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Transcritical CO_2 Heat Pump Simulation Model and Validation for Simultaneous Cooling and Heating

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***Abstract*—**In the present study, a steady-state simulation model has been developed to evaluate the system performance of a transcritical carbon dioxide heat pump system for simultaneous water cooling and heating. Both the evaporator (including both two-phase and superheated zone) and gas cooler models consider the highly variable heat transfer characteristics of CO_2 and pressure drop. The numerical simulation model of transcritical CO_2 heat pump has been validated by test data obtained from experiments on the heat pump prototype. Comparison between the test results and the model prediction for system COP variation with compressor discharge pressure shows a modest agreement with a maximum deviation of 15% and the trends are fairly similar. Comparison for other operating parameters also shows fairly similar deviation between the test results and the model prediction. Finally, the simulation results are presented to study the effects of operating parameters such as, temperature of heat exchanger fluid at the inlet, discharge pressure, compressor speed on system performance of CO_2 heat pump, suitable in a dairy plant where simultaneous cooling at 4°C and heating at 73°C are required. Results show that good heat transfer properties of CO_2 for both two-phase and supercritical region and efficient compression process contribute a lot for high system COPs.

***Keywords*—**CO_2 heat pump, dairy system, experiment, simulation model, validation.

I. Introduction

CO_2 has regained interest lately due to its eco-friendliness, low price, non-flammability, non-toxicity, compatibility with various common materials, compactness, excellent transport properties, etc. and several theoretical and experimental studies have been done on transcritical CO_2 systems within last fifteen years particularly in heat pump applications [1]. CO_2 heat pumps offer extensive possibilities in simultaneous cooling and heating applications due to the large temperature glide present in the gas cooler. Due to its transcritical nature, the performance of carbon dioxide system will not be exactly the same as the conventional subcritical vapour compression refrigeration and heat pump systems. Hence, simulation models developed for the conventional systems cannot be employed for this new system. But, there is a need for theoretical system simulation studies as experimental performance evaluation is difficult, expensive and time consuming. So, accurate computer simulation of the system to predict its steady state performance and effects of various design and operating parameters on the steady state performance will be very useful, although empirical nature of heat transfer and pressure drop correlations needs validation.

Recently, simulation studies on air-to-water CO_2 heat pumps were done for comparison with traditional solution [2] and study the influence of ambient temperature [3]. White et al. [4] have developed simulation model of CO_2 heat pump for high temperature heating incorporating the component performance parameter correlations based on the test conducted on CO_2 heat pump prototype. Kim et al. [5] conducted performance test and simulation studies on CO_2 heat pump with internal heat exchanger for water heating. Although, such studies on simultaneous water cooling and heating are scarce. Author with his coworkers [6] previously presented simulation study on CO_2 heat pump for simultaneous water cooling and heating and subsequently, Agrawal and Bhattacharyya [7] have done similar study using capillary tube as an expansion device.

In the present study, the previous simulation model has been modified by incorporating the superheated zone in the evaporator model and more recent heat transfer correlations. Validation of the present simulation model with author's own experimental data on transcritical CO_2 heat pump prototype for simultaneous water cooling and heating is presented as well. Finally, effects of operating parameters such as, water inlet temperatures and compressor speed at optimum discharge pressure on system performance are presented for dairy applications; in such systems simultaneous cooling and heating at 4°C and 73°C, respectively, are required.

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II. Simulation Model

The simulated carbon dioxide based heating and cooling system consists of compressor, expansion valve, evaporator and gas cooler. Water is taken as secondary fluid for both gas cooler and evaporator to give the useful cooling and heating outputs. Both these heat exchangers are of double-pipe counter flow type, where the refrigerant flows through the inner tube and water flows through the outer annular space. The corresponding temperature-entropy diagram with water flow lines is shown in Fig. 1.

The entire system has been modeled based on energy balance of individual components yielding conservation equations presented below. To consider the lengthwise property variation, all the heat exchangers have been discretized and momentum and energy conservation equations have been applied to each segment. The following assumptions have been made in the analysis:

1. Heat transfer with the ambient is negligible.
2. Only Single-phase heat transfer occurs for water (external fluid).
3. Compression process is adiabatic but not isentropic.
4. Pressure drop on waterside and in connecting pipes are negligible.
5. Changes in kinetic and potential energies are negligible.
6. Refrigerant is free from oil.

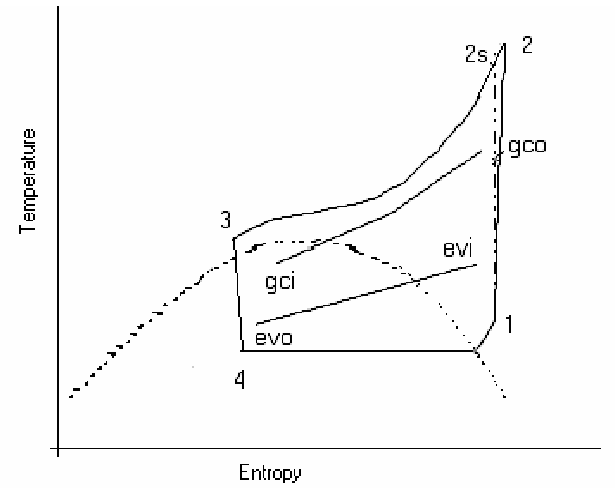

Fig. 1 Temperature-entropy diagram of a transcritical carbon dioxide system

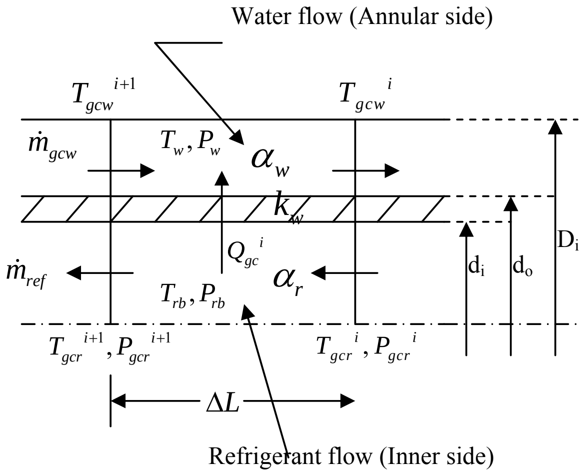

Fig. 2 A computational segment of gas cooler

A. Compressor Model

The refrigerant mass flow rate through the compressor is given by,

$$\dot{m}_r = \rho_1 \eta_v V_s \frac{N}{60} \tag{1}$$

where, volumetric efficiency η_v for the semi-hermetic compressor is estimated from [8]:

$$\eta_v = 0.9207 - 0.0756\left(\frac{P_{dis}}{P_{suc}}\right) + 0.0018\left(\frac{P_{dis}}{P_{suc}}\right)^2 \tag{2}$$

The isentropic efficiency of the compressor is estimated by employing the following correlation for the semi-hermetic compressor [8]:

$$\eta_{is,c} = -0.26 + 0.7952\left(\frac{P_{dis}}{P_{suc}}\right) - 0.2803\left(\frac{P_{dis}}{P_{suc}}\right)^2 + 0.0414\left(\frac{P_{dis}}{P_{suc}}\right)^3 - 0.0022\left(\frac{P_{dis}}{P_{suc}}\right)^4 \tag{3}$$

B. Gas Cooler Model

As mentioned earlier, the gas cooler is segmented lengthwise to accommodate the property variation. One of the computational segments of gas cooler of length ΔL is shown in Fig. 2. Employing LMTD expression, heat transfer in i^{th} segment of the gas cooler is given by,

$$Q_{gc}{}^{i} = (UA)_{gc}{}^{i} \frac{(T_{gcr}{}^{i} - T_{gcw}{}^{i}) - (T_{gcr}{}^{i+1} - T_{gcw}{}^{i+1})}{\ln\left(\dfrac{T_{gcr}{}^{i} - T_{gcw}{}^{i}}{T_{gcr}{}^{i+1} - T_{gcw}{}^{i+1}}\right)} \tag{4}$$

Additionally, energy balance in gas cooler for both the fluids yield:

$$Q_{gc}{}^{i} = \dot{m}_{ref}(h_{gcr}{}^{i} - h_{gcr}{}^{i+1}) = \dot{m}_{gcw} c_{pw}(T_{gcw}{}^{i} - T_{gcw}{}^{i+1}) \tag{5}$$

The overall heat transfer coefficient for the segment of gas cooler has been calculated using the fundamental equation for overall heat transfer coefficient yielding:

$$\frac{1}{UA_{gc}{}^{i}}=\frac{1}{\alpha_r A_r}+\frac{\ln\left(d_o/d_i\right)}{2\pi\Delta L k_w}+\frac{1}{\alpha_w A_w} \quad (6)$$

To estimate heat transfer rates, Gnielinski [9] equation is not suitable for normal tube (may be useful for micro-channel) due to large variation of fluid properties in the radial direction. To alleviate this deficiency, Pitla et al. [10] proposed a modification for supercritical in-tube carbon dioxide cooling, incorporating both bulk and wall properties. This correlation, used for gas cooler model, is given by;

$$Nu_r=\left(\frac{Nu_{rw}+Nu_{rb}}{2}\right)\frac{k_{rw}}{k_{rb}} \qquad \alpha_r=\frac{Nu_r}{d_i}k_{rb} \quad (7)$$

Here, Nu_{rb} and Nu_{rw} are the Nusselt numbers at bulk and wall temperature respectively, predicted by Gnielinski [9] equation within the range 2300 < Re < 10^6 and 0.6 < Pr < 10^5.

$$Nu=\frac{(f/8)(\mathrm{Re}-1000)\,\mathrm{Pr}}{1.07+12.7(f/8)^{1/2}(\mathrm{Pr}^{2/3}-1)} \quad (8)$$

where f is the friction factor given by: $f=(0.79\ln(\mathrm{Re})-1.64)^{-2}$

α_w is the waterside heat transfer coefficient and has been evaluated by the conventional Dittus-Boelter equation for annular flow. All water properties are assumed to be temperature dependent only, and polynomial expressions based on text book values have been used. Neglecting inertia effect, the refrigerant-side pressure drop in each hat exchanger segment is given by [11],

$$P_{gcr}{}^{i}-P_{gcr}{}^{i+1}=\frac{G_{gcr}{}^{2}}{2\rho_{rb}}\left(f\frac{\Delta L_{gc}}{d_i}+1.2\right) \quad (9)$$

where modified friction factor f is given by Petrov and Popov equation [11],

$$f=\left(1.82\ln(\mathrm{Re}_{rw})-1.64\right)^{-2}\frac{\rho_{rw}}{\rho_{rb}}\left(\frac{\mu_{rw}}{\mu_{rb}}\right)^{s} \quad (10)$$

where, the exponent s is given by, $s=0.023\left|\frac{Q_{gcr}{}^{i}}{G_{gcr}}\right|^{0.42}$.

C. Evaporator Model

Employing the LMTD-concept, heat transfer in each segment of the evaporator is given by,

$$Q_{ev}{}^{i}=(UA)_{ev}{}^{i}\frac{(T_{evw}{}^{i+1}-T_{evr}{}^{i+1})-(T_{evw}{}^{i}-T_{evr}{}^{i})}{\ln\left(\frac{T_{evw}{}^{i+1}-T_{evr}{}^{i+1}}{T_{evw}{}^{i}-T_{evr}{}^{i}}\right)} \quad (11)$$

Energy balance in the evaporator for the refrigerant (CO_2) and water, respectively, yields:

$$Q_{ev}{}^{i}=\dot{\mathrm{m}}_{\mathrm{ref}}(h_{evr}{}^{i+1}-h_{evr}{}^{i})=\dot{\mathrm{m}}_{\mathrm{evw}}c_{pw}(T_{evw}{}^{i+1}-T_{evw}{}^{i}) \quad (12)$$

The overall heat transfer coefficient for each segment of the evaporator has been calculated in the same way as for the gas cooler. In this analysis, the recently developed Yoon et al. [12] correlation has been employed to estimate the boiling heat transfer coefficient. For superheated zone, Gnielinski [9] equation has been used to estimate convective heat transfer coefficient of carbon dioxide. The waterside heat transfer coefficient has been evaluated by the conventional Dittus-Boelter equation for annular flow for both two-phase and superheated sections.

The refrigerant side pressure drop, $\Delta P_{ev,r}$, is given by (using Lockhart and Martinelli equation):

$$P_{evr}{}^{i}-P_{evr}{}^{i+1}=4\frac{\Delta L_{ev}}{d_i}\frac{f_r}{2}(1-x)^2\frac{G_{evr}^2}{\rho_l}\phi_l^2 \quad (13)$$

where, friction factor $f_r=0.0791\,\mathrm{Re}_l^{-0.25}$

and the two-phase frictional pressure drop multiplier is evaluated from:

$$\phi_l=\left(1.376+\frac{7.242}{X_{tt}{}^{1.655}}\right)^{1/2}$$

where X_{tt} is the Lockhart-Martinelli factor.

It can be noted that the evaporator consists of two zones: two-phase zone and superheated zone. Similar to the gas cooler, both zones in the evaporator are divided into a finite number of equal-length segments along the refrigerant flow direction. Each segment is treated as one counter-flow heat exchanger and the outlet conditions of each segment should become inlet conditions for the next segment. For each segment LMTD method is used and properties are evaluated based on mean temperature and pressure.

D. Expansion Device

The expansion process is considered to be isenthalpic under the assumption that the heat exchange with its surroundings is negligible, yielding:

$$h_4=h_3 \quad (14)$$

E. Numerical Procedure

A computer code, incorporating the subroutine 'CO2PROP' [6] for thermophysical and transport properties, has been developed to simulate the transcritical carbon dioxide system for simultaneous water cooling and heating at various operating conditions. Water inlet temperatures and water mass flow rates or outlet temperatures for both heat exchangers, compressor data, evaporator and gas cooler dimensions, compressor discharge pressure and degree of superheat are the input data for the simulation. As mentioned earlier, the property variations are encompassed by both evaporator and gas cooler models. Using discretization, the heat exchanger is made equivalent to a number of counter flow heat exchangers arranged in series and the combined heat transfer of all the segments is the total heat transfer of the heat exchanger. Therefore, fast changing properties of CO_2 have been modeled accurately in both evaporator and gas cooler. The code solves the system equations by suitable iterative method and tolerance has been maintained in the range of 10^{-3}. Pressure drop and heat loss in connecting lines are not considered; therefore, the outlet state of one component becomes the inlet state of the next component. By assuming suction pressure, refrigerant mass flow rate, compressor outlet conditions, refrigerant conditions as well as enthalpies (h_4 and h_3) at evaporator inlet and at gas cooler outlet are calculated based on mathematical model presented above. The suction pressure is adjusted by the iteration in order for the enthalpy of inlet and outlet expansion valves to converge within a prescribed tolerance and performances such as cooling and heating output, compressor work and COP are calculated. By varying the discharge pressure, maximum COP and corresponding optimum discharge pressure can be calculated.

III. Model Validation

The present numerical simulation model of transcritical CO_2 heat pump for simultaneous water cooling and heating applications has been validated by test data obtained from experiments on the prototype. The experimental CO_2 heat pump prototype consists of Dorin compressor (displacement is 2.2 m^3/h @ 2900 rpm), evaporator, gas cooler, manually controlled needle valve, receiver, accessories and instrumentation. Both the heat exchanger are tube-in-tube, coaxial, countarflow types, made of standard stainless steel, where refrigerant flows in inner tube and water in annulus. For evaporator, outer diameters of inner and outer tubes are 9.5 mm and 16 mm, respectively (thickness of 1 mm for both tubes) and total length is 7.2 m. For gas cooler, outer diameters of inner and outer tubes are 6.35 mm (thickness is 0.8 mm) and 12 mm (thickness is 1mm), respectively and total length is 14 m. Separate water circuits are used for both evaporator and gas to maintain constant inlet temperatures. Prototype description with instrumentations, testing, data reduction and error analysis, which shows the uncertainty range of ± 6%, have already reported earlier [13].

The experimental results clearly showed that superheating takes place in the evaporator ranging from 15-22 °C. Fig. 3 shows the comparison of model predicted and test data for system COP (combined heating and cooling outputs per compressor work), variation with the compressor discharge pressure, for water mass flow rates of 1.5 kg/min and 1 kg/min, and water inlet temperatures of 30 and 30.5°C in evaporator and gas cooler, respectively and evaporator pressure of 40 bar. Comparison between the test results and the model prediction shows a modest agreement with a maximum deviation of 15% and the trends are fairly similar. Comparison for other operating parameters also shows fairly similar deviation between the test results and the model prediction. Hence, the present simulation model can be used to predict the performance.

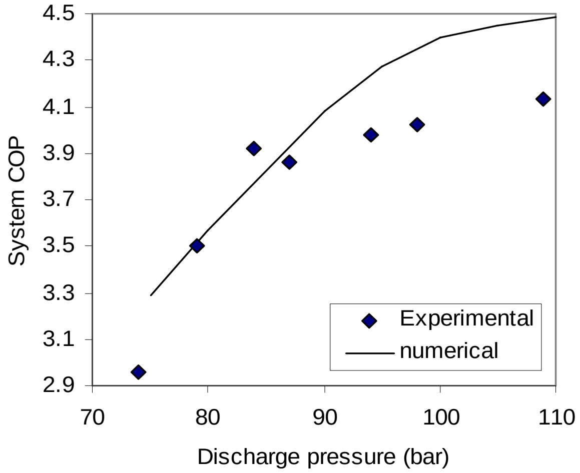

Fig. 3 Validation of numerical results against experimental data

IV. Effects of Operating Parameters

Effects of operating parameters on the system performance being studied for simultaneous water heating and cooling applications are evaluated on the basis of maximum system COPs at optimum discharge pressure. Gas cooler and evaporator dimensions, and compressor specifications, input to the simulation model, are same as for experimental prototype. It can be noted that as the water outlet temperatures of evaporator and gas cooler are fixed at 4°C and 73°C, respectively, water mass flow rates are assumed to be adjustable parameters in simulation, unlike to the experimental study. The degree of superheat is taken in the simulation as 10°C. The parameters varied are: compressor speed from 1500 to 3500 rpm, water inlet temperature from 20°C to 40°C for both evaporator and gas cooler. Unless otherwise specified, the mean values of these parameters are: compressor speed of 2900 rpm, water inlet temperature of 30°C.

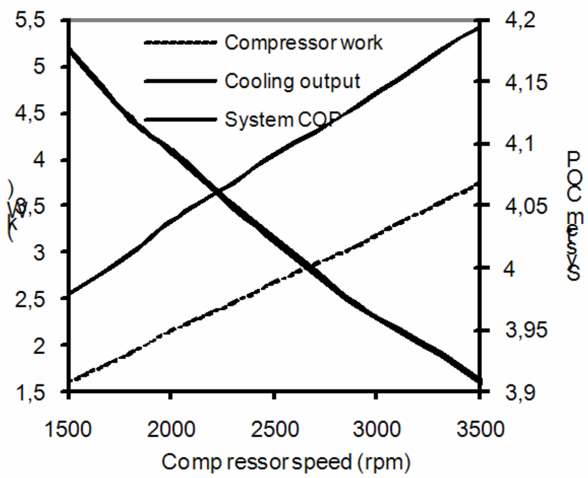

Fig. 4 Variation of performance with compressor speed

The effect of compressor speed on system performance at water inlet temperature of 30°C for both evaporator and gas cooler is presented in Fig. 4. It is observed that the system COP at optimum discharge pressure decreases as both compressor work and cooling output increase with compressor speed due to an increase in mass flow rate of refrigerant with compressor speed. However, the optimum discharge pressure was found to remain almost constant varying between 107 and 109 bar as the speed was modulated between 1500 and 3500 rpm.

The effect of water inlet temperature (same water inlet temperature for both evaporator and gas cooler) at a compressor speed of 2900 rpm is shown in Figs. 5 and 6. As the water inlet temperature increases, the cooling COP decreases due to the combined effect shifting of cooler exit refrigerant temperature to higher value that cause the degradation of heat transfer properties in gas cooler and decrease in two-phase region range. Water inlet temperature has a negligible effect on refrigerant mass flow rate as shown in Fig. 6. However, the optimum discharge pressure increases rapidly with increase in water inlet temperature due to rapid change of refrigerant outlet temperature as rapid changes in heat transfer properties in the gas cooler.

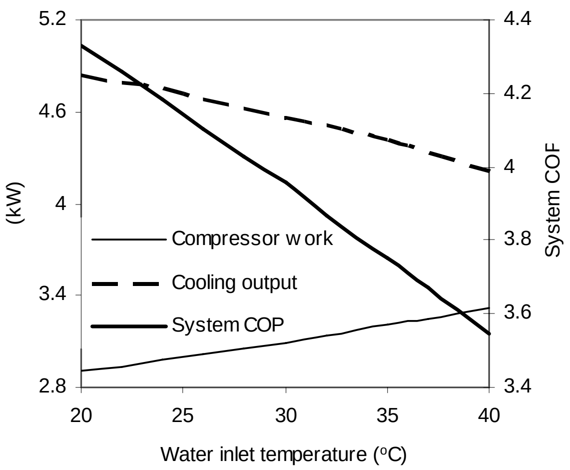

Fig. 5 Variation of performance with water inlet temperature

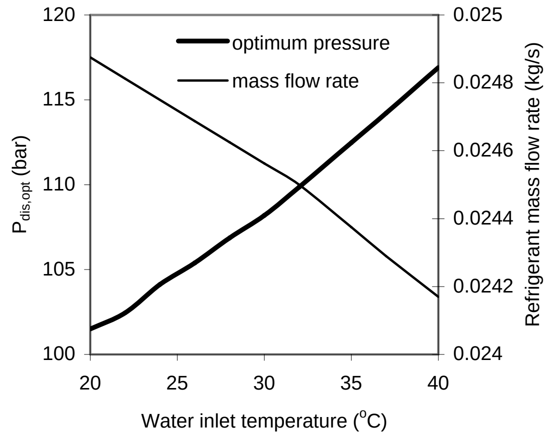

Fig. 6 Variation of optimum pressure and mass flow rate with water inlet temperature

V. Conclusion

The steady state performance of a carbon dioxide based transcritical heat pump for simultaneous water heating and cooling is presented here. The simulation model has been validated with the experimental data. Results are obtained by varying important operating parameters such as compressor speed and water inlet temperature over a given range. Comparison between the test results and the model prediction shows a modest agreement with a maximum deviation of 15% and the trends are fairly similar. Comparison for other operating parameters also shows fairly similar deviation between the test results and the model prediction. Effect of water inlet temperature on the optimum discharge pressure is very significant whereas effect of compressor speed is negligible. Results show that good heat transfer properties of carbon dioxide for both two-phase and supercritical region and efficient compression process contribute a lot for high system COPs.

Nomenclature

A	heat transfer area	(m^2)
c_p	specific heat capacity	(J/kgK)
d	inner tube diameter	(m)
D	outer tube diameter	(m)
G	mass velocity	(kg/m^2s)
h	specific enthalpy	(kJ/kg)
k	thermal conductivity	(W/mK)
k_w	wall thermal conductivity	(W/mK)
$\dot{m}$	mass flow rate	(kg/s)
N	compressor speed	(rpm)
Nu	Nusselt number	(-)
P	pressure	(bar)
Pr	Prandtl number	(-)
Q	heat transfer rate	(W)
Re	Reynolds number	(-)
T, t	temperatures	(K, °C)
U	overall heat transfer coefficient	(W/m^2K)

V_s	swept volume of compressor	(m^3)
x	quality of saturated carbon dioxide liquid vapor mixture	
α	heat transfer coefficient	(W/m^2K)
ΔL	segment length	(m)
f	friction factor	(-)
μ	viscosity	(kg/ms)
ρ	density	(kg/m^3)

Subscripts

1-4	statepoints
b	bulk
dis	compressor discharge
ev	evaporator
evr	refrigerant in evaporator
evw	evaporator water
gc	gas cooler
gcr	gas cooler refrigerant
i	inner
o	outer
l	liquid
opt	optimum
r	refrigerant
suc	suction
w	wall, water
wi	water inlet

Superscript

i	segmental step

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