

## PROSIMPLUS APPLICATION EXAMPLE

### CO<sub>2</sub> REFRIGERATION CYCLES

#### EXAMPLE PURPOSE

This example presents the simulation of refrigeration machines with transcritical CO<sub>2</sub>. Two transcritical cycles are presented, a simple cycle and a two-stage cycle. The cycles allow to provide temperatures below 0°C.

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CORRESPONDING PROSIMPLUS FILES	<p>PSPS_EX_EN-CO2-Refrigeration-Single-Stage.pmp3</p> <p>PSPS_EX_EN-CO2-Refrigeration-Two-Stages.pmp3</p>
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*Reader is reminded that this use case is only an example and should not be used for other purposes. Although this example is based on actual case it may not be considered as typical nor are the data used always the most accurate available. Fives ProSim shall have no responsibility or liability for damages arising out of or related to the use of the results of calculations based on this example.*

#### Energy

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# 1. PROCESS MODELING

## 1.1. Process description

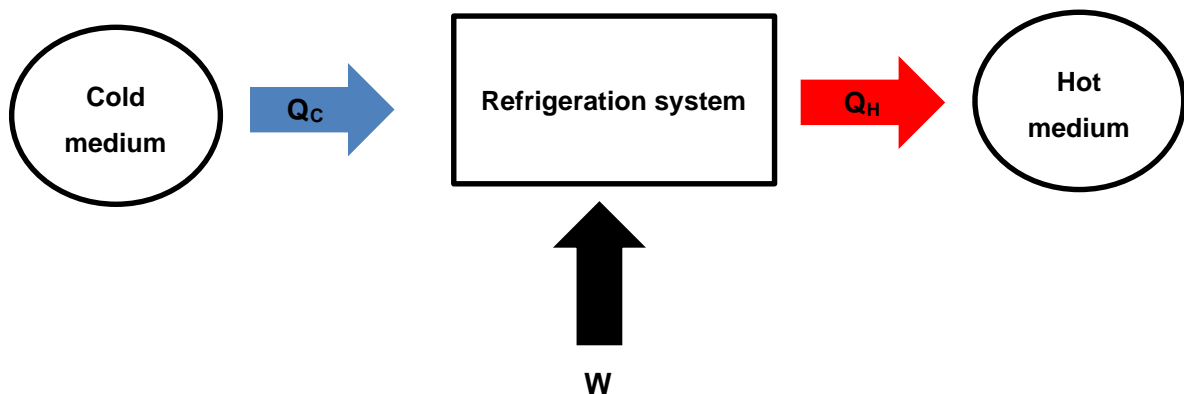
This example presents the simulations of transcritical cycles of refrigeration systems with CO<sub>2</sub>. The refrigeration system is defined as providing and maintaining temperatures below the immediate surrounding temperatures. The refrigerant extract heat from a low temperature medium and transfer it to a high temperature medium by receiving some external work (W).

Among other refrigerants, carbon dioxide (CO<sub>2</sub>) is a promising refrigerant and attracts many interests in the scientific and industrial sectors. The CO<sub>2</sub> (R744) is a very interesting fluid for a thermodynamic cycle: it is naturally available in the environment, its environmental impact is low (as opposed to CFCs and HCFCs, CO<sub>2</sub> (R744) has an Ozone Depletion Potential (ODP) of zero and a negligible Global Warming Potential (GWP)), it has a low density, it is non-corrosive, non-flammable, non-toxic, non-explosive and is miscible with some compressor oils. Because of its thermodynamic properties, especially its low critical temperature (31°C), for refrigeration purpose, CO<sub>2</sub> has to be employed in a transcritical cycle. This implies a supercritical regime in the operation where only gas cooling (*i.e.* no condensation) is possible.

In this example, two transcritical cycles are presented: a simple cycle (one stage) and a two-stages cycle. The simulation diagrams in paragraph 1.2 illustrate the process flowsheet of these two cycles.

The first transcritical cycle contains the following equipment: a compressor, a gas cooler, an expander and an evaporator. The two-stages cycle contains supplementary compressor and evaporator that work at a pressure lower than the critical pressure (subcritical pressure). However, there is a multitude of configurations for the two-stages cycles.

The simple cycle presented in this example can provide a temperature of  $\approx 0^{\circ}\text{C}$  ( $\approx 31.5^{\circ}\text{F}$ ) and has a COP of 2.7. The two-stages cycle is capable to distribute cold temperature of  $\approx 0^{\circ}\text{C}$  ( $\approx 31.5^{\circ}\text{F}$ ) and  $\approx -21^{\circ}\text{C}$  ( $\approx -7^{\circ}\text{F}$ ). Its COP value is 1.9.

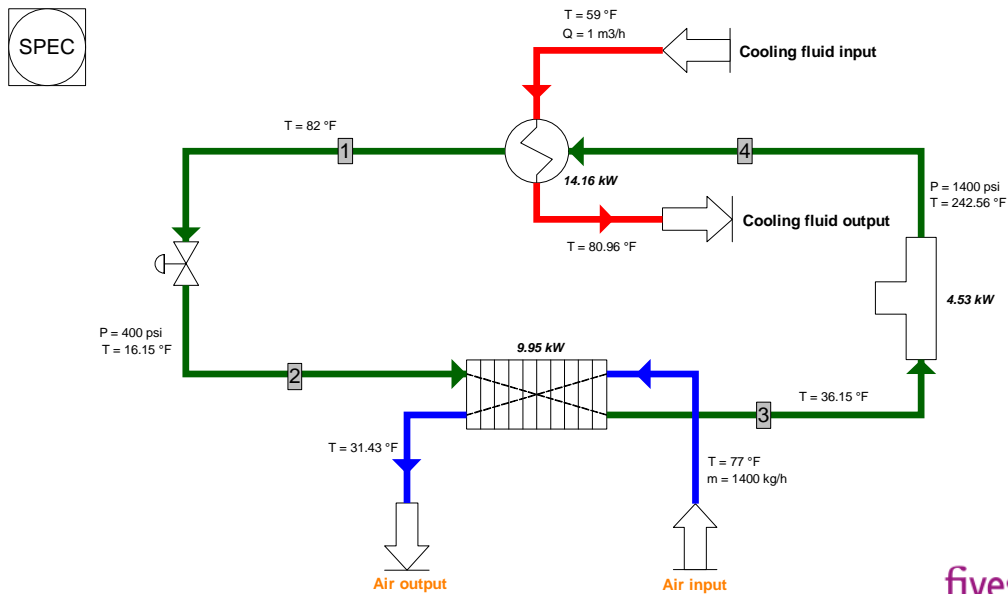


*Principle of refrigeration system*

## 1.2. Process flowsheet

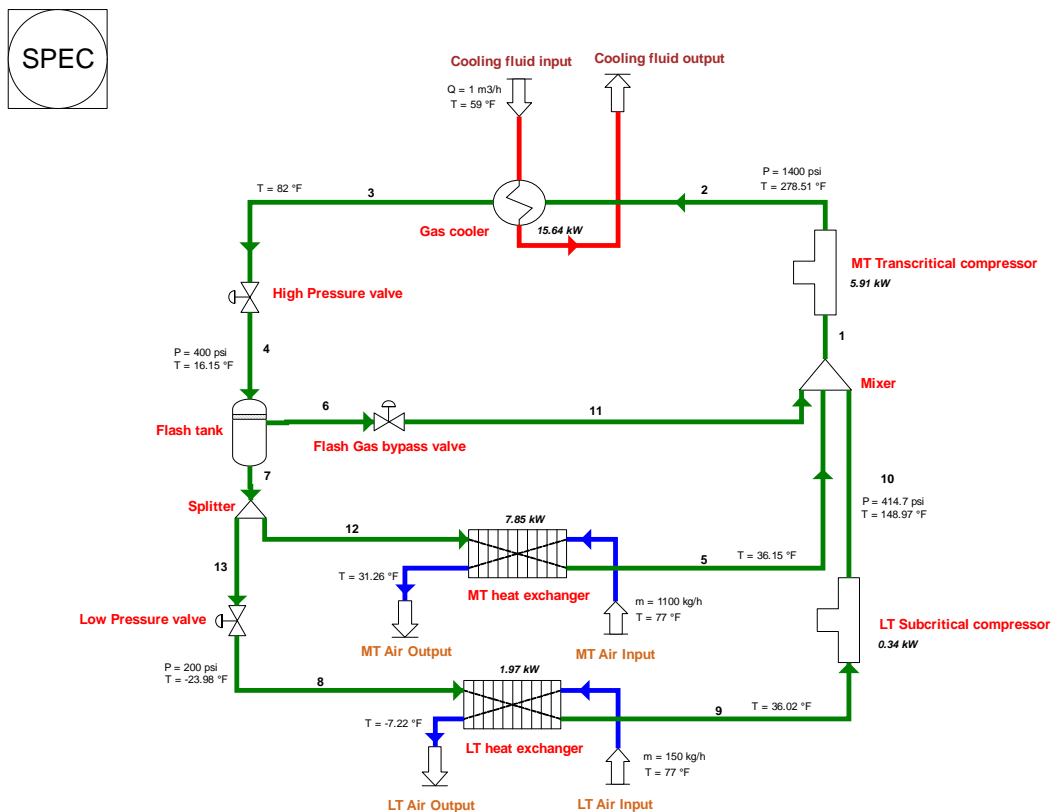
### 1.2.1 Simple cycle

This flowsheet is presented in: "PSPS\_EX\_EN-CO2-Refrigeration-Single-Stage.pmp3".



### 1.2.2. Two-stage cycle

This flowsheet is presented in: "PSPS\_EX\_EN-CO2-Refrigeration-Two-Stages.pmp3".



### 1.3. Components

The components taken into account in the simulation, their chemical formula and their CAS<sup>(\*)</sup> number are presented in the following table. Pure components physical properties are extracted from the ProSimPlus standard database [WIL19].

Component	Chemical formula	CAS number
Water	H <sub>2</sub> O	7732-18-5
Carbon dioxide	CO <sub>2</sub>	124-38-9
Oxygen	O <sub>2</sub>	7782-44-7
Nitrogen	N <sub>2</sub>	7727-37-9

### 1.4. Thermodynamic model

Three thermodynamic calculators are defined to simulate the simple cycle and the two-stage cycle of “CO<sub>2</sub> Refrigeration”:

- “Refrigerant”: this calculator only contains the carbon dioxide component. Given the nature of this compound, the thermodynamic model used to represent the phase's equilibria and the enthalpy calculations is the Soave Redlich and Kwong equation of state (SRK) [SOA72].
- “Water”: this calculator only contains the water component. Hence it uses the “pure water” thermodynamic model.
- “Air”: this calculator contains oxygen and nitrogen components. The thermodynamic model used is the “ideal” thermodynamic profile.

The thermodynamic models used are documented in the thermodynamic help accessible from the calculator definition window.

<sup>(\*)</sup>CAS Registry Numbers® are the intellectual property of the American Chemical Society and are used by ProSim SA with the express permission of ACS. CAS Registry Numbers® have not been verified by ACS and may be inaccurate

## 1.5. Operating conditions

### 1.5.1 Simple cycle

The operating conditions of the different modules in the simple cycle are the following:

✓ Process feed

Name	Cooling fluid input	Air input
Total volume flowrate (m <sup>3</sup> /h)	1	-
Total mass flowrate (kg/h)	-	1400
<b>Molar fractions:</b>		
Carbon dioxide	0	0
Water	1	0
Oxygen	0	0.21
Nitrogen	0	0.79
Temperature (°F)	59 (15°C)	77 (25°C)
Pressure (psi)	14.7 (1 atm)	14.7 (1 atm)

✓ Reciprocating compressor

Compressor type	Isentropic
Exhaust pressure (psi)	1400
Isentropic efficiency	0.8
Mechanical efficiency	0.95
Electrical efficiency	0.98
Constraints	Fixed vapor physical state

✓ Expansion valve "Thermostatic expander"

Constraint type	Pressure specification
Pressure (psi)	400

## ✓ Generalized heat exchanger "Condenser"

<b>Exchanger type</b>	Counter current or multipasses
<b>Specification type: "Hot stream"</b>	Outlet temperature
<b>Temperature (°F)</b>	82 (28°C)

Additional specifications applied on the condenser:

<b>Specification</b>	Heat exchange area calculation
<b>Clean overall heat transfer coefficient (W/m<sup>2</sup>/K)</b>	330
<b>Efficiency</b>	Pure counter current

## ✓ Plate and frame heat exchanger "Evaporator"

<b>Exchanger type</b>	Counter current or multipasses
<b>Specification type: "Cold stream"</b>	Superheated over its dew point temperature
<b>Temperature difference (°F)</b>	20

Additional specifications applied on the evaporator:

<b>Specification</b>	Heat exchange area calculation
<b>Heat transfer coefficients for 2-phase zones (W/m<sup>2</sup>/K):</b>	
<b>Liquid : Liquid</b>	500
<b>Liquid-vapor : Liquid</b>	1000
<b>Vapor : Liquid</b>	250
<b>Liquid : Liquid-vapor</b>	1000
<b>Liquid-vapor : Liquid-vapor</b>	1500
<b>Vapor : Liquid-vapor</b>	500
<b>Liquid : Vapor</b>	250
<b>Liquid-vapor : Vapor</b>	1000
<b>Vapor : Vapor</b>	100
<b>Efficiency</b>	Pure counter-current

## ✓ Constraints and recycles (SPEC)

The Constraints and recycles module is necessary in the flowsheet because the CO<sub>2</sub> is fed in loop. The parameters used in the SPEC module are presented below:

Constraints and Recycles (\$SPEC)

Name: Constraints and Recycles 1

Desc:

Identification Parameters Scripts Report Streams Notes Advanced parameters

☒ Module enabled

Numerical methods: Default

Convergence criterion: Criterion: 1E-8

Stop Test

Non evolution of criterion: 1E-7

Non evolution of variables: 1E-6

Maximum number of passages in the MCN: 100

Maximum number of iterations: 20

Print

Print every: 10 iterations

Tear streams iterative variables

☒ Enthalpies

☐ Pressures

Resume

☐ Use of values obtained at convergence of the previous problem

Damping strategy

Initial damping factor: 1

Sensitivity analysis

Step size of the recycle streams variables proportional to...: the difference between 2 itera

Proportionality factor: 0.1

Step size of the adjusted variables proportional to...: the difference between 2 itera

Proportionality factor: 0.1

Constraints: Parameters...

Tear streams: Parameters...

OK Cancel

The refrigeration cycle is composed of pure component (CO<sub>2</sub>) which changes its physical state in the heat exchangers. In these conditions, it is more relevant to set the enthalpy as the iterative variable instead of the temperature.



## 1.5.2 Two-stage cycle

The operating conditions of the different modules in the two-stage cycle are the following:

✓ Process feed

Name	Cooling fluid input	MT Air Input	LT Air Input
Total volume flowrate (m <sup>3</sup> /h)	1	-	-
Total mass flowrate (kg/h)	-	1100	150
Molar fractions:			
Carbon dioxide	0	0	0
Water	1	0	0
Oxygen	0	0.21	0.21
Nitrogen	0	0.79	0.79
Temperature (°F)	59 (15°C)	77 (25°C)	77 (25°C)
Pressure (psi)	14.7 (1 atm)	14.7 (1 atm)	14.7 (1 atm)

✓ Reciprocating compressor

Name	MT Transcritical compressor
Type of compressor	Isentropic
Exhaust pressure (psi)	1400
Isentropic efficiency	0.8
Mechanical efficiency	0.95
Electrical efficiency	0.98
Constraints	Fixed vapor physical state

Name	LT Transcritical compressor
Type of compressor	Isentropic
Exhaust pressure (psig)	400
Isentropic efficiency	0.8
Mechanical efficiency	0.95
Electrical efficiency	0.98
Constraints	Fixed vapor physical state

## ✓ Expansion valve

Name	Constraint type	Pressure (psi)
High Pressure valve	Pressure specification	400
Low Pressure valve	Pressure specification	200
Flash Gas bypass valve	Pressure specification	300

## ✓ Generalized heat exchanger "Gas cooler"

Exchanger type	Counter current or multipasses
Specification type: "Hot stream"	Outlet temperature
Temperature (°F)	82 (28°C)

Additional specifications applied on the gas cooler:

Specification	Heat exchange area calculation
Clean overall heat transfer coefficient (W/m <sup>2</sup> /K)	330
Efficiency	Pure counter current

## ✓ Plate and frame heat exchanger

Name	MT heat exchanger	LT heat exchanger
Exchanger type	Counter current or multipasses	Counter current or multipasses
Specification type: "Cold stream"	Superheated over its dew point temperature	Superheated over its dew point temperature
Temperature difference (°F)	20	60

The additional specification "Heat exchange area calculation" applied on the heat exchangers are identical to those applied on the evaporator in the simple cycle.

## ✓ Liquid-vapor separator

This module is defined with default operating parameters like shown below:

Flash type	Constant pressure and enthalpy flash
Pressure specification	The lowest of the feed streams
Pressure drop (psi)	0
Heat duty specification	Adiabatic

## ✓ Stream splitter "Splitter"

Streams	Splitting ratio	Outlet pressure
12	0.81	Equal to the feed pressure

*Remark: the mixer "Mixer" is defined with default operating parameters (the outlet pressure is equal to the lowest of the feeds pressures).*

## ✓ Constraints and recycles (SPEC)

The parameters used in the SPEC module are presented below:

Constraints and Recycles (\$SPEC)

Name: Constraints and Recycles 1

Desc:

Identification Parameters Scripts Report Streams Notes Advanced parameters

☒ Module enabled

Numerical methods: Default

Convergence criterion

Criterion: 1E-8

Stop Test

Non evolution of criterion: 1E-7

Non evolution of variables: 1E-6

Maximum number of passages in the MCN: 100

Maximum number of iterations: 20

Print

Print every: 10 iterations

Tear streams iterative variables

☒ Enthalpies

☐ Pressures

Resume

☐ Use of values obtained at convergence of the previous problem

Constraints: Parameters...

Tear streams: Parameters...

OK Cancel

The refrigeration cycle is composed of pure component (CO<sub>2</sub>) which changes its physical state in the heat exchangers. In these conditions, it is more relevant to set the enthalpy as the iterative variable instead of the temperature.

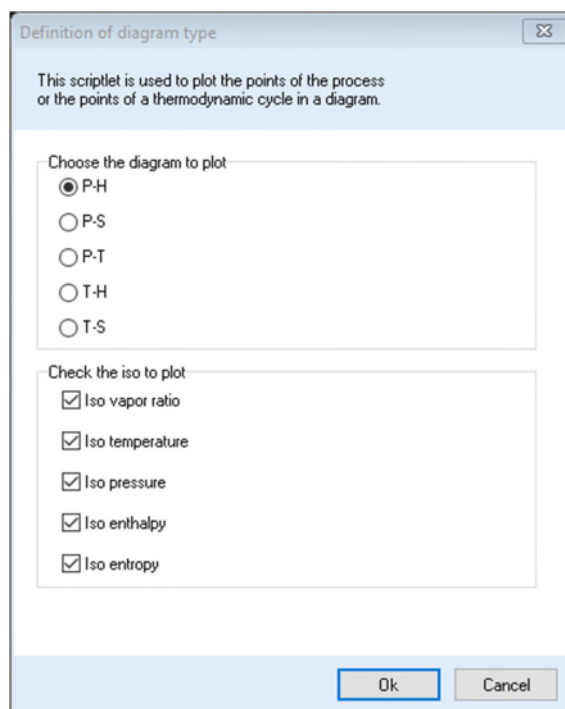
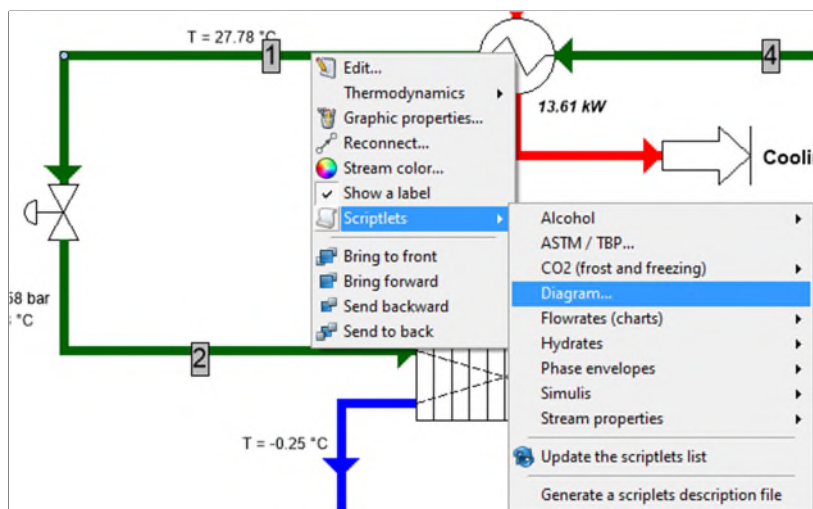
## 1.6. Initialization

The calculation sequence is automatically determined by ProSimPlus. Only one tear stream was detected: the material stream “2” (inlet of the evaporator) in the simple cycle and the material stream “1” (inlet of the compressor “MT Transcritical Compressor”) in the two-stage cycle. The following initializations of these streams are used:

	Simple cycle	Two-stage cycle
Stream	“2”	“1”
Mass fractions:		
Carbon dioxide	1	1
Water	0	0
Oxygen	0	0
Nitrogen	0	0
Total mass flowrate (kg/h)	200	200
Temperature (°F)	77 (25°C)	77 (25°C)
Pressure (psi)	400 (27.2 atm)	14.7 (1 atm)

## 1.7. “Tips and tricks”

The thermodynamic cycle in Pressure (P) – Enthalpy (H) diagram can be visualized using the “Scriptlets” functionality by right-clicking on one of the material streams of the cycle:



Scriptlet parameters

Choose the type (enthalpy and entropy)

☒ Molar

☐ Mass

Do you want to connect the points?

☐ No

☒ Yes

Do you want to modify the number of iso?

☒ No

☐ Yes

Ok Cancel

For the points of the cycle to be connected, it is necessary to number the material streams in the required order.

Streams definition

This scriptlet is used to plot the points of the process or the points of a thermodynamic cycle in a diagram.

Choose the streams used to plot the diagram

☐ Selected streams (during scriptlet execution)

☒ Streams numbered (from 1 to NB)

☐ Streams used in the previous configuration

Ok Cancel

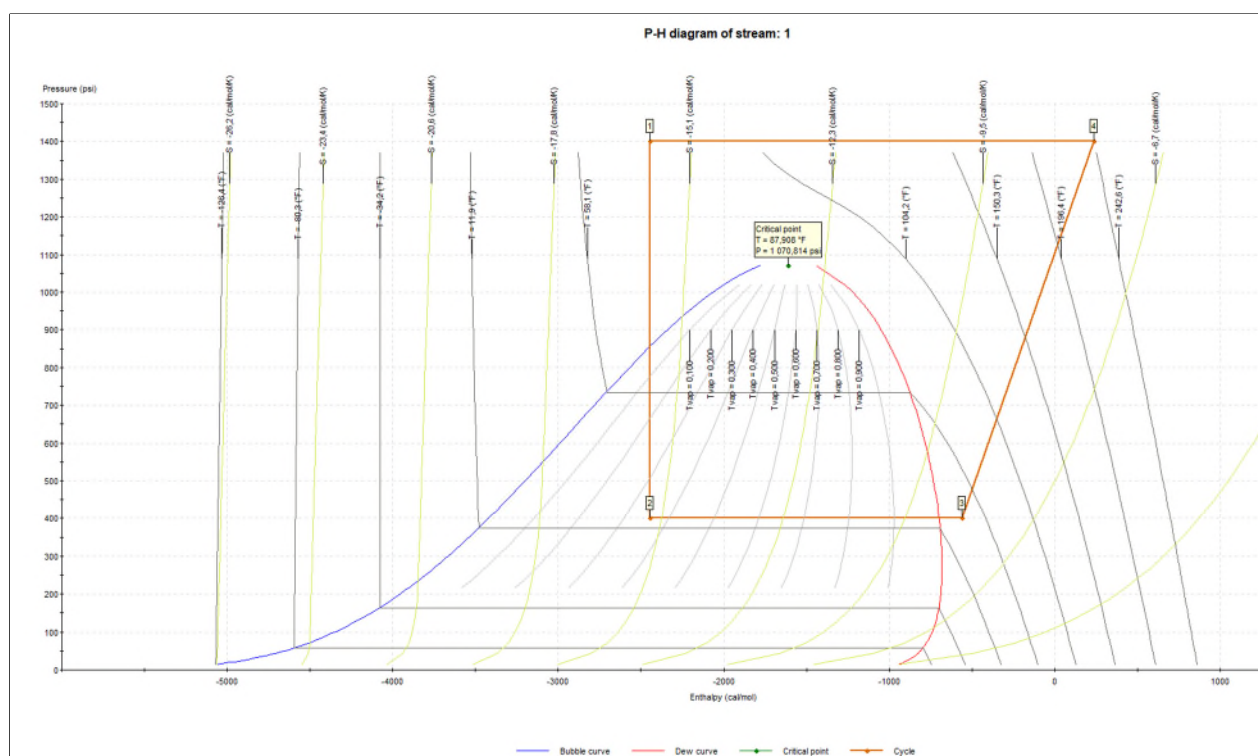
Scriptlet parameters

The streams added to the diagram must be numbered (from 1 to NB). It is therefore necessary to change the streams names by a number on your flowsheet.

Number of points (NB)

4

Ok Cancel



## 2.RESULTS

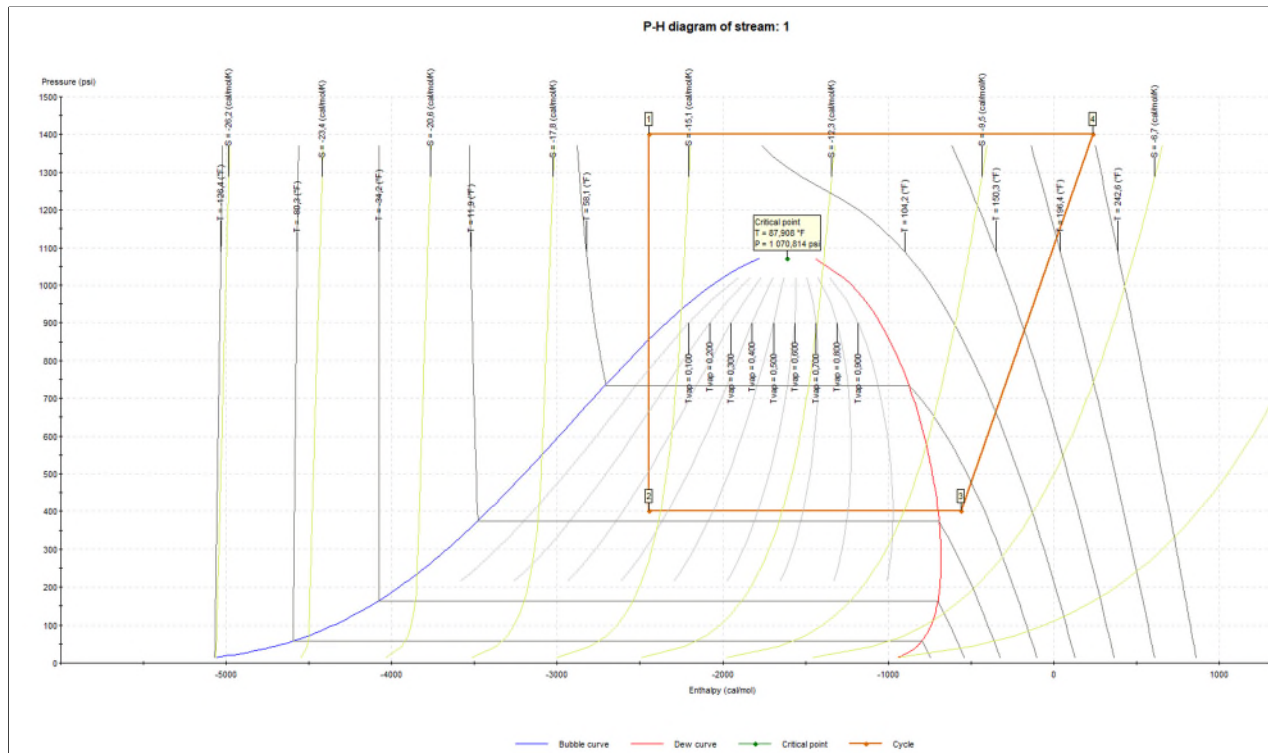
### 2.1. Process Performance

Simulation result	Notation	Simple cycle
Air temperature at the process outlet (°F)	A	31.4 (≈ 0°C)
Reciprocating compressor (kW)	B	4.5
Evaporator (kW)	C	10
COP	D (=C/B)	2.2

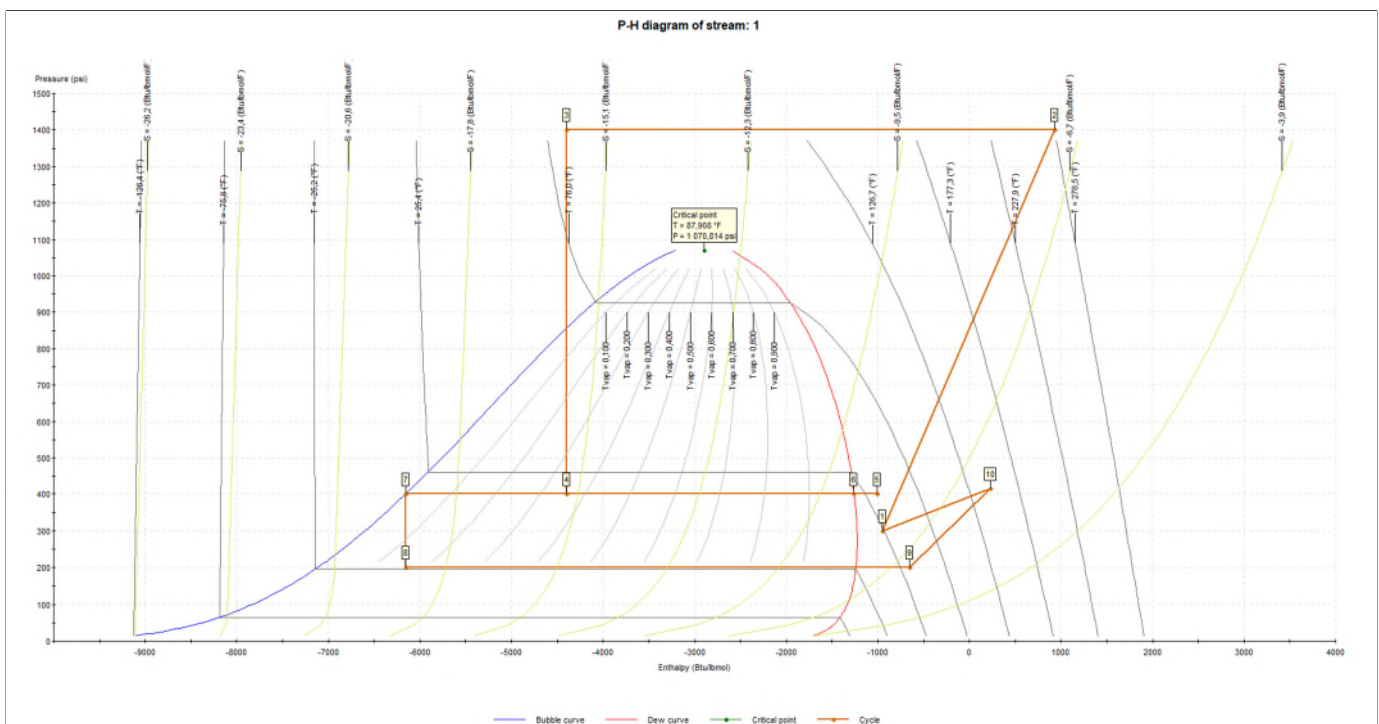
Simulation result	Notation	Two-stage cycle
Air temperature at the “MT heat exchanger” outlet (°F)	E	31.3 (≈ 0°C)
Air temperature at the “LT heat exchanger” outlet (°F)	F	-7.2 (≈ -21°C)
MT Transcritical compressor (kW)	G	5.9
LT Transcritical compressor (kW)	H	0.3
MT heat exchanger (kW)	I	7.9
LT heat exchanger (kW)	J	2
COP	K (=(I+J)/(G+H))	1.6

## 2.2. Thermodynamic cycles

The transcritical cycle for the simple cycle is presented below:



Regarding the two-stage cycle, the transcritical cycle from the material stream “1” to material stream “10” is presented below:





### 3. REFERENCES

- [SOA72] SOAVE G., "Equilibrium constants from a modified Redlich-Kwong equation of state", C.E.S., 27, 6,1197-1203 (1972)
- [WIL19] Wilding, W. V.; Knotts, T. A.; Giles, N. F.; Rowley, R. L. DIPPR Data Compilation of Pure Chemical Properties; Design Institute for Physical Properties, AIChE: New York, NY (2019)