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Flipping the switch: carbon-negative and water-positive data centers through waste heat utilization

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Artificial intelligence (AI) growth poses major electricity, emissions, and water challenges. Globally, AI data centers are projected to demand Gigawatts of electricity, leading to Gigatons of carbon dioxide emissions and trillions of gallons of water consumed per year. With increasing deployment of high efficiency chip cooling, which in turn raises the waste heat temperature, data center waste heat could become a Gigawatt-scale energy resource. In this perspective, we analyze the various options for using data center heat from a thermodynamic, revenue, and emissions perspective. We show that direct air capture and thermal water purification are highly promising due to their ability to efficiently capture/avoid CO_2 while producing a valuable product. Using data center heat for other purposes such as heating, cooling, electricity conversion, or atmospheric water production, are shown to have lower potential for emissions reduction and economic benefit. We then discuss the advantages of waste heat-powered direct air capture and water production compared to incumbent carbon capture and desalination approaches. Importantly, we highlight key technological and scientific opportunities that can enable these impactful end uses. Lastly, we propose a new data center metric, the Energy Use Efficiency (EUE), which incentivizes waste heat reuse and shows that data centers with heat utilization can be carbon-negative and water-positive, addressing major sustainability challenges of AI.

Broader context

The unprecedented growth of data centers and artificial intelligence poses major energy and environmental challenges due to large requirements of energy and water, with significant accompanying carbon dioxide emissions. On the other hand, data centers present a massive, underutilized opportunity as essentially all the power consumed at a data center is rejected as heat, opening an unused Gigawatt-scale thermal energy resource. Here, we analyze various options for data center heat use from a thermodynamic, revenue, and emissions perspective. We show that capture of atmospheric carbon dioxide and thermal water purification, which have been rarely considered in literature, are highly promising due to their ability to efficiently remove/avoid CO_2 while producing a valuable product. Conventional heat uses such as heating, cooling, or electricity conversion have lower potential for emissions reduction and economic benefit. We discuss advantages of waste heat-powered direct air capture and water production compared to incumbent approaches and highlight key technological and scientific opportunities to enable these impactful end uses. Lastly, we show that data centers with heat utilization can be water-positive and carbon-negative, inverting the paradigm of data centers and addressing major sustainability challenges of AI.

Introduction

The explosive growth of data centers for Artificial Intelligence (AI) poses major risks for energy, water security, and climate.[1,2] Data centers are expected to grow from ≈2% of global energy demand to 3–4% by 2030 (55 GW to ≈150 GW),[3] while consuming ≈5 billion cubic meters of water globally by 2027, equivalent to half the water consumption of the United Kingdom.[4] The growth is even more prominent in the United States, where data centers could consume over 10% of all electricity by 2028[5–7] and ≈2.4 billion cubic meters of water.[7] The primary bottleneck to AI data center expansion is the available power supply[8] which is spurring the growth of fossil fuels and leading to high carbon dioxide emissions associated with data center computing.[9–11] In light of this massive expected growth, it is critical to reimagine data centers to improve their efficiency and reduce their environmental impact.

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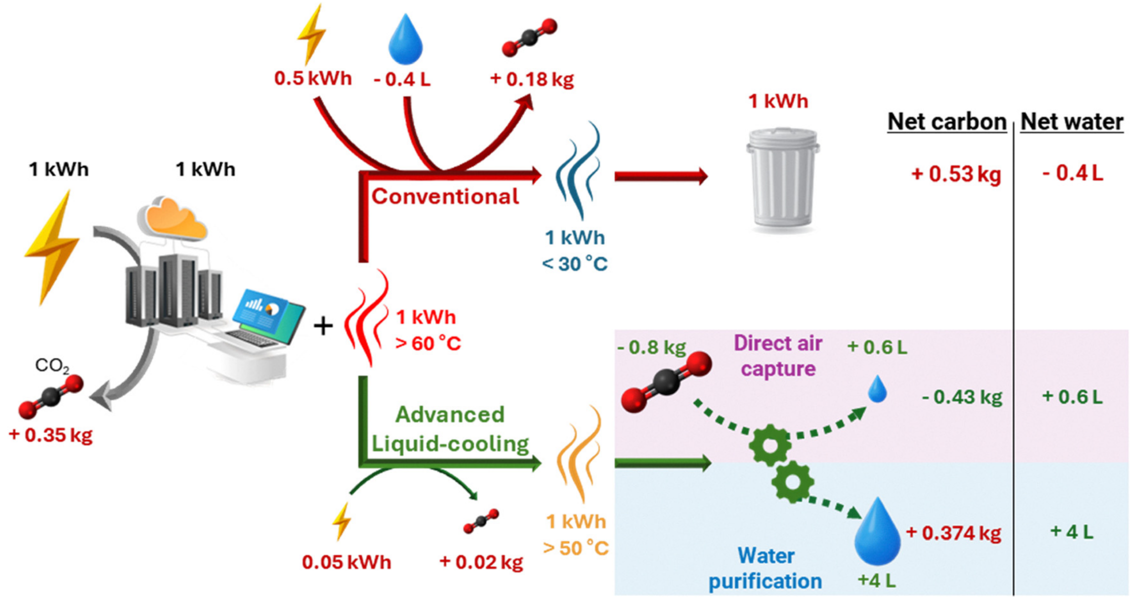

Fig. 1 Representative data center carbon, water, and energy balance and potential to revert the paradigm with waste heat utilization. One kWh of electricity consumed by a US data center produces 1 kWh worth of computation, which then becomes 1 kWh of heat, and produces 0.35 kg CO_2. A data center air cooling system dissipates the kWh of heat at near-ambient temperatures ($\approx$30 °C), requiring significant water consumption ($\approx$0.4 L) for cooling and additional energy ($\approx$0.5 kWh). High-performance, liquid or two-phase cooling requires lower energy, no water consumption, and dissipates heat at higher temperatures (>30 °C). This higher temperature waste heat could be used to simultaneously capture carbon and water from the air ($\approx$0.8 kg CO_2 kWh^{-1} and $\approx$0.8 kg water kWh^{-1}) or thermally purify water ($\approx$4 L kWh^{-1}), boosting data center productivity and sustainability.

Data centers rely on servers and chips that are effectively large resistive heaters that also compute, converting a kWh of electricity for computation into a kWh of heat (Fig. 1). Therefore, per kWh of electricity, a data center could extract one unit of energy for computing, first, and then use an equivalent unit of heat for another purpose. Instead of using this heat, data centers consume additional electricity and water to dissipate their heat to the environment (*i.e.*, waste heat).

Data center energy efficiency is commonly quantified through the power use effectiveness (PUE), which measures the ratio of total data center energy consumption to the server energy consumption (*i.e.*, IT equipment Energy):

$$\begin{aligned} \text{PUE} &= \frac{\text{Total facility energy}}{\text{IT equipment energy}} \\ &= \frac{\text{IT equipment energy} + \text{Non IT equipment energy}}{\text{IT equipment energy}} \end{aligned} \tag{1}$$

The industry average PUE is 1.44,[7] meaning that for every kWh of electricity used to power a server, 0.44 kWh are used for all other data center uses, but mainly cooling (Fig. 1).[7,12,13] Rather than converting 1 kWh of electricity into 1 unit of computational energy and 1 unit of useful heat, the average data center only extracts 0.69 kWh ($1 \div 1.44 = 0.69$) of computational energy. This is the result of poor heat rejection from the chips to the ambient as well as the lack of widespread heat utilization. We note that PUE has limitations as a metric,[14,15] but we use since it is the mostly widely used in literature and practice.[16]

Data center energy efficiency can be improved by (1) increasing computational efficiency, (2) improving cooling and chip thermal management, and (3) utilizing the waste heat. Significant efforts are underway towards increasing computation efficiency by chip manufacturers and software developers.[17–20] These efforts have reduced in >100× the energy consumption per computation operations and could play a major role in limiting the growth of AI energy use.[21] Similarly, advanced cooling technologies are of growing interest, driven by the need to cool increasingly energy-intensive AI chipsets (increasing from $\approx$200 W now to >1000 W in the coming years).[22–25] There is extensive ongoing work in this field, aimed at reducing the cooling thermal resistance from the chip to the environment by replacing the nearly universal air cooling with liquid and two-phase approaches and integrating better thermal interface materials.[26–29] These approaches, which must ensure reliable dissipation of increasingly larger heat fluxes, have high potential to reduce data center energy use through a lower PUE. Additionally, efficient cooling can increase the dissipated heat temperature from $\approx$30 °C for air cooling to >50 °C (Fig. 1), enabling waste heat utilization. Therefore, the deployment of advanced cooling for AI growth is leading to >100 Gigawatts of heat at increasingly higher and more useful temperatures. This opens the possibility for widespread waste heat utilization, a crucial step towards sustainable data centers and AI.

Although low-grade waste heat is rarely used, there is a unique opportunity to utilize data center waste heat given its magnitude as well as the sustainability risks of AI. However, this utilization must be economically viable. Recent studies on data center heat utilization have focused on residential/commercial district heating, heat to power, and heat upgrading.[30–32] However, several studies show unfavorable economic potential

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with long payback periods for these end uses,[33–35] because space heating is inexpensive, despite being a highly efficient end use. The key to utilizing any source of waste heat, including from data centers, is finding the most valuable end uses.

In this perspective, we analyze the merits of data center waste heat utilization enabled by advanced cooling technologies. We first analyze various possible end uses of low-grade waste heat from thermodynamic, revenue, and emissions perspectives. With this analysis, we demonstrate that carbon removal, which to our knowledge has not been discussed in the academic literature as a data center waste heat end use, and evaporative water purification, which has been rarely considered, are the most appealing options due to their large potential to capture/avoid carbon and produce a valuable resource. Next, we demonstrate advantages of waste heat-powered carbon capture and water purification over incumbent approaches and identify key research gaps that must be addressed to enable these novel end uses. Finally, we show through a new, simplified energy metric, Energy Use Efficiency (EUE), that waste heat utilization increases the energy effectiveness of data centers, extracting >1 units of computation and heat for every unit of electricity. This demonstrates the large opportunity to utilize data center heat to reverse the conventional paradigm of carbon-positive and water-negative data centers.

Possible uses of data center waste heat

Over 70% of the world's primary energy is lost as heat[36] because it is notoriously difficult to valorize.[37,38] Waste heat utilization is uniquely difficult to rationalize economically because the capital costs of the infrastructure to use waste heat can outweigh the low cost of common heating sources such as natural gas and coal.[32,39] Other hurdles include co-location and regulation.[39] To overcome these challenges, data centers need end uses that (i) require costly forms of heat, (ii) use low-grade heat, and (iii) are geographically flexible.

We consider six applications that are compatible with the temperature ranges expected from data center waste heat (30–70 °C):[40–42] (i) direct use of heat for space, water, or process heating either onsite or through a district heat network (Fig. 2a),[31,42] (ii) conversion of heat to electricity (Fig. 2b),[31,43] (iii) conversion of heat to cold through a chiller (Fig. 2c),[42,44] (iv) thermal purification of water through evaporation-condensation (Fig. 2d),[42,45] (v) water production from humidity *via* thermal sorption-desorption (Fig. 2e),[46,47] and (vi) direct air capture (DAC) of carbon dioxide from the air *via* thermal sorption–desorption (Fig. 2f).[48,49]

We evaluate the data center waste heat potential for these end uses by estimating the respective economic benefit, E, and the carbon dioxide emissions benefit, C. For these applications, E is the revenue from selling the product/service of each application (eqn (2)) and C is the total carbon dioxide avoided/removed (eqn (3)):

$$E = Q \cdot \eta \cdot P \tag{2}$$

$$C = Q \cdot \eta \cdot I \tag{3}$$

where Q is the total data center waste heat. We consider Q = 200 TWh, corresponding to a moderate projection of data center electricity consumption in the United States by 2030.[6] Therefore, E and C represent the near future potential of data center waste heat utilization in the United States. Importantly, since E represents the revenue, it does not account for capital and operational expenses in each end use. For each end use to be economically viable it is critical that E exceeds the levelized cost of the respective product. η is the amount of product obtained per unit of heat for each application. For instance, for heat-to-electricity conversion, η, corresponds to the conversion efficiency (*i.e.*, the electricity produced per unit heat), which is bounded by the Carnot limit. For carbon capture, η is the amount of captured CO_2 per unit heat. P is the economic value from each output, *e.g.*, the electricity price for electricity conversion or the revenue per ton of CO_2 captured for carbon capture. I is the product carbon intensity, *e.g.*, the CO_2 amount emitted per unit of product. For carbon capture, I = 1, reflecting how a ton of CO_2 is removed per ton of CO_2 captured. High η, P, and I are desirable as they indicate high energy utilization, high product economic value, and large amount of carbon dioxide removed/avoided in each application, respectively. In particular, we note that η is a key performance metric for each application and that significant efforts have been made to improve this energy utilization. To capture current performance as well as the potential for improvement within thermodynamic bounds, we have considered a range of values for η from the currently demonstrated performance to the thermodynamic limit. SI S1 details the η, P, and I values considered.

Fig. 2g shows our analysis results comparing different waste heat uses. Notably, from our results, carbon capture is a promising waste heat reuse application. DAC with waste heat has high economic benefit E (>1 billion USD) due to providing a high value service (clean heat) for a high value product (>\$100 per ton CO_2).[50,51] It also has the potential to remove large amounts of atmospheric CO_2 (≈50–1000 Megatonnes per year). Remarkably, this carbon capture potential is comparable to the United States' goal of annually capturing 400–1800 CO_2 Megatonnes by 2050[52] highlighting how data center waste heat could significantly contribute towards this goal. Relative to other waste heat uses, the decarbonization potential of waste heat-powered DAC exceeds in about an order of magnitude that of evaporative water purification, direct heat use, cooling, and conversion to electricity, reflecting comparatively low carbon intensities for water and heat and low efficiencies for cooling and electricity production (see SI S1).

The economic potential in Fig. 2g can be explained by (i) the value of the product, P, and (ii) the productivity per unit heat, η. The most economically attractive end uses have high η and produce valuable products. Fig. 2g shows that atmospheric water production is the least economically attractive end use due to the high energy intensity (low η) and low product value (P). For electricity, although it is highly valuable, the low heat-to-electricity conversion efficiency (η < 10%) at these

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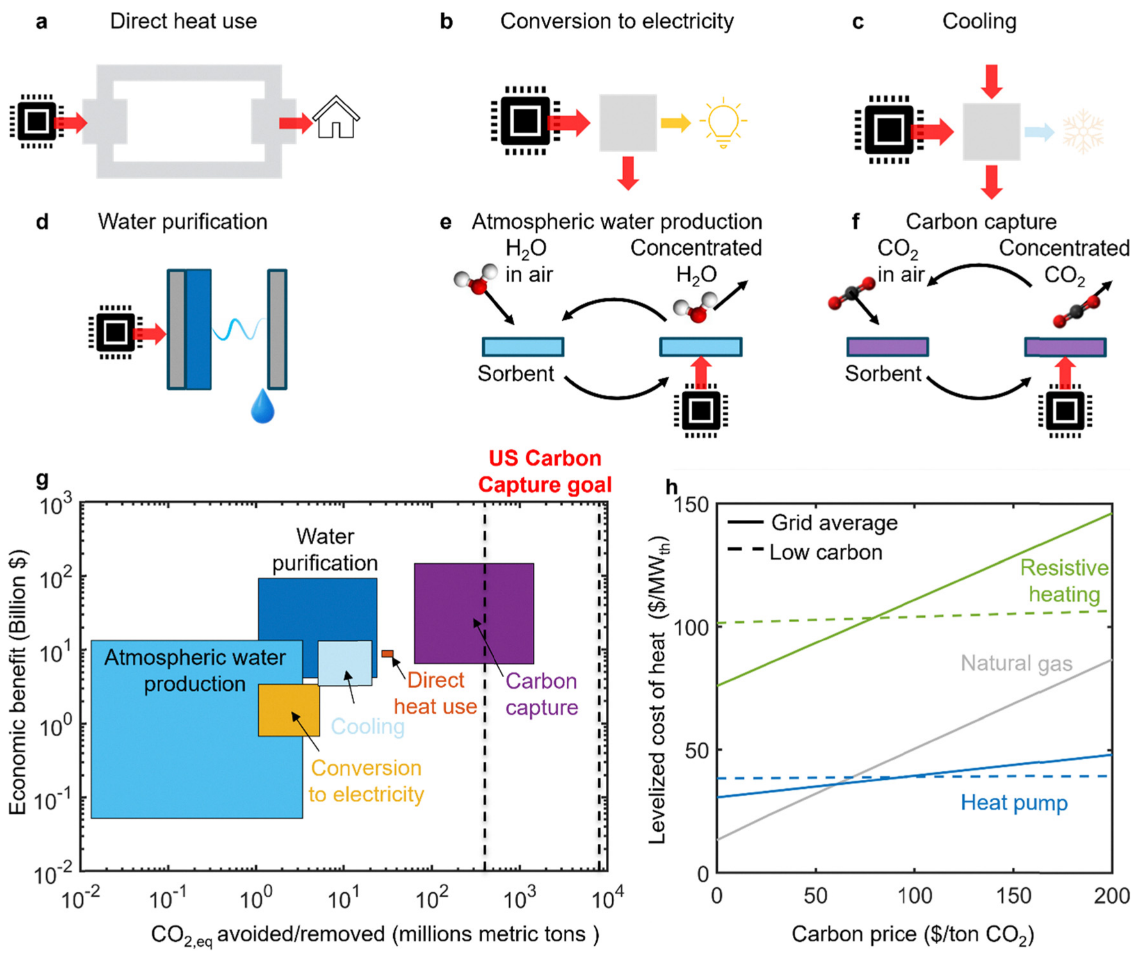

Fig. 2 Data center waste heat utilization options and potential. Waste heat end uses considered of (a) direct heat use, (b) heat-to-electricity conversion, (c) cooling through waste heat-powered sorption chillers, (d) thermal evaporation-condensation water purification, (e) atmospheric water production using sorbents, and (f) carbon capture using sorbents. (g) Economic benefit and CO_2 abatement potential for each application. Carbon capture and water purification have the highest potential for economic benefit, while carbon capture has the highest CO_2 abatement potential, comparable to the United States' 2050 carbon capture goal.[52] (h) Levelized cost of heat for different sources as a function of carbon price. Applications using unabated heat will tend to favor fossil sources, such as natural gas. Applications using abated heat, such as DAC, have higher levelized cost of heat (LCOH), providing a better opportunity for data center waste heat.

temperatures makes it a less economically viable option. To elucidate the other alternatives, we show the levelized cost of heat (LCOH) for various sources as a function of carbon price in Fig. 2h (see SI S2 for details). Sorption cooling and direct heating are the next most valuable applications, ranging from \$1–\$10 billion. The efficiency of delivering waste heat to its end use is relatively high. However, traditional low-temperature heat uses such as space heating and drying are inexpensive ($\approx$\$20 per MWh_{th}) because they typically rely on unabated, cheap fossil fuels (*i.e.*, carbon price = \$0 per ton, Fig. 2g). Therefore, switching from fossil fuels to waste heat has relatively low economic potential, in addition to requiring co-location. Both hinder the potential of data center waste heat use for direct heat, as also noted in previous studies.[33–35] Analogously, sorption cooling faces many of the same nontechnical hurdles. Although cooling is more valuable than heat, the relatively low conversion efficiency of heat to cooling combined with the need for colocation renders cooling a challenging end use.

Conversely, thermally-regenerated DAC and evaporative water purification are the two most appealing options for data center waste heat utilization with an estimated economic potential of \$3–\$100 billion. Thermal DAC systems use expensive heat to regenerate sorbents, often from electricity or abated natural gas.[53] High associated emissions increase the cost of heat for carbon removal (Fig. 2h). To address this, some DAC systems use low-carbon electricity, energy storage, hourly matching of renewable energy, and/or a clean baseload electricity source (*e.g.*, nuclear and geothermal) – all of which can be >3× more expensive than unabated fossil fuels.[54] Alternatively, heat pumps can efficiently provide heat for DAC but at the expense of high additional CAPEX, potentially increasing the cost of carbon capture.[55,56] The heat used in thermal DAC is uniquely valuable because a carbon price increases its value. Therefore, the value proposition of using waste heat for DAC is not only in the value of carbon removal, but also in its low emissions. For water purification, the heat is more efficiently used to produce a product – potable water – compared to

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atmospheric water production. Additionally, like electricity, purified water could be more easily transported to end users compared to heat owing to the existing expansive and long-distance infrastructure for electricity and water transport. This stands in contrast with the challenging transport of heat over long distances.[57] The relative geographical flexibility of DAC and thermal water purification is a distinct advantage compared to other options. A complete analysis of our economic and emissions results can be found in SI S1.

Altogether, our results show that carbon capture and evaporative water purification have great promise as end-uses of data center waste heat due to high carbon avoided/removed and economic potential. These conclusions hold even for higher temperature waste heat (Fig. S1) and other regions, such as China (Fig. S2) and Europe (Fig. S3). In our analysis, we considered each heat use application independently. However, hybrid approaches that use the heat for multiple purposes based on geographic, temporal, and economic constraints could also hold promise for heat valorization.

Data center waste heat-powered carbon capture (DC-DAC): potential and challenges

As shown in Fig. 2, data center waste heat-powered DAC (DC-DAC) could represent an impactful, yet underexplored, opportunity to remove atmospheric CO_2 and generate an economic benefit by selling it. DC-DAC could be achieved by thermal swing adsorption or thermal vacuum swing adsorption, where a solid sorbent is cycled between two temperatures.[58] At low temperatures, the sorbent captures dilute CO_2 ($\approx$400 ppm concentration) from air that is blown past the sorbent (Fig. 3a). The sorbent is then heated to higher temperatures using the data center heat, where it releases concentrated CO_2. After desorption, the sorbent cools down and it can readsorb CO_2, completing the cycle. Altogether, this process could source heat from the computing chips to power the energy-intensive thermal desorption step (Fig. 3b), replacing the expensive alternatives discussed earlier (*c.f.* Fig. 2h). Since only a small portion of the total energy input in temperature swing DAC is electricity ($\approx$10–20%),[59,60] data center heat could replace the largest and most expensive energy need. The concentrated CO_2 can later be compressed and transported offsite to be sequestered, used for enhanced oil recovery, or converted into carbon-based materials such as fuels or plastics (Fig. 3b). Additionally, this system would likely co-produce water as a byproduct, as ambient moisture is typically co-adsorbed and co-desorbed with CO_2 by the sorbents.[61] DC-DAC could then reverse the conventional paradigm, turning data centers into carbon-negative and water-producing systems which can help address major global challenges.

DC-DAC can benefit from free heat with data center co-location but may need to transport the produced CO_2 far distances for storage or utilization. Fig. 3c and 3d compare the free heat economic and carbon capture efficiency benefits, with the transport penalty against conventional systems that

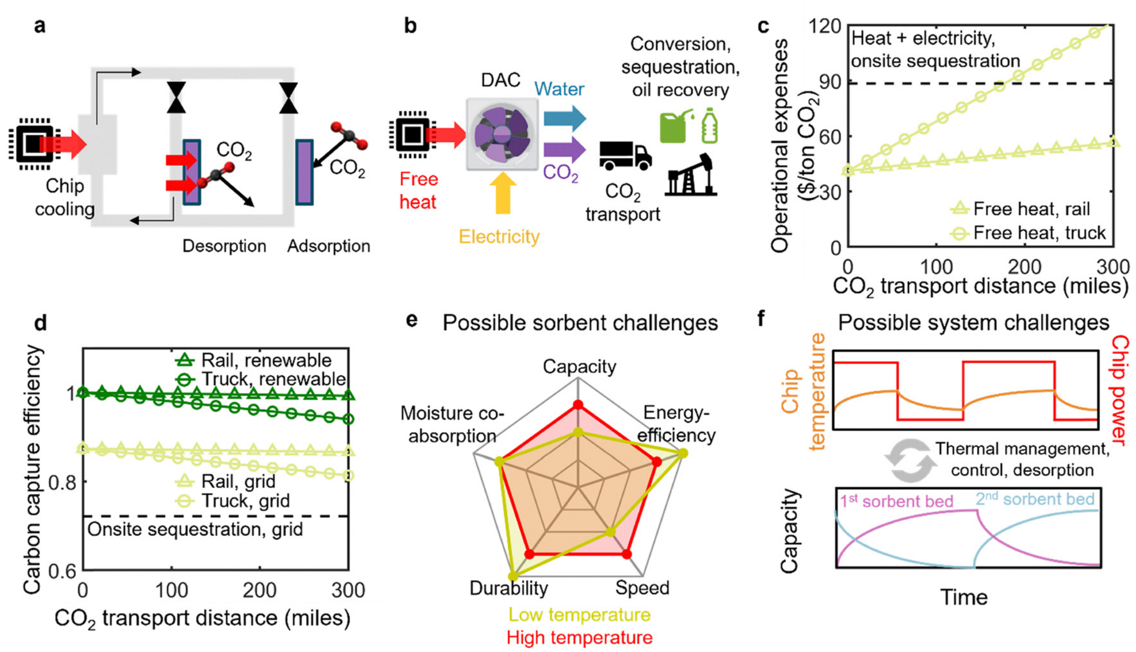

Fig. 3 Data center waste heat-powered DAC (DC-DAC) benefits and opportunities. (a) Potential system that uses data center waste heat generated in the computing chips to drive cyclic CO_2 adsorption–desorption. (b) Such a system can produce water and concentrated CO_2 from air. CO_2 can be transported offsite for end use. (c) DC-DAC can have lower operational expense, even when accounting for the cost of offsite transport, compared to onsite use but with heat and electricity consumption. (d) Similarly, DC-DAC can have high carbon capture efficiency, even when accounting for the offsite transport emissions, when compared with onsite use but with electricity consumption from the grid. (e) Conventional sorbents operate at high temperatures (>80 °C). Operating these sorbents at lower temperatures leads to lower sorption capacity and slow desorption, but higher durability and energy efficiency. Enabling DC-DAC, requires sorbents that overcome the low temperature operation challenges. (f) Chip power use variability, due to temporal variations in computing tasks, must be optimally coupled with the sorption-desorption dynamics through software and hardware (*e.g.*, thermal storage) for maximum heat utilization.

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consume electricity and heat but use the CO_2 onsite (see SI S3 for details). Firstly, there is an economic benefit from using waste heat despite the transport cost (Fig. 4c). DAC electricity and heat can demand $\approx$ \$90 per ton CO_2. Waste heat can reduce this cost to $\approx$\$40 per ton CO_2. However, cost increases proportionally to the CO_2 transport distance such that it reaches >\$120 and $\approx$\$60 per ton CO_2 for 300 miles of truck and rail transport, respectively. Naturally, a shorter transport is cheaper, but additionally, it releases less carbon dioxide. DC-DAC can still achieve high carbon capture efficiency (CCE) despite the emissions from transport, particularly if using rail over trucking (Fig. 3d). For instance, a DAC system in the United States that consumes grid electricity and heat produces on average $\approx$0.3 kg CO_2 per kg CO_2 captured due to the electricity and heat-related emissions. This translates into a $\mathrm{CCE} = \frac{\mathrm{Captured\,CO_2} - \mathrm{Produced\,CO_2}}{\mathrm{Captured\,CO_2}} \approx 0.7$. However, by using waste heat, CCE > 0.8 is possible even if the CO_2 is transported by truck or rail for 300 miles (Fig. 3d). If the electricity for DAC is obtained from renewable sources, the CCE can exceed 0.9. Altogether, this analysis shows that data center waste heat can reduce DAC operational cost and increase carbon capture efficiency even when transporting the produced CO_2 for <150 miles (for truck transport) and <300 miles (rail transport).

Realizing the potential of DC-DAC requires overcoming material-level and system-level challenges. Firstly, DAC sorbents typically desorb at >80 °C.[59] Sorbents have lower performance at lower temperatures, as some (and potentially all) CO_2 molecules remain bonded to the sorbent, and due to slower desorption (Fig. 3e).[62,63] Temperatures >80 °C might exceed data center waste heat since chips operate at <90 °C due to reliability concerns[42,59] and thermal resistances from the chip to the DAC system will further decrease the heat temperature. Despite major ongoing efforts in reducing these thermal resistances through high efficiency cooling and improved thermal interfaces, DC-DAC might require high performance sorbents that overcome the capacity and speed challenges of low temperature desorption. On the other hand, achieving low temperature desorption can have additional benefits beyond enabling data center waste heat-powered DAC, such as longer sorbent lifetimes and higher efficiencies due to lower sensible heating needs (Fig. 3e). Moisture co-adsorption, which can improve or lower performance, should also be considered when developing novel materials to ensure high performance across a wide range of humidity conditions.[61,64]

Some recent amine-based solid sorbents have achieved promising performance at temperatures relevant for DC-DAC. For instance, covalent organic framework-polyamine sorbents have been shown to release $\approx$2 mmol CO_2 g^{-1} sorbent at 60 °C.[48] Hydrogel-polyethylenimine sorbents have been shown to release $\approx$4.5 mmol CO_2 g^{-1} sorbent and $\approx$1.9 mmol CO_2 g^{-1} sorbent at 70 and 50 °C, respectively.[62] Further improvements on desorption capacity at low temperatures could be possible through even higher amine efficiencies, amine loadings, and by tuning the amine type to maximize low-temperature desorption.[65] Ideally, this reduction of desorption temperature should not come at the expense of additional vacuum, as this can lead to higher system-level costs.[66] In parallel, a mechanistic understanding of the sorption performance (CO_2 capacity, moisture sorption, and kinetics) as a function of material properties and its conditions (humidity, sorption temperature, desorption temperature, pressure) is critical towards material-level and system-level optimization.[67]

Secondly, DC-DAC poses system-level challenges due to the magnitude (>100 MW/data center) and nature (low temperature, possibly intermittent) data center heat. For instance, utilizing >100 MW of heat would lead to the largest DAC facility currently demonstrated. This could pose challenges such as area-dense DAC plant design that ensures high CO_2 concentrations (~400 ppm) entering the system and demanding massive scaling of the sorbents and contactors. Similarly, different desorption approaches might be necessary as commonly considered steam stripping could be incompatible with the low waste heat temperatures (<70 °C).[67] Liquid-sorbent heat exchangers could potentially be used; however, they should be carefully designed by coupling material properties with heat and mass transfer to ensure maximum heat utilization.[68] Lastly, strategies to dynamically match the data center heat with the cyclic adsorption–desorption DAC could also be required (Fig. 3f). Data center computation, which produces the heat, can have high temporal variability due to varying task complexity, arrival times, and resource utilization.[69] This will lead to a variable heat generation profile. Ideally, all this heat is utilized for carbon capture, demanding software and hardware tools that dynamically source the heat for the DAC desorption. For instance, software tools that schedule computation tasks accounting for the availability of sorbents for desorption or that control sorption times through variable airflows can help maximize waste heat utilization.[70] Similarly, physical components, such as energy-dense systems that store excess heat and release it later to power desorption, can enable further flexibility and improved heat use.

Data center waste heat-powered evaporative water purification (DC-W): potential and challenges

Evaporative water purification is another major opportunity for data center waste heat reuse. By utilizing waste heat, this process avoids carbon dioxide emissions associated with conventional water desalination and produces an economic stream by selling water. A schematic of a possible data center waste heat-powered evaporative water purification (DC-W) system, similar to membrane distillation,[71] is shown in Fig. 4a. This system transfers heat from the data center chips to water that will be purified, which can be seawater or brackish groundwater, *via* a coolant. The hot coolant heats the brackish water, which evaporates leaving behind a concentrated brine. The vapor is then condensed on a cold surface, producing clean water. Furthermore, the condensation heat released can be reutilized to evaporate more brackish water in a subsequent

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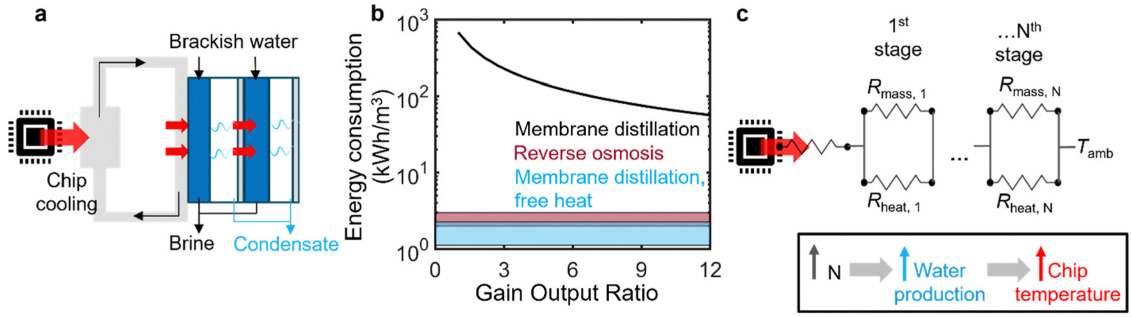

Fig. 4 Data center waste heat-powered thermal water purification (DC-W) benefits and opportunities. (a) Potential system that uses data center waste heat generated on the computing chips to purify water *via* evaporation-condensation. Heat is removed from the chips and used to evaporate brackish water and then condense it to produce clean water. The condensation heat can be reutilized in subsequent evaporative stages. (b) By using free heat, this system can have lower energy requirements than reverse osmosis and conventional membrane distillation without waste heat use. (c) DC-W systems should be optimized to ensure maximum water production and safe chip operating temperatures.

stage (Fig. 4a), increasing the water production for a given heat input. Heat reutilization and energy efficiency can be quantified by the gain output ratio = $m_w h_{lv}/Q_{in}$,[72] where m_w is the mass of water treated, h_{lv} is the water latent heat of vaporization, and Q_{in} is the heat provided to the system. As the Gain Output Ratio of a membrane distillation system increases, its energy consumption decreases (Fig. 4b). Even for typical values of Gain Output Ratio (~2–12),[72] the energy consumption of membrane distillation exceeds in over an order of magnitude that of reverse osmosis (Fig. 4b, see SI S4 for details). However, by utilizing "free" data center waste heat, evaporative water treatment systems can have lower energy requirements than reverse osmosis. This lower energy consumption, combined with low system cost and enhanced fouling resistance relative to reverse osmosis,[72] make DC-W a promising technology for water treatment which can turn data centers into water-positive systems.

Maximizing water production using data center waste heat requires system-level heat and mass transfer optimization. As shown in Fig. 4c, while increasing the number of stages generally increases water production due to higher heat reutilization, it also adds heat and mass transfer resistances. Consequently, the chip temperature will tend to increase with higher number of stages.[45,71] Therefore, DC-W systems must be carefully designed to ensure safe chip operation (<90 °C)[59] while maximizing water production through optimized number of stages, high efficiency chip cooling, and heat and mass transfer-optimal separation distances between evaporation and condensation surfaces. From an operational perspective, heat utilization can also be maximized through computer load task scheduling.[70] These system-level opportunities can transform data centers into systems that address the critical water scarcity challenge by enabling high efficiency water purification.

A new data center metric: energy use efficiency

We propose a new metric to emphasize extracting as much benefit as possible, in the form of compute and useful heat, from data center electricity. We note that there are numerous other data center energy and sustainability metrics, and we refer readers to other reviews that cover them in more detail.[73–75]

We start with the total-power usage effectiveness (TUE):[76]

$$\mathrm{TUE} = \frac{\text{Total facility energy}}{\text{Energy into compute components}} \tag{4}$$

Energy into compute components is closer to the 'computational work' that we define in Fig. 1 as it only includes energy use by CPUs, GPUs, memory, and drives, and excludes server fan energy. Energy into compute components also reflects the heat generated at the chips that can be utilized. In contrast, IT equipment energy, as used in eqn (1) for the PUE, includes server fan energy. We build onto TUE by incorporating our reframing of data centers from Fig. 1. We propose a new metric called energy use efficiency (EUE):

$$\mathrm{EUE} = \frac{\text{Energy into compute components} + \text{reuse energy}}{\text{Total facility energy}} \tag{5}$$

EUE incentivizes data center waste heat use, reuse energy, which can lead to EUE > 1. We note that EUE is a function of TUE and a less common energy reuse metric, energy reuse factor (ERF):[77]

$$\mathrm{ERF} = \frac{\text{Reuse energy}}{\text{Total facility energy}} \tag{6}$$

$$\begin{aligned}\mathrm{EUE} &= \frac{\text{Energy into compute components}}{\text{Total facility energy}} + \frac{\text{Reuse energy}}{\text{Total facility energy}} \\ &= \frac{1}{\mathrm{TUE}} + \mathrm{ERF}\end{aligned} \tag{7}$$

There are fundamental issues with energy management metrics in data centers, such as EUE and PUE, because better values do not necessarily reflect higher efficiency.[78] For example, energy into compute components does not measure the computational work done, but rather all the power supplied to the compute components. Even an idle CPU (*i.e.*, no computational work) draws power, idle power. If an energy efficient chipset consumes 90% less power while idle, energy into compute components decreases by 90%, but total facility energy decreases less

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since there are other data center energy demands. Therefore, both TUE and PUE will increase while EUE will decrease, suggesting a lower data center energy effectiveness despite lower data center energy consumption. For these reasons, we agree with others about the importance of incorporating energy utilization into data center metrics.[15,78] We can overcome this and more accurately reflect our framework in Fig. 1 with a more comprehensive version of our proposed metric, EUE^+:

$$\text{EUE}^+ = \frac{\text{Computational work} + \text{reuse energy}}{\text{Total facility energy}} \tag{8}$$

where computational work = energy into compute components − idle power is defined as the power a component draws while serving a computational task. While similar to EUE, the distinction is that the EUE^+ numerator only includes useful work (*i.e.*, it excludes idle power)– utilization is inherently factored into EUE^+. If a chipset draws 500 W of power while computing, 500 W are added to both the numerator and denominator. If that chipset draws 50 W of power while idle, that is 0 W of useful work and the 50 W is only added to the denominator, decreasing EUE^+ and penalizing idle power.

Flipping the switch: achieving carbon-negative and water-positive data centers

Using this framework, our analysis in Fig. 2, and our proposed metric, we estimate the potential impact of using data center waste heat for carbon capture and water purification in terms of carbon, water, and energy efficiency. Fig. 5 shows the carbon and water efficiency of various data center operators including Google (red), Meta (blue), and Microsoft (yellow). We also include the industry average (black). SI S5 provides further details on the data.

The *y*-axis on Fig. 5 is a variant of water use efficiency (WUE*):

$$\text{WUE}^* = \frac{\text{Net annual water production}}{\text{IT equipment energy}} \tag{9}$$

in units of L kWh^{-1} and defined such that a positive value corresponds to water production. The x-axis on Fig. 5 is the carbon use efficiency (CUE):

$$\text{CUE} = \frac{\text{Total GHG emissions}}{\text{IT equipment energy}} \tag{10}$$

in units of kg CO_2 kWh^{-1}, where a positive value represents carbon production. Fig. 5 shows that existing data centers are in the bottom right quadrant since they all consume water and produce CO_2 (using location-based carbon emissions). The size of the circles also indicates the EUE of each data center – the smaller the circle, the smaller the EUE.

Typical data centers are in the lower right quadrant as they produce carbon and consume water, partially due to the prevalence of air cooling. Liquid and two-phase cooling can improve the CUE and WUE^+ by reducing cooling energy and

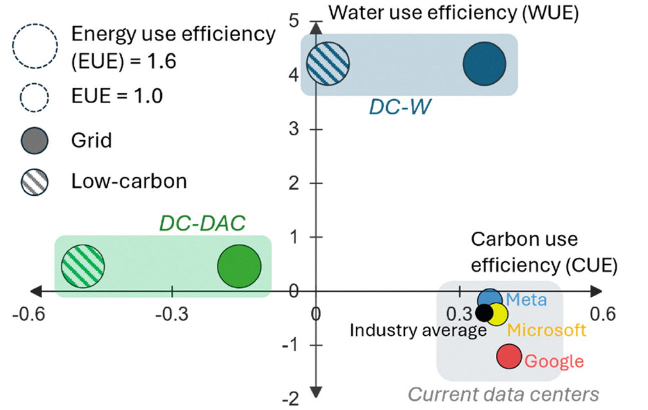

Fig. 5 Carbon (CUE), water (WUE*), and energy (EUE) use efficiencies of data centers. Utilizing waste heat from data centers increases the size of the dot (improves EUE). Utilizing this waste heat for DC-W or DC-DAC moves the dot towards the top left. The CUE was calculated based on the location-based electricity emissions.

enabling the use of dry cooling, in contrast with evaporative processes. However, efficient cooling only moves the point closer to the origin, not past it. To move data centers to the upper left quadrant (*i.e.*, flipping the switch), they must use their waste heat.

Fig. 5 also shows our estimate for the CUE and WUE* of a DC-DAC data center. Complete details of our analysis are in SI S6. Importantly, we assume TUE < 1.05 and a 65 °C facility water outlet temperature. Using our assumptions, DC-DAC powered by green electricity removes 0.5 kg of CO_2 (CUE = −0.43) and produces 0.5 kg of water (WUE* = 0.38) for every kWh of electricity into the data center. Assuming the data center is operating at full capacity, the EUE is 1.6. Even if powered entirely by a natural gas combined cycle plant, the data center still removes net carbon (CUE = −0.03). If the data center instead uses its waste heat to thermally produce water (DC-W), the WUE* increases significantly to 3.9, but the CUE remains the same as before. Regardless, either end use moves data centers from the lower right quadrant (undesirable) to either deep into the top right (evaporative water production) or slightly into the upper left (carbon removal).

Conclusion

Waste heat utilization offers a crucial opportunity to boost data center sustainability, critical amid ongoing AI-driven data center growth. From a thermodynamic, revenue, and emissions perspective waste heat-powered carbon capture and water purification are promising waste heat end uses, capable of removing/avoiding large amounts of carbon dioxide (>100 MT CO_2 per year for carbon capture) while producing a valuable output (>$1 B per year in produced water or carbon). This potential exceeds that of conventional waste heat use applications, including power generation and direct heat use. Enabling these underexplored DAC and water applications demands scientific and engineering innovations, which can help realize

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carbon capture and water production with improved performance over incumbent approaches. Through these novel end uses, data centers can become carbon-negative and water-positive while achieving high efficiency, as captured by our proposed metric, the Energy Utilization Efficiency, EUE. This can reverse the conventional data center paradigm, turning this rapidly growing infrastructure in a tool to address major emissions and water challenges. Ultimately through combined and parallel efforts in heat reuse, improved chip computation efficiency, and advanced cooling technologies AI sustainability can be achieved.

Author contributions

C. D. D. conceptualization, investigation, formal analysis, writing – original draft, and writing – review & editing. Z. B. conceptualization, investigation, formal analysis, writing – original draft, and writing – review & editing.

Conflicts of interest

There are no conflicts of interest to declare.

Data availability

The data supporting this article have been included as part of the SI.

(S1) Conversion efficiency, economic value, and product carbon intensity of heat use applications; (S2) Effect of emissions on carbon price; (S3) Parameters for data center waste heat-powered direct air capture (DC-DAC) analysis; (S4) Parameters for data center waste heat-powered evaporative water purification (DC-W) analysis; (S5) Data center environmental metrics; and (S6) Combined analysis of data centers with waste heat-powered thermal water purification (DC-W) and direct air capture (DC-DAC). See DOI: **https://doi.org/10.1039/d5ee02676h**

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