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Techno-Economic Analysis for Early-Stage Assessment of Chemical Looping Heat Pump Technology

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ABSTRACT

Heating, ventilation, air conditioning, and refrigeration (HVAC&R) in buildings is responsible for a significant portion of the U.S. primary energy consumption. To address energy and climate issues, technological breakthroughs for next generation HVAC&R technologies are expected to enable high energy efficiency and decarbonization targets. Among the novel technologies, the chemical looping heat pump (CLHP) has been proposed as a promising and valuable alternative to conventional vapor compression (VC) systems. Previous analyses have shown that CLHPs can achieve 20-30% performance improvements with significant cost savings opportunities. However, there has been no direct comparison of economics between CLHP and existing technologies.

In this work, a modeling framework to estimate levelized cost of energy (LCOE) for space conditioning applications is developed to enable a direct early-stage comparison of emerging technologies with conventional VC systems. The LCOE is composed of two contributions, levelized operating expenditures (OPEX) and levelized capital expenditures (CAPEX), that are helpful in understanding the influence of key factors such as unit utilization (annual cooling and heating delivered, kWh_t/yr) and price of electricity (POE, \$/kWh_e). The LCOE model was used to evaluate various scenarios (e.g., different utilizations, utility costs, and unit performance improvements) with the goal of determining target markets for initial CLHP products across the United States.

Keywords: HVAC&R, CLHP, cost models, LCOE

1. INTRODUCTION

Developing highly efficient heat pumping technologies will play an important role in addressing climate issues and energy consumption. It is expected that nearly half of the energy usage in the building sector is due to space heating, cooling, and refrigeration (U.S. EIA, 2022). Developing cost-effective and energy efficient heat pumps will accelerate the decarbonization of the U.S. energy system. Several non-vapor compression technologies have been investigated as alternatives to conventional vapor compression (VC) equipment due to their potential superior performance and the ability to use more favorable working fluids (U.S. DOE, 2016). Chemical heat pump systems have gained attention over the last few years as potential alternatives to conventional vapor compression cycles. Within the family of chemical heat pumps, chemical looping heat pumps (CLHP) have the potential for 20-30% performance improvements with low-GWP refrigerants (James et al., 2019; Kim et al., 2022). However, James et al. (2019) and Kim et al. (2022) have not provided economic comparisons between CLHP and vapor compression technologies, which is a key factor towards actual commercialization.

In this work, a framework for determining the levelized cost of energy (LCOE) for space conditioning applications was derived to allow direct comparisons of the economics of new and VC heat pumping technologies. Key components of the LCOE model are operating (OPEX) and capital expenditures (CAPEX). In particular, the OPEX depends strongly on the price of electricity (POE, \$/kWh_e) and unit utilization (annual cooling and heating delivered, kWh_t/yr) that vary with location in the U.S. With this in mind, LCOEs were evaluated across the U.S. under reasonable operating conditions to identify the best scenarios for initial CLHP products in terms of commercial viability.

2. CHEMICAL LOOPING HEAT PUMP

Figure 1 shows a schematic of a CLHP system consisting of a portion of a vapor compression cycle (e.g., expansion valve, evaporator) integrated with a liquid pump and an electrochemical cell. The electrochemical reaction occurring in the cell changes the fluid properties to a less volatile fluid and the phases from gas to liquid before a compression process. This process allows the fluid to be pressurized in the liquid phase (between state ⑤ and state ①) and be converted back into the original fluid (between state ② and state ③), which decouples fluid compression from the heat pumping cycle. Although additional electrical work is needed to drive the reaction, the coefficient of performance (COP) of the system could outperform that of the conventional vapor compression system by nearly 25%. In addition to system efficiency improvements, a scalable CLHP system could be easily realized by using multiple membrane electrode assemblies (MEAs) stacked in series similar to fuel cell industries (Kim et al., 2020). Modular architectures consisting of multi-fuel cell stacks will further broaden the range of applications (Rajalakshmi et al., 2008).

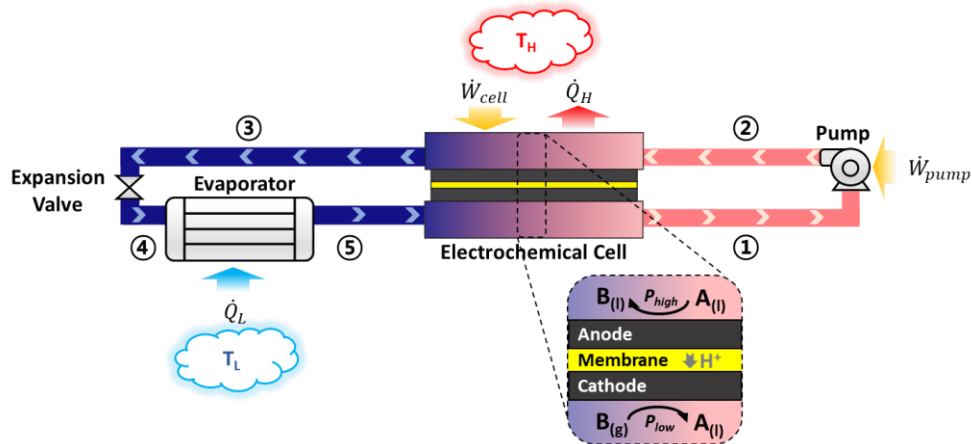


Figure 1: Schematic of Chemical Looping Heat Pump (CLHP) in cooling mode operation. The CLHP system consists of vapor compression cycle components (e.g., expansion valve and evaporator) combined with a liquid pump and an electrochemical cell. Electrochemical redox reaction enables the transformation of fluid properties and phases (Anode: $Fluid A_{(l)} \rightarrow Fluid B_{(l)}$; Cathode: $Fluid B_{(g)} \rightarrow Fluid A_{(l)}$) by changing the degree of hydrogen bonds (e.g., hydrogenation and dehydrogenation). This allows for fluid compression in the liquid phase.

3. COST MODELING AND ANALYSIS

3.1 Methodology

A framework of the cost modeling includes the approaches used to estimate levelized operating costs and capital costs. The goal was to understand the effect of unit utilization, price of electricity and unit efficiency on the overall economics with an index that can be directly compared with current energy costs. Generally, the levelized cost associated with the purchase of the capital equipment decreases when the amount of cooling and heating delivered over the lifetime ($Q \cdot LT$) is high. Also, the influence of operating costs on the overall LCOE increases when the price of electricity is high or the efficiency is low. The following assumptions were made to simplify the levelized cost analysis that are only appropriate for early-stage technology evaluation:

- Constant price of electricity (POE) is used for predicting the utility costs of the cell and pump operation.
- POEs do not include time-of-use energy or demand charges.
- Operation and maintenance costs are not included.
- The technology is purchased with cash that does not include interest payments.
- Tax rebates for purchasing high efficiency equipment are not included.
- The inflation rate is equal to the discount rate (neglect the time value of money).
- An average COP_{VC} of 2.9 (-) is assumed for both cooling and heating that is kept constant over the lifetime.
- A lifetime (LT) of 10 years was assumed for the unit.

The LCOE is defined as a sum of operating and capital costs normalized by the total delivered output (of value) for end-users over the life cycle (Odukamaiya et al., 2021). Since the "value" for space conditioning applications is the

thermal energy delivered (either cooling or heating), the LCOE is estimated as the ratio of capital and operating costs to cooling and heating delivered over the lifetime ($Q \cdot LT$) as indicated in Eq. (1).

$$LCOE = \frac{C \cdot \dot{Q} + POE \cdot W \cdot LT}{Q \cdot LT} \quad (1)$$

where LT (yr) is a lifetime of a unit, r (-) is a discount rate to calculate the present value of future cash flow of the system, and POE ($\$/kWh_e$) is the current price of electricity. W (kWh_e/yr) is the annual electrical energy consumption for operating the space conditioning system and Q (kWh_t/yr) is the amount of annual cooling and heating delivered. C ($\$/kW_t$) is a capital cost per unit rated cooling capacity and \dot{Q} (kW_t) is a rated cooling capacity (heating capacity is in the range of cooling capacity). The subscripts t and e in kW or kWh correspond to thermal energy and electrical energy, respectively. Eq. (1) captures materials selections and costs (C), unit cooling capacity, durability (\dot{Q} , LT), and weather/regional conditions (Q , W , POE). Both operating and capital costs are key components of the leveled cost analysis. This study defines leveled costs associated with both operating (OPEX) and capital expenditures (CAPEX) based on operating and capital costs normalized by the cooling or heating delivered over the lifetime of the unit. Mathematically, OPEX and CAPEX are defined as:

$$OPEX = \frac{POE}{COP} \quad (2)$$

$$CAPEX = \frac{C \cdot \dot{Q}}{Q \cdot LT} \quad (3)$$

LCOE is simply the sum of OPEX and CAPEX. Figure 2(a) shows the influence of POE (x-axis) and CLHP cell efficiency (blue color codes) on OPEX. The solid lines represent OPEX values of the CLHP as a function of POE, where COPs are predicted as a function of various cell efficiencies by using a thermodynamic cycle model (James et al., 2019). The black dashed line represents the data of a conventional 4-component vapor compression (VC) cycle using similar operating conditions reported in James et al. (2019) and it serves as a reference to compare CLHP and VC cycle (Kim et al., 2022). The breakeven cell efficiency for comparable COP with VC is about 55%, which is readily achievable. Also, cell efficiencies up to 75% might be possible leading to COP improvements of up to 50% compared to VC. Given the potential for performance improvements, regions having a high POE are beneficial for the initial products to maximize cost savings and reduce the payback periods. Figure 2(b) shows the impact of annual production volumes (units/yr) and the amount of cooling and heating delivered (kWh_t/yr) on CAPEX. The relationship between a capital cost per unit rated cooling capacity and production volumes was adopted from Kim et al. (2022) and a unit cooling capacity (\dot{Q}) of 10.55 kW_t (3 RT) was used as a reference case. The results indicate that high production volume and unit utilization (amount of cooling and heating demands) could enable significant CAPEX reductions.

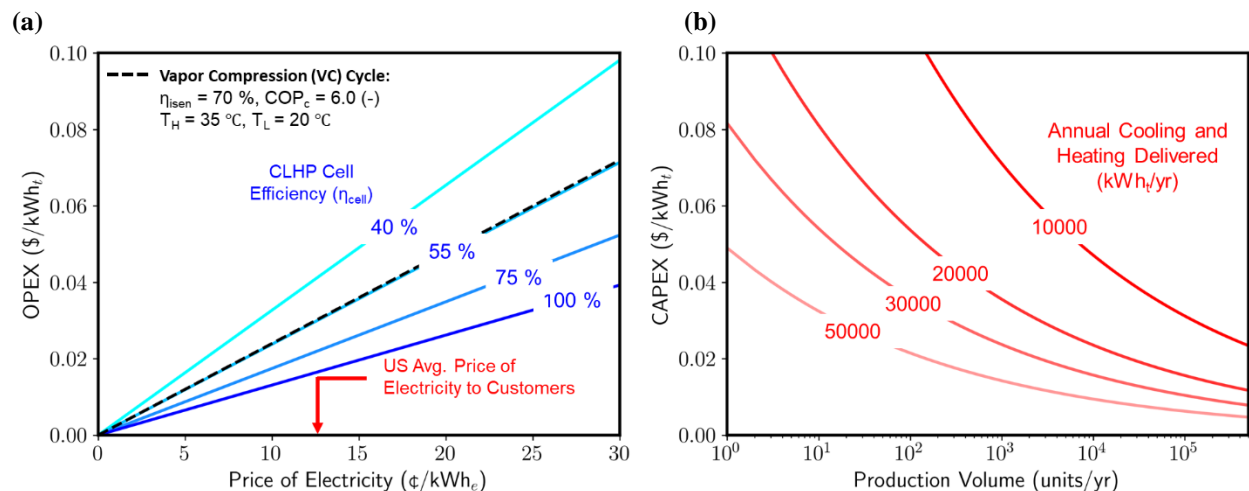


Figure 2: (a) Operating expenditures (OPEX) as a function of the price of electricity and various cell efficiencies. The black dash line represents a reference case using a vapor compression unit; (b) Capital expenditures (CAPEX)

as a function of production volumes with annual cooling and heating delivered (kWh_t/yr). A total area of 35 m² for 10.55 kW_t (3 RT) unit was employed based on the results published by Kim et al. (2022).

3.2 Case Study Description

Table 2 summarizes the baseline parameters used in this study. Finding a suitable range of capital costs for each technology is important as capital costs have a significant impact on LCOE analysis. Unlike vapor compression technologies, estimating the capital cost of the CLHP system was challenging due to lack of published data. To minimize uncertainties, the capital costs were chosen in the range \$5,000 to \$10,000 based on the results published by Kim et al. (2022). These cost values were then normalized with respect to the unit rated cooling capacity (10.55 kW_t in this case), providing the cost ranges from 500 \$/kW_t to 1,000 \$/kW_t. Similarly, retail costs of 10.55 kW_t air source heat pumps ranging from \$2,550 to \$4,550 were adopted as a reference case, resulting in normalized capital costs in the range of 250 \$/kW_t to 450 \$/kW_t (U.S. EIA, 2018). An average vapor compression cycle COP_{VC} of 2.9 (-) was selected as a reasonable value based on typical values for heating COP_{h,VC} of 3.3 (-) and cooling COP_{c,VC} of 2.5 (-) (Lee et al., 2021).

Table 2: Parameters used in LCOE analysis

Parameter	Description	Value(s)	Reference
C _{CLHP}	CLHP capital cost per unit rated cooling capacity	500 \$/kW _t ~ 1,000 \$/kW _t	Kim et al. (2022)
C _{VC}	VC capital cost per unit rated cooling capacity	360 \$/kW _t ~ 460 \$/kW _t	U.S. EIA (2018)
COP _{VC}	Average COP _{VC} for both cooling and heating (reference)	Average: 2.9 (-) Heating: 3.3 (-); Cooling: 2.5 (-)	Lee et al. (2021)
COP _{CLHP} /COP _{VC}	Average COP improvement for both in cooling and heating	1.1 ~ 1.3 (-)	James et al. (2019); Kim et al. (2022)
\dot{Q}	Unit cooling capacity (heating capacity is in the range of 10.55 kW _t)	10.55 kW _t	-
Q	Amount of annual cooling and heating delivered	10,000 kWh _t /yr ~ 40,000 kWh _t /yr	-
LT	Lifetime of the system	10 yrs	-
POE	Price of electricity	0.13 \$/kWh _e and 0.23 \$/kWh _e	U.S. EIA (2021)
r	Discount rate	3%	-

As discussed in Section 3.1, annual cooling and heating delivered (kWh_t/yr) and POE (\$/kWh_e) are the important factors that influence LCOE and determined as a function of building loads and weather data. Figure 3(a) shows building load profiles for cooling and heating predicted based on Table 3, which is adapted from AHRI Standard 210/240 (2023). For example, for cooling mode, the desired cooling capacity is 10.55 kW_t (3 RT) at T_H = 35 °C and T_L = 20 °C, which is denoted as $\dot{q}_{A,Full}$ that is also used in heating load calculation. The predicted load profiles were then combined with the weather data (e.g., bin hours) for cooling and heating, as illustrated by bar plots in Figure 3(b) (example weather data from Washington, D.C.). Figure 4 shows annual bin hour map, where the data were collected from 130 weather stations across the contiguous United States and used for estimating the annual cooling and heating delivered (see calculation examples in Kim et al. (2022)).

Table 3: Building heating and cooling load predictions based on AHRI Standard 210/240 (2023).

Mode	Expression	Description
Cooling	$BL_c = \left(\frac{t_j - 65}{95 - 65} \right) \left(\frac{\dot{q}_{A,Full}}{1.1} \right)$	$\dot{q}_{A,Full} = 10.55 \text{ kW}_t$ at T _H = 35 °C, T _L = 26.67 °C
Heating	$BL_h = \left(\frac{t_{zl} - t_j}{t_{zl} - t_{OD}} \right) \cdot C \cdot \dot{q}_{A,Full}$	Region I: t _{OD} = 37 °F, C = 1.10, t _{zl} = 58 °F Region II: t _{OD} = 27 °F, C = 1.06, t _{zl} = 57 °F Region III: t _{OD} = 17 °F, C = 1.30, t _{zl} = 56 °F Region IV: t _{OD} = 5 °F, C = 1.15, t _{zl} = 55 °F Region V: t _{OD} = -10 °F, C = 1.16, t _{zl} = 55 °F Region VI: t _{OD} = 30 °F, C = 1.11, t _{zl} = 57 °F

Outdoor Design Temp. (t_{OD}); Heating Load Line Eq. Slope Factor (C); Zero-Load Temp (T_{zl})

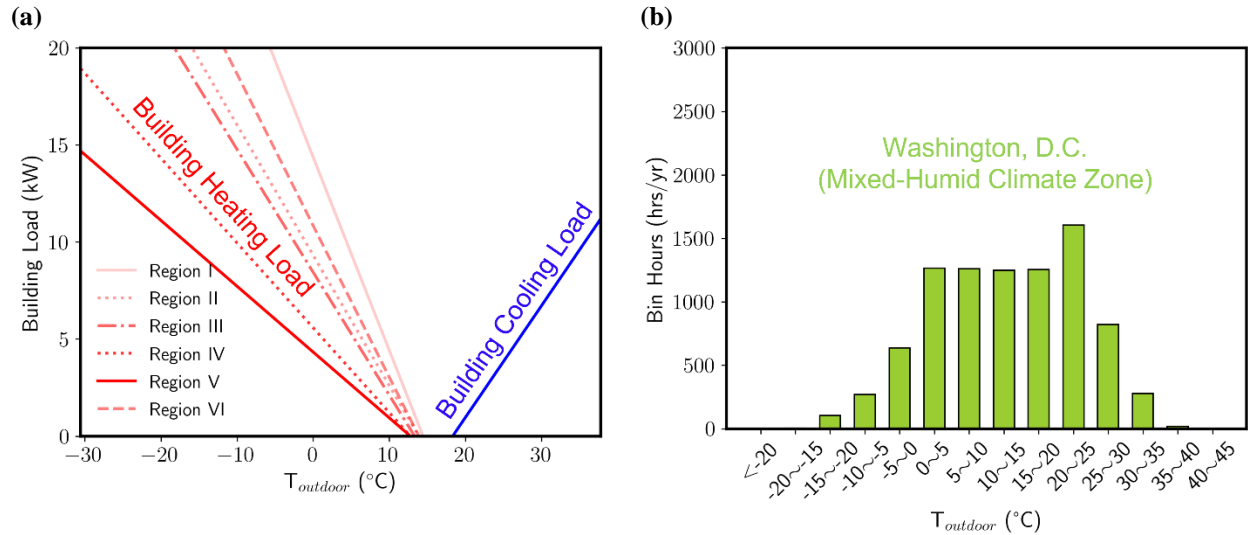


Figure 3: (a) Estimated building load of 10.55 kW_t (3 RT) unit based on AHRI Standard 210/240 (2023); (b) Bin weather data from Washington, D.C. (Mixed-Humid Climate Zone) was selected as an example.

Figure 5(a) shows predictions of the cooling and heating needs with a unit capacity of 10.55 kW_t. It was assumed that the air conditioning operated at ambient temperatures above 20 °C and the heat pumping at temperatures below 15 °C. Cities located on the west coast of the U.S. are the regions where annual cooling and heating delivered are relatively lower than others ($\leq 10,000$ kWh_t/yr). For example, units in San Francisco (CA) (marine climate) mostly operate in mild weather conditions between 20 °C and 25 °C for cooling (548 hours/year) and 10 °C and 15 °C for heating operation (4588 hours/year). Unlike a marine climate, the demands for cooling and heating tend to increase in cities under extreme weather conditions (*e.g.*, 30,000 ~ 40,000 kWh_t/yr) due to the long duration of hot/dry weather conditions or Midwest regions having a both cooling and heating loads. One example is Phoenix (AZ), which has nearly 2,800 hours/year of conditions for $T_{outdoor} \geq 30$ °C or Minneapolis (MN) where heating equipment would run 2,680 hours/year for $T_{outdoor} \leq 0$ °C. In a mixed-humid climate, the cooling and heating loads are nearly 25,000 kWh_t/yr. Lastly, Figure 5(b) shows average monthly U.S. average POE across the contiguous United States. The U.S. average POE value of 0.13 \$/kWh_e and relatively high 0.23 \$/kWh_e were selected for LCOE analysis.

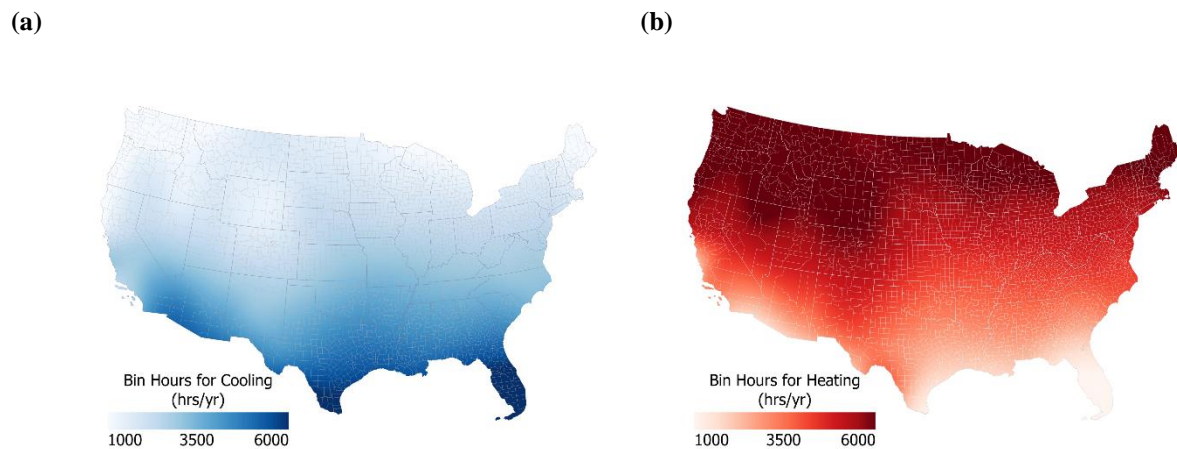


Figure 4: (a) Annual bin hours for cooling (b) and heating across the contiguous United States. The data were collected from the typical meteorological year (TMY3) data sets with 130 data points.

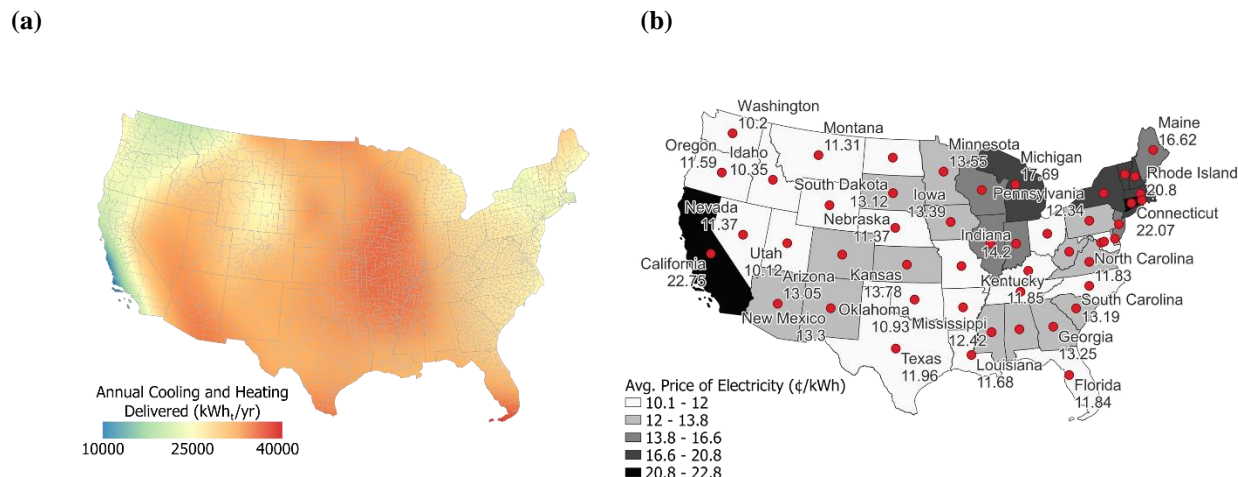


Figure 5: (a) Annual cooling and heating delivered (kWh_t/yr) across the contiguous United States. A 10.55 kW_t (3 RT) unit was employed for the predictions; (b) Average monthly price of electricity (¢/kWh_e) across the contiguous United States. Figure 5(b) was adapted with permission from the reference (Kim et al., 2022).

3.3 Results

Figure 6 shows LCOEs for both CLHP and VC as a function of capital costs (C), coefficient of performance ratio (COP_{CLHP}/COP_{VC}), annual cooling and heating delivered (Q), and the price of electricity (POE). Table 4 summarizes four different scenarios used in plots of Figure 6. The scenarios could give LCOE estimates that are representative for various cities in the U.S. For example, assuming 10% or 30% performance improvements with POE of 0.13 \$/kWh_e, potential cities are Phoenix (AZ) and Chicago (IL) as depicted in Figure 5(b) and the LCOEs of CLHP of those cities are nearly 0.05 \$/kWh_t since the annual cooling and heating delivered are close to 40,000 (kWh_t) as indicated in Figure 5(a).

In some scenarios, LCOEs of CLHP technology could be less than that of VC. Since LCOE is highly dependent on unit utilization ($Q \cdot LT$), POE , and COP_{CLHP}/COP_{VC} , the right combination of these factors leads to LCOE values for CLHP that are economically competitive. In the case of Figure 6(b), the LCOE could be economically feasible only when the annual cooling and heating demand is higher than nearly 40,000 kWh_t. In high utilization ($Q \cdot LT$), POE and the unit efficiency are dominant factors in influencing the LCOEs of CLHP (see Eq. (1)). The more extreme climate zones (Boston (MA) in winter or Phoenix (AZ) in summer) or Midwest would be more suitable for realizing competitive LCOE due to high cooling and heating demands. Figure 6(d) shows that the economics of CLHP could easily be competitive with VC in regions having high $POEs$ and COP improvements. Examples of this scenario are Boston (MA) with high utility costs (0.21 ~ 0.23 \$/kWh_e) and moderate cooling and heating needs (20,000 ~ 25,000 kWh_t/yr). The expected LCOE in these cities is nearly 0.06 ~ 0.08 \$/kWh_t for CLHP.

However, in the situation of less than 10% COP improvement (Figure 6(a) and Figure 6(c)), the economic feasibility of the CLHP would be limited. For example, there might be no cities that would have sufficiently high POE and cooling and heating needs. One of the potential solutions for mitigating this problem is to reduce the capital costs of the CLHP (C_{CLHP}). The capital costs will be decreased by using non-precious metal catalysts and improving electrodes and flow fields for compact sizing. Addressing both the material- and system-level challenges will help increase the CLHP technology readiness level.

Table 4: Description of Scenarios in Figure 6 for LCOE Predictions

Figure 6	COP_{CLHP}/COP_{VC}	POE (\$/kWh _e)	Description
(a)	1.1	0.13	10% performance improvement in a region with an average price of electricity in the US (e.g., Chicago, IL or Phoenix, AZ)
(b)	1.3	0.13	30% performance improvement in a region with an average price of electricity in the US (e.g., Chicago, IL or Phoenix, AZ)

(c)	1.1	0.23	10% performance improvement in a region with a high price of electricity (e.g., Boston, MA or San Diego, CA)
(d)	1.3	0.23	30% performance improvement in a region with a high price of electricity (e.g., Boston, MA or San Diego, CA)

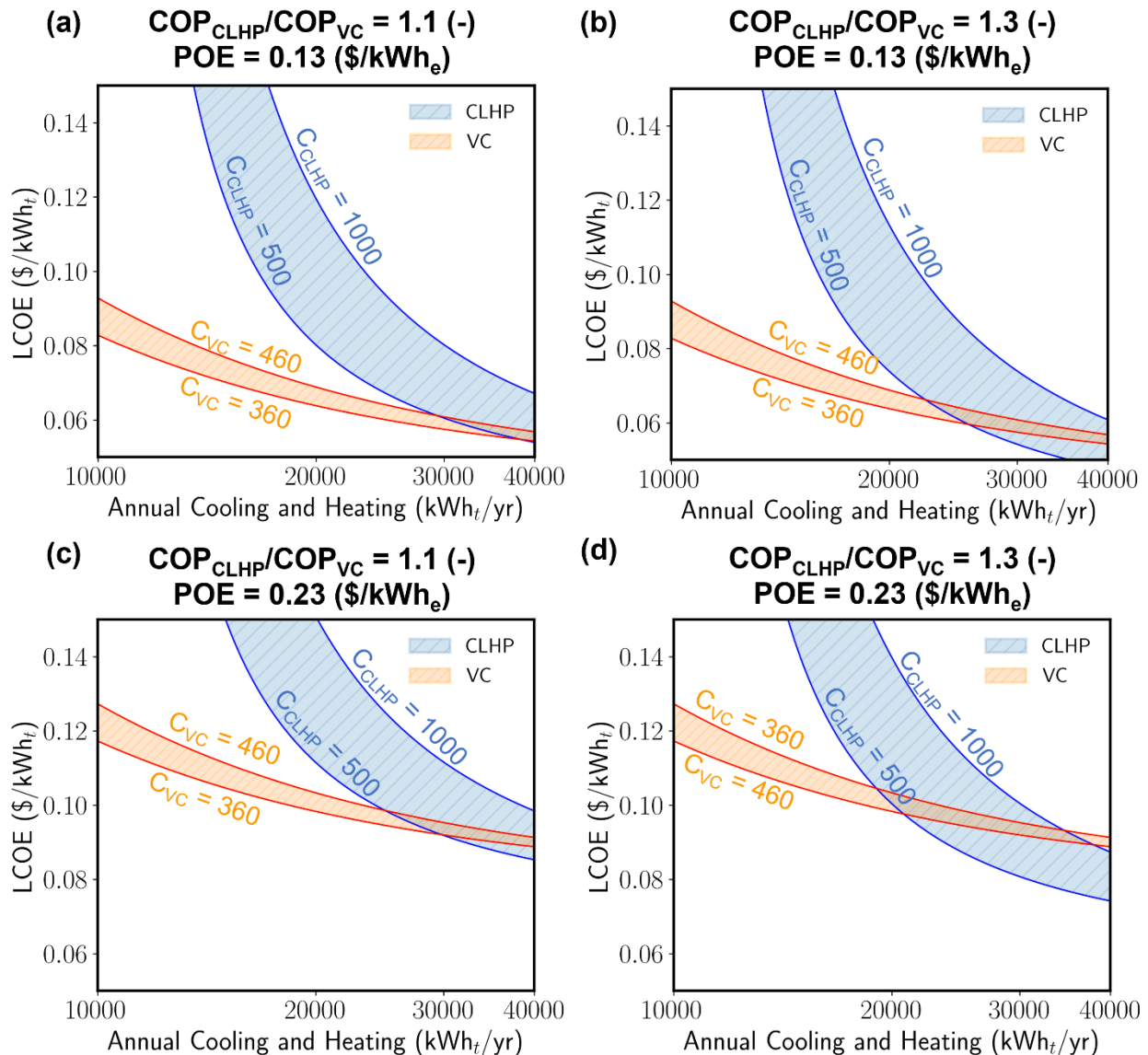


Figure 6: Levelized cost of energy (LCOE) for space conditioning comparison of chemical looping heat pump (CLHP) to vapor compression (VC) based on a set of assumptions: $\text{COP}_{\text{CLHP}}/\text{COP}_{\text{VC}} = 1.1$ and 1.3 (-), the price of electricity (POE) = 0.13 and 0.23 ($\$/\text{kWh}_e$), unit capacity (\dot{Q}) = 10.55 kW_t , lifetime (LT) = 10 (yr), $C_{\text{CLHP}} = 500 \sim 1,000$ $\$/\text{kWh}_t$, and $C_{\text{VC}} = 360 \sim 460$ $\$/\text{kWh}_t$.

Figure 7 shows estimated LCOE for CLHP technology across the contiguous United States based on Figure 5 and LCOE expressions for CLHP presented in the previous section. Each graph provides a LCOE map for different potential COP improvements (10% and 30%) with fixed unit capacity, lifetime, and capital costs (average value of 750 $\$/\text{kWh}_t$). As discussed in Figure 6, the economics of CLHP technology could be comparable to VC when the LCOE is less than nearly 0.06 $\$/\text{kWh}_t$. To meet this target, CLHP technology must achieve 30% COP improvement for heating or cooling, leading to LCOE in the range of $0.04 \sim 0.07$ $\$/\text{kWh}_t$, as shown in Figure 7(b). Figure 7(a) represents the scenario of 10% improvements, where the expected LCOE is in range from $0.07 \sim 0.11$ $\$/\text{kWh}_t$.

Increasing the lifetime (LT) of the system or decreasing the capital costs (C) would also enable significant LCOE reductions for the initial products.

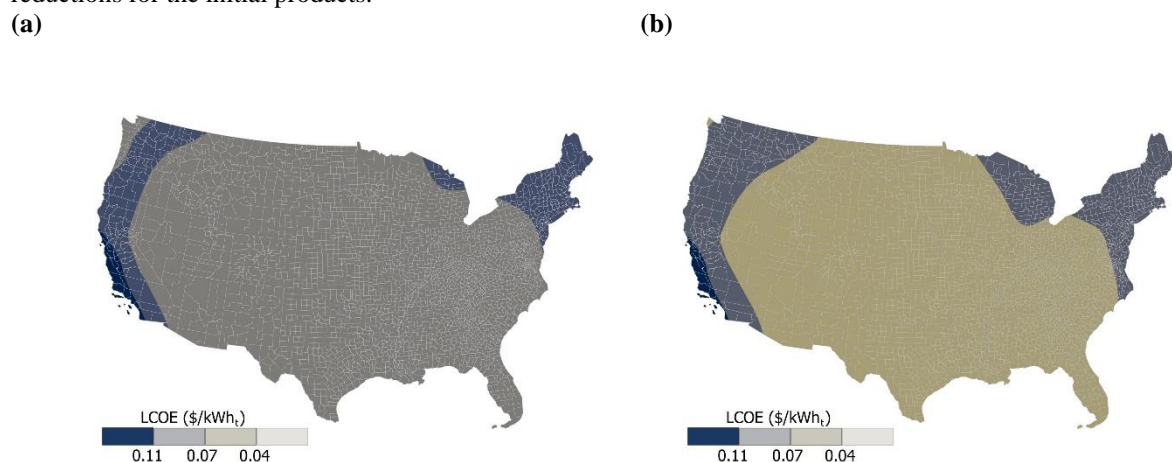


Figure 7: Levelized cost of energy (LCOE) of chemical looping heat pump (CLHP) based on a set of assumptions: $COP_{CLHP}/COP_{VC} =$ (a) 1.1 (-) and (b) 1.3 (-), $(\dot{Q}) = 10.55 \text{ kW}_t$, lifetime (LT) = 10 (yr), $C_{CLHP} = 750 \text{ \$/kWh}_t$

4. CONCLUSIONS

This study covered quantitative techno-economic analyses to evaluate early-stage economic feasibility of CLHP technology. The levelized cost of energy (LCOE) for this technology was used to enable a direct comparison with vapor compression (VC) technology. LCOE composed of levelized operating expenditures (OPEX) and levelized capital expenditures (CAPEX). This breakdown is useful in understanding the influence of individual parameters on LCOE, such as unit utilization (annual cooling and heating delivered, kWh_t/yr) and price of electricity (POE, $\text{\$/kWh}_e$). The LCOEs for CLHP and conventional VC technology were evaluated under various scenarios (e.g., different utilizations, utility costs, and unit performance improvements) to determine target markets for initial products across the United States.

The amount of unit utilization and performance improvement are particularly important when the capital cost of the unit is relatively high. For example scenarios, the LCOE of CLHP could be less than that of VC in the case of high utilization ($\geq 20,000 \text{ kWh}_t$) with high performance improvements ($COP_{CLHP}/COP_{VC} = 1.3$) even though the capital cost of the CLHP is nearly 1.5~2 times higher than VC. However, in the case of less than 10% COP improvement, the LCOE of the system might not be comparable to existing technologies. Addressing both materials- and system-level challenges for CLHP will enable an increase in the economic feasibility of the system.

NOMENCLATURE

A	area (cm^2) or fluid A	P	pressure (kPa)
B	fluid B	PEM	polymer electrolyte membrane
C	capital cost per rated capacity ($\text{\$/kW}_t$) or slope factor	POE	price of electricity ($\text{\$/kWh}_e$)
COP	coefficient of performance (-)	\dot{q}	unit cooling capacity
LCOE	levelized cost of energy ($\text{\$/kWh}_t$)	Q	annual cooling and heating delivered (kWh_t/yr)
LT	lifetime (yrs)	r	discount rate (%)
MEA	membrane electrode assembly	T, t	temperature ($^\circ\text{C}$)
n	number	VC	vapor compression
η	efficiency		

Subscript

A_{full} test condition at $T_H = 35 \text{ }^\circ\text{C}$ and $T_L = 20 \text{ }^\circ\text{C}$ (AHRI Standard 210/240, 2023)

c	cooling	j	temperature bin
cell	electrochemical cell	low, L	low-side pressure or temp.
CLHP	chemical looping heat pump	h	heating
e ⁻	electron	(l)	liquid
e	electrical	mix	mixture
endplate	electrochemical cell plate	OD	outdoor temp.
t	thermal or total	VC	vapor compression
(g)	gas	endplate	electrochemical cell plate
high, H	high-side pressure or temp.	zl	Zero-Load Temp

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