TRANSCRITICAL CARBON DIOXIDE DIRECT-EXPANSION GROUND COUPLED HEAT PUMP: MODELING AND APPLICATION

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Abstract: Although geothermal heat pumps have been attracting more attention these days due to several energy efficiency and environmental benefits, they might be criticized over the fact that the performance decreases significantly over seasonal operation due to the unbalance loading in the ground. However, in direct-expansion geothermal heat pumps using carbon dioxide the performance drop is relatively small due to less sensitive operation to evaporating temperature, elimination of the secondary loop, efficient compression and relatively low pressure drop in the ground loop portion.
In this study, a theoretical quasi-transient model is developed to quantify the performance drop of a CO_2 direct-expansion geothermal heat pump over time. The system under study consists of a compressor, gas cooler, internal heat exchanger, expansion valve and a vertical geothermal borehole. Steady-state thermodynamic and heat transfer calculations of system components are coupled with transient heat transfer model in the ground.
The model is used to simulate a relatively small heat pump over 48 hours. Results show that the coefficient of performance decreases slightly by 4.9% over the first 12 hours and only by 1.8% over the next 36 hours due mainly to less sensitive performance to evaporating temperature. It is also shown that the evaporator temperature decreases only by about 2°C due to relatively low pressure drop in the borehole attributed to significantly low kinematic viscosity and surface tension of CO_2.

Key words: ground coupled heat pump, transient simulation, transcritical, carbon dioxide

1 INTRODUCTION

Carbon Dioxide (CO_2) has been attracting more attention as a refrigerant for heat pumps these days as it is environmentally friendly and it offers interesting thermodynamic characteristics and superior thermophysical properties. This, together with the established energy efficiency advantage of ground coupled heat pumps (GCHPs), makes the geothermal CO_2 heat pump a promising environmentally energy efficient option.
In order to link CO_2 heat pumps to the ground, geothermal boreholes should be either an integral part of the heat pump called direct-expansion ground-coupled heat pump (DX-GCHP) or linked indirectly to the heat pump, like the typical secondary-loop ground-coupled heat pump (SL-GCHP). DX systems offer thermodynamic and system efficiency advantages over secondary loop (SL) systems, due to the elimination of the secondary heat transfer fluid heat exchanger

and the circulating pump (Guo et al. 2012). However, the scarcity of related technical knowledge has significantly slowed its widespread use.

In general, modeling of direct-expansion geothermal heat pumps has been rarely studied. Most of the existing studies experimentally evaluated the whole system performance using typical refrigerants (Guo et al. 2012, Wang et al. 2009, Lenarduzzi and Bennet 1991, Goulburn and Fearon 1983 and Johnson 2002), some other studies were performed to establish some guides and improvements for the design (Mei and Baxter 1990 and Wang et al. 2013) and Beauchamp et al. 2013 developed a numerical model to analyse the performance of a ground heat exchanger used as an evaporator.

Very few works have recently studied geothermal heat pumps using CO_2. Recent studies by Eslami Nejad et al. 2014 focused only on numerical modeling of CO_2-filled vertical geothermal boreholes. Austin and Sumathy 2011 is one of the few studies that simulate the whole cycle. They developed a numerical model to analyze the thermodynamic performance of a DX-GCHP using horizontal borehole. However, they applied a cylindrical steady-state thermal resistance for conduction in the ground and they did not account for dynamic characteristics of the system.

In the present study, a theoretical model is developed to analyse the quasi-transient performance of a CO_2 DX-GCHP. Steady-state thermodynamic and heat transfer calculations of the system components are coupled with one-dimensional (1D) transient heat transfer model in the ground. The model accounts for the dynamic temperature variation in the ground and can be used to investigate the system performance over time.

2 NOMENCLATURE

c_p	Specific heat (J/kgK)
h	CO_2 enthalpy (kJ/kg)
k	Thermal conductivity (W/mK)
$\dot{m}_c$	CO_2 mass flow rate (kg/s)
$\dot{m}_w$	Water mass flow rate (kg/s)
P	Pressure (MPa)
q''_b	Heat flux at the borehole wall (W/m^2)
Q_e	Total heat transfer rate in boreholes (W)
Q_{gc}	Heat transfer rate in gas cooler (W)
Q_{IHE}	Heat transfer rate in internal heat exchanger (W)
r	Radial direction in the ground perpendicular to the borehole depth (m)
r_b	Borehole radius (m)
r_p	Borehole pipe external radius (m)
t	Time (s)
T	Temperature (°C)
T_g	Undisturbed ground temperature (°C)
$T_{w,in}$	Inlet water temperature to gas cooler (°C)
$T_{w,out}$	Outlet water temperature to gas cooler (°C)
UA	Overall heat transfer coefficient (W/K)
$\dot{V}_{swept}$	Swept volume rate of compressor (m^3/hr)
Greek symbols	
α	Thermal diffusivity (m^2/day)
ε	Heat exchanger effectiveness
η_v	Volumetric efficiency
η_{isen}	Isentropic efficiency

ρ	Density (kg/m^3)

Subscripts

1 to 6	Thermodynamic states shown in Figure 2
gt	Grout
c	CO_2
g	Ground
gc	Gas cooler
IHE	Internal heat exchanger
in	Inlet
isen	Isentropic
out	Outlet
sh	Superheat
w	Water

3 SYSTEM DESCRIPTION

As shown in Figure 1, the DX-GCHP under this study consists of five main system components including the compressor (1-2), the gas cooler (2-3), the internal heat exchanger (3-4), the expansion valve (4-5) and the geothermal borehole (5-6). In this system CO_2 (Refrigerant) is flowing directly down to the borehole, changing direction at the bottom (U connection) and coming up to extract heat from the ground by evaporation. Then it enters the internal heat exchanger to exchange heat with the gas at the gas cooler exit in order to be superheated to a certain degree. The gas is then compressed by the compressor to supercritical pressure with a corresponding temperature rise. The high pressure/high temperature vapor enters the gas cooler to heat the water. Finally, after the internal heat exchanger, low temperature/high pressure CO_2 gas is throttled to the lower pressure level of the cycle.

Table 1: System characteristics

Parameters	unit	value
k_g	W/mK	2.65
α_g	m^2/day	0.08
k_{gt}	W/mK	2.0
r_b	cm	3.9
$r_{p,in}$	cm	0.32
$r_{p,out}$	cm	0.4
$2D$	cm	2.32
L	m	4x30
ΔTsh	°C	5
$T_{gc,out}$	°C	35
$T_{w,in}$	°C	20
T_g	°C	10
UA_{IHE}	W/K	58.5
ε_{gc}		0.78
$\dot{V}_{swept}$	m^3/hr	1.12
$\dot{m}_w$	Kg/s	0.03

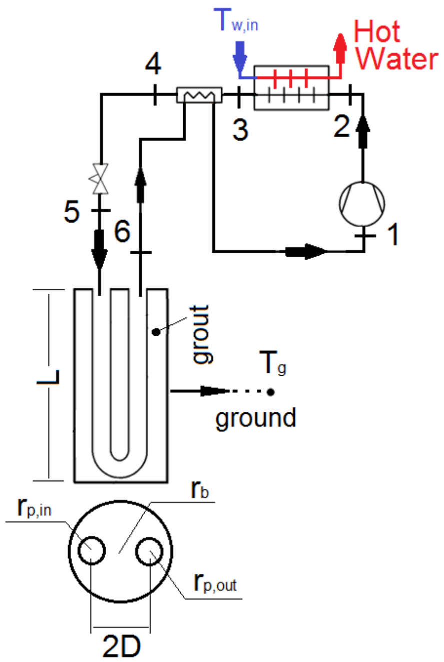

Figure 1: Schematic presentation of the system

The steady-state borehole model is coupled to 1D transient heat conduction in the ground. This model is then used along with simple steady-state thermodynamic and heat transfer calculations of other system components to analyse the system for water heating under quasi-transient conditions. A brief explanation of each system component, along with important governing equations, is given in the theoretical model section.

4 THEORETICAL MODEL

The performance of the system described in the previous section is analyzed using a combined steady-state numerical model for the borehole, a transient analytical model for the ground and some simple heat transfer and thermodynamic models for the expansion valve, the compressor and the heat exchangers. Some general assumptions to develop the theoretical models are:

- All the system components are operating under steady-state conditions
- Pressure drop in connecting tubes is neglected
- Flow for the CO_2 inside tubes is one-dimensional
- Heat loss to the environment is ignored, except in the boreholes where CO_2 exchanges heat with the ground. This process is transient.
- Changes in kinetic and potential energy are negligible.

The theoretical analysis of each model is discussed separately as follows:

4.1 Geothermal borehole

The geothermal borehole consists of a long copper U-tube (two pipes) embedded in a solid material (grout). In this study, a detailed numerical steady-state model developed by Eslami-Nejad et al. (2014) is used. The model is based on 1D fluid heat transfer in the axial direction (along borehole depth) as well as two-dimensional (2D) thermal resistances between the borehole wall and the fluid in the pipes. The model can predict two-phase temperature, pressure and vapor quality profiles of CO_2 along the borehole.
Four boreholes with relatively small diameters (78 mm) are considered to extract the required heat from the ground (Q_e). They are connected in parallel and located far enough from each other, with negligible thermal interaction. It is assumed that the grout material is homogeneous and the heat capacity of the grout as well as the heat conduction in the axial direction is negligible. Borehole dimensions and the grout thermal conductivity (k_{gt}) are listed in Table 1.

4.1.1 Heat transfer in the ground

It is well known (Marcotte et al. 2010) that axial effects in boreholes heat transfer become important only after several years of operation, however; only radial dependence is taken into account. In that case, the basic problem is to find the temperature distribution (T) in the direction perpendicular to the borehole (r) satisfying the heat conduction equation.

$$\frac{1}{\alpha_g}\frac{\partial T}{\partial t}=\frac{\partial^2 T}{\partial r^2}+\frac{1}{r}\frac{\partial T}{\partial r} \tag{1}$$

for the domain from the borehole wall to the far field ($r > r_b$) and the following boundary conditions,

$$T(r,0)=T_g \quad , \quad T(\infty,t)=T_g \quad , \quad -k_g \left.\frac{\partial T}{\partial r}\right|_{r=r_b} = q_b''(t) \text{ at } r=r_b \tag{2}$$

where q_b'' is the heat flux at the borehole wall and T_g is the undisturbed ground temperature. The solution of Equation (1) is classical and it can be found in several classic books (Ozisik ,1993). However, in the context of borehole design, the solution is evaluated at $r=r_b$, and for a constant heat pulse ($q_b''=const.$). This special case is the classical infinite cylindrical source (ICS). For a variable heat pulse, the solution is usually found by superposing the heat pulses response. This form of solution is basically the discrete convolution of the variable heat load with the heat pulse response. The calculation of discrete convolution is known to be very time consuming. Lamarche and Beauchamp (2007) proposed a non-history scheme, valid for the ICS solution which can solve the problem in a very rapid way. It assumes that the heat flux is known at the borehole. Here the fluid temperature at the inlet or outlet of the borehole is imposed, so the initial scheme has to be modified. The details of the scheme are described in the reference. For the present study, 6 min time step is used. The undisturbed ground temperature is equal to 10℃ and the ground thermal conductivity and diffusivity are listed in Table 1.

4.2 Compressor

A semi-hermetic compressor is used in this study and the mass flow rate of CO_2 through the compressor is given by:

$$\dot{m}_c = \rho_1 \eta_v \dot{V}_{swept} \tag{3}$$

The volumetric and isentropic efficiency correlations developed by Oritz et al. 2003 for semi-hermetic compressors are used:

$$\eta_v = -0.9207 - 0.0756\left(\frac{P_2}{P_1}\right) + 0.0018\left(\frac{P_2}{P_1}\right)^2 \tag{4}$$

$$\eta_{isen} = -0.26 + 0.7952\left(\frac{P_2}{P_1}\right) - 0.2803\left(\frac{P_2}{P_1}\right)^2 + 0.0414\left(\frac{P_2}{P_1}\right)^3 - 0.0022\left(\frac{P_2}{P_1}\right)^4 \tag{5}$$

The change in CO_2 enthalpy over compression in the compressor is calculated as:

$$\left(h_2 - h_1\right) = \frac{(h_{2,isen} - h_1)}{\eta_{isen}} \tag{6}$$

4.3 Gas cooler

The ε-NTU method is used to model the gas cooler. Although the heat transfer in the gas cooler is reported as highly non-linear by number of studies, the whole gas cooler is taken as one segment to simplify the calculations. However, in order to account for the rapid change in specific heat through the supercritical region, the mean values are taken over the temperature range in the gas cooler.

$$Q_{gc} = \varepsilon_{gc} \cdot C_{\min} \cdot \left(T_2 - T_{w,in}\right) \tag{7}$$

where, C_{min} is the smaller heat capacity rate of the two fluids (water and CO_2) in the gas cooler. Since the heat released by CO_2 is taken by the water, the energy balance is added as follows:

$$Q_{gc} = \dot{m}_c \cdot (h_2 - h_3) = \dot{m}_w \cdot c_{p,w} \cdot (T_{w,out} - T_{w,in}) \quad (8)$$

Water inlet temperature ($T_{w,in}$), water mass flow rate ($\dot{m}_w$) and gas cooler effectiveness (ε_{gc}) are assumed to be constant at 20℃, 0.03 (*kg/s*) and 0.78 respectively. Furthermore, the pressure drop of both water and CO_2 sides is assumed to be negligible. In order to get the best efficiency in the specified conditions, the CO_2 exit temperature from the gas cooler is set to 35℃.

4.4 Internal heat exchanger

The LMTD method is employed for the internal heat exchanger. Like the gas cooler the entire heat exchanger is taken as one calculation segment.

$$Q_{IHE} = UA \cdot \frac{(T_3 - T_1) - (T_4 - T_6)}{\ln[(T_3 - T_1)/(T_4 - T_6)]} \quad (9)$$

Relatively low temperature/high pressure supercritical region after the gas cooler (state 3 to 4) internally transfers the heat to the subcritical region after the evaporator to fully evaporate CO_2 and guarantees a few degrees of superheat at the inlet of the compressor. The heat balance equation is written as:

$$Q_{IHE} = \dot{m}_c \cdot (h_3 - h_4) = \dot{m}_c \cdot (h_1 - h_6) \quad (10)$$

The degree of superheat (ΔT_{sh}) is an input to the calculation which is 5℃ in this study. The overall heat transfer coefficient is assumed to be constant equal to 58.5 W/m^2, corresponding to a heat exchanger efficiency of 80%. The pressure drop in both supercritical and subcritical sides of the heat exchanger is ignored.

4.5 Expansion valve

The expansion valve process is considered to be isenthalpic:

$$h_4 = h_5 \quad (11)$$

5 SIMULATION PROCEDURE

A computer code has been developed to simulate the quasi-transient operation of a transcritical carbon dioxide heat pump. The operating parameters used to start a simulation include: degree of super heat, temperature of CO_2 at the exit of the gas cooler, water inlet temperature and mass flow rate, compressor speed, borehole dimensions and characteristics of both the internal heat exchanger and the gas cooler. They are all listed in Table 1. At each time step, three main iterative numerical procedures are used to determine the steady-state operating conditions of the system components, as well as the ground thermal condition for the next time step. In the last iterative loop, the borehole wall temperature is updated, using the transient heat transfer calculation in the ground. Based on the convergence criteria for each loop, all three loops iterate interactively until they all converge. The CO_2 properties required throughout the simulation procedure are evaluated by REFPROP version 9.0 (Lemmon et al, 2013).

6 RESULTS AND DISCUSSION

Geothermal heat pumps are criticized over the fact that the performance decreases over time due to the temperature change in the ground. For example, for systems operating in heating mode, the ground temperature in the vicinity of the borehole decreases due to the heat extracted by the borehole from the ground. Therefore, transient simulation of geothermal heat pumps is very important to capture the dynamic characteristics of the system. The quasi-transient model developed in this study accounts for transient heat transfer in the ground giving the possibility of investigating the performance of a transcritical DX-GCHP over time. In this study the model is used to simulate a heat pump that produces hot water for low-energy buildings (passive buildings) where hot water load is comparable to space heating load.
Figure 2 presents the cycle diagram (P-h) of the heat pump after 1 hour and 48 hours of operation, respectively in dash and solid lines. The cycle consists of 6 thermodynamic states (points) and in Table 2 is listed the CO_2 temperature corresponding to each point.
In both cycles, 5°C superheat is considered at the inlet of compressor (point 1) and gas cooler exit temperature is fixed at 35°C.
Although geothermal heat pumps are not sized to work continuously for 48 hours, what is shown in Figure 2 is that even over long operation, heat pump operating condition does not differ significantly. As shown in Figure 2, the pressure in the evaporator decreases by about 0.2 MPa (3.95 MPa to 3.75 MPa at point 5) from 1 hr to 48 hrs of operation. This represents 2°C drop in temperature presented in Table 2 (4.8°C to 2.8°C at point 5). The reduction in pressure causes a drop in density of point 1, leading to a slight decrease in the mass flow rate of CO_2 by about 8 % (from 0.025 kg/s to 0.023 kg/s). Since the water mass flow rate is constant (0.03 kg/s) and CO_2 mass flow rate decreases, inlet temperature of gas cooler increases to maintain 35°C at the exit of the gas cooler.

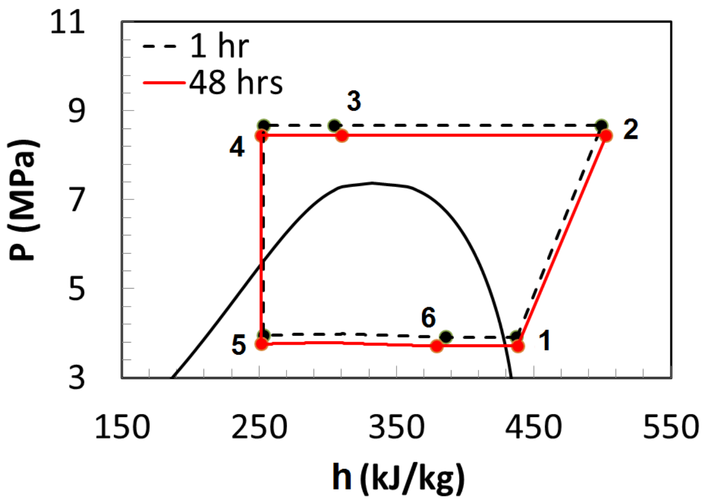

Figure 2: Cycle diagram (P-h) after 1 hour operation and after 48 hours operation

Table 2: Temperature of thermodynamic states presented in Figure 2

	Temperature (°C)	
Point	**1 hr**	**48 hrs**
1	9.4	7.4
2	89.4	90.3
3	35.0	35.0
4	22.7	22.0
5	4.8	2.8
6	4.4	2.4

Figure 3 and Figure 4, present vapor quality and temperature profiles respectively in the evaporator (borehole) after 1 hour and after 48 hours of operation. Although temperature decreases by about 2°C (from 1 hr to 48 hrs), very slight changes are observed in the vapor quality. As shown in Figure 3, CO_2 enters the borehole at quality of 0.19 and 0.2 and it exits at

0.81 and 0.78 after 1 hour and 48 hours respectively. It is interesting to mention that from the beginning to the end of the simulation; about 55% of heat is extracted by the second leg of the U-tube which is not the case in the secondary loop GCHP systems with noticeable performance drop from the first leg to the second leg (Zeng et al. 2003). The performance increase in DX systems is basically due to the overall temperature drop of refrigerant over the pipe length (Figure 4). As shown in Figure 4, CO_2 temperature decreases from 4.8 to 4.4 and from 2.8 to 2.4 due to corresponding pressure drop of 35.3 and 40.7 after 1 hour and after 48 hours of operation respectively. Temperature rise at the beginning of the borehole is due to the fact that the gravitational pressure increase is the dominant part that can increase the global pressure for the down flowing fluid. However, in the second leg where the fluid is flowing upwards, the temperature drop, as well as the pressure drop is more pronounced since the gravity is in the opposite direction of the flow.

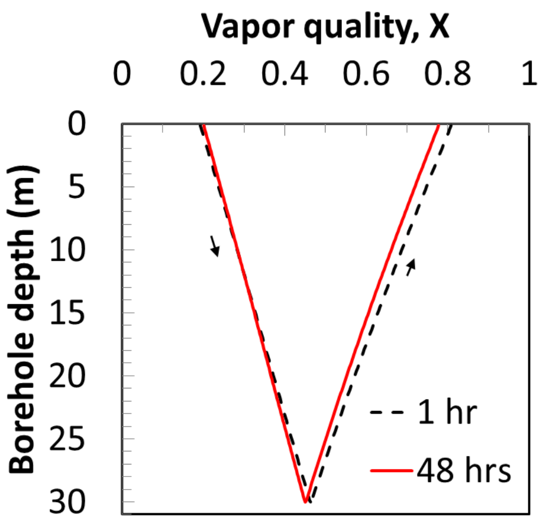

Figure 3: Vapor quality profile of CO_2 in the borehole

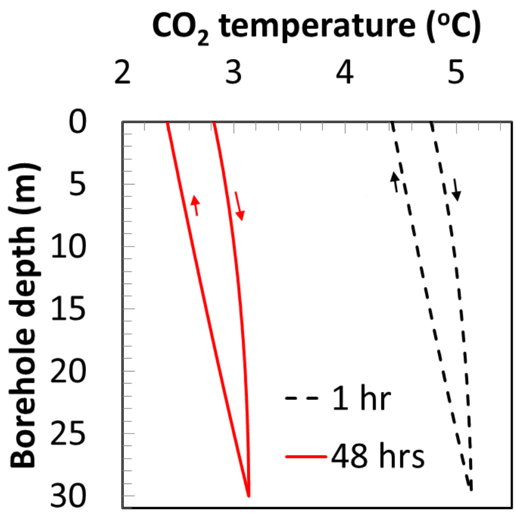

Figure 4: Temperature profile of CO_2 in the borehole

Figure 5 presents the evolution of hot water temperature ($T_{w,out}$) over time at the exit of the gas cooler. The gas cooler is sized to heat water from 20°C to 60°C. As shown in Figure 5, when the heat pump starts, $T_{w,out}$ reaches 60°C, however; it decreases to 55.7°C after 48 hours of operation as the heat pump capacity drops. This may not be the case as in real application hot water temperature is kept constant at 60°C (to prevent legionella growth) and either water mass flow rate or heat pump capacity may change.

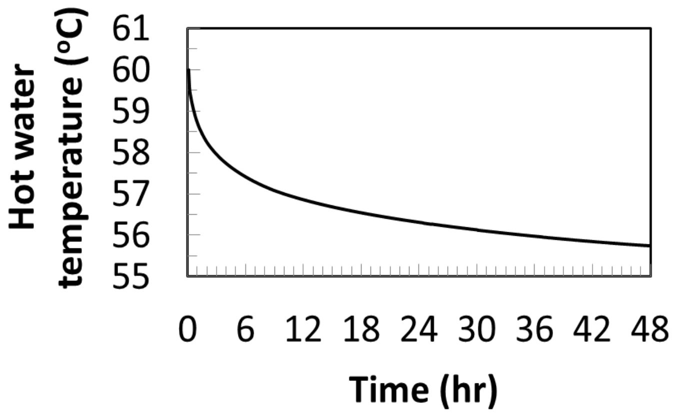

Figure 5: Hot water exit temperature ($T_{w,out}$) as a function of time

Figure 6 presents the evolution of three parameters including the heat pump coefficient of performance (COP), the extracted heat from the ground (Q_e) and the heating capacity of the heat pump (Q_{gc}) over 48 hours of operation.

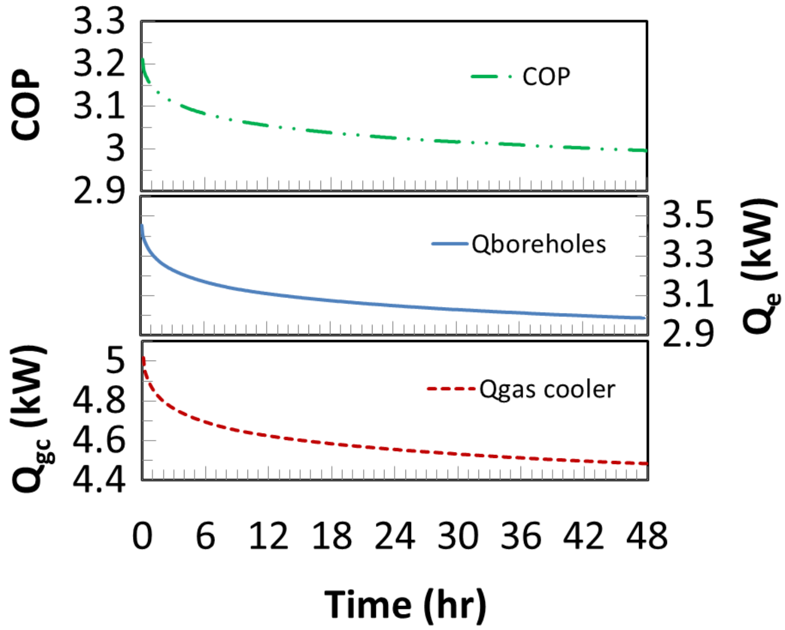

Figure 6: Heat pump COP (top), extracted heat from the ground (middle) and heating capacity of the heat pump (bottom) over simulation time

As shown in Figure 6, at start up, the heat pump is able to deliver 5 kW with a COP of 3.2 to heat the water to 60℃. This performance is superior to both DX-GCHP and conventional systems using typical refrigerants (Lenarduzzi and Bennet 1991, Goulburn and Fearon 1983 and Nekså 2002). After 12 hours of operation COP decreases by 4.9% representing a drop of 7.8 % in the heat pump capacity. However, over the next 36 hours, COP and heat pump capacity drop slightly by only 1.8% and by 2.8 % respectively. The relatively small performance and capacity drop of CO_2 can be explained by low sensitivity of its performance to evaporating temperature (Kim et al. 2004).

In addition, borehole performance decreases by less than 10% from extracting 864 W per borehole at the beginning to 778 W after 12 hours. However, for the last 36 hours, borehole performance decreases only by 3.5%. This is due to significantly small pressure drop of CO_2 along the borehole that would maintain relatively constant temperature deference between the fluid and the ground all over the borehole.

6 CONCLUSION

In this study, a theoretical model has been developed to analyze the quasi-transient performance of a transcritical direct-expansion ground coupled heat pump, using CO_2. Steady-state thermodynamics and heat transfer calculations of system components including compressor, gas cooler, expansion valve, internal heat exchanger and geothermal boreholes are linked to 1D transient heat transfer model in the ground.
In order to analyse the system performance for water heating application, a relatively small heat pump with characteristics listed in Table 1 is simulated for 48 hours. In general, it can be concluded that the CO_2 heat pumps can offer relatively higher COP for water heating compared to other refrigerants. Furthermore, even over long operation time, heat pump operating condition does not change significantly due to the less sensitive performance to evaporating temperature, efficient compression, relatively low pressure drop in evaporator and superior thermophysical and thermodynamic characteristics of CO_2.
Detailed dynamic analysis showed that the COP, the heat pump capacity and the heat extracted by the boreholes decreased over the first 12 hours of operation by 4.8%, 6.8% and 10% respectively, while they significantly diminished over the next 36 hours to 1.9%, 2.8% and 3.5%. It is also shown that the evaporator temperature drops only by 2℃ due to the temperature reduction of the ground in the borehole vicinity; however, the vapor quality profile along the borehole experiences very small changes over simulation time.
It is worth mentioning that the 48-hour continuous operation is exaggerated here to evaluate the performance of geothermal CO_2 heat pump under long operating condition. However, in real applications, heat pumps are sized to cycle more often and geothermal heat pumps can recover quite fast from the last operation period.
Finally, it is recommended that a detailed modeling of the internal heat exchanger and the gas cooler be incorporated to perform a thorough comparative analysis between different refrigerants and CO_2.

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