PROSIMPLUS APPLICATION EXAMPLE

CO$_2$ REFRIGERATION CYCLES

EXAMPLE PURPOSE

This example presents the simulation of refrigeration machines with transcritical CO$_2$. Two transcritical cycles are presented, a simple cycle and a two-stage cycle. The cycles allow to provide temperatures below 0°C.

ACCESS	☑ Free Internet	☐ Restricted to ProSim clients	☐ Restricted	☐ Confidential

CORRESPONDING PROSIMPLUS FILES	*PSPS_EX_EN-CO2-Refrigeration-Single-Stage.pmp3*
	PSPS_EX_EN-CO2-Refrigeration-Two-Stages.pmp3

www.prosim.net

TABLE OF CONTENTS

1. PROCESS MODELING

1.1. Process description

This example presents the simulations of transcritical cycles of refrigeration systems with CO_2. 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_2) is a promising refrigerant and attracts many interests in the scientific and industrial sectors. The CO_2 (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, CO2 (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_2 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 ≈0°C (≈31.5°F) and has a COP of 2.7. The two-stages cycle is capable to distribute cold temperature of ≈0°C (≈31.5°F) and ≈-21°C (≈-7°F). Its COP value is 1.9.
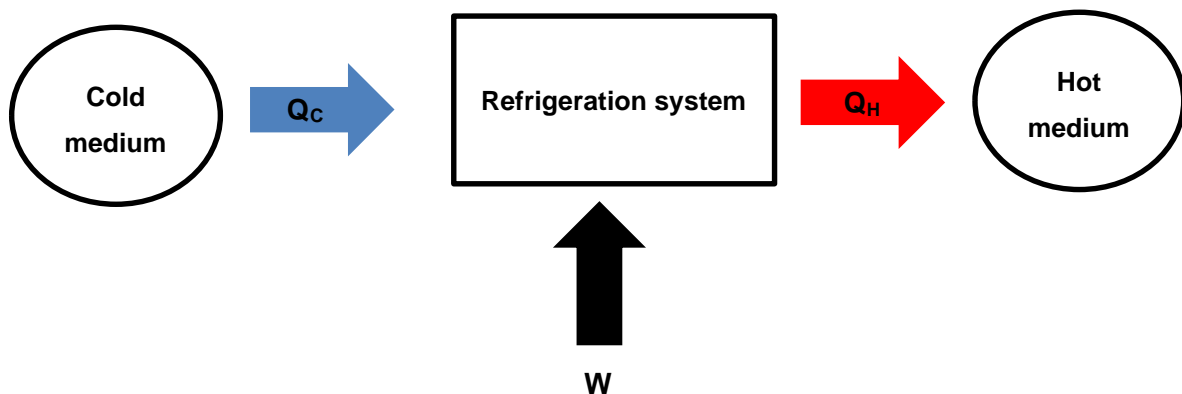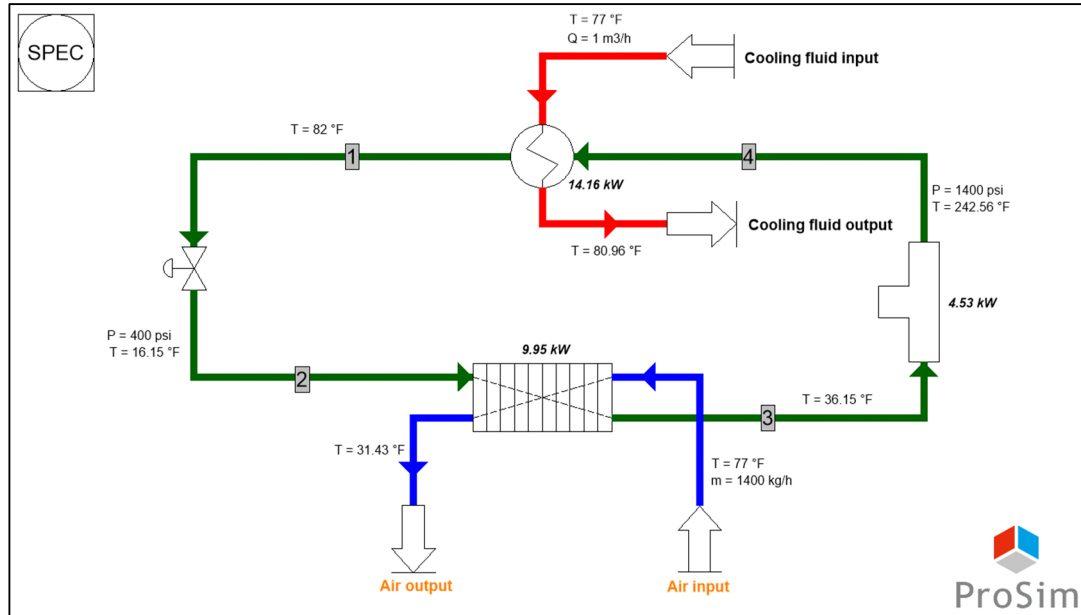

Principle of refrigeration system

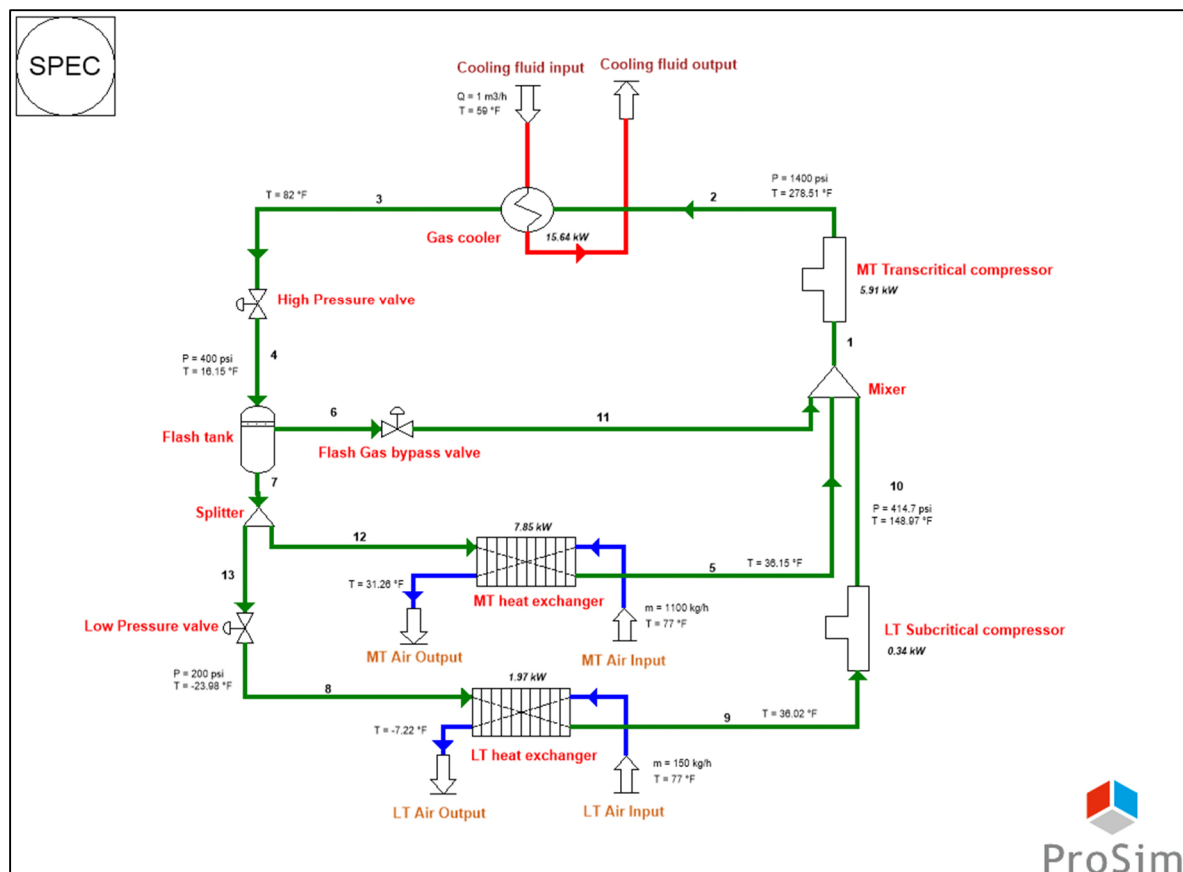## 1.2.   **Process flowsheet**

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. <u>Components</u>

The components taken into account in the simulation, their chemical formula and their CAS[(*)] 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_2O	7732-18-5
Carbon dioxide	CO_2	124-38-9
Oxygen	O_2	7782-44-7
Nitrogen	N_2	7727-37-9

1.4. <u>Thermodynamic model</u>

Three thermodynamic calculators are defined to simulate the simple cycle and the two-stage cycle of "CO₂ 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.

[(*)]*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. <u>Operating conditions</u>

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 (m³/h)	1	-
Total mass flowrate (kg/h)	-	1400
Molar fractions:		
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

www.prosim.net

✓ Generalized heat exchanger "Condenser"

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

Additional specifications applied on the condenser:

Specification	Heat exchange area calculation
Clean overall heat transfer coefficient (W/m²/K)	330
Efficiency	Pure counter current

✓ Plate and frame heat exchanger "Evaporator"

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

Additional specifications applied on the evaporator:

Specification	Heat exchange area calculation
Heat transfer coefficients for 2-phase zones (W/m²/K):	
Liquid : Liquid	500
Liquid-vapor : Liquid	1000
Vapor : Liquid	250
Liquid : Liquid-vapor	1000
Liquid-vapor : Liquid-vapor	1500
Vapor : Liquid-vapor	500
Liquid : Vapor	250
Liquid-vapor : Vapor	1000
Vapor : Vapor	100
Efficiency	Pure counter-current

✓ Constraints and recycles (SPEC)

The Constraints and recycles module is necessary in the flowsheet because the CO_2 is fed in loop. The parameters used in the SPEC module are presented below:

The refrigeration cycle is composed of pure component (CO_2) 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 (m³/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/m²/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:

The refrigeration cycle is composed of pure component (CO_2) 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. <u>Initialization</u>

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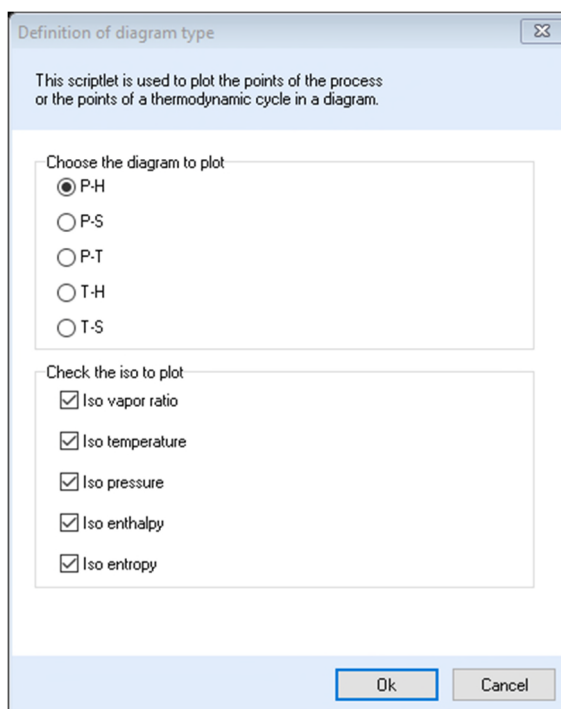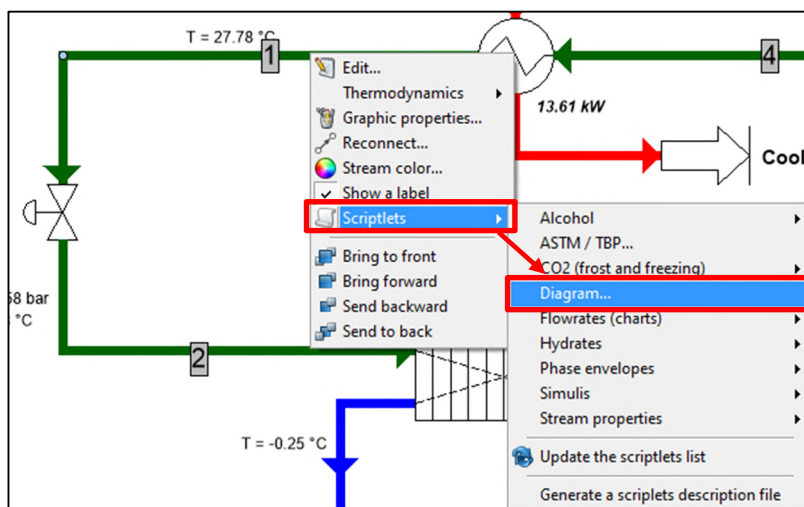
For the points of the cycle to be connected, it is necessary to number the material streams in the required order.
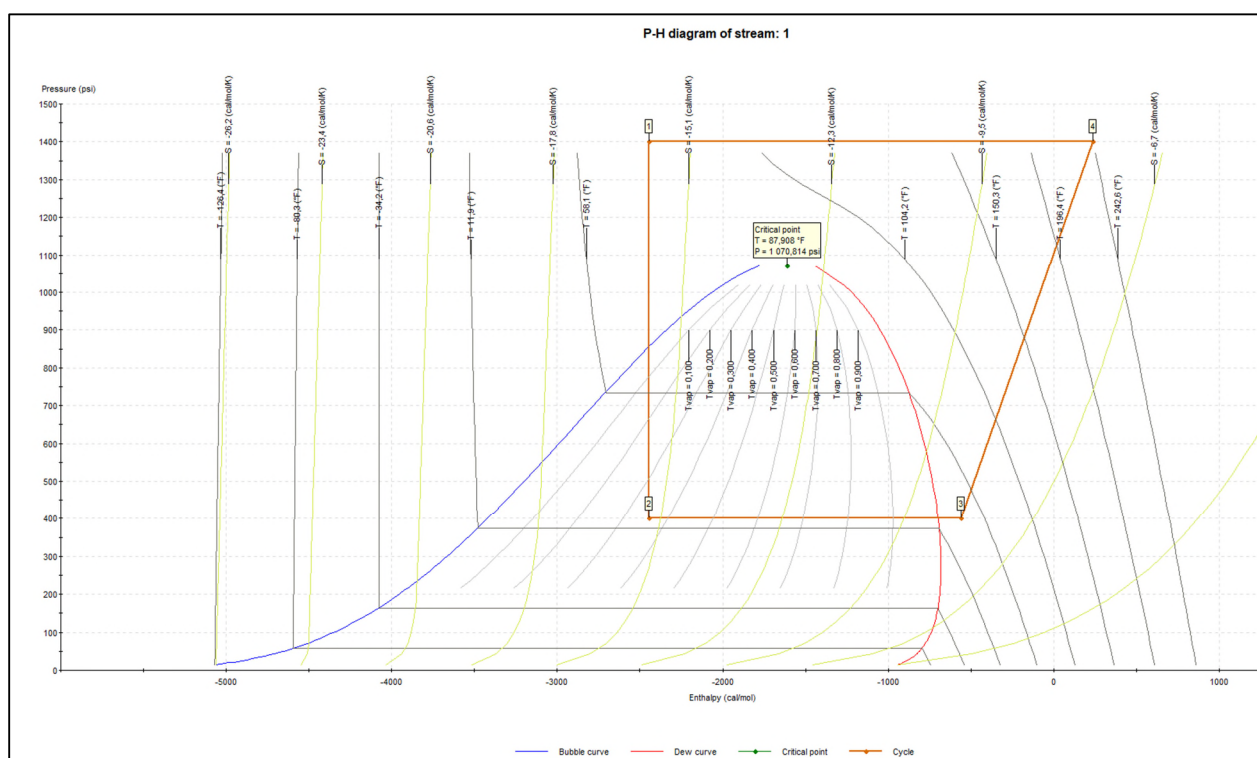
2. RESULTS

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:
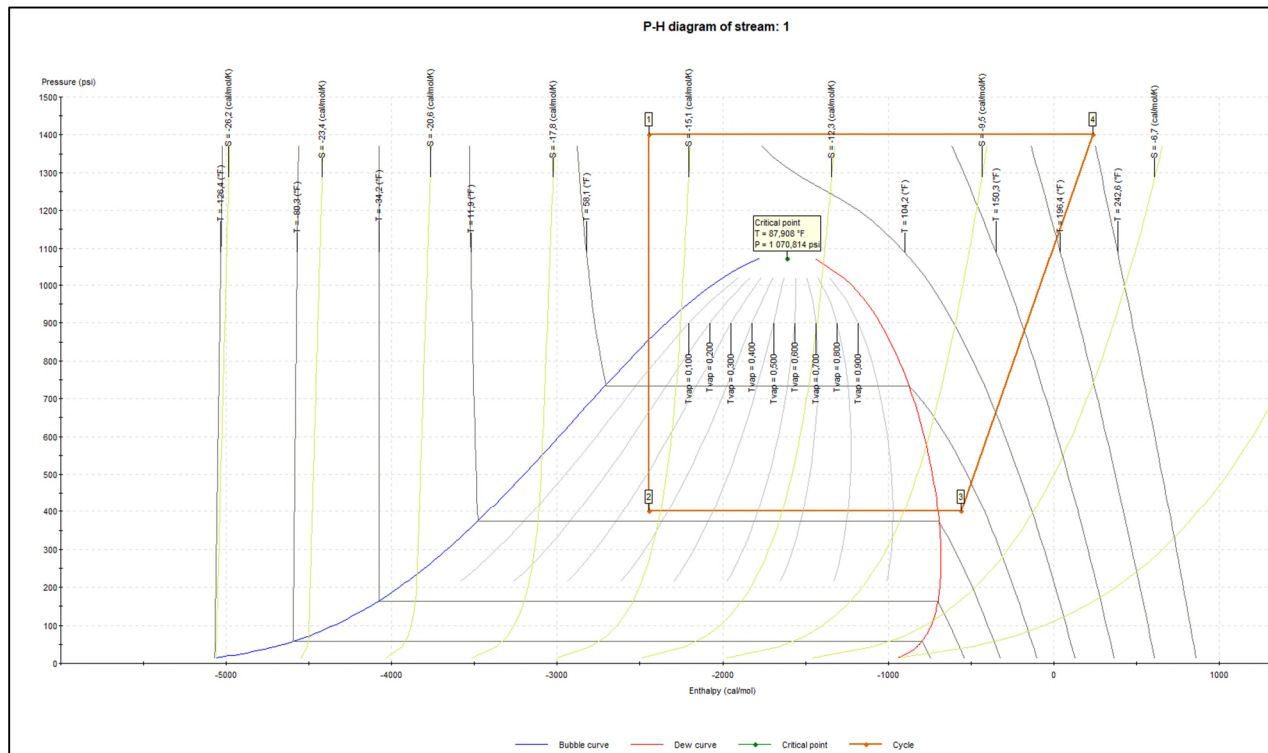
Regarding the two-stage cycle, the transcritical cycle from the material stream "1" to material stream "10" is presented below:
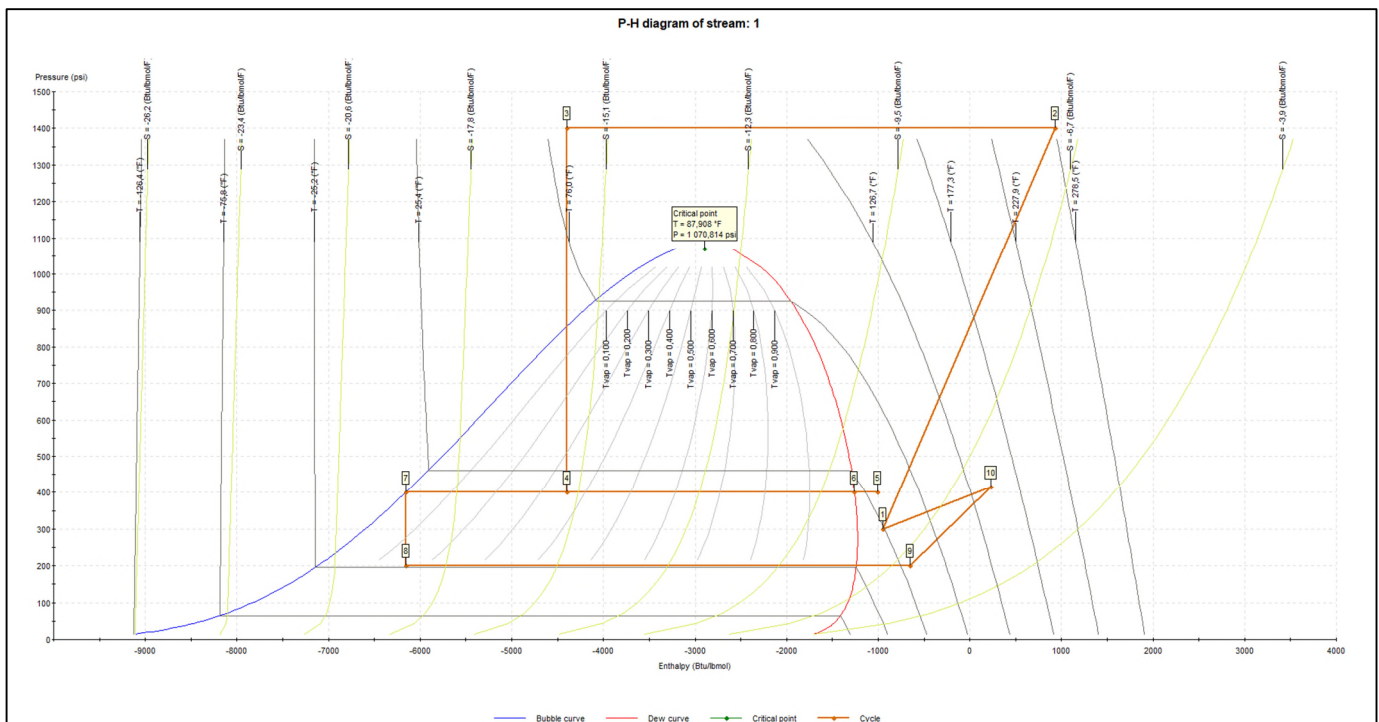
3. REFERENCES

[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)