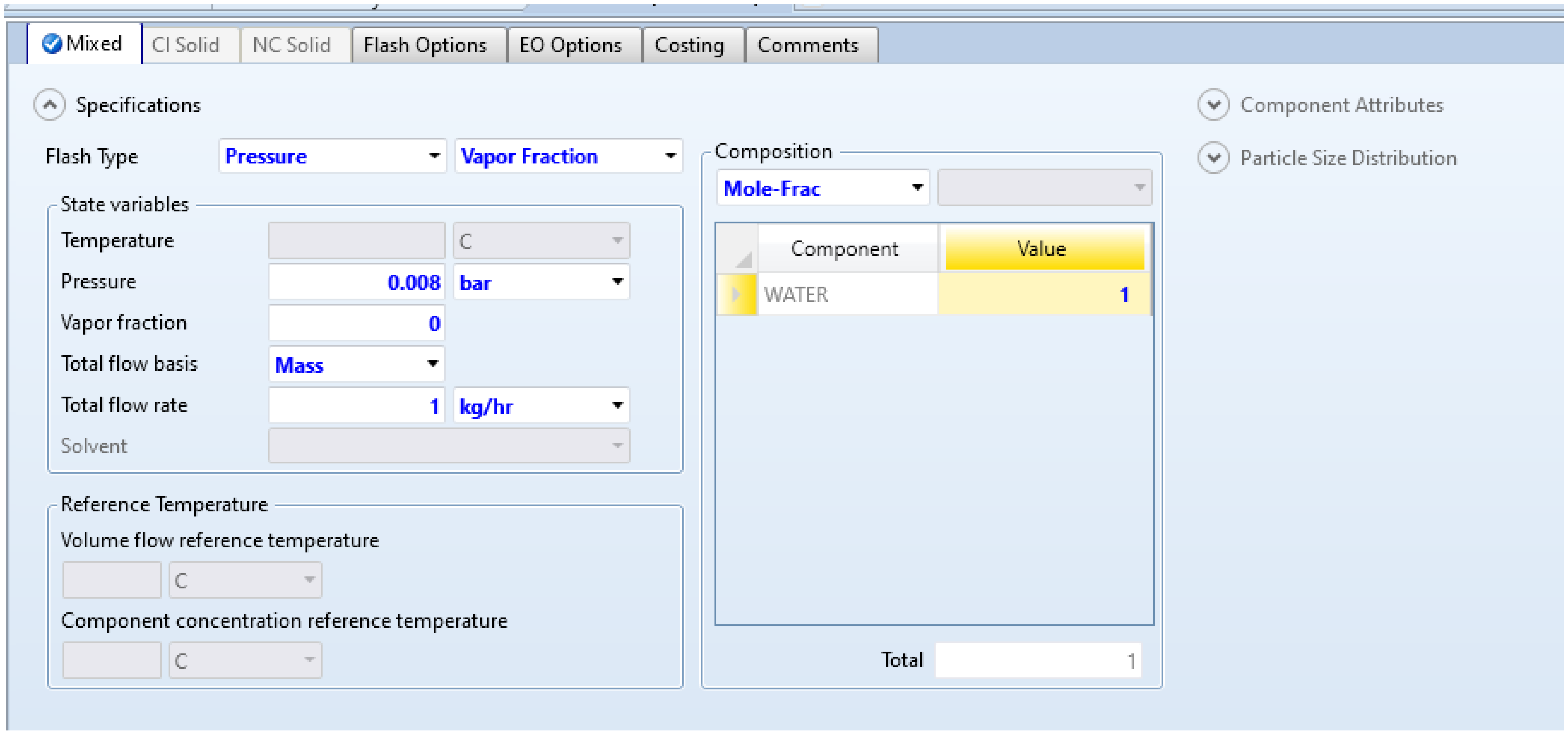




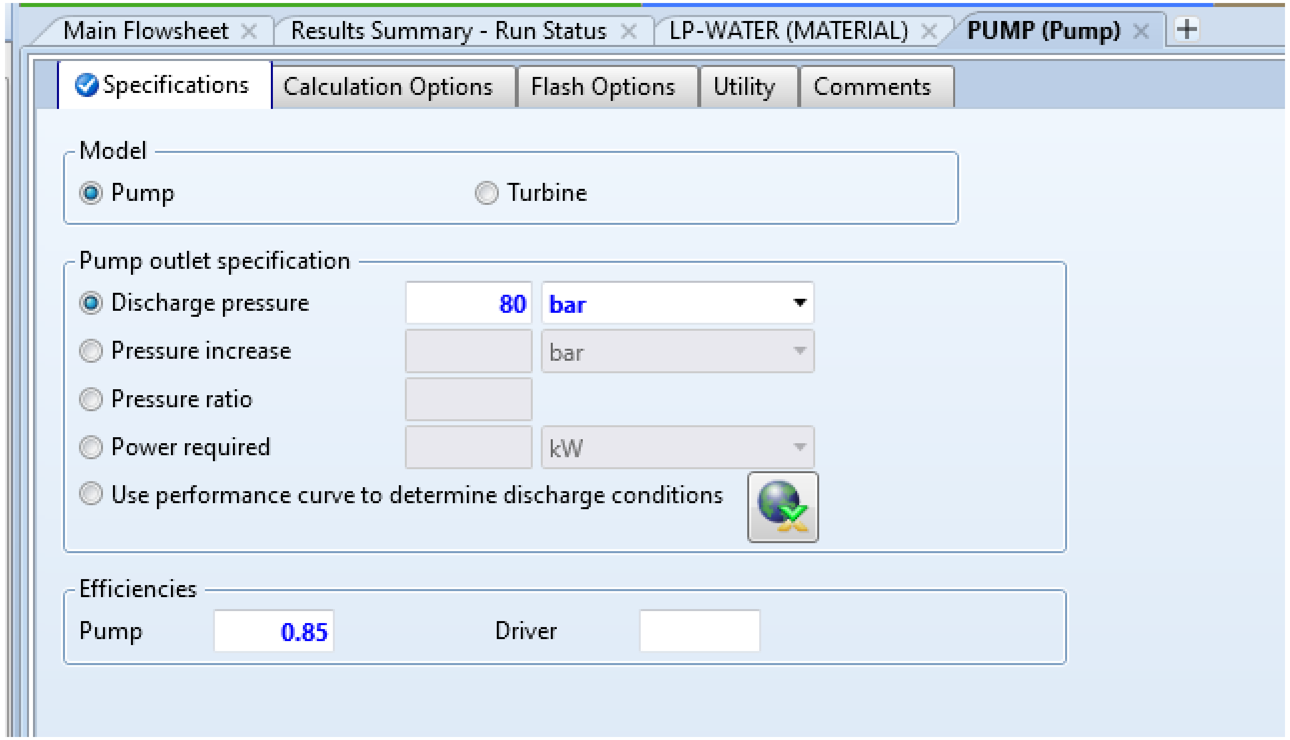
Definizione del flowsheet



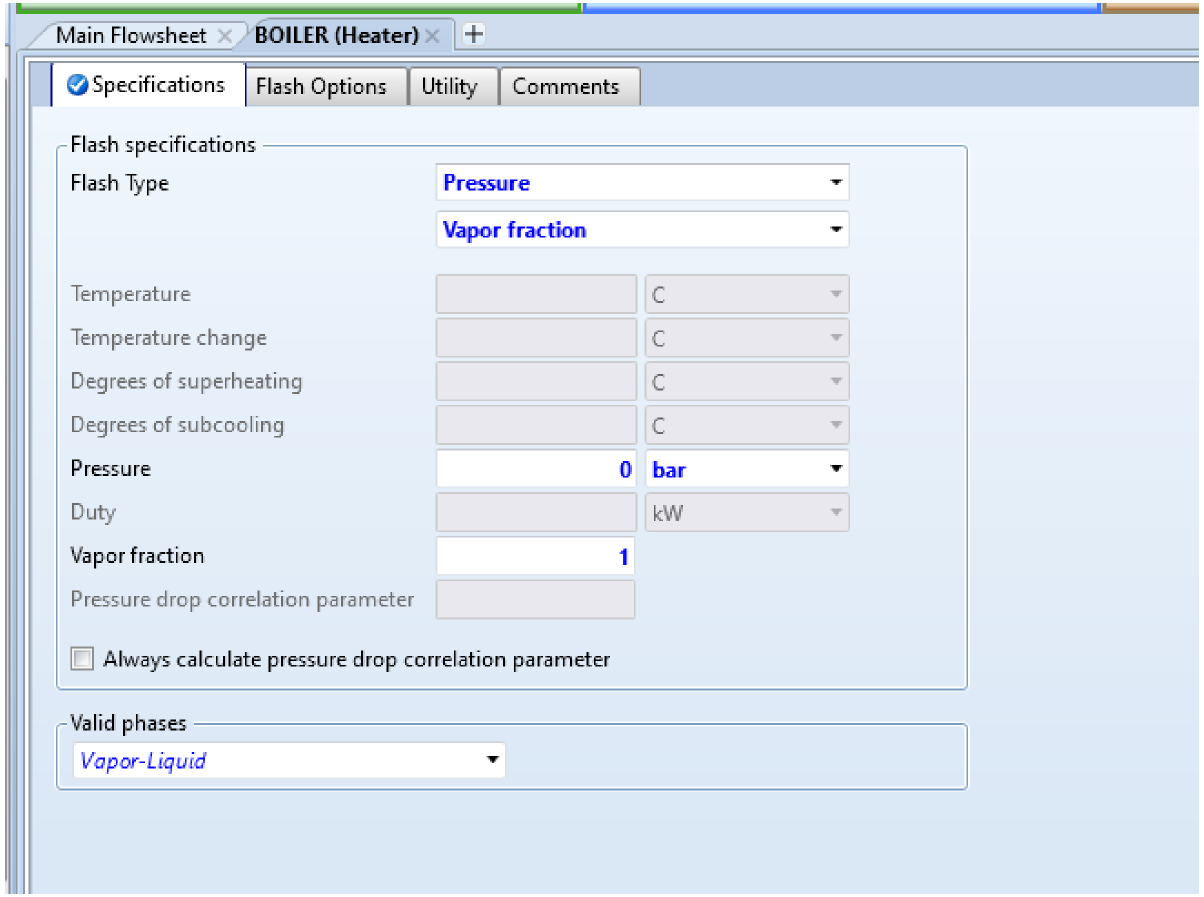
LP-WATER stream definition



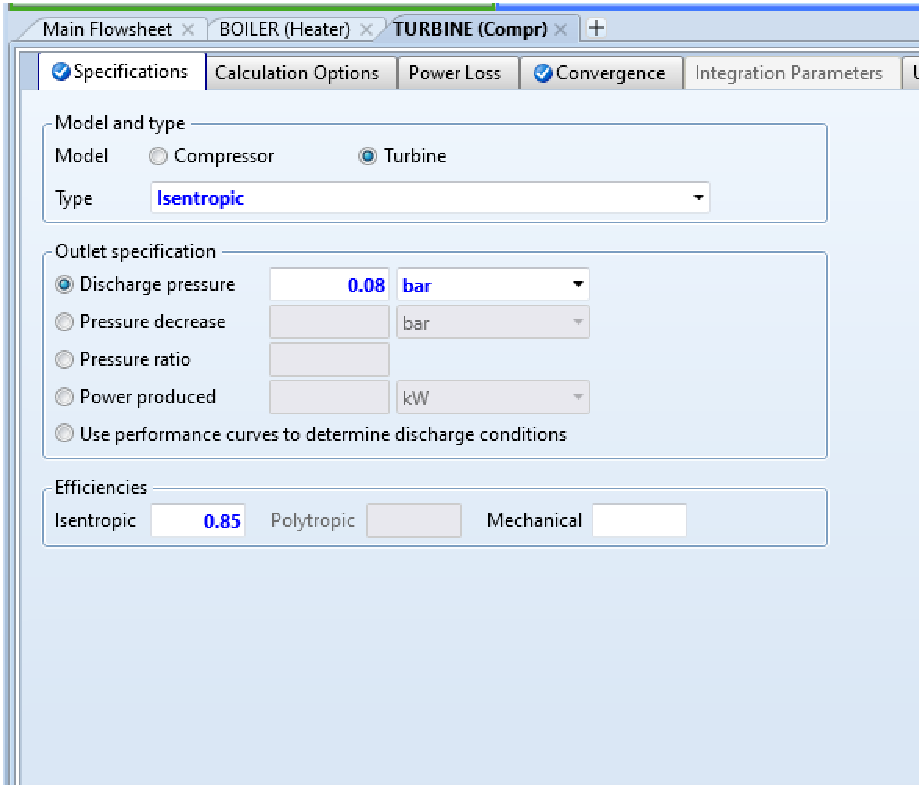
PUMP block definition

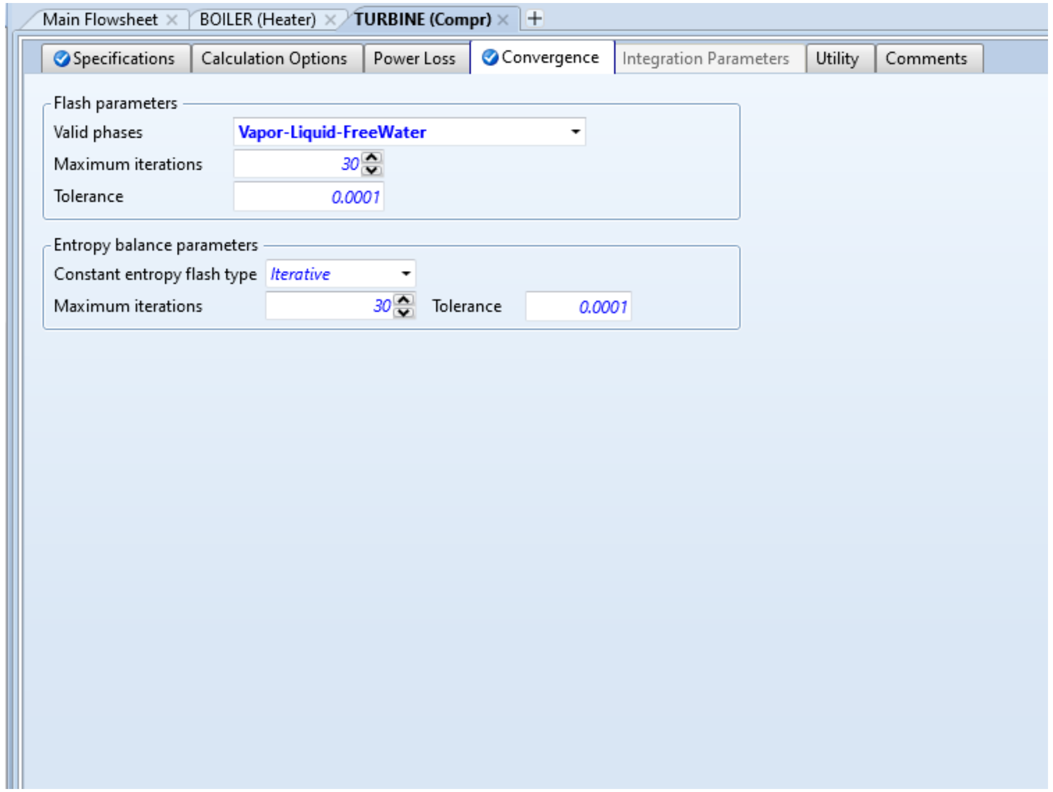


BOILER block definition



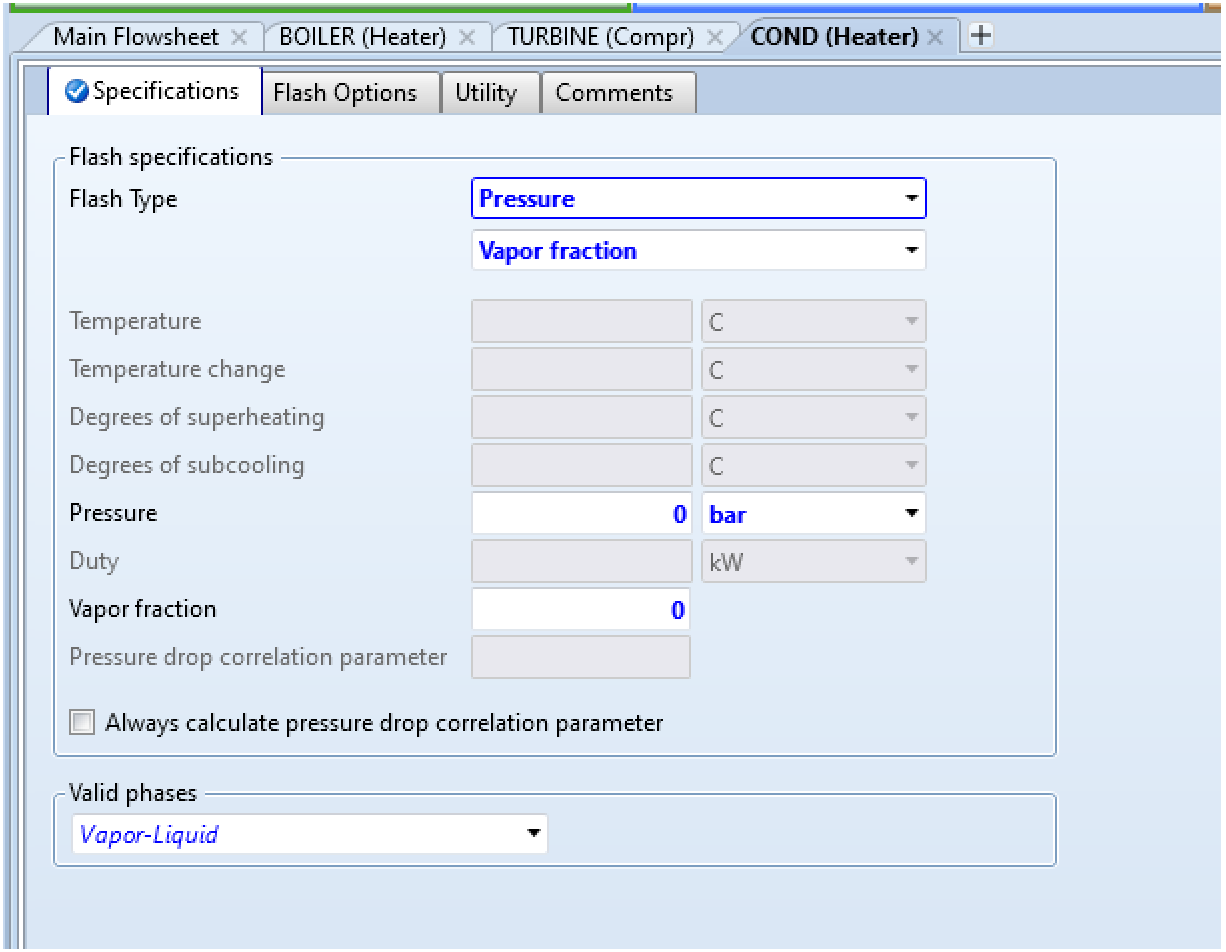
TURBINE block definition



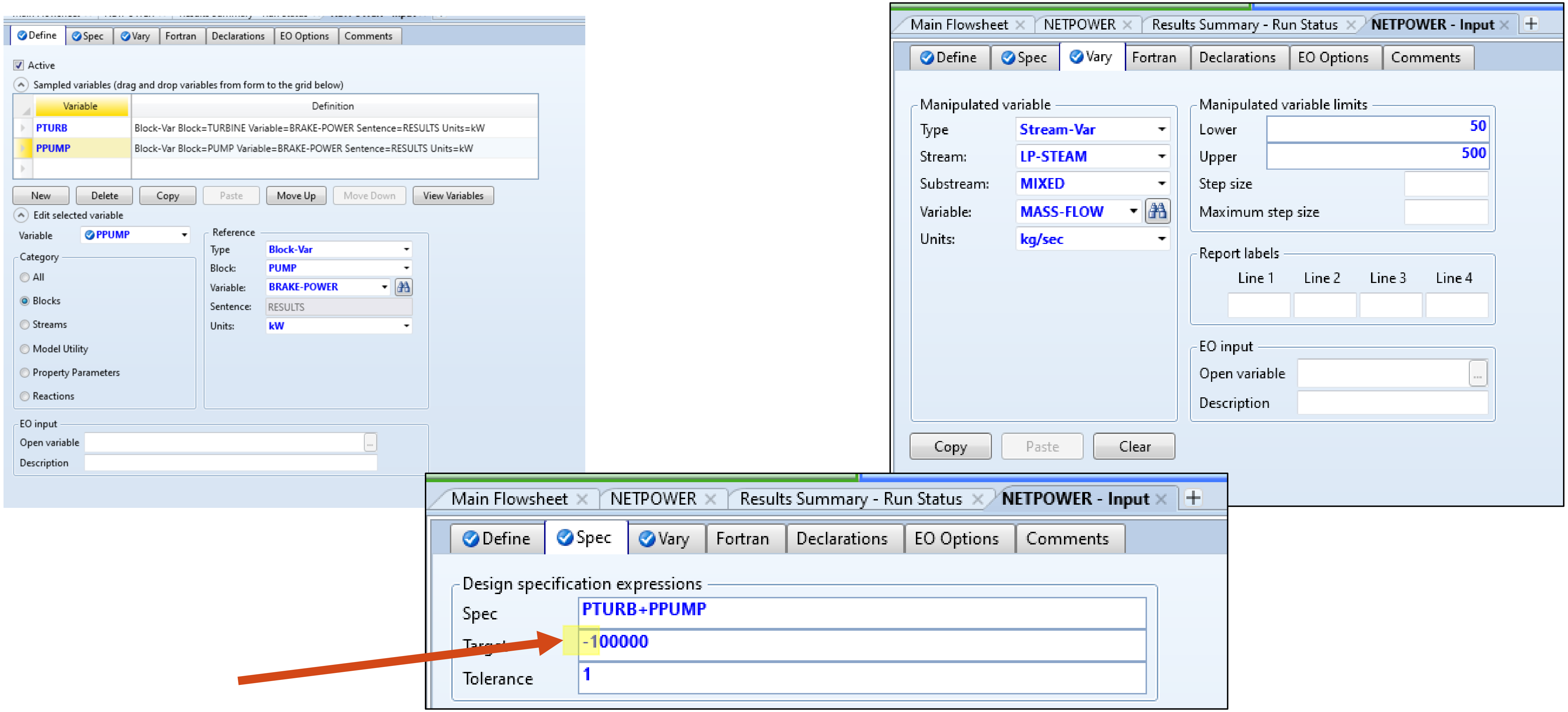


Free water: this represents any unbound, uncondensed liquid water that may be present in the system. It refers to water that is not associated with the vapor-liquid equilibrium but exists as a separate phase. This phase could occur, for example, in systems where water droplets are suspended in a gas stream

CONDENSER block definition

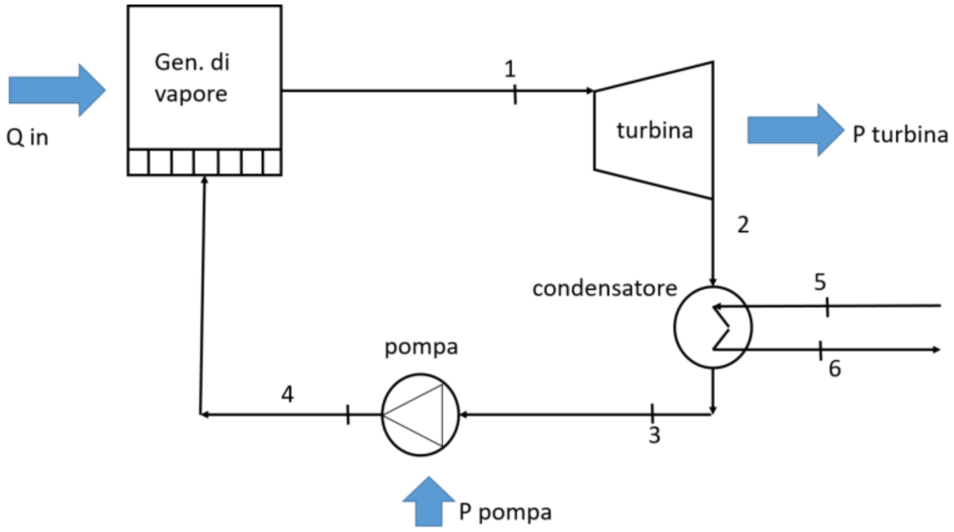


DESIGN SPECIFICATION
Net power output



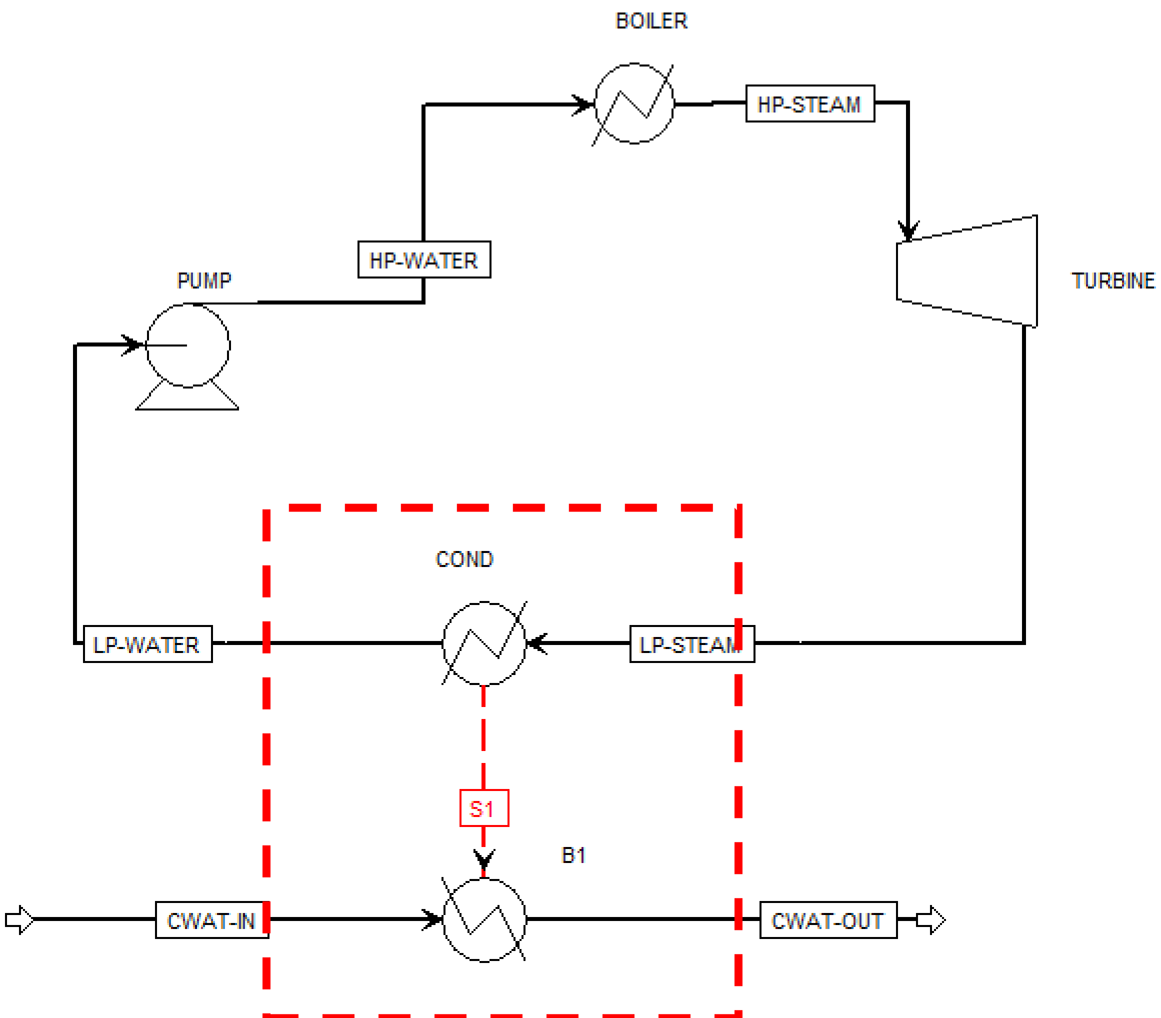
Risultati attesi (calcolati con EES, Engineering Equation Solver)

	1 h_i [kJ/kg]	2 p_i	3 s_i [kJ/kg-K]	4 T_i [C]	5 x_i	6 $h_{is;i}$ [kJ/kg]	7 $s_{is;i}$ [kJ/kg-K]
[1]	2758	80	5,743	295	1		
[2]	1939	0,08	6,202	41,49	0,7348	1794	5,743
[3]	173,7	0,08	0,5921	41,49	0		
[4]	183,2	80	0,5967	42,07		181,8	0,5921

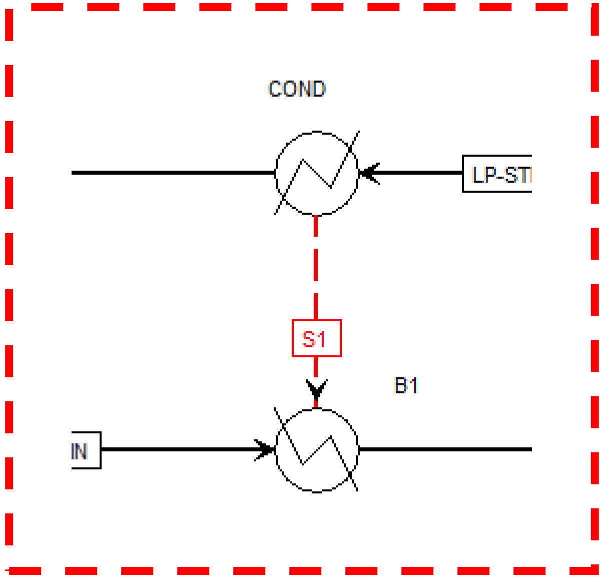


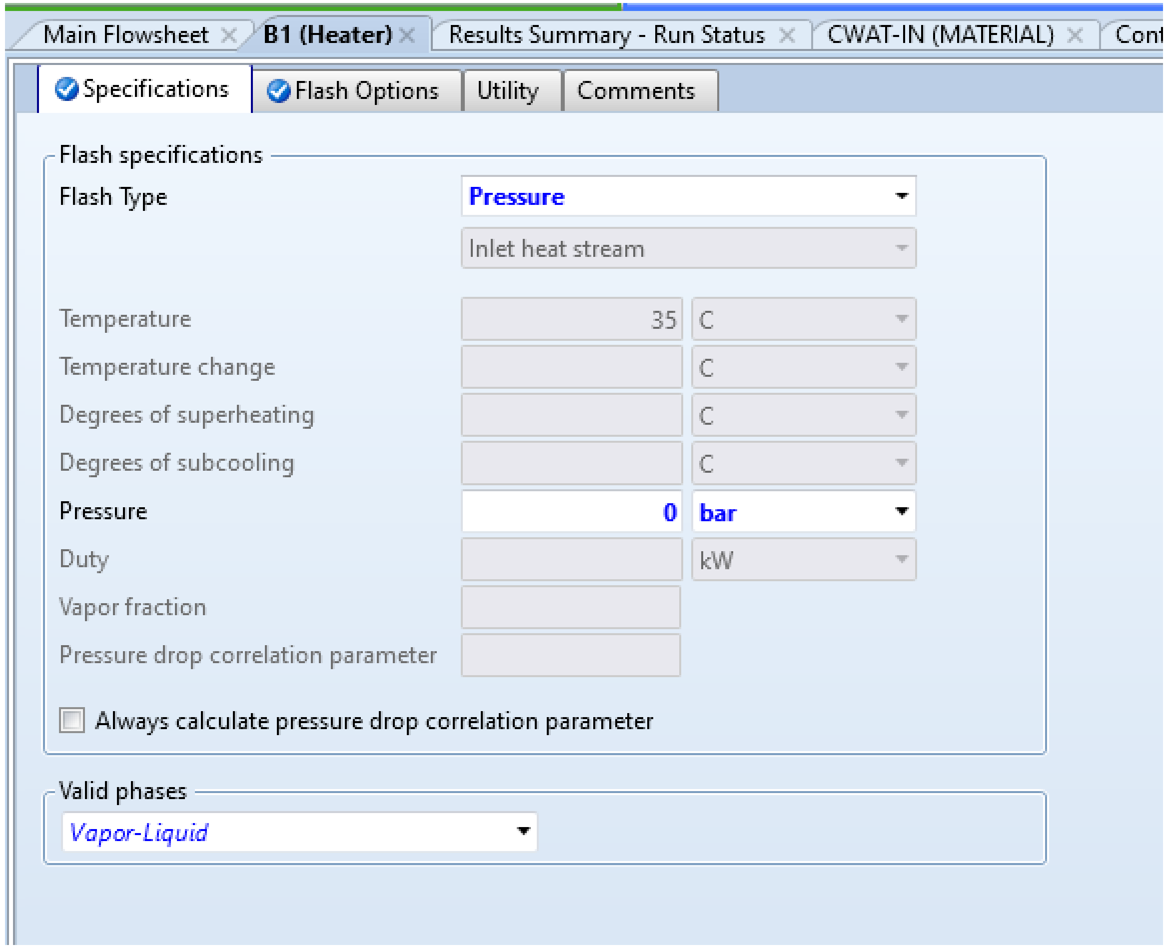
BKP SLIDES

DESIGN SPECIFICATION
Cooling water flow rate



Condenser cold side block definition

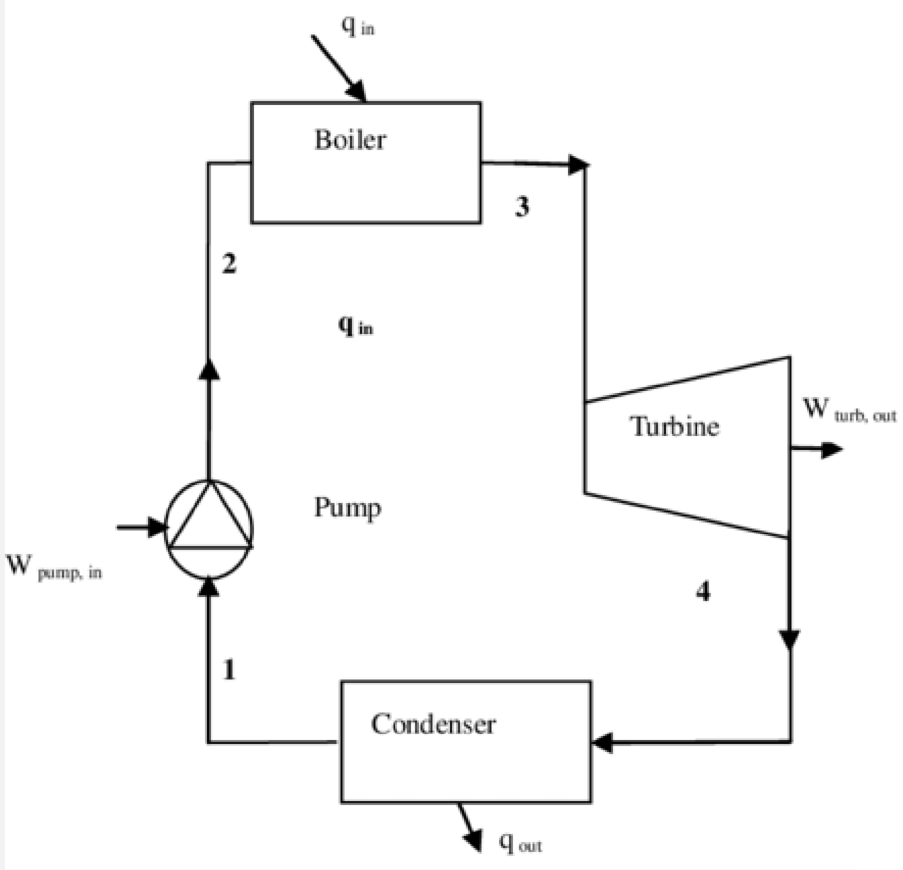




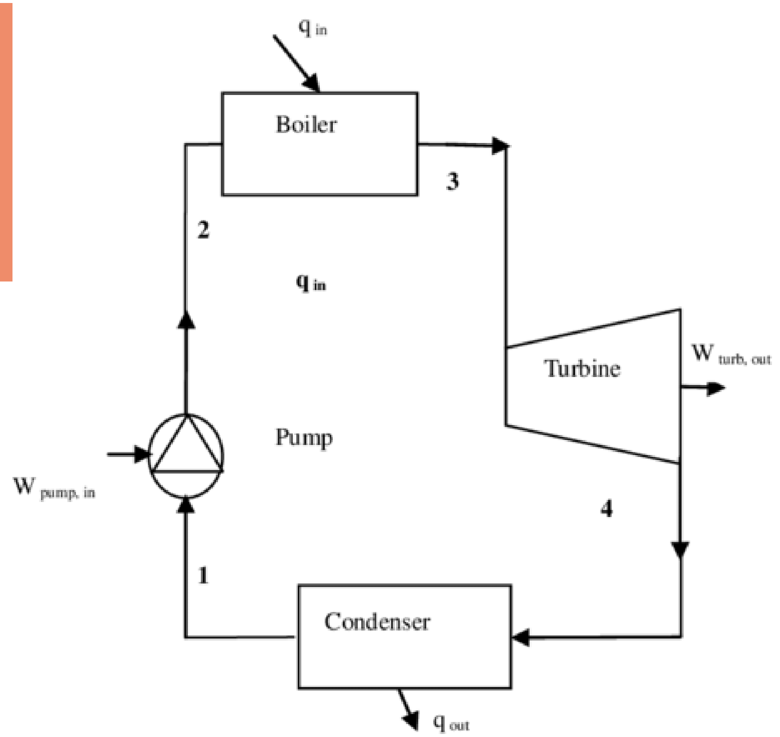
Process simulation example with Aspen Plus: Rankine cycle

Rankine cycle data and aim

- Data
  - 1 kg/s water
  - 600 °C steam temperature @ 3 MPa
  - Turbine discharge pressure @ 101325 Pa
  - Condenser @ 100 °C liquid phase
- Aim
  - Heat required
  - Work produced



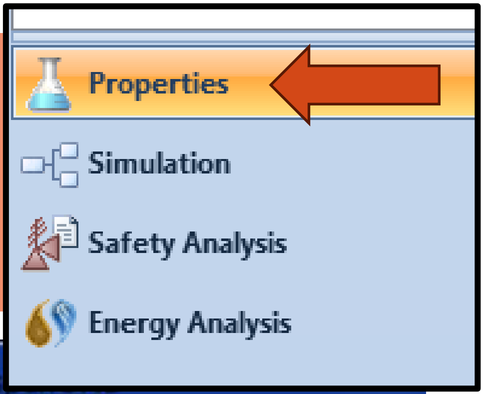
Rankine cycle

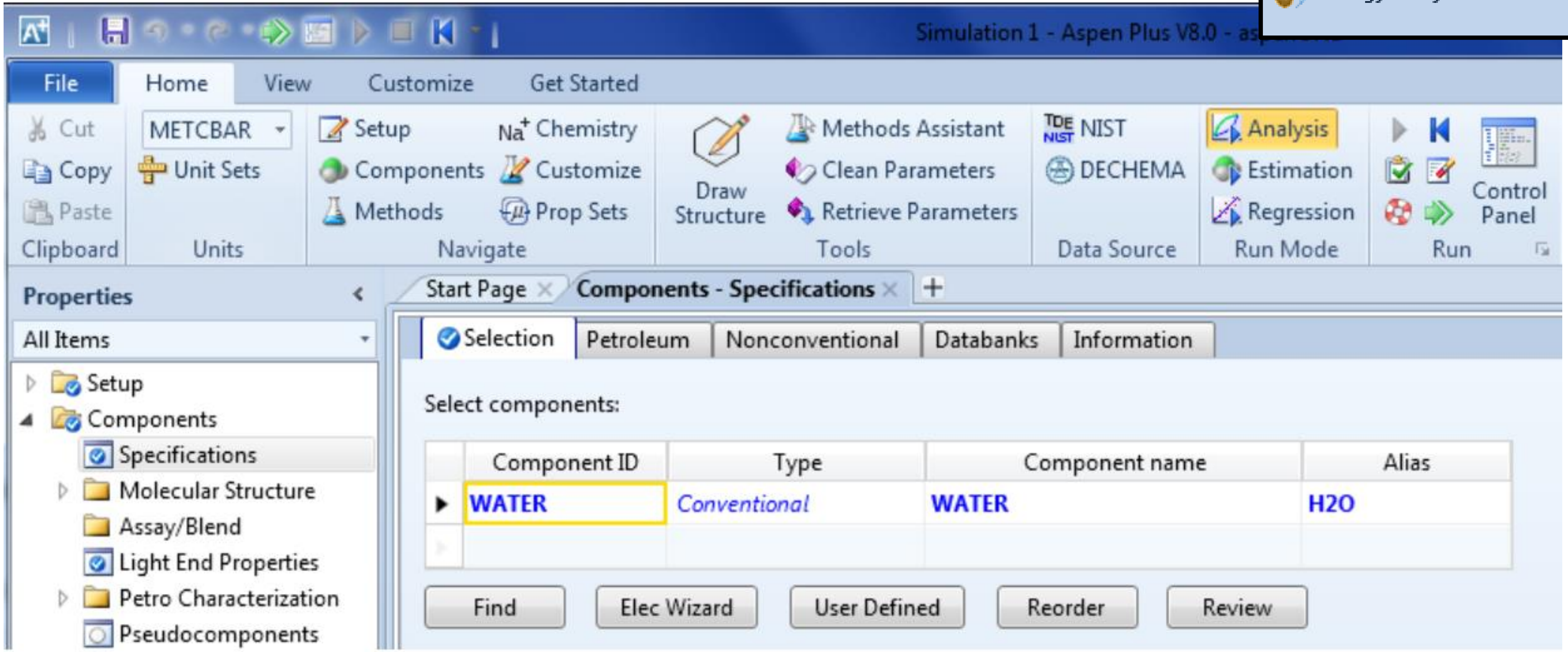


A steam engine consists of the following steps:

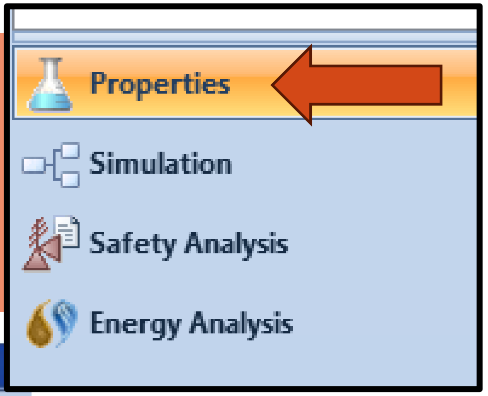
- Water is pumped into a boiler using a pump.
- Water is vaporized in a boiler and becomes high temperature and pressure steam.
- Steam flows through a turbine and does work. The pressure and temperature go down during this step. The steam is also partially condensed.
- The steam is further cooled to be condensed completely. Then, it is fed to the pump mentioned in the first step to be re-used.

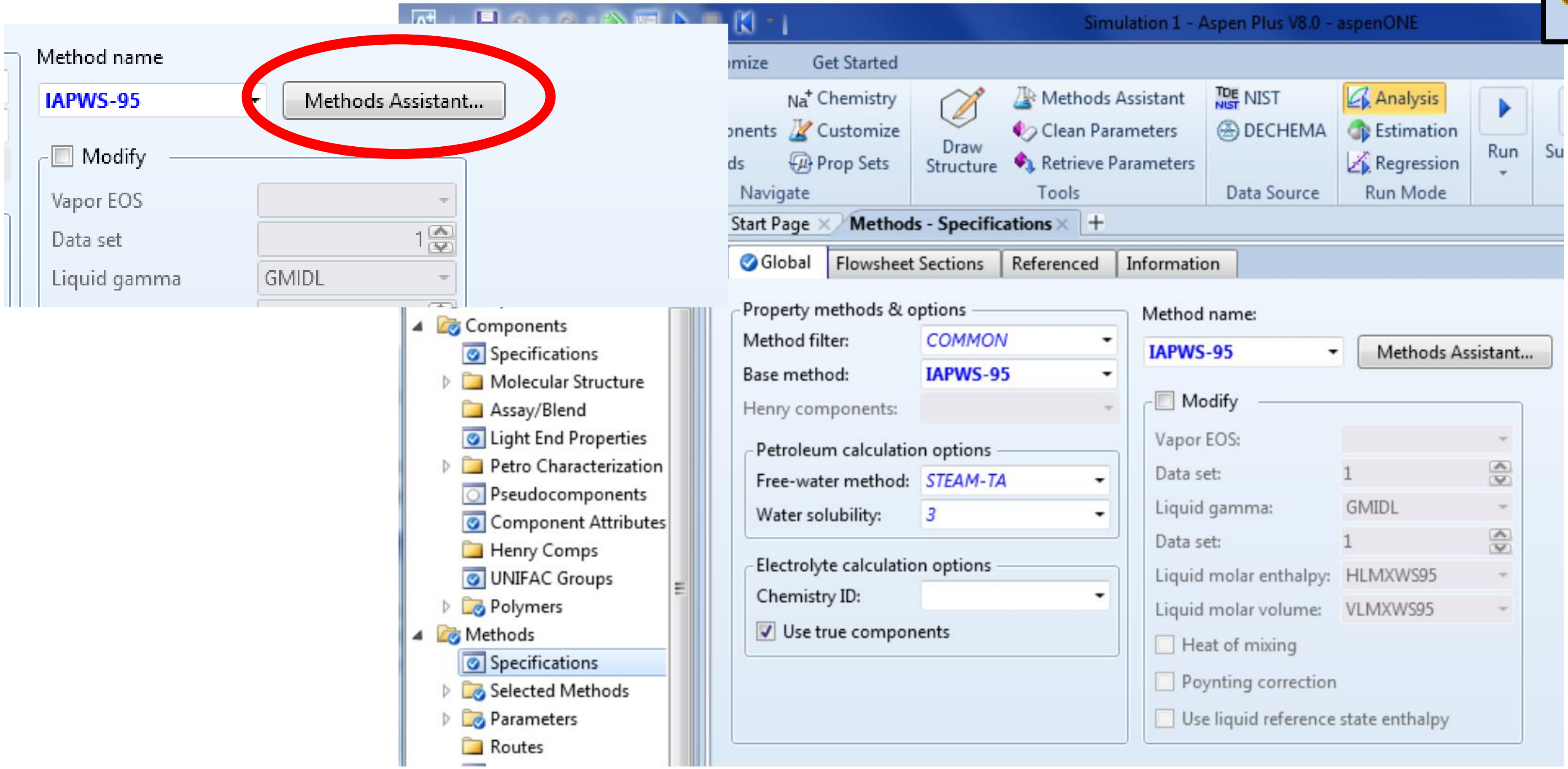
Components


Properties
Simulation
Safety Analysis
Energy Analysis


Simulation 1 - Aspen Plus V8.0
File
Home
View
Customize
Get Started
Cut
Copy
Paste
Clipboard
METCBAR
Unit Sets
Units
Setup
Components
Methods
Chemistry
Customize
Prop Sets
Navigate
Draw Structure
Methods Assistant
Clean Parameters
Retrieve Parameters
Tools
NIST
DECHEMA
Data Source
Analysis
Estimation
Regression
Run Mode
Control Panel
Run
Properties
All Items
Setup
Components
Specifications
Molecular Structure
Assay/Blend
Light End Properties
Petro Characterization
Pseudocomponents
Start Page
Components - Specifications
Selection
Petroleum
Nonconventional
Databanks
Information
Select components:
Component ID
Type
Component name
Alias
WATER
Conventional
WATER
H2O
Find
Elec Wizard
User Defined
Reorder
Review

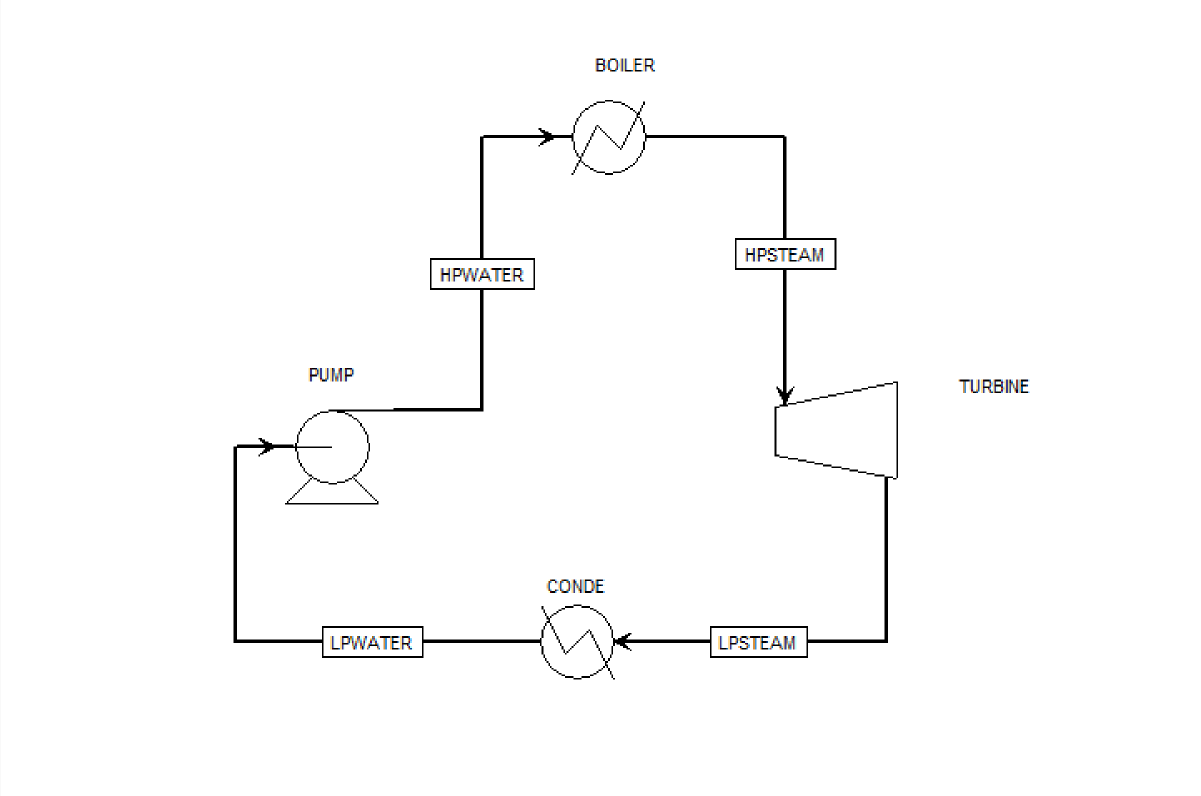
Method



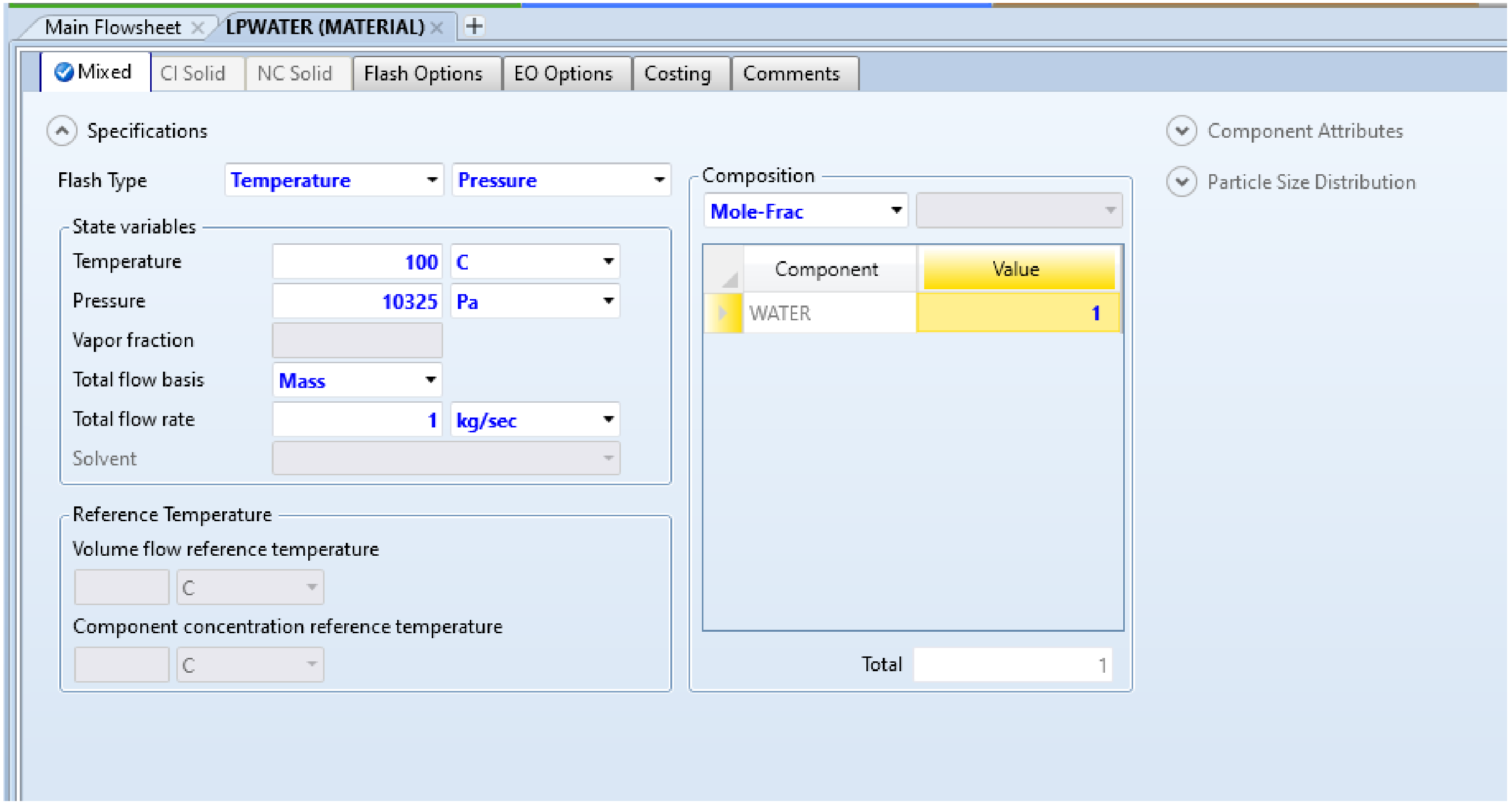


IAPWS: International Association for the Properties of Water and Steam

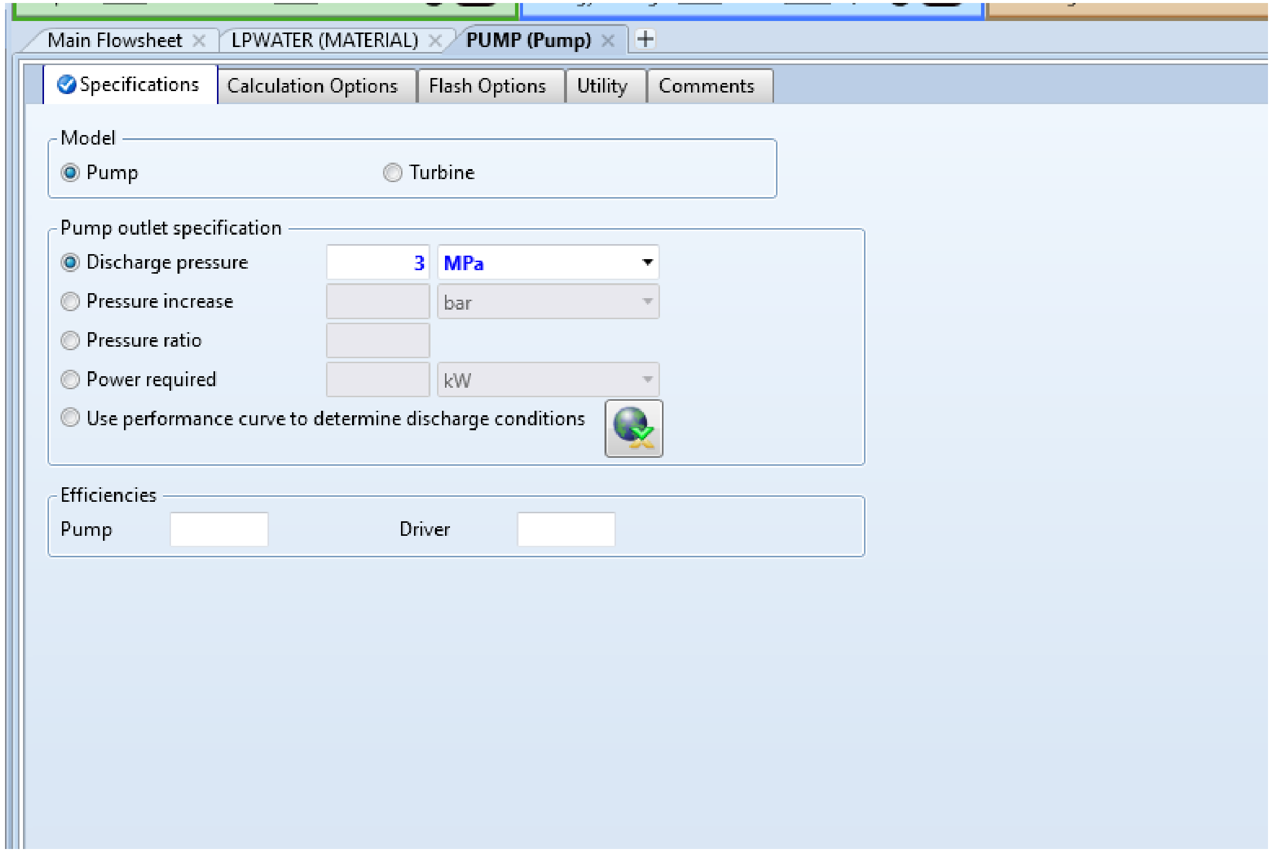
Flowsheet definition



LPWATER

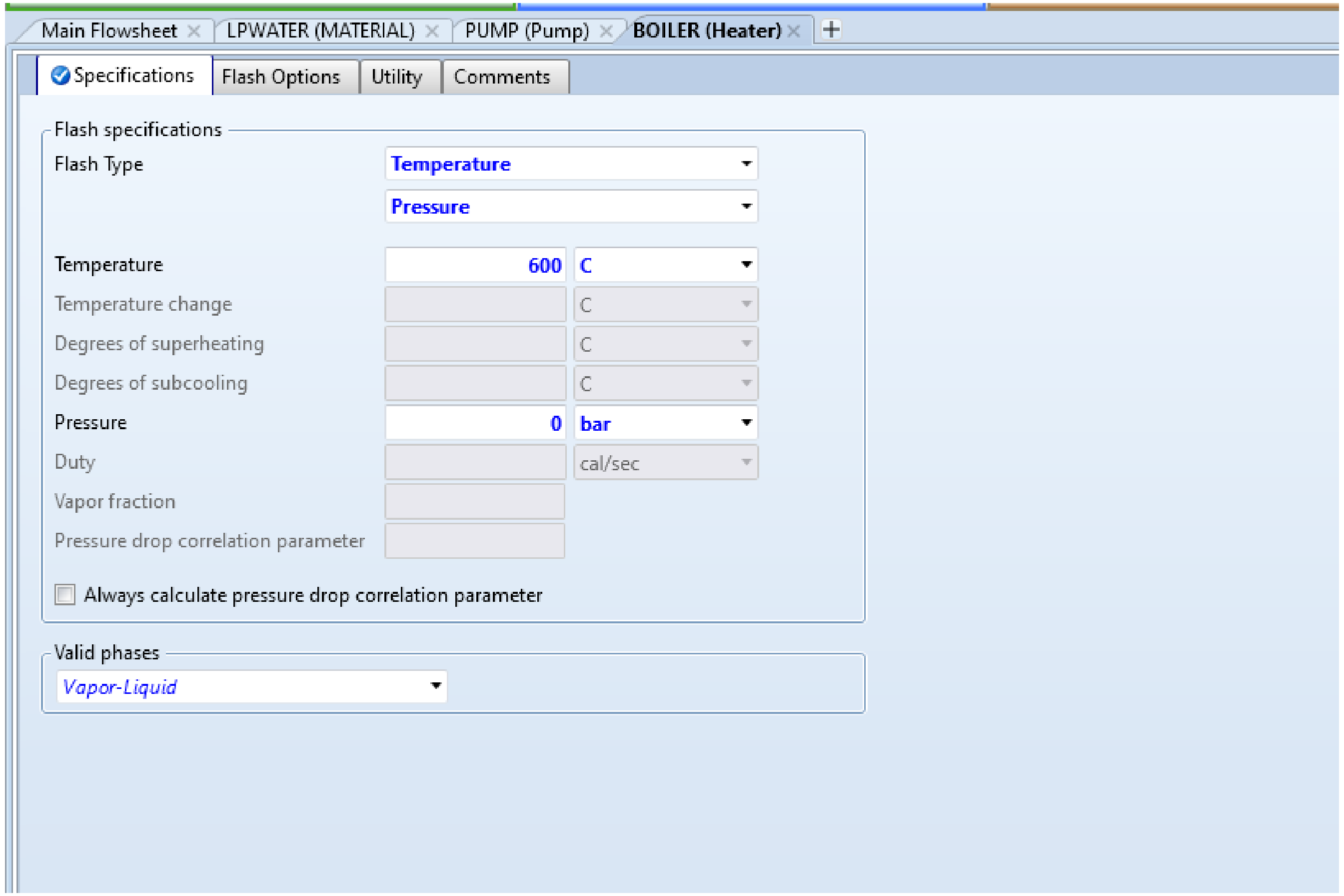

Main Flowsheet
LPWATER (MATERIAL)
Mixed
CI Solid
NC Solid
Flash Options
EO Options
Costing
Comments
Specifications
Flash Type
Temperature
Pressure
State variables
Temperature
100
C
Pressure
10325
Pa
Vapor fraction
Total flow basis
Mass
Total flow rate
1
kg/sec
Solvent
Reference Temperature
Volume flow reference temperature
C
Component concentration reference temperature
C
Composition
Mole-Frac
Component
Value
WATER
1
Total
1
Component Attributes
Particle Size Distribution

PUMPè



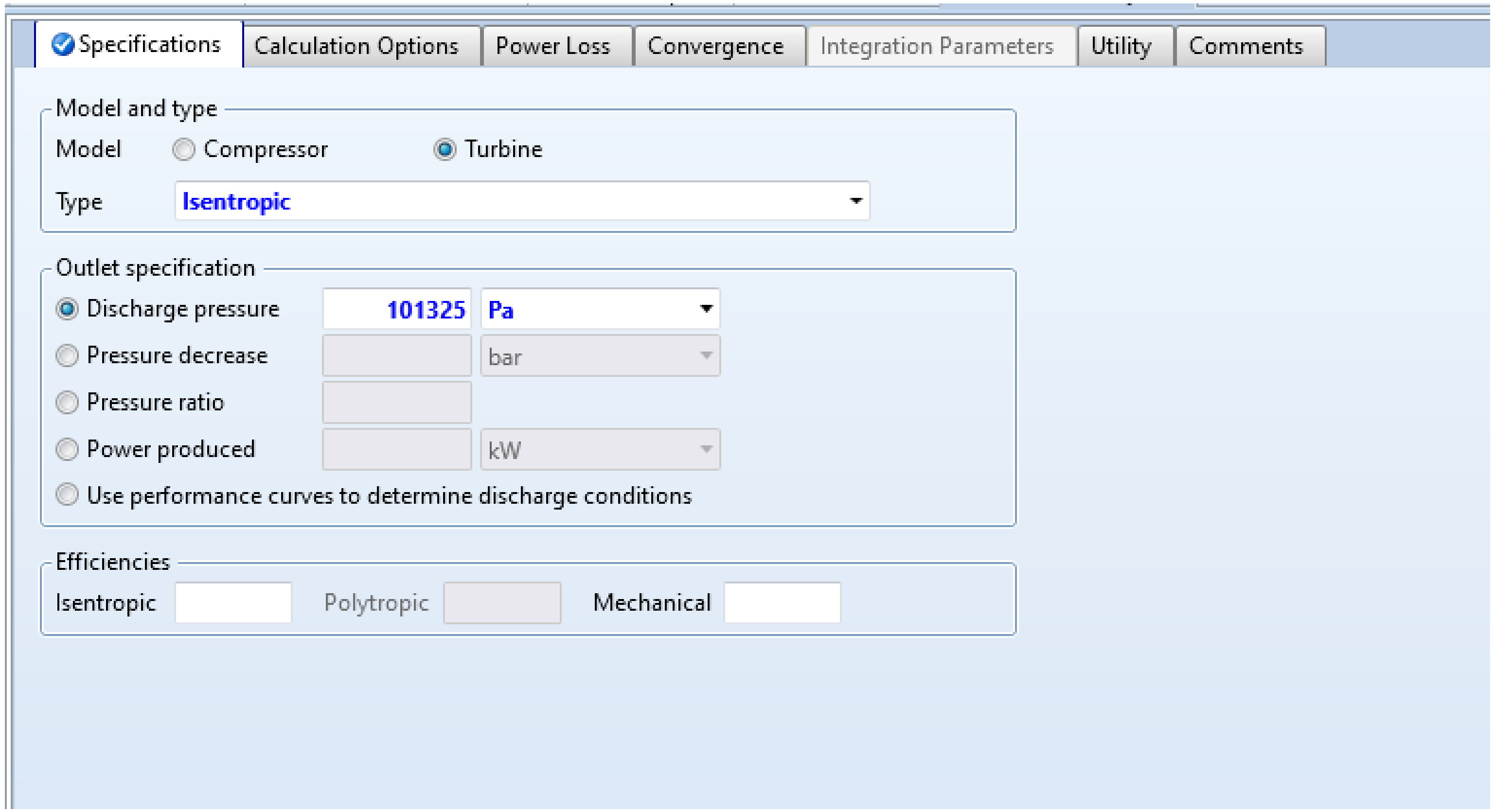
Main Flowsheet
LPWATER (MATERIAL)
PUMP (Pump)
Specifications
Calculation Options
Flash Options
Utility
Comments
Model
Pump
Turbine
Pump outlet specification
Discharge pressure
3
MPa
Pressure increase
bar
Pressure ratio
Power required
kW
Use performance curve to determine discharge conditions
Efficiencies
Pump
Driver

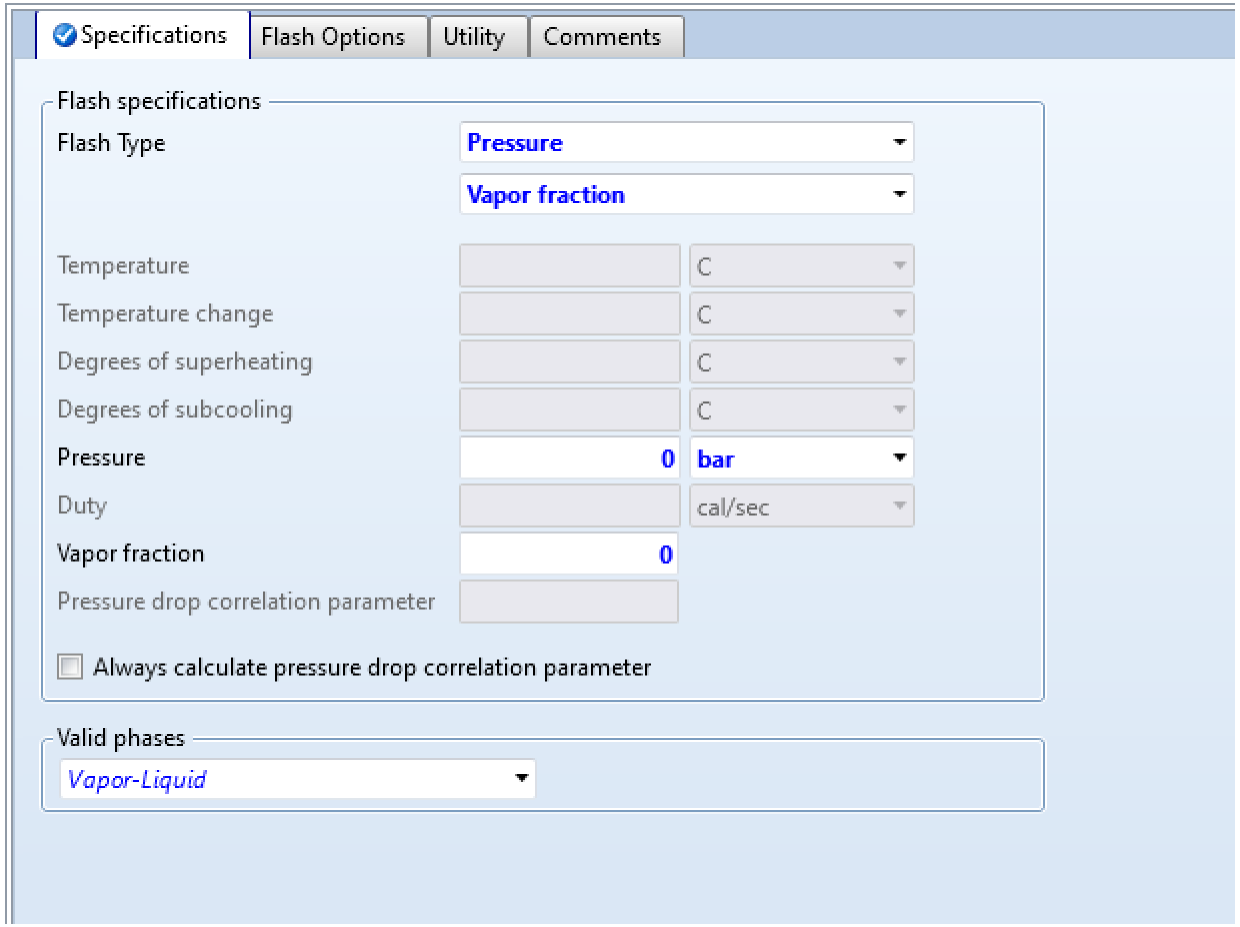
BPOILER

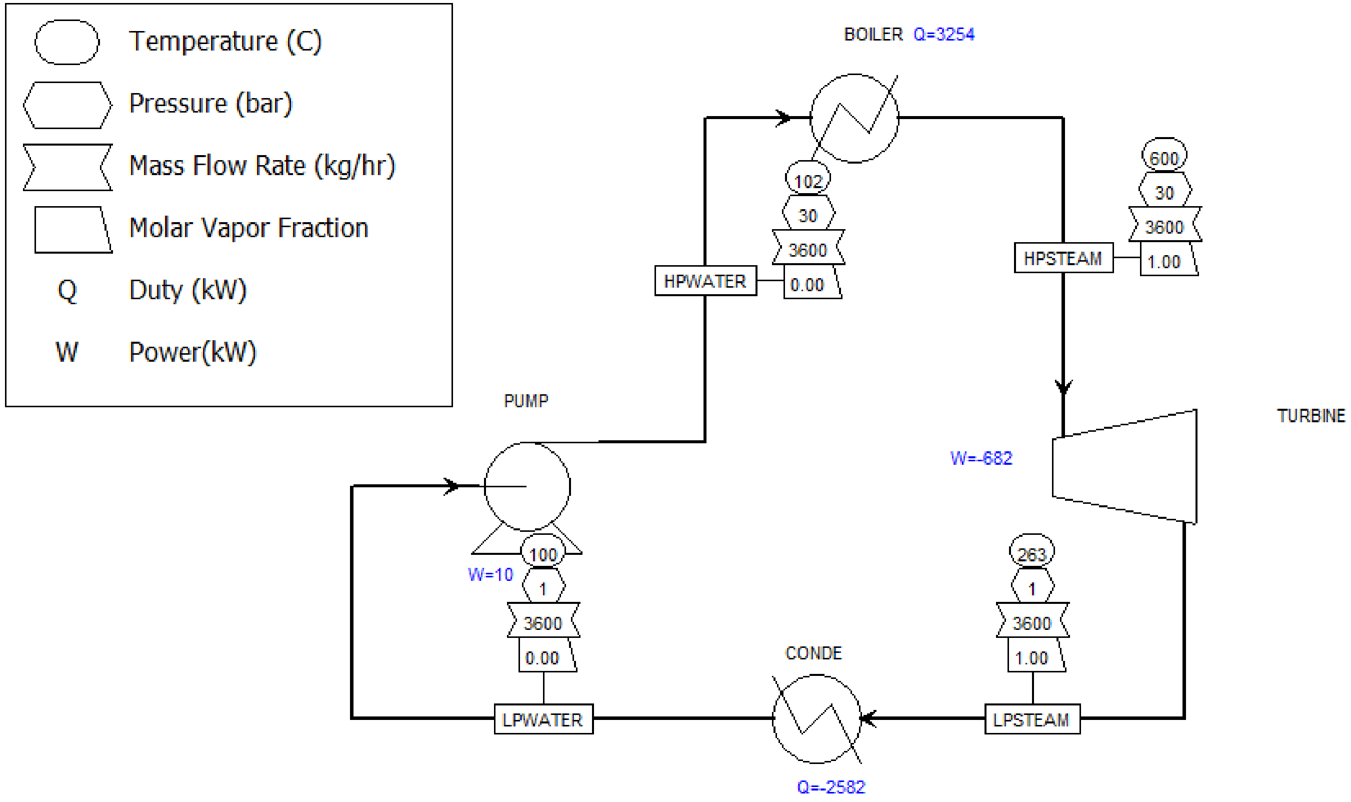


Main Flowsheet
LPWATER (MATERIAL)
PUMP (Pump)
BOILER (Heater)
Specifications
Flash Options
Utility
Comments
Flash specifications
Flash Type
Temperature
Pressure
Temperature
600
C
Temperature change
C
Degrees of superheating
C
Degrees of subcooling
C
Pressure
0
bar
Duty
cal/sec
Vapor fraction
Pressure drop correlation parameter
Always calculate pressure drop correlation parameter
Valid phases
Vapor-Liquid

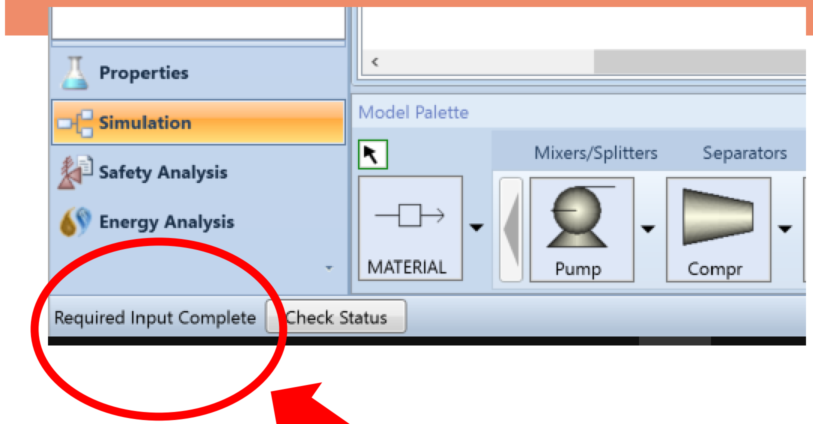
TURBINE

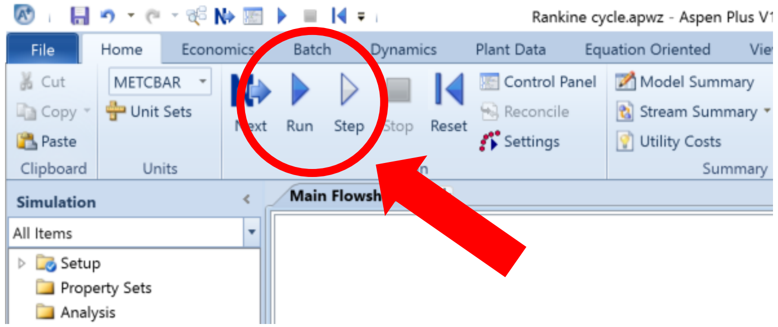

Specifications
Calculation Options
Power Loss
Convergence
Integration Parameters
Utility
Comments
Model and type
Model
Compressor
Turbine
Type
Isentropic
Outlet specification
Discharge pressure
101325
Pa
Pressure decrease
bar
Pressure ratio
Power produced
kW
Use performance curves to determine discharge conditions
Efficiencies
Isentropic
Polytropic
Mechanical

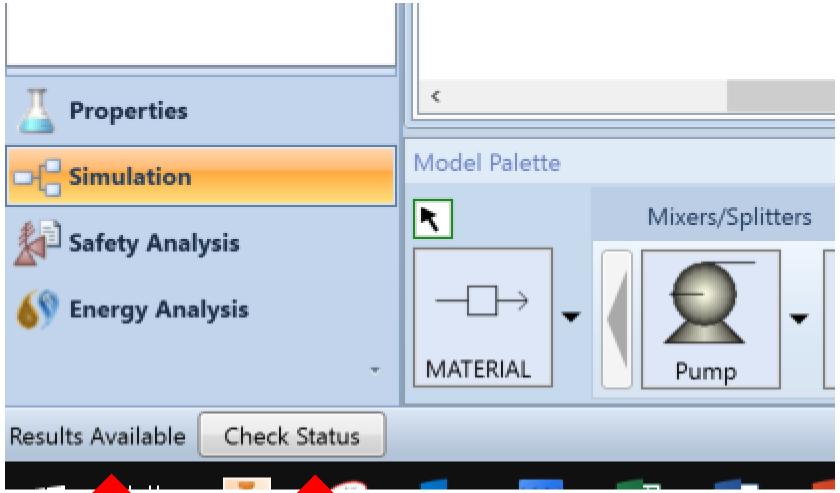

Specifications
Flash Options
Utility
Comments
Flash specifications
Flash Type
Pressure
Vapor fraction
Temperature
C
Temperature change
C
Degrees of superheating
C
Degrees of subcooling
C
Pressure
0
bar
Duty
cal/sec
Vapor fraction
0
Pressure drop correlation parameter
Always calculate pressure drop correlation parameter
Valid phases
Vapor-Liquid


Temperature (C)
Pressure (bar)
Mass Flow Rate (kg/hr)
Molar Vapor Fraction
Q Duty (kW)
W Power(kW)
BOILER Q=3254
102
30
3600
0.00
HPWATER
600
30
3600
1.00
HPSTEAM
PUMP
TURBINE
W=-682
100
1
3600
0.00
W=10
LPWATER
CONDE
Q=-2582
263
1
3600
1.00
LPSTEAM

Run the simulation







Warnings – Errors check

Stream result summary

Main Flowsheet | LPWATER (MATERIAL) | PUMP (Pump) | BOILER (Heater) | TURBINE (Compr) | CONDE (Heater) | Unit Sets - METCBAR | Results Sum

Material | Heat | Load | Work | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids

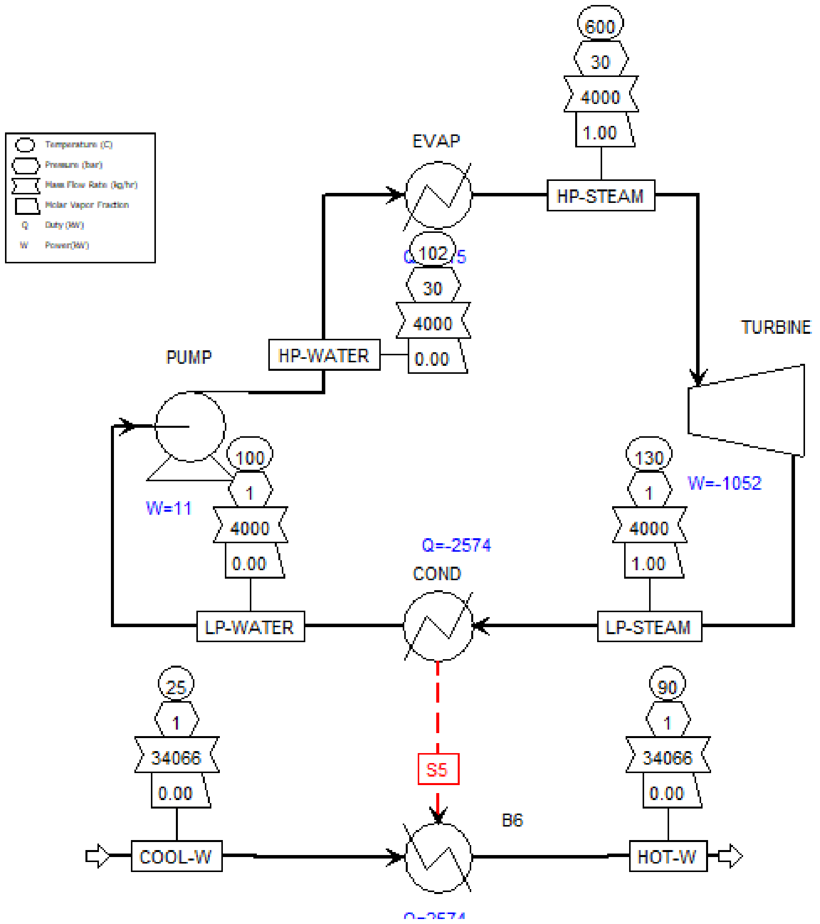
	Units	HPSTEAM	HPWATER	LPSTEAM	LPWATER
Description					
From		BOILER	PUMP	TURBINE	CONDE
To		TURBINE	BOILER	CONDE	PUMP
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN
Maximum Relative Error					
Cost Flow	$/hr				
− MIXED Substream					
Phase		Vapor Phase	Liquid Phase	Vapor Phase	Liquid Phase
Temperature	C	600	101.887	263.353	99.9743
Pressure	bar	30	30	1.01325	1.01325
Molar Vapor Fraction		1	0	1	0
Molar Liquid Fraction		0	1	0	1
Molar Solid Fraction		0	0	0	0
Mass Vapor Fraction		1	0	1	0
Mass Liquid Fraction		0	1	0	1
Mass Solid Fraction		0	0	0	0
Molar Enthalpy	cal/mol	-52874.1	-66873.7	-55807.6	-66917.7
Mass Enthalpy	cal/gm	-2934.96	-3712.05	-3097.79	-3714.5
Molar Entropy	cal/mol-K	-8.25163	-34.861	-5.80591	-34.9438
Mass Entropy	cal/gm-K	-0.458035	-1.93508	-0.322277	-1.93968
Molar Density	mol/cc	0.000419103	0.0531964	2.27868e-05	0.0531975
Mass Density	gm/cc	0.00755026	0.958348	0.00041051	0.958368
Enthalpy Flow	kW	-12288.1	-15541.6	-12969.8	-15551.9

Model Palette

Link to Excel: calculator

Aim:

Calculated cycle efficiency value

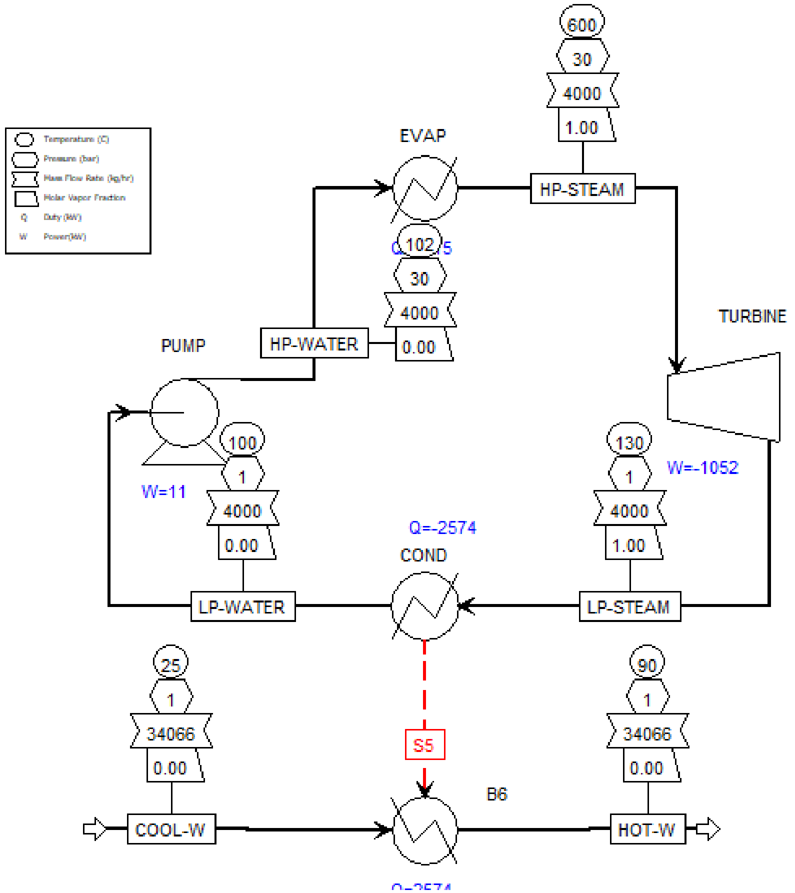


Design specification:
calculate water flow rate at condenser

Aim:

Calculate the cooling water flow rate to the condenser.

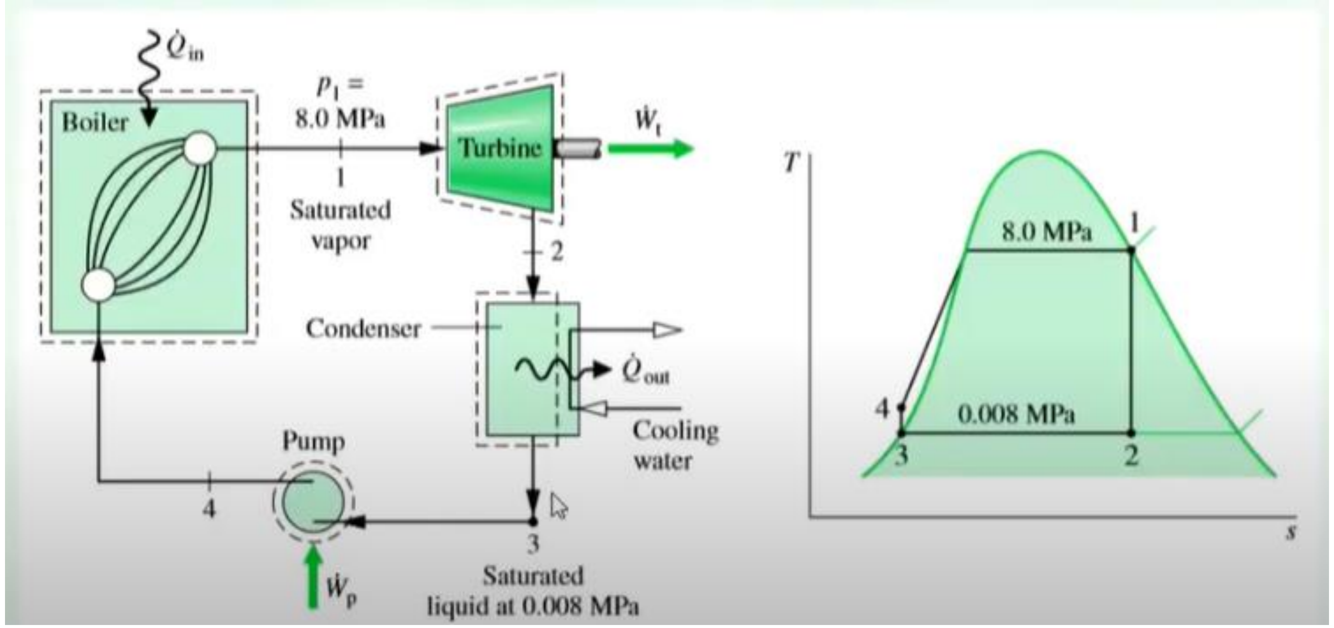
Exit water at condenser should be for example 40 °C



Exercise

EXAMPLE 8.1 Ideal Rankine Cycle

Steam is the working fluid in an ideal Rankine cycle. Saturated vapor enters the turbine at 8.0 MPa and saturated liquid exits the condenser at a pressure of 0.008 MPa. The *net* power output of the cycle is 100 MW. Determine for the cycle (a) the thermal efficiency, (b) the back work ratio, (c) the mass flow rate of the steam, in kg/h, (d) the rate of heat transfer, $\dot{Q}_{in}$, into the working fluid as it passes through the boiler, in MW, (e) the rate of heat transfer, $\dot{Q}_{out}$, from the condensing steam as it passes through the condenser, in MW, (f) the mass flow rate of the condenser cooling water, in kg/h, if cooling water enters the condenser at 15°C and exits at 35°C.



Thermodynamic and transport component property analysis

It is possible to use Aspen Plus to retrieve thermodynamic component properties

Tutorials:

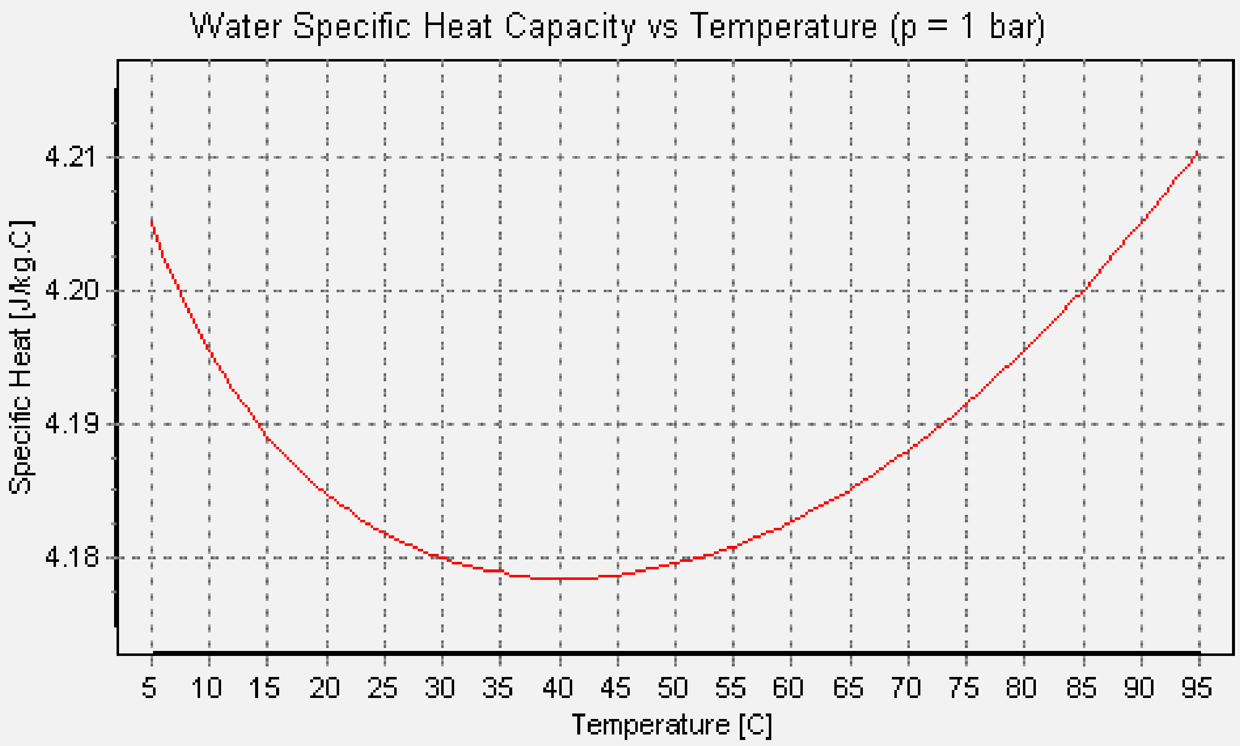
- find the *specific heat capacity (CP-M mass constant pressure heat capacity)* variation with temperature for water between 20 and 95°C using the properties tool
- find the *viscosity (CP-M mass constant pressure heat capacity)* variation with temperature for water between 20 and 95°C using the properties tool

For water → IAPWS-95 method

(International Association for the Properties of Water and Steam)

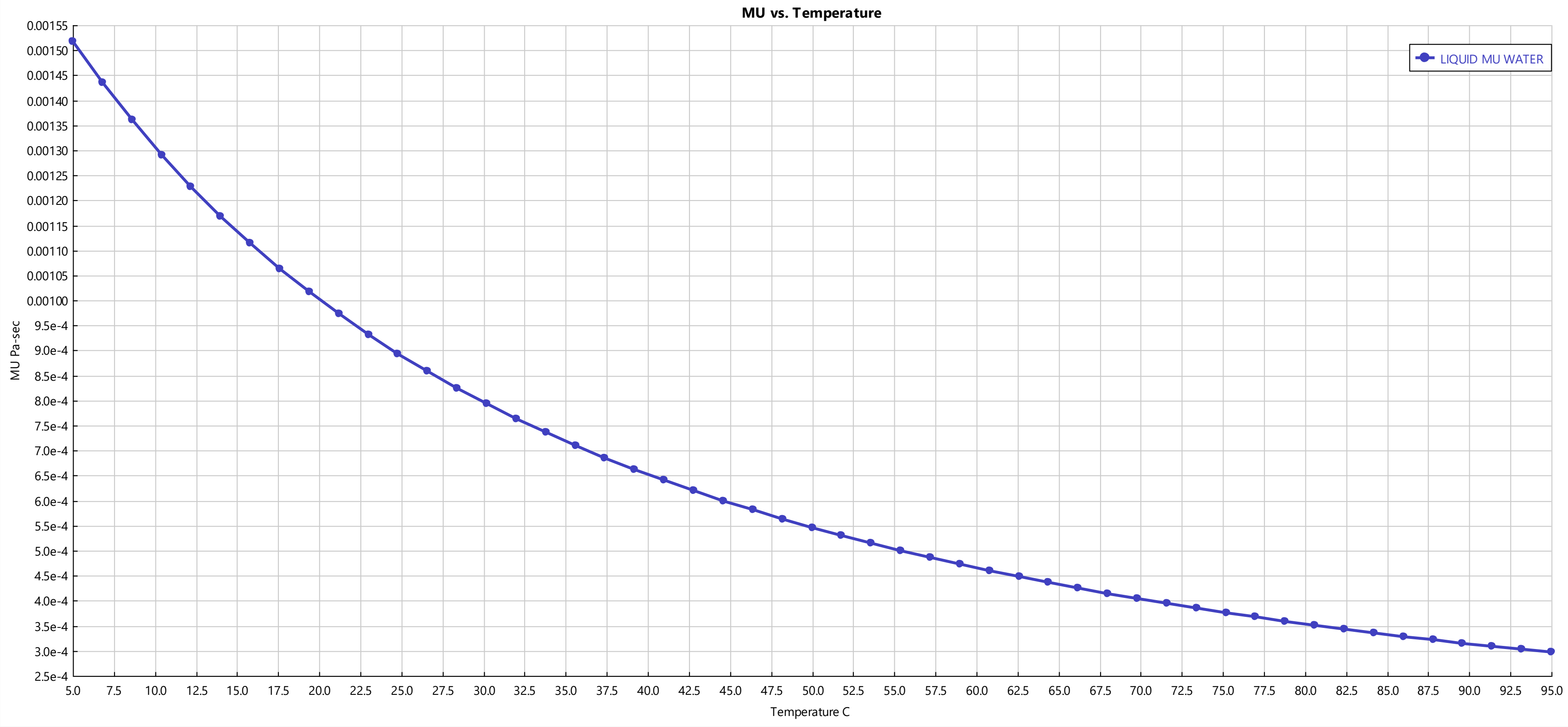
Thermodynamic and transport component property analysis

- Water c_p variation , 5 ÷ 95 °C result



Thermodynamic and transport component property analysis

- Water viscosity, 5 ÷ 95 °C result



Blk slides

Analisi del ciclo reale

Condizioni ambientali	
Temperatura e umidità relativa ambiente	15°C, 60%
Pressione ambiente	101325 Pa
Compressore	
Δp filtro aspirazione	1 kPa
Δh_{is} per ogni stadio	27 kJ/kg
Massa trafilamenti allo scarico compressore	0.8%
Rendimento politropico	
SP < 1: $\eta_p = 0.895 \cdot [1 - 0.07108 \cdot \log_{10}^2 (SP)]$	
SP ≥ 1: $\eta_p = 0.895$	
Rendimento organico	99.7%
Combustore	
Combustibile: gas naturale (93% CH_4 - LHV=44.14 MJ/kg)	
Temperatura combustibile	15°C
Pressione combustibile	30 bar
$\Delta p/p$ combustibile (min.)	33%
$\Delta p/p$ aria	3%
Perdite termiche (% del calore sviluppato)	0.4%
Temp.totale ingresso 1°rotore (TIT)	1280°C
Turbina	
Δh_{is}, stadi raffreddati	300 kJ/kg
Δh_{is}, stadi non raffreddati	100 kJ/kg
Rendimenti politropici	
SP < 1: $\eta_p = \eta_{p,\infty} \cdot [1 - 0.02688 \cdot \log_{10}^2 (SP)]$	
SP ≥ 1: $\eta_p = \eta_{p,\infty}$	
$\eta_{p,\infty}$: 0.89 (stadi raffr.), 0.925 (stadi non raffr.)	
Rendimento politropico 1°ugello	0.95
Rendimento organico	0.997
Temperatura massima palettature 1°ugello	830°C
Temperatura massima pale di altre schiere	800°C
$\Delta p/p$ medio refrigerante	40%
Numero di Mach assiale allo scarico	0.45
Rendimento del diffusore	0.50
Δp scarico	1 kPa
Generatore elettrico	
Rendimento:	vedi fig.2.15

Il parametro SP usato nella valutazione di η_p è definito come $V^{0.5}/\Delta h_{is}^{0.25}$, dove V è la portata volumetrica all'uscita per gli stadi di turbina e la portata volumetrica media per il compressore.

Tab.3.1: *Esempio di assunzioni necessarie per il calcolo di una moderna turbina a gas. Questi valori saranno utilizzati nello sviluppo degli esempi del presente testo, quando non specificato diversamente.*

Ciclo reale

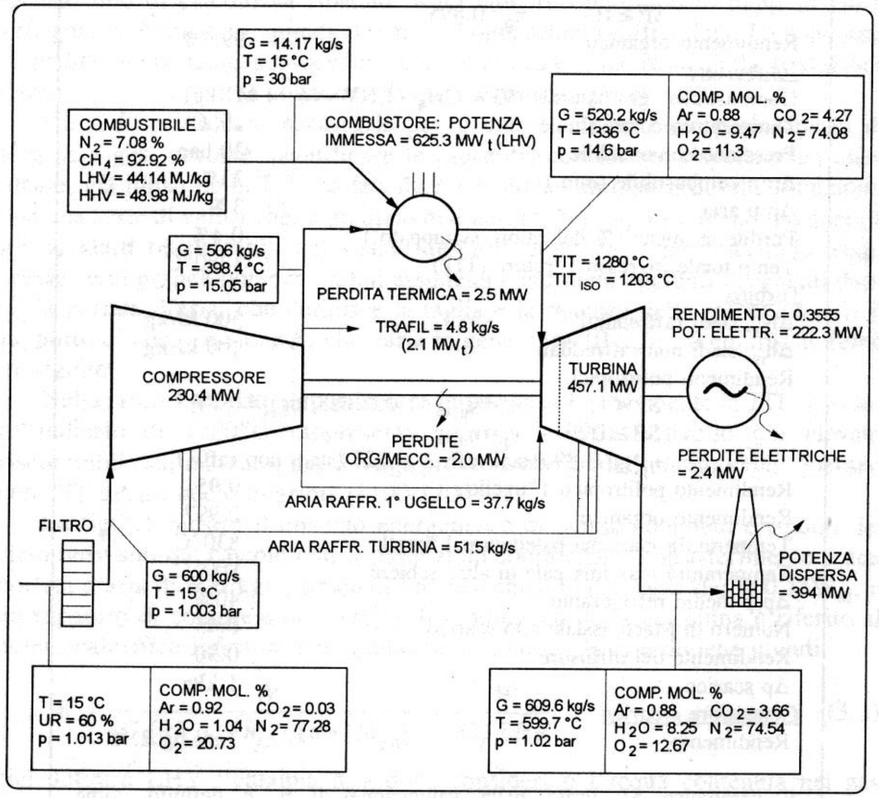


Fig.3.1: *Bilancio termico completo di una turbina a gas in ciclo semplice con β=15, TIT=1280°C, portata aria 600 kg/s. Assunzioni di calcolo da Tab.3.1.*