SEMI-THEORETICAL SIMULATION MODEL FOR A TRANSCRITICAL CARBON DIOXIDE MOBILE A/C SYSTEM

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ABSTRACT

This paper describes a semi-theoretical simulation model, CYCLE11_CO2, for a transcritical carbon dioxide vapor-compression refrigeration cycle. CYCLE11_CO2 is based on an earlier simulation model, CYCLE11-UA, developed at the National Institutes of Standards and Technology for evaluating alternative refrigerants and refrigerant mixtures. Here we describe CYCLE11_CO2, its inputs, its outputs, and present some typical simulation results. The simulation results are compared to experimental data.

INTRODUCTION

The worldwide refrigeration and air conditioning industries are undergoing major changes brought on by the global environmental crisis. The discovery that chlorine atoms contained in chlorofluorcarbon (CFC) and hydrochlorofluorocarbon (HCFC) refrigerants can act as catalysts repeatedly combining with and breaking apart stratospheric ozone molecules led to the Montreal Protocol (1987) and its amendments, London (1990), Copenhagen (1992), Vienna (1995), and Montreal (1997). These international agreements have put in place a timetable to phase out the production of CFC and HCFC refrigerants. As a result, the refrigeration and air conditioning industries are now in the process of introducing hydrofluorocarbon (HFC) refrigerants as replacements. This transition took place in the United States automotive industry in the early 1990's when CFC-12 was replaced with HFC-134a. HFC's, however, have relatively large global warming potentials compared to natural fluids (e.g. ammonia, hydrocarbons, carbon dioxide, air, water), i.e. they directly contribute to the so-called greenhouse effect by trapping the earth's infrared radiation. This negative impact on the global environment has let to an increased interest in natural fluids as refrigerants [1-5] with carbon dioxide receiving significant consideration as a possible refrigerant for mobile air conditioning systems [6-15]. Researchers worldwide are actively pursuing the question of whether carbon dioxide is a good refrigerant in mobile air-conditioning applications; however, the question remains to be definitively answered. To this end, more studies are needed which shed light on the advantages and disadvantages of carbon dioxide as a refrigerant in mobile air conditioning. The objective of this paper is to present CYCLE11_CO2, a semi-theoretical simulation model for a transcritical carbon dioxide vapor-compression system. The simulation results obtained by CYCLE11_CO2 are compared to experimental data presented by McEnaney et al. [14].

BACKGROUND

The simulation model used to generate the results presented in this paper is based on a vapor-compression simulation model developed at the National Institutes of Standards and Technology [16-18]. CYCLE11 simulates the theoretical vapor-compression refrigeration cycle using eleven refrigerant state points. The thermodynamic and transport properties are calculated using REFPROP [19]. There are two versions of CYCLE11: (a) CYCLE11-ΔT and (b) CYCLE11-UA. The major difference between these two versions is the way in which the heat exchangers are modeled. In CYCLE11-ΔT, the evaporator and the condenser are represented by ΔT, an average effective temperature difference between the refrigerant and the external heat transfer fluid (HTF). In CYCLE11-UA, the evaporator and the condenser are represented by the product of their overall heat-transfer coefficients and their heat-transfer areas. In addition, CYCLE11-UA includes inputs for compressor speed and compressor displacement volume, whereas, CYCLE11-ΔT performs calculations based on a unit mass of circulating refrigerant. The solution logic aims to obtain

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agreement between the ΔT calculated using refrigerant and HTF properties, and the inputted ΔT (ΔT version) or the ΔT calculated from the basic heat transfer relation given in Eq. (1) (UA version).

$$\dot{Q}_{hx} = \dot{m}_{ref}\,\Delta h_{ref} = UA\Delta T_{hx} \tag{1}$$

where $\dot{Q}_{hx}$ is the heat transfer rate, $\dot{m}_{ref}$ ie refrigerant mass flow rate, Δh_{ref} change in the refrigerant specific enthalpy between the inlet and the outlet of the heat exchanger, UA is the product of the overall heat-transfer coefficient and the heat transfer area. ΔT_{hx} and is the average effective temperature difference for the heat exchanger.

The results presented in this paper are generated from a modified version of CYCLE11-UA, entitled CYCLE11_CO2. The details describing CYCLE11_CO2 will be forthcoming in a future publication.

CYCLE11_CO2

INPUTS AND FEATURES – Sample model inputs are shown in Fig. 1. In particular, we would like to call attention to the input used to describe the three heat exchangers, namely, the evaporator, the gas cooler, and the liquid-line/suction-line heat exchanger (llsl hx). The evaporator and the gas cooler can be either of the counter-flow, the parallel-flow, or the cross-flow type. Of obvious interest to passenger vehicle applications are heat exchangers of the cross-flow type. The evaporator and the gas cooler are described by their UA values (product of the overall heat-transfer coefficient and heat transfer area) and by the refrigerant pressure drops through the respective heat exchangers. The input data include the inlet and outlet temperatures of the HTF for each heat exchanger. The llsl hx is of the counter-flow type and is described by the pressure drop on each side of the heat exchanger, by its effectiveness, and by the refrigerant temperature at the compressor inlet (i.e. the outlet from the low-pressure side of the llsl hx). [Note: in a given simulation, the user has the option of either specifying the UA values and the pressure drops or the user can allow the program to simulate these values through the transport properties option.]

Since both the coefficient of performance (COP) and the refrigeration capacity are functions of the high-side (i.e. outlet of the gas cooler) pressure [6], the user has the option of either (a) selecting the high-side pressure or (b) allowing the program to select the high-side pressure to optimize the COP. Figure 2 shows an example of the high-side pressure input screen. Additionally as can be seen in Fig. 2, the user can limit the maximum refrigerant temperature in the system. This option is available since the optimum pressure may lead to excessively high compressor discharge temperatures for some compressor applications. This was noted by McEnaney, et al. [14]; the maximum temperature that their prototype compressor could withstand was 140 °C. Thus, if the user chooses to limit the maximum refrigerant temperature, the program will select the high-side pressure that maximizes the COP subject to the maximum refrigerant temperature constraint.

Electric motor efficiency [0.900].........................:
Compressor swept volume (m^3) [0.000021]......:
Compressor RPM [1800.0]................................:
G.Cool HX (1=Count, 2=Parallel, 3=Cross) [3]....:
HTF temp. entering gas cooler (C) [42.9]..........:
HTF temp. exiting gas cooler (C) [53.1]............:
UA for gas cooler (kW/K)..... [3.919E-01]...........:
Evap. HX (1=Counter, 2=Parallel, 3=Cross) [3]...:
HTF temp. entering evaporator (C) [32.7].........:
HTF temp. exiting evaporator (C) [12.8]............:
UA for evaporator (kW/K)..... [5.142E-01]...........:
Pressure drop thru gas cooler (kPa) [130.0]........:
Pressure drop thru evaporator (kPa) [130.0].......:
Suction line heater ? (Y OR N) [Y] ....:
Press drop on liquid side of h.e. (kPa) [125.0]...:
Press drop on suction side of h.e. (kPa) [125.0].:
Effectiveness of the suction h.e. [0.60].............:
Refrig temp at compressor inlet (C) [31.9].......:

Figure 1. Sample model input.

Do you want to optimize the COP by having the program find the optimum gas cooler outlet pressure? Or do you want to input the gas cooler outlet pressure yourself?

1 = Optimize 2 = User Input Default = [1]..........:

Do you want to limit the max comp temp? Y/N [Y] ....:

Maximum compressor temp (C) [140.0] ....:

Do you want to involve transport properties (Y/N) [N]....:

Figure 2. Sample model input for the high-side pressure.

The user also has the option of involving transport properties. See Fig. 3 for example user input. The user is able to impose (options 0 and 1) or to simulate (option 2) the pressure drop and UA values. If option 0 is chosen, the transport properties are not used to calculate the simulation results. If option 1 is chosen, the transport properties are used to calculate results for this base case. These base results are then used in later simulations when option 2 is selected. That is, the base results, along with the transport properties, are used to calculate the simulation results for option 2. Thus, option 2 can be used, for example, to simulate other operating conditions (e.g. different ambient temperatures or different compressor speeds) or to simulate other refrigerant choices once the base condition (through option 1) has been simulated. For a more detailed description see Domanski and McLinden [16] and Domanski et al. [17]. [Note: the user does not explicitly input the number of refrigerant circuits. The program uses the baseline refrigerant mass flux and the simulated mass flow rate to determine the number of circuits.]

```
Do you want to optimize the COP by having the program
find the optimum gas cooler outlet pressure? Or do you
want to input the gas cooler outlet pressure yourself?

1 = Optimize   2 = User Input    Default = [1]..........: 2

Gas Cooler Exit Pressure [10000.0 kPa] ....................:

Do you want to involve transport properties (Y/N) [N]..: Y

dP (0=imposed, 1=reference, 2=simulated) [0]........: 1
UA (0=imposed, 1=reference, 2=simulated [0].........: 1
U for the evaporator ( kW/K-m2 ) [ 0.10]...............:
A_ref side/A_air side for the evaporator [0.1]..............:
U for the gas cooler ( kW/K-m2 ) [ 0.10].................:
A_ref side/A_air side for the gas cooler [0.1]...............:
Evaporator tube diameter (mm) [0.790]......................:
Gas cooler tube diameter (mm) [0.790].......................:
Dia of high-pressure side of suction hx (mm) [ 6.00]....:
Dia of low-pressure side of suction hx (mm) [ 6.00]......:
Refrigerant mass flux (kg/m2-s ) [0.32500E+03].........:
```

Figure 3. Sample model input when imposing transport properties.

OUTPUT – The simulation output includes calculations for the heat exchangers, the compressor, key refrigerant state points, and the overall system performance.

For the gas cooler the calculations are: the average effective temperature difference, the refrigerant state at the inlet to the gas cooler, the refrigerant state at the outlet of the gas cooler, and the overall heat transfer rate.

For the evaporator the calculations are: the average effective temperature difference, the refrigerant state at the inlet to the evaporator, the refrigerant state at the outlet of the evaporator, and the overall heat transfer rate.

For the llsl hx the calculations are: the superheat from the evaporator outlet to the compressor inlet, the temperature drop from the gas cooler outlet to the expansion device inlet, and the heat transfer between the two refrigerant streams.

For the compressor the calculations are: the compressor work, the volumetric efficiency and the isentropic efficiency. Both of these parameters are determined from a curve fit of the experimental data provided in McEnaney et al. [14].

The system performance parameters calculated are: the compressor work, refrigeration capacity, refrigerant mass flow rate, and COP.

RESULTS

For the data shown in Figs. 4-6 and in Tbl. 1, the heat exchanger input is: UA values, pressure drops, and temperatures of the HTF at the inlets and outlets of the heat exchangers.

Figure 4 shows simulation results for test point M3 given in McEnaney et al. [14]. This particular test point has a compressor speed of 1800 rpm, a gas cooler inlet air temperature of 42.9 °C, an evaporator inlet air temperature of 32.7 °C, and a gas cooler outlet pressure of 11280 kPa. Figures 5 and 6 show the results of Fig. 4 plotted on T-s and P-h state diagrams, respectively.

Table 1 shows validation results for four tests points (I11, I17, M3, H3) taken from McEnaney et al. [14]. The table shows, in summary form, both the experimental data of McEnaney et al. [14] and the simulation results from CYCLE11_CO2. In all cases shown here, the high-side pressure has been provided as input (i.e. the program's optimization routine was not used to select the high-side pressure). However, for example if the program's optimization routine is used for test point M3, the high-side pressure that results is 12347 kPa (with a corresponding COP of 1.76) versus the baseline value of 11280 kPa (with a corresponding COP of 1.72). For all cases shown here, the pressure drop values have also been provided as input. However, if the user simulates the test point M3 at a compressor speed of say 3000 rpm instead of the baseline speed of 1800 rpm, then the program would calculate a refrigerant mass flow rate of 61.9 g/s versus the baseline value of 43.9 g/s. The resulting pressure drops through the gas cooler and evaporator would be 252 kPa and 285 kPa, respectively, versus the baseline values of 131 kPa for both heat exchangers. Likewise, for all the cases shown here, the UA values have been provided as input. However, if the user simulates the test point M3 at a compressor speed of say 3000 rpm instead of the baseline value of 1800 rpm, the simulated UA values would increase by approximately 3% over the baseline values.

The way in which the data in Tbl. 2 (test point M5) were generated is different from the way in which the data in Figs. 4-6 and in Tbl. 1 were generated. The data in Tbl. 2 were simulated based on a reference case (in this case, test point I11), and thus demonstrate the powerful capabilities of CYCLE11_CO2. Unlike the data in Figs. 4-6 and in Tbl. 1, for the data of Tbl. 2, the only information inputted for the heat exchanger is the temperature of the HTF at the inlets to the heat exchangers. The other parameters, namely, the UA values, the pressure drops, and the temperatures of the HTF at the outlets of the heat exchangers have all been simulated. Tables 3a and 3b show percentage errors between the experimental data and the simulation results for the test points shown in Tbls. 1 and 2, respectively. More complete simulation results will appear in a forthcoming publication.

CONCLUSIONS

We have developed a robust simulation model for a transcritical carbon dioxide vapor-compression refrigeration cycle. The model's capabilities include counter-flow, parallel-flow, or cross-flow representations of the evaporator and the gas cooler. The simulation results presented show good agreement with experimental data provided in McEnaney et al. [14].

This simulation model should prove useful in highlighting the advantages and disadvantages of using carbon dioxide as a refrigerant in mobile air conditioning applications.

As the automotive industry moves toward shorter and shorter product development cycles, it is becoming increasingly more important for design engineers to rely on simulation models, such as the one described in this paper, to aid them in their design efforts.

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DEFINITIONS, ACRONYMS, ABBREVIATIONS

LATIN SYMBOLS AND ABBREVIATIONS

A: area [m^2]
COMP: compressor
COOL: gas cooler
COP: coefficient of performance [-]
COPh: coefficient of performance in heating mode [-]
COPr: coefficient of performance in cooling mode [-]
dens: density [kg/m^3]
EFFV: volumetric efficiency [-]
EVAP: evaporator
h: specific enthalpy [kJ/kg]
HTF: external heat transfer fluid
llsl hx: liquid-line/suction-line heat exchanger
$\dot{m}$: refrigerant mass flow rate [kg/s]
P: pressure [kPa]
Q: heat transfer [kJ/kg]
$\dot{Q}$: heat transfer rate [kW]
rms: refrigerant mass flow rate [kg/s]
rpm: compressor speed [revolutions/min]
s: specific entropy [kJ/kg-K]
T: temperature [°C]
ΔT: average effective temperature difference between refrigerant and HTF [°C]
U: overall heat transfer coefficient [kW/m^2-K]

SUBSCRIPTS

hx: heat exchanger
ref: refrigerant

Cycle analysis by CYCLE11_CO2, Version 1.0 of August 9, 1999

INPUT DATA:

HX stream temps:	Source (in, out):	32.7,	12.8 C	Cross flow HX
	Sink (in, out):	42.9,	53.1 C	Cross flow HX

Compressor RPM = 1800.0 Compressor ambient temperature= 32.2 C
El. motor eff = 1.000; Vswept = 0.207E-4 m^3

UA (kW/K).....: Evaporator = 0.5142 Gas Cooler = 0.4566
Imposed pressure drops (kPa).: Evap = 131.0 Gas Cooler = 131.0
Imposed dP for suction h.e. (kPa).:Liq Side = 150.0 Suction Side = 150.0
Effectiveness of the suction heat exchanger = 0.8131

RESULTS:
Avg. eff. temperature differences (cool,evap): 17.56 9.88 C
Superheat due to h.t. with outlet from gas cooler = 22.7
Temp drop from gas-cool-out to exp-dev-in due to h.t. w/ suction side = 11.1 C
Q (suction heat exchanger) = 51.75 kJ/kg

Entropy prod.:	Evap = 4.152E-02	Cool = 4.972E-02	Tot = 9.124E-02 kJ/kg K
	Source = -3.902E-01	Sink = 5.684E-01	Tot = 1.782E-01 kJ/kg K

State	T (C)		P	H	DENS	S	QUALITY
	HTF	REF	(kPa)	(kJ/kg)	(kg/m^3)	(kJ/kg K)	
1 COMP IN	n/a	31.9	4258.8	-40.7	96.4	-0.79956	1.000
2 COMP OUT	n/a	126.6	11410.0	26.4	190.1	-0.75303	1.000
3 COOL IN	53.1	126.6	11410.0	26.4	190.1	-0.75303	1.000
4 COOL OUT	42.9	50.4	11279.0	-156.2	521.8	-1.27173	1.000
5 SUCHX OUT	n/a	39.4	11129.0	-207.9	697.1	-1.43350	1.000
6 EVAP I	12.8	10.3	4539.8	-207.9	291.4	-1.39280	0.369
7 EVAP OUT	32.7	9.2	4408.8	-92.5	136.9	-0.98236	0.953
8 SUCHX OUT	n/a	31.9	4258.8	-40.7	96.4	-0.79956	1.000

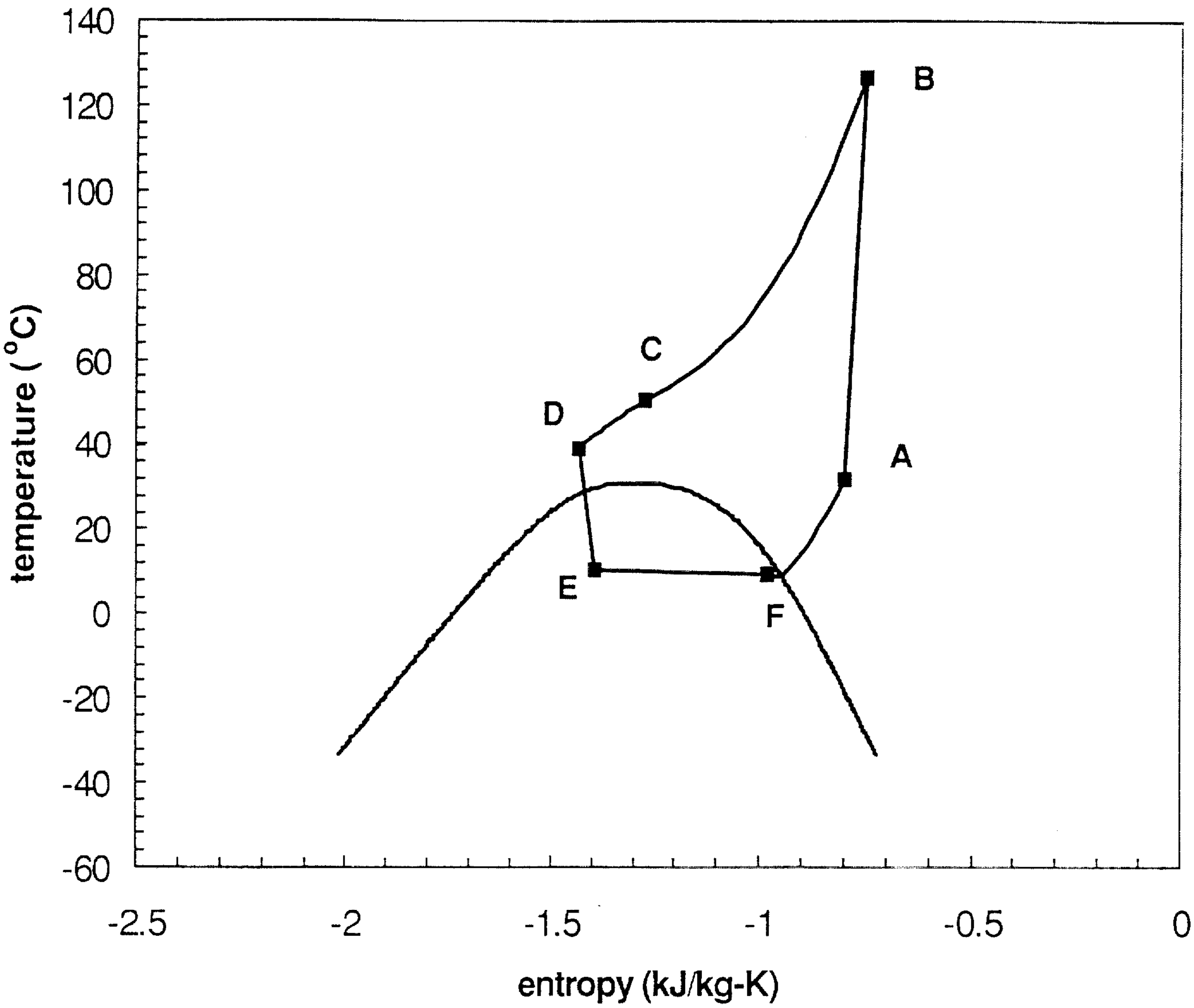
Volumetric Efficiency = 0.734% Isentropic Efficiency = 0.727

Performance:	Cycle	System		
Work:	67.10 kJ/kg	2.948	kW	RMS (kg/s) = .4393E-01
Refrig. capacity:	115.41 kJ/kg	5.070	kW	COPr = 1.720
Heating capacity:	182.53 kJ/kg	8.018	kW	COPh = 2.720

General performance data:	Refrigerating	Heating
Vol. capacity @ EffV = 1.000	11121.8 kJ/m^3	17589.8 kJ/m^3
Vol. capacity @ EffV = 0.734	8164.0 kJ/m^3	12911.9 kJ/m^3

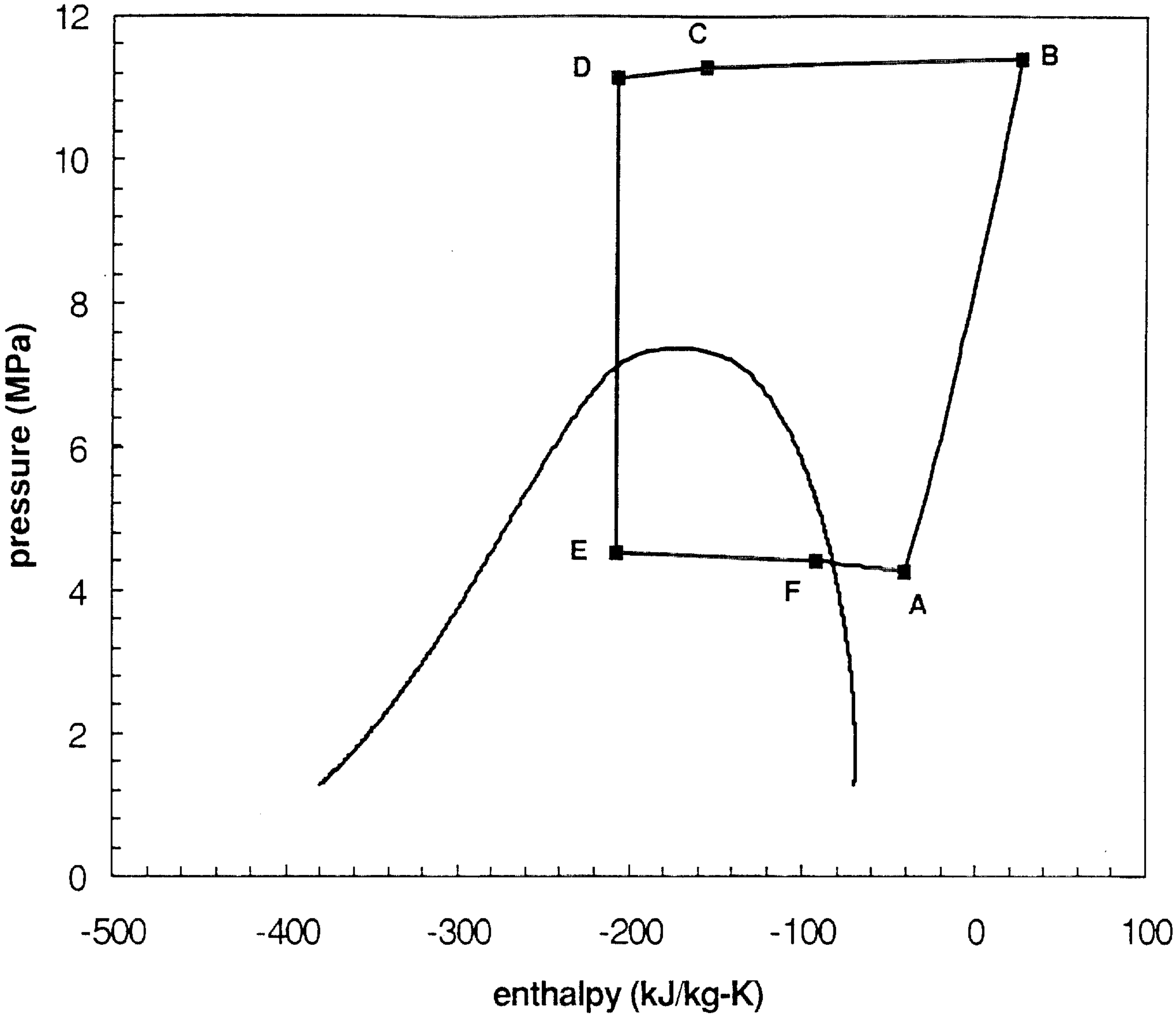
Pressure Ratio = 2.68

Figure 4. Simulation results for test point M3 given in McEnaney et al. [14]. (High-side pressure is 11280 kPa.)



Point A: outlet from low-pressure side of llsl hx/inlet to compressor
Point B: outlet from compressor/inlet to gas cooler
Point C: outlet from gas cooler/inlet to high-pressure side of llsl hx
Point D: outlet from high-pressure side of llsl hx/inlet to expansion device
Point E: outlet from expansion device/inlet to evaporator
Point F: outlet from evaporator/inlet to low-pressure side of llsl hx

Figure 5. Results for test point M3 shown in Fig. 4 plotted on a temperature-entropy state diagram.



Point A: outlet from low-pressure side of llsl hx/inlet to compressor
Point B: outlet from compressor/inlet to gas cooler
Point C: outlet from gas cooler/inlet to high-pressure side of llsl hx
Point D: outlet from high-pressure side of llsl hx/inlet to expansion device
Point E: outlet from expansion device/inlet to evaporator
Point F: outlet from evaporator/inlet to low-pressure side of llsl hx

Figure 6. Results for test point M3 shown in Fig. 4 plotted on a pressure-enthalpy state diagram.

Table 1. Comparison between experimental data taken from McEnaney et al. [14] and CYCLE11_CO2 simulation results.

Test Point	**I11**		**I17**		**M3**		**H3**	
	Test Conditions		**Test Conditions**		**Test Conditions**		**Test Conditions**	
Compressor Speed (rpm)	950		950		1800		3000	
Gas Cooler Air Flow Rate (m^3/ min)	22.7		22.7		26.9		35.4	
Evaporator Air Flow Rate (m^3/ min)	7.08		7.08		7.08		7.08	
Gas Cooler Air Inlet Temperature (°C)	43.3		43.3		43.3		43.3	
Evaporator Air Inlet Temperature (°C)	26.7		21.1		32.2		32.2	
Relative Humidity (%)	40		40		40		40	
	I11		I17		M3		H3	
	Experi-mental Data [14]	Simula-tion Results	Experi-mental Data [14]	Simula-tion Results	Experi-mental Data [14]	Simula-tion Results	Experi-mental Data [14]	Simulation Results
T (point A) (°C)	31.0	**31.0**	34.5	**34.5**	31.9	**31.9**	32.8	**32.8**
T (point B) (°C)	110.1	**116.0**	111.1	**122.7**	124.1	**126.6**	153.5	**159.0**
T (point C) (°C)	46.7	**47.1**	45.8	**46.0**	50.1	**50.4**	50.7	**51.6**
T (point D) (°C)	38.4	**39.4**	39.4	**39.6**	41.0	**39.4**	39.0	**36.9**
T (point E) (°C)	9.3	**9.2**	6.0	**5.9**	10.9	**10.3**	6.3	**5.1**
T (point F) (°C)	9.0	**8.8**	5.7	**5.5**	9.7	**9.2**	4.2	**3.1**
Comp Pressure Ratio	2.54	**2.46**	2.59	**2.49**	2.78	**2.68**	3.59	**3.45**
$\dot{Q}_{evap}$ (kW)	2.78	**2.85**	2.29	**2.35**	4.67	**5.07**	6.32	**7.22**
$\dot{Q}_{gascool}$ (kW)	3.68	**4.28**	3.04	**3.69**	7.13	**8.02**	11.72	**12.42**
$\dot{m}$ (kg/s)	0.0226	**0.024**	0.020	**0.021**	0.0423	**0.044**	0.0501	**0.054**
$\dot{W}_{comp}$ (kW)	1.39	**1.43**	1.30	**1.34**	2.93	**2.95**	5.15	**5.20**
COP	2.005	**1.99**	1.763	**1.76**	1.593	**1.72**	1.226	**1.39**
Quality at evap in	0.38	**0.40**	0.46	**0.47**	0.39	**0.37**	0.36	**0.34**
Quality at evap out	0.99	**0.99**	1.0	**0.99**	0.96	**0.95**	0.96	**0.96**

Point A: outlet from low-pressure side of llsl hx/inlet to compressor
Point B: outlet from compressor/inlet to gas cooler
Point C: outlet from gas cooler/inlet to high-pressure side of llsl hx
Point D: outlet from high-pressure side of llsl hx/inlet to expansion device
Point E: outlet from expansion device/inlet to evaporator
Point F: outlet from evaporator/inlet to low-pressure side of llsl hx

Table 2. Comparison between experimental data taken from McEnaney et al. [14] and CYCLE11_CO2 simulation results. (Test point I11 used as the reference case.)

Test Point	M5	
	Test Conditions	
Compressor Speed (rpm)	1800	
Gas Cooler Air Flow Rate (m^3/min)	26.9	
Evaporator Air Flow Rate (m^3/min)	7.080	
Gas Cooler Air Inlet Temperature (°C)	43.3	
Evaporator Air Inlet Temperature (°C)	26.7	
Relative Humidity (%)	40	
	Experimental Data [14]	Simulation Results
T (point A) (°C)	31.9	**31.9**
T (point B) (°C)	136.7	**153.3**
T (point C) (°C)	48.8	**48.0**
T (point D) (°C)	28.1	**33.7**
T (point E) (°C)	4.6	**1.8**
T (point F) (°C)	3.6	**0.7**
Comp Pressure Ratio	3.23	**3.32**
$\dot{Q}_{evap}$ (kW)	4.23	**4.45**
$\dot{Q}_{gascool}$ (kW)	6.74	**7.37**
$\dot{m}$ (kg/s)	0.033	**0.032**
$\dot{W}_{comp}$ (kW)	2.88	**2.92**
COP	1.47	**1.53**
Quality at evap in	0.38	**0.33**
Quality at evap out	0.96	**0.95**

Point A: outlet from low-pressure side of llsl hx/inlet to compressor
Point B: outlet from compressor/inlet to gas cooler
Point C: outlet from gas cooler/inlet to high-pressure side of llsl hx
Point D: outlet from high-pressure side of llsl hx/inlet to expansion device
Point E: outlet from expansion device/inlet to evaporator
Point F: outlet from evaporator/inlet to low-pressure side of llsl hx

Table 3a. Percentage differences between experimental and simulated values for data of Table 1.

Test point	I11	I17	M3	H3
	|% difference|	**|% difference|**	**|% difference|**	**|% difference|**
Comp Pressure Ratio	3.1	3.9	3.6	3.9
$\dot{Q}_{evap}$	2.5	2.6	8.6	14.2
$\dot{Q}_{gascool}$	16.3	21.4	12.5	6.0
$\dot{m}$	6.2	5.0	4.0	7.9
$\dot{W}_{comp}$	2.9	3.1	0.7	1.0
COP	2.9	0.2	8.0	13.4
Quality at evap in	5.3	2.2	5.1	5.6
Quality at evap out	0.0	1.0	1.0	0.0

Table 3b. Percentage differences between experimental and simulated values for data of Table 2.

Test point	M5
	|% difference|
Comp Pressure Ratio	2.8
$\dot{Q}_{evap}$	5.2
$\dot{Q}_{gascool}$	9.3
$\dot{m}$	3.0
$\dot{W}_{comp}$	1.4
COP	4.1
Quality at evap in	13.2
Quality at evap out	1.0

NOTE: % difference = (experimental value - simulation value)/(experimental value) x 100%