Climate- and Technology-Specific PUE and WUE Predictions for U.S. Data Centers using a Physics-Based Approach

Nuoa Lei (✉ nuoaLei2021@u.northwestern.edu)

Northwestern University

Eric Masanet

University of California, Santa Barbara

Research Article

Keywords: Data centers, Water, Energy analysis, Water-energy nexus, Water usage effectiveness, Power usage effectiveness

Posted Date: August 3rd, 2021

DOI: <https://doi.org/10.21203/rs.3.rs-769999/v1>

License: © ⓘ This work is licensed under a Creative Commons Attribution 4.0 International License.

[Read Full License](#)

Climate- and Technology-Specific PUE and WUE Predictions for U.S. Data Centers using a Physics-Based Approach

Highlights

- An open model is presented for simultaneous data center PUE and WUE predictions
- Credible PUE and WUE ranges are presented across U.S. data center types and locations
- Variance analysis indicates potentially large PUE and WUE improvement potentials
- Sensitivity results identify PUE and WUE improvement strategies and data priorities
- PUE and WUE values can be used by energy analysts for water footprint analysis

Abstract

The onsite water use of data centers (DCs) is becoming an increasingly important consideration within the policy and energy analysis communities, but has heretofore been difficult to quantify in macro-level DC energy models due to lack of reported water usage effectiveness (WUE) values by DC operators. This work addresses this important knowledge gap by presenting thermodynamically-compatible power usage effectiveness (PUE) and WUE values for a wide range of U.S. DC archetypes and climate zones, using a physics-based model that is validated with real-world data. Results enable energy analysts to more accurately analyze the onsite energy and water use of DCs by size class, cooling system type, and climate zone under many different operating conditions including operational setpoints. Sensitivity analyses further identify the variables leading to best-achievable PUE and WUE values by climate zone and cooling system type—including operational set points, use of free cooling, and cooling tower equipment and operational factors—which can support DC water- and energy-efficiency policy initiatives. The consistent PUE and WUE values may also be used in future work to quantify the indirect water use of DCs occurring in electrical power generating systems.

Keywords

Data centers; Water; Energy analysis; Water-energy nexus; Water usage effectiveness; Power usage effectiveness.

1. Introduction

Data centers (DCs) are an increasingly important component of global electricity use, and this electricity use may grow in the near-term due to rising demand for DC services as the world becomes increasingly interconnected and as compute-intensive applications like artificial intelligence and blockchains become more commonplace (Lei et al., 2021b; Masanet et al., 2020a; Patterson et al., 2021). As a result, the electricity use of DCs has become a more frequent topic of research within the energy analysis community (Hintemann and Hinterholzer, 2019; Shehabi et al., 2018). DC electricity use can generally be divided into two primary categories: the electricity use of information technology (IT) equipment (i.e., servers, storage devices, and network devices) and the electricity use of power provision and cooling (i.e., infrastructure) equipment (Lei, 2020; Masanet et al., 2020a; Shehabi et al., 2016). Many energy analysts model infrastructure equipment energy use by assuming an average power usage effectiveness (PUE) value, where PUE is defined as the dimensionless ratio of a DC's total electricity use (in kilowatt-hours, or kWh) to its IT electricity use (in kWh) (Jauregui, 2011). The analyst's assumed PUE value is then multiplied

by modeled IT electricity use to arrive at a total electricity use estimate for a DC or for DCs within a given region (European Commission, 2020; Koomey, 2011; Shehabi et al., 2016).

However, the onsite water use of DCs is also an important environmental consideration (Mytton, 2021; Siddik et al., 2021), and can even pose barriers to DC siting in water stressed regions. Onsite water use is predominantly driven by the water used in DC space conditioning systems, which are comprised of cooling systems and air humidification systems (Lei and Masanet, 2020). The major types of cooling systems that require onsite water are water-cooled chiller systems and direct evaporative cooling systems (Evans, 2004). Yet analysis of water use is currently less common compared to electricity use within the energy analysis community, in part due to lack of reliable data on the onsite water use of DCs and its relation to different space conditioning systems. The onsite water use of a DC can be expressed as its water usage effectiveness (WUE), which is defined as the ratio of a DC's total onsite water use to its IT electricity use (Patterson et al., 2011), expressed in units of liters per kilowatt-hour (kWh). Despite the growing importance of onsite water use, few DC operators regularly report their WUE values, with Facebook (Facebook, 2014) and Scaleway (Scaleway, 2021) being notable exceptions.

To incorporate onsite water use estimation into DC energy models, analysts require credible estimates of WUE values that correspond not only to specific cooling system types, but also to specific local climate conditions. Local climate conditions can be important factors because they affect a DC's ability to utilize economizers for "free cooling" in lieu of mechanical cooling; also, local air temperatures and relative humidity (RH) will affect space conditioning requirements. Moreover, because WUE and PUE values are interrelated on the basis of mass and energy balances that are governed by thermodynamic principles, for accurate modeling of onsite water use, analysts must be careful to choose WUE values that are thermodynamically-compatible with their assumed PUE values. To date, however, no thermodynamically-compatible WUE and PUE values have been published for use by energy analysts across a range of typical DC space conditioning types and climatic conditions. Therefore, the DC energy analysis community has been limited in its ability to accurately estimate onsite water use.

This paper fills this important knowledge gap by presenting a physics-based model for predicting thermodynamically-compatible WUE and PUE values with reasonable accuracy for different DC types and locations, and which only relies on publicly-available data and reasonable assumptions about key system parameters.

More specifically, this paper makes the following contributions to the literature:

- i. Expands a previous and proven physics-based DC PUE model (Lei and Masanet, 2020) to generate thermodynamically-compatible WUE estimates.
- ii. Constructs 10 different DC archetypes on the basis of detailed technology and operating parameters, which broadly represent most types of air-cooled DC operations in the United States.
- iii. Applies the model to generate predicted PUE and WUE ranges for each DC archetype within 16 different U.S. climate zones (Baechler et al., 2015), which can be used by the DC energy analysis community for estimating onsite water use under many different conditions and locations.
- iv. Presents and discusses the model's sensitive variables, which are those that future analysts should focus on for improving the accuracy of the model when applied to any specific DC.

Furthermore, the model is made freely available for use and further improvements by the research community. As such, this paper fills important quantitative knowledge gaps on DC WUE and its main climate, technological, and operational determinants and provides a new method for predicting both PUE and WUE in future DC modeling exercises with both reasonable accuracy and spatial specificity. This paper does not address the indirect water use of DCs, which is associated with water consumed within the power grids that provide DCs with electricity (Shehabi et al., 2016; Siddik et al., 2021). However, the WUE predictions presented here for assessing the onsite water use of DCs can be important inputs into future studies that estimate the total (i.e., onsite plus indirect) DC water footprints.

2. Previous WUE analyses

Unlike the DC energy usage that has attracted much attention from academic research and mainstream media, water is another key resource for DC operations, but it has only recently attracted public attention due to local water stress issues (GILLIN, 2021; SATTIRAJU, 2020). However, as the demand for digital services continues to grow, the importance of DC direct water use is also growing. One obvious reason is that the use of energy and water within a DC is coupled. Therefore, increasing DC power capacity may lead to increased direct water consumption, which could compete with local communities for stressed water resources. For example, due to expanded digital services and organizational growth, Google's overall direct water consumption increased from 2.5 billion gallons in 2016 to 4.17 billion gallons in 2018 (Google, 2019). As a result, some DC facilities have been scrutinized by local communities, public utilities, and water conservation groups for requiring too much water (SATTIRAJU, 2020). To help facilitate awareness and reporting of DC water use, The Green Grid (TGG) proposed the WUE metric in 2011 as a standardized method for DC operators to calculate and report their direct water use performance (Patterson et al., 2011).

To date, only a few published studies have attempted to quantify DC water use performance (i.e., WUE) in the peer-reviewed literature, and most current water analyses are based on limited measurement data or unvalidated assumptions. The earliest studies were published by Sharma et al., who analyzed measured water and energy data from a single DC cooled by a hybrid cooling system employing air-cooled and water-cooled chillers operating on a rotational basis. The authors analyzed data from two representative days to evaluate the tradeoffs between the DC's water use and energy efficiency, concluding that water-cooled chillers are much more energy efficient than air-cooled chillers although the former drives significant cooling tower water consumption (Sharma et al., 2009, 2008). The same authors later extended their analysis to include the use of an airside economizer, and compared its water and energy use performance to a water-cooled chiller system and an air-cooled chiller system using energy and water use estimations based on manufacturer data (Sharma et al., 2010). By extending their analysis, the authors found that compared with using a water-cooled chiller, using an air-cooled chiller can reduce the DC water consumption at the expense of increasing the electricity cost, while using outside air cooling could reduce both the DC's water and power use at the same time. A 2016 report by Lawrence Berkeley National Laboratory (LBNL) analyzed the direct water use of DCs at the national level, estimating that the total direct water usage of U.S. DCs amounted to 126 billion liters in 2014 (Shehabi et al., 2016). To arrive at this estimate, the authors assumed a nationwide average DC on-site water consumption of 1.8 liters per kWh of total DC site energy use. More recently, Sharma et al. performed a time-series analysis of the energy and direct water use of a DC employing a water-cooled chiller system with a waterside economizer in western Massachusetts using monitored data (Sharma et al., 2017). The authors observed clear seasonal variations in the DC's on-site PUE and WUE values (both of which peaked during the summer

season), highlighting the significance climate effects on the DCs' power and water use. A study by Gozcu et al. is one of the only studies that attempted to model DC PUE and WUE values, which also expanded the regional coverage considerably by analyzing the energy and direct water saving potentials of different DC free cooling technologies (including airside economizers, indirect evaporative coolers, waterside economizers) in 19 cities, underscoring the importance of economizer choices in DC operations (Gozcu et al., 2017). However, the modeling methodology of this study was not clearly documented, and the modeling results were not verified using real DC operation data.

There is another category of studies that conducted secondary data analysis for DC water use based on extrapolation or data aggregation. Ristic et al. (Ristic et al., 2015) extrapolated a global average DC overall water footprint based on the direct water use of four different cooling technologies (air- or water-cooled chiller with or without an airside economizer using adiabatic cooling) in Phoenix, a worldwide DC energy use estimate in 2010 (Koomey, 2011), and the global average water footprint per unit of electricity generation, which resulted in a large DC overall water footprint range of 1,047 to 151,061 m³/TJ. Siddik et al. investigated the environmental footprint of U.S. DCs in 2008 (Siddik et al., 2021), based on the nationwide average DC on-site water use estimated by LBNL (Shehabi et al., 2016), average DC PUE values reported in (Masanet et al., 2020b), and an estimated geographical distribution of U.S. DCs (Ganeshalingam et al., 2017), revealing that around 1/5 of the U.S. DC servers are cooled by water drained from water stressed watersheds.

While all of these studies have provided valuable insights into the water intensities associated with different cooling system types in different locations, none answer our proposed research questions due to several important limitations (Table 1). First, direct water use estimates are typically limited to cooling tower water use only, which neglects potentially non-trivial water consumption by adiabatic cooling and humidification systems. Second, direct water use estimates have mostly been limited to a small set of cooling technologies in a few specific locations without revealing important technical parameters that may impact WUE in those locations, such as equipment efficiencies and set points. Third, all but one study (Gozcu et al., 2017) analyzed the direct water use of single DCs in specific locations, and using data from a small number of representative days, which prohibits exploration of how climate variations by location would affect WUE. Even so, the study by Gozcu et al. applied static equipment power and water use profiles and did not explore how DC facility system variations would affect WUE. Fourth, while some studies presented corresponding PUE values, others did not, which overlooks an important consideration for estimating both direct and indirect water use intensities in a thermodynamically-consistent manner. Finally, the overall lack of generalizable models prohibits extension of results to other cooling system types, operating conditions, or locations, which is necessary for energy analysts and policy makers to estimate DC water use and identify improvement pathways under the many different conditions associated with existing DCs.

Table 1. Summary of previous studies of DC water use.

Study	Study scope (direct and/or indirect ?)	Direct water scope (cooling tower, adiabatic cooling, space humidification?)	Were PUE values reported?	Were WUE values reported ?	DC locations considered	Cooling variants considered?	Study type (empirical data or modeled estimate)	Temporal basis (single day, multiple day, annual)	Level of technical detail reported (equipment efficiency, setpoints, etc.)	If a model was used, is it available and generalizable?
(Sharma et al., 2009, 2008)	Direct	Cooling tower	No	No	No	No	Empirical data	Multiple day	No	n/a
(Sharma et al., 2010)	Direct + indirect	Cooling tower	No	No	Palo Alto, California	✓	Empirical data	Multiple day	No	n/a
(Shehabi et al., 2016)	Direct + indirect	Cooling tower	✓	No	United States	n/a	Empirical data	Annual	No	n/a
(Sharma et al., 2017)	Direct	Cooling tower	✓	✓	Holyoke, Massachusetts	No	Empirical data	Annual	Supply air temperature (26.7 °C)	n/a
(Gozcu et al., 2017)	Direct	Cooling tower + adiabatic cooling	✓	✓	19 cities	✓	Modeled estimate	Annual	Chiller efficiency (COP=4.0), Supply air temperature (15 or 25 °C)	Not available
(Ristic et al., 2015)	Direct + indirect	Cooling tower + adiabatic cooling	No	No	Phoenix, Arizona	✓	Empirical data	Annual	Supply air temperature (27 °C)	n/a
(Siddik et al., 2021)	Direct + indirect	Cooling tower	✓	No	United States	n/a	Empirical data	Annual	No	n/a

Note: n/a = not applicable.

3. Methodology

3.1. Modeling scope and system definitions

In this paper we focus on modeling the WUE and PUE of DCs under different space conditioning technology, operations, and climate conditions. We report both WUE and PUE values since the latter can be useful in future studies for estimating indirect water use and both values can vary significantly with climate and technology assumptions. Importantly, WUE and PUE are directly related by physics, so it is important that compatible values are used together in future studies to avoid introducing errors that can be made when predicting WUE and PUE independently.

A DC's space conditioning technologies, operating characteristics, and climate conditions influence both its PUE and WUE values. Thus, simultaneous modeling of PUE and WUE values under the same technology, operations, and climate conditions is necessary for accurate quantification of a DC's overall water footprint. In our analysis, we selected seven different space conditioning technology configurations consisting of different combinations of refrigeration units, cooling towers, direct evaporative (i.e., adiabatic) coolers, and space humidification options as summarized in Table 2. These seven configurations were identified as most representative of present-day DC space conditioning systems globally based on (Capozzoli and Primiceri, 2015; Evans, 2012; Joshi and Kumar, 2013; Lei and Masanet, 2020) and are schematically depicted in Figure 1. For further information and technical details on these systems, readers are referred to (Evans, 2012; Lei and Masanet, 2020).

To assess differences in operating characteristics that affect WUE and PUE, including equipment efficiencies and internal temperature and humidity set points, we further defined three different DC size classes based on the taxonomy in (Shehabi et al., 2016). Small-scale DCs represent spaces typically less than 1000 ft², which generally operate with low uninterruptible power supply (UPS) and airflow efficiencies and narrow allowable temperature and humidity ranges (Ni and Bai, 2017) and include server rooms. Large-scale DCs can occupy more than 20,000 ft², inclusive of hyperscale DCs, and tend to operate with high UPS and airflow efficiencies with wider allowable temperature and humidity ranges, leading to frequent use of free cooling (Barroso et al., 2013; Jay Park, 2011; Miller, 2009). In between these two extremes lie midsize DCs, which are representative of many on-premise enterprise and colocation DCs ranging from 1000-20,000 ft² and with average operating efficiencies (Lawrence et al., 2019).

In total, we considered 10 different cases representing different size classes and space conditioning technology configurations, covering a wide swath of typical DC technology and operating conditions.

Table 2. DC size class and space conditioning cases considered

Case	DC Size	Cooling system configuration ⁽¹⁾	Direct water use equipment included		
			Direct evaporation	Space humidification ⁽²⁾	Cooling tower
1	Large-scale	Airside economizer + adiabatic cooling + (water-cooled chiller)	✓	✓ (adiabatic)	✓
2	Large-scale	Waterside economizer + (water-cooled chiller)	n/a	✓ (adiabatic)	✓
3	Midsize	Airside economizer + (water-cooled chiller)	n/a	✓ (adiabatic)	✓

4	Midsize	Waterside economizer + (water-cooled chiller)	n/a	✓ (adiabatic)	✓
5	Midsize	Water-cooled chiller	n/a	✓ (adiabatic)	✓
6	Midsize	Airside economizer + (air-cooled chiller)	n/a	✓ (adiabatic)	n/a
7	Midsize	Air-cooled chiller	n/a	✓ (adiabatic)	n/a
8	Small	Water-cooled chiller	n/a	✓ (isothermal)	✓
9	Small	Air-cooled chiller	n/a	✓ (isothermal)	n/a
10	Small	Direct expansion system	n/a	✓ (isothermal)	n/a

Note: (1) parentheses indicate a supplemental cooling system (e.g., in case 1, a water-cooled chiller will be used only when the airside economizer and adiabatic cooling system cannot satisfy the DC cooling requirement); (2) parentheses indicate the type of humidifiers being used for space humidification (i.e., adiabatic humidifier or isothermal humidifier).

Finally, to consider how local climate conditions affect WUE and PUE values for our 10 different cases, we focused our analysis on the United States given its wide variety of climate zones. Specifically, we analyzed each DC case within sixteen distinct U.S. climate zones designated by the International Energy Conservation Code (IECC) and the American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE) (ASHRAE, 2013; Baechler et al., 2015). The IECC/ASHRAE climate zones include eight major temperature-oriented zones and three moisture subcategories (A: moist; B: dry; C: marine.) as depicted in Figure 2. For each IECC/ASHRAE climate zone, we chose a representative city designated by the U.S. Department of Energy (Department of Energy, 2020), shown in brackets in Figure 2. For each city, meteorological data containing hourly air temperature, RH, and atmospheric pressure in a typical meteorological year were compiled (EnergyPlus, 2016), which were then used to simulate WUE and PUE values for each DC case for each hour over the entire meteorological year.

In the next section, we briefly introduce the hourly DC PUE and WUE model used in our framework. Our DC PUE and WUE simulation code (in Python) is available through the link provided in Appendix A.

Figure 1. Schematic diagrams of considered DC cooling system configurations (CRAH = computer room air handler).

Figure 2. United States IECC/ASHRAE climate zones (circles represent climate zone representative cities).

3.2. DC PUE and WUE model

Our combined PUE and WUE model is derived from a physics-based PUE model previously published in (Lei and Masanet, 2020). Below, we describe the governing equations and key parameters in the model for calculating both WUE and PUE for a given set of space conditioning system technology, operating, and climate conditions. For a more detailed description of the model and calculation approach, readers are referred to Appendix A and (Lei and Masanet, 2020). The numerical values assigned to each parameter in our DC case simulations are described in the next section.

Eq (1) expresses the DC on-site water use rate (w^{DC} , kg/s) which is a function of the water used by three equipment types (see Table 2): (1) cooling towers (including evaporated water (w_e^{CT} , kg/s), windage loss of water (w_w^{CT} , kg/s), and draw-off water (w_d^{CT} , kg/s)); (2) adiabatic cooling (also called as direct evaporative cooling) (w^{AC} , kg/s); and (3) space humidification (w^{SH} , kg/s).

$$w^{DC} = w^{CT} + w^{AC} + w^{SH} = (w_e^{CT} + w_w^{CT} + w_d^{CT}) + w^{AC} + w^{SH} \quad (1)$$

Cooling tower water use rates in Eq (1) depend on the amount of heat generated in the data center (Q^{DC} , kW) and the power use of the DC (p^{DC} , kW), which is calculated using Eqs. (2) and (3). These two equations are also fundamental for simultaneously calculating both WUE and PUE for the same system conditions on the basis of underlying system physics. Further details on the calculation of total DC power use in Eq (3) can be found in (Lei and Masanet, 2020).

$$Q^{DC} = p^{IT} + p_{loss}^{UPS} + p_{loss}^{PD} + p^L + p^{IS} \quad (2)$$

$$p^{DC} = p^{IT} + p_{loss}^{UPS} + p_{loss}^{PD} + p^L + p^{IS} + \sum p^{PUMPS} + \sum p^{FANS} + p^{CH} \quad (3)$$

where p^{IT} , p_{loss}^{UPS} , p_{loss}^{PD} , p^L , p^{IS} , p^{PUMPS} , p^{FANS} , and p^{CH} are respectively the power use of IT equipment, power loss of UPS system, power loss of power transformation and distribution system, and the power used by the lighting system, isothermal humidifier, pumps (which includes the humidification pumps used for adiabatic cooling and in adiabatic space humidifiers), fans, and mechanical chiller (direct expansion cooling units were classified into the chiller category in this paper for simplicity).

The energy flow across the cooling tower (Q^{CT} , kW) is calculated via Eq (4).

$$Q^{CT} = Q^{DC} + Q_s^{CH} / (SHR * COP_{L,T}) \quad (4)$$

where Q_s^{CH} is the quantity of sensible cooling supplied by a mechanical chiller (kW), governed by the DC heat generation and the amount of free cooling supplied by the economizer (the amount of free cooling being exploited is a function of outdoor air condition and the DC indoor air setpoints, which is determined by the enthalpy difference of supply and outside air for case 1, temperature difference of supply and outside air for other cases employing airside economizer, and temperature difference between the return facility water temperature and the outdoor wet bulb temperature for cases employing a waterside economizer (Joshi and Kumar, 2013; Lei and Masanet, 2020)); SHR is the sensible heat ratio (kW/kW), defined as the sensible cooling load divided by the total cooling load of a mechanical chiller; $COP_{L,T}$ is the chiller's coefficient of performance (COP) (kW/kW), parametrized by the chiller load factor and an outdoor temperature-related variable using Gaussian process regression based on data from (Gullo et al., 2017; Squillo, 2018; Yu and Chan, 2007).

Thereafter, the three different cooling tower water use parameters were calculated using an established cooling tower energy and mass balance model (Environmental Protection Agency and program, 2017), expressed by Eqs. (5)-(7).

$$w_e^{CT} = Q^{CT} / H_{vap} \quad (5)$$

$$w_w^{CT} = \phi_w * Q^{CT} / (c_w * \Delta T_{CT}) \quad (6)$$

$$w_d^{CT} = w_e^{CT} / (CC - 1) - w_w^{CT} \quad (7)$$

where H_{vap} is the latent heat of vaporization of water (kJ/kg), which is a function of cooling tower water temperature; ϕ_w is the windage loss of water as a percentage of cooling tower mass flow rate of water; c_w is the specific heat of water ($kJ/kg \cdot ^\circ C$); ΔT_{CT} is the cooling tower supply and return temperature difference ($^\circ C$); CC is the cycles of concentration, describing the levels of dissolved solids in the cooling tower water.

Our case 1 considers the use of airside economizers with adiabatic cooling, with reliance on a water-cooled chiller for hours when climate conditions are not favorable. This configuration can deliver both low WUE

and low PUE values, especially in cooler climates where reliance on mechanical chillers can be substantially reduced or even eliminated completely as demonstrated by several hyperscale DC operators (Amazon, 2020; Jay Park, 2011; Morgan, 2016). These operators also tend to use high temperature set points to maximize adiabatic cooling use hours (Jay Park, 2011; Miller, 2009). The amount of water use for adiabatic cooling is determined by both the DC outdoor air conditions and the indoor air set points (i.e., dry bulb temperature, RH, and dew point) and is calculated using Eq. (8).

$$w^{AC} = m_{cd,dry} * (d_{cd} - d_{oa}) \quad (8)$$

where $m_{cd,dry}$ is the mass flow rate of dry air that goes through the adiabatic process (kg/s); d_{cd} is the absolute humidity of humidified air (kg/kg), see (Joshi and Kumar, 2013) for the calculation method; d_{oa} is the absolute humidity of outdoor air (kg/kg).

Lastly, to compensate for humidity loss within the internal DC space and avoid electrostatic discharge (ASHRAE, 2015), humidification of the DC indoor air is occasionally required. Applying the law of mass conservation, the water use of space humidification is modeled as a function of the latent heat removed by the chiller system (Evans, 2008), which is expressed as Eq. (9). Note that the amount of water used for space humidification is not influenced by the choice of DC humidifier in the model (i.e., adiabatic humidifier or isothermal humidifier); however, this choice can result in a different PUE value given that these two humidification technologies have different effect on the supplied DC air temperature (Energy Star, 2020).

$$w^{SH} = (Q_s^{CH} / SHR - Q_s^{CH}) / H_{cond} \quad (9)$$

where H_{cond} is the latent heat of condensation of water (kJ/kg).

Consequently, the hourly PUE (PUE_i^{DC} , kWh/kWh) and hourly WUE (WUE_i^{DC} , kg/kWh or $liters/kWh$) is calculated in the model as follows:

$$PUE_i^{DC} = p^{DC} / p^{IT} \quad (10)$$

$$WUE_i^{DC} = 3600 * w^{DC} / p^{IT} \quad (11)$$

where the subscript i indicates the power or water use in the i th hour of a year.

Finally, the annual average PUE (PUE^{DC} , kWh/kWh) and WUE (WUE^{DC} , kg/kWh or $liters/kWh$) are calculated as follows:

$$PUE^{DC} = \sum_i PUE_i^{DC} / N \quad (12)$$

$$WUE^{DC} = \sum_i WUE_i^{DC} / N \quad (13)$$

where N is the total number of hours across a year (typically 8760 hours).

3.3. Model inputs and data sources

To analyze a given DC case in a given climate zone, the combined PUE and WUE model requires two major categories of model inputs: (1) DC facility system parameters (i.e., equipment specifications, system efficiency variables, and indoor environment setpoints); and (2) ambient climate data. Table 3 summarizes

the ranges assumed for major facility system parameters in each DC case, which were determined based on best available data sources and engineering estimations. Importantly, high and low values were established for each parameter to facilitate model sensitivity and uncertainty analyses, with values corresponding to best-case and worst-case conditions for each parameter gleaned from the data sources and engineering estimation process. Hourly ambient climate data were collected for each representative city (see Figure 2) based on meteorological data acquired from EnergyPlus Weather Data (EnergyPlus, 2016), which included hourly dry bulb temperature, RH, and atmospheric pressure in a typical meteorological year.

Table 3. Ranges of input values for major DC facility system parameters.

Input variables	Unit	Large-scale DC			Midsize DC				Small DC			References
		Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8	Case 9	Case 10	
UPS efficiency	%	90–99	90–99	80–94	80–94	80–94	80–94	80–94	77–85	77–85	77–85	(Barroso et al., 2013; Greenberg, S., E. Mills, B.Tschudi, P. Rumsey, 2006; Jay Park, 2011)
Percentage of power loss in power transformation and distribution system	%	0–2	0–2	2–5	2–5	2–5	2–5	2–5	2–4	2–4	2–4	(Barroso et al., 2013; Jay Park, 2011; Rasmussen, 2011)
Lighting power to IT power ratio	%	0–0.2	0–0.2	2–5	2–5	2–5	2–5	2–5	2–4	2–4	2–4	(Barroso et al., 2013; Lei and Masanet, 2020; Rasmussen, 2011)
Supply air dry bulb setpoint (lower bound)	°C	10–18	10–18	15–18	15–18	15–18	15–18	15–18	18–22.5	18–22.5	18–22.5	(ASHRAE, 2015)
Supply air dry bulb setpoint (higher bound)	°C	27–35	27–35	27–32	27–32	27–32	27–32	27–32	22.5–27	22.5–27	22.5–27	(ASHRAE, 2015; Miller, 2012)
Supply air dew point setpoint (lower bound)	°C	-12 – – 9	-12 – – 9	-12 – – 9	-12 – – 9	-12 – – 9	-12 – – 9	-12 – – 9	-9.9 – – 8.1	-9.9 – – 8.1	-9.9 – – 8.1	(ASHRAE, 2015)
Supply air dew point setpoint (higher bound)	°C	15–27	15–27	15–27	15–27	15–27	15–27	15–27	13.5–16.5	13.5–16.5	13.5–16.5	(ASHRAE, 2015)
Supply air relative humidity setpoint (lower bound)	%	60–95	60–90	60–80	60–80	60–80	60–80	60–80	54–66	54–66	54–66	(ASHRAE, 2015; Newman, 2013)
Supply air relative humidity setpoint (higher bound)	%	8–20	8–20	10–30	10–30	10–30	10–30	10–30	20–30	20–30	20–30	(ASHRAE, 2015)
Sensible heat ratio (SHR)	%	95–99	95–99	95–99	95–99	95–99	95–99	95–99	95–99	95–99	95–99	(EMERSON, 2010; Evans, 2010)

Temperature difference (supply/return CRAH air)	°C	13.9–19.4	13.9–19.4	5–10	5–10	5–10	5–10	5–10	5–8	5–8	5–8	(Joshi and Kumar, 2013; Lei and Masanet, 2020)
Temperature difference (supply/return facility system water)	°C	5–10	5–10	5–10	5–10	5–10	5–10	5–10	5–10	5–10	n/a	(ASHRAE, 2015, 2014)
Temperature difference (supply/return cooling tower water)	°C	4–6	4–6	4–6	4–6	4–6	n/a	n/a	4–6	n/a	n/a	(ASHRAE, 2014)
Fan pressure (CRAH)	Pa	300–1000	300–700	400–1000	400–900	400–900	400–1000	400–900	400–900	400–900	400–600	(Joshi and Kumar, 2013; Lei and Masanet, 2020; Patankar, 2010)
Fan efficiency (CRAH)	%	65–90	65–90	60–80	60–80	60–80	60–80	60–80	60–75	60–75	60–75	(Schild and Mysen, 2009)
Fan pressure (cooling tower)	Pa	100–400	100–400	200–400	200–400	200–400	n/a	n/a	200–400	n/a	n/a	(Lei and Masanet, 2020)
Fan efficiency (cooling tower)	%	65–90	65–90	60–80	60–80	60–80	n/a	n/a	60–75	n/a	n/a	(Schild and Mysen, 2009)
Pump pressure (humidification pump)	kPa	6300–7700	6300–7700	6300–7700	6300–7700	6300–7700	6300–7700	6300–7700	6300–7700	6300–7700	n/a	(Condair, 2020; Lei and Masanet, 2020)
Pump efficiency (humidification pump)	%	60–80	60–80	60–80	60–80	60–80	60–80	60–80	60–70	60–70	n/a	(DoE, 2006)
Pump pressure (chiller pump)	kPa	114.9–172.4	114.9–172.4	114.9–172.4	114.9–172.4	114.9–172.4	114.9–172.4	114.9–172.4	114.9–172.4	114.9–172.4	n/a	(Lei and Masanet, 2020)
Pump efficiency (chiller pump)	%	60–80	60–80	60–80	60–80	60–80	60–80	60–80	60–70	60–70	n/a	(DoE, 2006)
Pump pressure (cooling tower)	kPa	166.9–250.4	166.9–250.4	166.9–250.4	166.9–250.4	166.9–250.4	n/a	n/a	166.9–250.4	n/a	n/a	(Lei and Masanet, 2020)
Pump efficiency (cooling tower)	%	60–80	60–80	60–80	60–80	60–80	n/a	n/a	60–70	n/a	n/a	(DoE, 2006)

Pump pressure (waterside economizer pump)	kPa	n/a	114.9–172.4	n/a	114.9–172.4	n/a	n/a	n/a	n/a	n/a	n/a	(Lei and Masanet, 2020)
Pump efficiency (waterside economizer pump)	%	n/a	60–80	n/a	60–80	n/a	n/a	n/a	n/a	n/a	n/a	(DoE, 2006)
Approach temperature (cooling tower)	°C	2.8–6.7	2.8–6.7	2.8–6.7	2.8–6.7	2.8–6.7	n/a	n/a	2.8–6.7	n/a	n/a	(ASHRAE, 2015)
Approach temperature (economizer heat exchanger)	°C	n/a	1.7–2.8	n/a	1.7–2.8	n/a	n/a	n/a	n/a	n/a	n/a	(ASHRAE, 2015)
Chiller partial load factor	-	0.2–0.8	0.2–0.8	0.1–0.5	0.1–0.5	0.1–0.5	0.1–0.5	0.1–0.5	0.1–0.5	0.1–0.5	n/a	(Gullo et al., 2017; Lei and Masanet, 2020; Squillo, 2018; Yu and Chan, 2007)
Liquid-gas ratio (cooling tower)	-	0.2–4	0.2–4	0.2–2	0.2–2	0.2–2	n/a	n/a	0.2–2	n/a	n/a	(Asvapoositkul and Treeutok, 2012; Lemouari et al., 2009)
COP relative error to regressed value	%	-11 – 11	-11 – 11	-40 – 0	-40 – 0	-40 – 0	-40 – 25	-40 – 25	-60 – 20	-45 – 30	-45 – 20	(Gullo et al., 2017; Lei and Masanet, 2020; Squillo, 2018; Yu and Chan, 2007)
Heat exchanger effectiveness (CRAH cooling coils)	-	n/a	0.7–0.9	n/a	0.65–0.9	0.65–0.9	0.65–0.9	0.65–0.9	0.65–0.8	0.65–0.8	n/a	(Lei and Masanet, 2020; Sammeta et al., 2011)
Windage loss of water as a percentage of cooling tower mass flow rate	%	0.005–0.5	0.005–0.5	0.005–0.5	0.005–0.5	0.005–0.5	n/a	n/a	0.05–0.5	n/a	n/a	(Environmental Protection Agency and program, 2017; Ramzy, 2020)
Cycles of concentration	-	3–15	3–15	3–12	3–12	3–12	n/a	n/a	3–12	n/a	n/a	(Environmental Protection Agency and program, 2017)

Note: uniform distributions of the input variable ranges were assumed in the uncertainty and sensitivity analysis (see section 3.4).

3.4. Uncertainty and sensitivity analysis

Parameter uncertainty is one of the major uncertainty sources in physics-based engineering models (Doukas et al., 2018). Because DCs are complex systems with considerable variations in design and system operation, simulation runs with all possible DC facility system parameters is critical for understanding uncertainties. In this study, the Latin hypercube design-of-experiments approach was applied for efficient parameter stratification, and for reducing simulation runs of the computationally expensive model (McKay et al., 2000). For a given climate zone and a DC case defined in section 3.1, to balance the computation time and the convergence in the variance of the simulation results, 50 samples of the DC facility system parameters summarized in Table 3 were generated using Latin hypercube sampling. Each of the generated samples represents one possible DC design and operation scenario and was used for the one-hour-timestep PUE and WUE simulation across the year under the representative climates. As a result, the 50 one-year-round simulation results provide reasonable uncertainty ranges of the DCs' annual average PUE and WUE values for a given climate zone.

In addition, Sobol's sensitivity analysis was performed to give the parameter importance ranking for the proposed model, by decomposing the variance of the model's outputs (i.e., WUE and PUE values) to additive terms attributed to the model's input variables (Sobol, 2001). Two different sensitivity metrics of Sobol's method are typically employed by the sustainability modeling community to inspect complicated models: the main-effect index, and the total-effect index (Nossent et al., 2011). Given the high-level interactions of the model's input variables in affecting a DC's power and water use (e.g., climate condition and DC indoor environment setpoints jointly determine its economizer use, hence its power and water use), the total-effect index was chosen here as a more robust sensitivity measure. A Monte Carlo estimator with Saltelli's sampling scheme was used in this study to numerically approximate the Sobol's total-effect index, and the associated sensitivity analysis computer experiments were conducted using the Python's SALib package (Herman and Usher, 2017). The detailed sensitivity analysis results are presented in Section 4.4.

4. Results and discussion

4.1. Model validation

The model was validated using the reported annual average PUE and WUE values from specific DC operators (Facebook, 2020a, 2020b, 2020c, 2020d; Sharma et al., 2017). The validity of the PUE model has been demonstrated in (Lei and Masanet, 2020), and the main focus here is to show that the model can concurrently produce reasonable PUE and WUE values. Figure 3 shows the model validation results. For both PUE and WUE, all the reported annual average values lie within the prediction intervals, which demonstrates that the model provides reasonably accurate results. However, most of the reported values locate around the lower to medium quantiles of the prediction intervals, which may indicate that energy and water efficient DCs are more likely to report their PUE and WUE values publicly. In addition, reported values for large-scale DCs with adiabatic cooling systems indicate a preference for low PUE values, which is represented in Figure 3 by the fact that the reported PUE values lie very close to the prediction minimum while this is not necessarily the case for the reported WUE values. The reason is that adiabatic humidification sprays water into air (resulting in a larger WUE value), in return for decreased supply air temperature and hence a lower PUE value. On the other hand, the prediction interval is much larger for the midsize DC than the large-scale DCs due to the wider uncertainties in facility system variables, and the nature of the cooling technologies chosen by large-scale DCs (see section 4.2). Finally, it can be clearly

observed that model captures the decreasing trends of the PUE and WUE values when moving toward the more efficient large-scale DCs and cooler climates, which is also discussed with more details in the next section.

Figure 3. PUE and WUE prediction intervals versus reported values.

4.2. On-site PUE and WUE simulation results

Figure 4 and Figure 5 respectively show the predicted ranges of annual average PUE and WUE values for the 10 different DC cases and 16 different climate zones.

Figure 4. Annual average PUE simulation results across DC cases and climate zones (1A~8).

Figure 5. Annual average WUE simulation results across DC cases and climate zones (1A~8).

As expected, predicted PUE ranges are lower in cooler climates. For almost all the cases, the highest PUE values were observed in 1A (hot moist) and the lowest values were observed in 8 (subarctic). There are three minor exceptions. In case 10, for which we assumed isothermal humidifiers for space humidification, the highest PUE value was identified in 2B (hot dry) because the required isothermal humidification gives rise to an additional DC cooling load and thus increases the PUE value. In cases 3 and 6, airside economizers (no adiabatic cooling) were used, and the lowest PUE values were predicted in 4C (marine) because of its suitability of the outdoor air temperature and humidity for direct air cooling. In cases 2 and 4, waterside economizers were used, and the lowest PUE values were associated with 3C (marine) because its dry summer season is beneficial for indirect evaporative cooling. However, these exceptions are insignificant, and the general trends still hold well.

However, the magnitudes of the PUE values differ significantly by DC size due to different efficiency practices implemented, from a median of 1.12-1.25 for large-scale DCs (case 1 and 2), to a median of 1.39-1.98 for midsize DCs (case 3-7), and to a median of 1.71-2.22 (case 8-10) for small DCs. The median simulated ranges for different sizes of DCs are very similar to the values reported by LBNL (Shehabi et al., 2016), industry PUE survey data from the Uptime Institute (Lawrence, 2019), the reported values by hyperscale operators (Facebook, 2020c, 2020d, 2020b, 2020a; Google, 2020), and values presented in recent academic studies (Li et al., 2020; Ni and Bai, 2017), which indicate the validity of the model.

Likewise, the WUE values vary by DC size due to different efficiency practices implemented but show a much greater variation across different cooling system types. For water-cooled chiller systems, DCs with no economizer use were expected to have the highest WUE values (case 5 and 8) due to significant amounts of cooling tower water use. Within this category, the WUE values were smaller in cooler climates due to the reduced amount of heat rejected by condensers (because of higher chiller COP in cooler climates). However, the reduced heat from the chiller compressor was not comparable with the internal heat generated by DCs. Hence, the decreasing trends of WUE values were less pronounced when moving to the cooler climates. The same reason could explain the comparatively smaller but still considerable WUE values for DCs with waterside economizers (cases 2 and 4), where the use of the economizers eliminates or reduces the heat from the compressors but the massive internal heat from DCs still needs to be removed by the cooling towers, and hence a still considerable cooling tower water consumption.

Furthermore, DCs with airside economizers (cases 1 and 3) can have much lower WUE values when outside weather conditions allow direct air cooling and the shutdown of the chilled water systems, which frequently occurs in cooler climates. Note that, although the combination of the adiabatic cooling systems with the airside economizers (case 1) incurs additional water use for humidification, it reduces the probability of running more water-intensive supplemental cooling systems. As a result, the water uses of case 1 is evidently lower compared to that of case 3. Moreover, the direct water uses of air-cooled chillers and direct expansion systems (cases 6, 7, 9, and 10) are very small and only driven by sporadic humidification needs. However, air-cooled chillers and direct expansion systems are generally less energy-efficient (in terms of PUE values) than water-cooled chiller systems. Hence, if the water embodied in the DCs' electricity use (indirect water use) was considered, such systems may have significantly higher overall water footprints than the others, which is beyond the scope of this paper.

Although the DC WUE values are climate-dependent, unlike the obvious relationship between the annual average PUE values and the climate zone as shown in Figure 4, the annual average WUE values in Figure 5 are less climate zone sensitive except for cases 1, 3, 5, and 8. For cases 1 and 3, the considerable difference in the whole year free cooling hours between the climate zones explain the changes in the associated WUE values. For cases 5 and 8, the climate effect on the annual average WUE value is still visible but to a lesser extent. This is because a large portion of the cooling tower water use is attributable to the DC's internal heat generation, which is DC workload-dependent and climate-independent, which obscures the water use part that is climate-dependent (i.e., the water use caused by the heat from chiller compressor). Thus, this trend is solely determined the climate's effect on the chiller COP, and the decreasing trends is small given the large portion of climate-independent water use (see Eq. (4)). For cases 2 and 4, the climate effect still exists but becomes obscured due to the use of the waterside economizer, which reduces or even eliminates the climate-dependent water use part contributed by the chiller compressor. For the remaining cases 6, 7, 9 and 10, the effect of climate on the WUE values are negligible due to the small magnitude in DC water use and large margin of error in the simulation results.

As discussed above, under a given climate, the magnitude of the PUE and WUE values could differ significantly by different DC cases, illuminating the energy and water saving potentials available through climate-wise DC design and cooling system selection. However, even for the same climate zone and DC case, large uncertainty in the PUE and WUE value could exist, which represents the large existing variabilities in DCs' operations and indicates major opportunities for DC water and energy savings through efficiency improvement. It can be seen that the variance of the PUE and WUE values is much larger for small and midsize DCs than that of the large-scale DCs. The reason is that the large-scale DCs are more optimized for their systems' operation, where the use of advanced control techniques such as machine learning (Gao and Jamidar, 2014) result in less variabilities in their systems' efficiencies and setpoints, while the small and midsize DCs may or may not implement such strategies, and thus have larger variations in their systems' operational parameters. On the other hand, compared to the variance of the PUE values, the variance of the WUE values can be large especially for cases that involve cooling tower operations (cases 2, 3, 4, 5, and 8, and case 1 under hot climates), which highlights the large water saving potentials associated with efficient cooling tower operational strategies, such as choosing energy-efficient chillers to reduce the controllable part of cooling tower water evaporation, installing windage drift eliminators to reduce cooling tower windage water losses, and increasing the cooling tower water's dissolved mineral level within the acceptable range to reduce cooling tower draw-off water use.

4.3. Climate dependent practical minimum PUE and WUE values

This section discusses the achievable practical minimum PUE and WUE values by different DC cases, represented by the 5th quantiles of the simulation results, which could serve as a useful benchmark to assess a DCs' energy and water use efficiency under different climates, and to quantify the remaining PUE and WUE improvement potentials for DCs.

It can be clearly observed that locations with higher latitude generally have lower practical minimum PUE and WUE values due to lower dry bulb temperatures (Figure 2, 4, 5). The outdoor humidity level is another determining factor that affects the practical minimum PUE and WUE values, manifested by the different values between the marine, dry, and moist climate zone categories. Those PUE and WUE values of DCs do not necessarily have to be high in dry regions but are usually high in hot-humid regions. The reason is that DCs could make use of the direct or indirect evaporative free cooling under dry climates, but the dehumidification process occurs more frequently under hot-humid climates, where extra cooling needs to be supplied by the mechanical chillers to process the air to the dew point.

While we acknowledge that the climate parameters are one of the most influential factors affecting PUE and WUE values (see section 4.4), some of the cases show very little variation (in magnitude) in PUE and WUE by climate zone (e.g., PUE of case 1 and case 2, and WUE of case 2, 4, 5, and 8). This observation conforms to the publicly documented locational-distributed PUE values from Google (Google, 2020). However, this does not contradict with our findings in the next section because the values here correspond to the annual averages, where the averaging effect of the DC PUE and WUE under normal and favorable weather conditions (such as those during night and winter) across the year could explain those small climate zone variations. Nonetheless, the inner-year extreme hot weather conditions could significantly increase a DC's capital cost, where expensive supplemental cooling infrastructure systems must be built for reliable cooling, which is beyond the scope of this research and should be a subject of future investigation.

Finally, achieving the practical minimum PUE and WUE values requires DCs to aggressively improve every aspect of their facility systems' efficiency, some of which could be very difficult without the help of advanced control technologies or proper operations and expert trouble shooting. One of the most useful strategies is to focus on measures that could bring the largest saving potentials, which are identified by the sensitivity analysis results discussed in the next section.

4.4. Sensitivity analysis results

Figure 6 summarizes the total-effect indices of Sobol's sensitivity analysis. A parameter with a larger total-effect index has greater contribution to the variance of the predicted PUE or WUE values, demonstrating its importance for the DC PUE or WUE simulation, and as a focus to improve the DC's energy or water use efficiency. Similarly, a variable with a large total-effect index also indicates that it is the variable for which the energy analyst should try to obtain the most accurate value for more accurate PUE and WUE predictions.

It can be clearly observed that the variance in both the PUE and WUE predictions are attributable to a few key parameters. Outdoor climates (dry bulb temperature and relative humidity) are one of the most common and influential parameters for the predicted PUE and WUE values. This applies to nearly all the cases' PUE values, and the WUE values of cases where airside economizers were used (cases 1, 3, and 6), justifying our use of the one-hour-timestep annual simulations in this research, given free cooling resources vary at this timescale. For DCs that mainly use cooling towers for heat removal (cases 2, 4, 5,

and 8), variance in the windage water loss percentage and cycles of concentration are the largest contributors to variance in the predicted WUE values, reinforcing the importance of proper cooling tower operations for DC water efficiency. And for the cases 7, 9, and 10, the variance in the predicted WUE values is almost solely attributable to the variance in the sensible heat ratio because space humidification is the only source of water use in these cases.

When the climate conditions are given, meaning that the climate parameters do not contribute to the simulation variance, the most common important variables for the DC PUE predictions become the UPS efficiency, chiller partial load factor, and a parameter describing the variabilities between different DCs' chiller efficiencies (i.e., COP relative error to regressed value (Lei and Masanet, 2020)), demonstrating the importance of energy-efficient equipment for DC energy savings. As for the WUE predictions, the most important parameters remain the same for cases that rely on cooling towers for heat removal, and for cases that only implement space humidification. Furthermore, the variance in the DC indoor air setpoints altogether play as one large contributor to the variance in both the PUE and WUE predictions (note that Sobol's sensitivity indices can be additive), which affect the DCs' water and energy use through influencing the amount of free cooling that can be exploited by DCs, a similar PUE and WUE influencing mechanism with that of the climate parameters. These facility system parameters are the largest PUE and/or WUE variance contributors when the climate parameters are deterministic. On one hand, they indicate the primary focuses for the DCs' PUE and WUE improvements. On the other hand, they represent the major sources of modeling uncertainties in macro-level DC energy and water use estimation. These uncertainties will be challenging to reduce without empirical data on these parameters being reported by existing data centers. Thus, improved data reporting from DC operators is imperative for more accurate PUE and WUE predictions.

Figure 6. Sobol' total-effect indices for DC on-site PUE and WUE values.

5. Conclusions

This work addressed a key knowledge gap for energy analysts seeking to analyze the direct energy and water use of DCs, which are a rapidly growing sector. The physics-based approach produced thermodynamically-compatible PUE and WUE ranges for a wide variety of air-cooled DC archetypes in all major U.S. climate zones, whereas the model has been validated by annual data from real DC operations. This work provides energy analysts with PUE and WUE values that have greater technology and climate zone specificity than previous analyses, and enables them to consider best and worst case values for more robust DC onsite energy use and water use estimates as well as PUE and WUE improvement potentials. Moreover, the consistent PUE and WUE values presented here can facilitate more accurate modeling of indirect water use, for which PUE is the key driving variable.

Results reflect how DCs typically have lower PUE values in cooler climates, but further showed that PUE values vary greatly by DC size due to varied operating practices. Similarly, WUE values are lower in cooler climates, but show significant greater variations across different DC cooling system types. The case-by-case sensitivity analyses identified the most effective measures for PUE and WUE improvement. Results reinforced the significance of climates and indoor setpoints in determining PUE and WUE values, highlighted the importance of water-efficient operations (such as installing windage drift eliminators, or proper water dissolved mineral management) if cooling towers were used, and also underscore the

necessity of deploying energy efficient equipment (including energy-efficient chillers and UPS systems). The sensitivity analysis also identified major sources of uncertainties, enabling energy analysts to target better data for specific variables in future analyses.

Future model accuracy also hinges on improved PUE and WUE reporting by more DCs, which would enable reduction of prediction uncertainties. Such reporting should be encouraged by policy makers to improve external understanding of DC water use but also stimulate greater combined PUE and WUE improvements.

Although this study focused on U.S. DCs, it could be easily extended to other regions with the relevant meteorological data. The proposed modeling framework can be a valuable tool for DC multi-objective resource use optimization through energy- and water- efficient facility system management (Lei and Masanet, 2021). It could also provide granular data to further investigate the environmental benefits of DC workload mitigation/shifting (Lei et al., 2021a; Zheng et al., 2020).

The results can also provide insights for climate-wise DC siting. However, capital investment is another important aspect correlating with the climate condition for DC site selection, which is not considered in this study and should be subject to more future research. For example, a DC with an airside economizer and adiabatic cooling could have both lower capital costs and less operational resource consumption (i.e., water and electricity) in area cooler than that in a hot-humid region, due to the reduced cost for supplemental mechanical cooling system and the lowered PUE and WUE value. In addition, we only focused on WUE as a means for estimating absolute water use quantities; future work should consider quantities, required qualities, and local stress issues associated with DC water use.

Acknowledgements

The authors acknowledge financial support provided by Leslie and Mac McQuown.

Appendix A. Simulation code availability

The datasets and codes associated with this study are available at: <https://github.com/nuoaleon/Data-Center-Water-footprint>

References

- Amazon, 2020. Reducing Water in Data Centers [WWW Document].
- ASHRAE, 2015. Thermal Guidelines for Data Processing Environments, 4th ed, ASHRAE Datacom Series. ASHRAE, Atlanta.
- ASHRAE, 2014. Liquid Cooling Guidelines for Datacom Equipment Centers, 2nd ed, ASHRAE Datacom Series. Atlanta.
- ASHRAE, 2013. Climatic data for building design standards. ASHRAE Stand.
- Asvapoositkul, W., Treeutok, S., 2012. A simplified method on thermal performance capacity evaluation of counter flow cooling tower. Appl. Therm. Eng. <https://doi.org/10.1016/j.applthermaleng.2012.01.025>
- Baechler, M.C., Gilbride, T.L., Cole, P.C., Hefty, M.G., Ruiz, K., 2015. High-Performance Home Technologies: Guide to Determining Climate Regions by County. Pacific Northwest Natl. Lab. Oak Ridge Natl. Lab.
- Barroso, L.A., Clidaras, J., Hölzle, U., 2013. The datacenter as a computer: An introduction to the design of warehouse-scale machines, second edition, Synthesis Lectures on Computer Architecture. <https://doi.org/10.2200/S00516ED2V01Y201306CAC024>
- Capozzoli, A., Primiceri, G., 2015. Cooling systems in data centers: State of art and emerging technologies, in: Energy Procedia. <https://doi.org/10.1016/j.egypro.2015.12.168>
- Condair, 2020. Cool, Clean and Comfortable [WWW Document]. Condair HP-Series.
- Department of Energy, 2020. Reference Buildings by Climate Zone and Representative City [WWW Document].
- DoE, 2006. Improving Pumping System Performance: A Sourcebook for Industry. U.S. Dep. Energy.
- Doukas, H., Flamos, A., Lieu, J., 2018. Understanding risks and uncertainties in energy and climate policy: Multidisciplinary methods and tools for a low carbon society. Springer International Publishing. <https://doi.org/10.1007/978-3-030-03152-7>
- EMERSON, 2010. Precision versus comfort cooling choosing a cooling system to support business-critical IT environments. Business-Critical Contin.
- Energy Star, 2020. Make Humidification Adjustments | Products | ENERGY STAR [WWW Document]. Energy Star.
- EnergyPlus, 2016. Weather Data – EnergyPlus [WWW Document]. US Department Energy.
- Environmental Protection Agency, U., program, W., 2017. Water Efficiency Management Guide Mechanical Systems Mechanical Systems.
- European Commission, 2020. Energy-efficient Cloud Computing Technologies and Policies for an Eco-friendly Cloud Market | Shaping Europe’s digital future.
- Evans, T., 2012. The Different Technologies for Cooling Data Centers. Schneider Electr.
- Evans, T., 2010. How and Why Mission-Critical Cooling Systems Differ From Common Air Conditioners

White Paper #56. Schneider Electr.

Evans, T., 2008. Humidification Strategies for Data Centers and Network Rooms, White Paper #58. Schneider Electr.

Evans, T., 2004. The different types of air conditioning equipment for IT environments. APC White Pap. 24.

Facebook, 2020a. Prineville Data Center | Facebook [WWW Document].

Facebook, 2020b. Forest City Data Center - Home | Facebook [WWW Document].

Facebook, 2020c. Altoona Data Center | Facebook [WWW Document].

Facebook, 2020d. Luleå Data Center | Facebook [WWW Document].

Facebook, 2014. Open sourcing PUE/WUE dashboards [WWW Document]. Faceb. Eng. URL <https://engineering.fb.com/2014/03/14/data-center-engineering/open-sourcing-pue-wue-dashboards/> (accessed 7.13.21).

Ganeshalingam, M., Shehabi, A., Desroches, L.-B., 2017. Shining a Light on Small Data Centers in the USA 1–31.

Gao, J., Jamidar, R., 2014. Machine Learning Applications for Data Center Optimization. Google White Pap.

GILLIN, P., 2021. Tackling Data Center Water Usage Amid Historic Droughts, Wildfires [WWW Document]. datacenterfrontier. URL <https://datacenterfrontier.com/data-center-water-usage/> (accessed 7.15.21).

Google, 2020. Efficiency – Data Centers [WWW Document]. Google Data Centers.

Google, 2019. Environmental Report.

Gozcu, O., Ozada, B., Carfi, M.U., Erden, H.S., 2017. Worldwide energy analysis of major free cooling methods for data centers, in: Proceedings of the 16th InterSociety Conference on Thermal and Thermomechanical Phenomena in Electronic Systems, ITHERM 2017. <https://doi.org/10.1109/ITHERM.2017.7992592>

Greenberg, S., E. Mills, B.Tschudi, P. Rumsey, and B.M., 2006. Best Practices for Data Centers : Lessons Learned from Benchmarking 22 Data Centers. Aceee.

Gullo, P., Tsamos, K., Hafner, A., Ge, Y., Tassou, S.A., 2017. State-of-the-art technologies for transcritical R744 refrigeration systems - A theoretical assessment of energy advantages for European food retail industry, in: Energy Procedia. Elsevier Ltd, pp. 46–53. <https://doi.org/10.1016/j.egypro.2017.07.283>

Herman, J., Usher, W., 2017. SALib: An open-source Python library for Sensitivity Analysis. J. Open Source Softw. 2, 97. <https://doi.org/10.21105/joss.00097>

Hintemann, R., Hinterholzer, S., 2019. Energy consumption of data centers worldwide: How will the internet become green?, in: CEUR Workshop Proceedings.

Jaureguiualzo, E., 2011. PUE: The Green Grid metric for evaluating the energy efficiency in DC (Data Center). Measurement method using the power demand, in: International Telecommunications

- Energy Conference (Proceedings). <https://doi.org/10.1109/INTLEC.2011.6099718>
- Jay Park, 2011. Designing a Very Efficient Data Center [WWW Document].
- Joshi, Y., Kumar, P., 2013. Energy efficient thermal management of data centers, *Energy Efficient Thermal Management of Data Centers*. <https://doi.org/10.1007/978-1-4419-7124-1>
- Koomey, J., 2011. Growth in Data Center Electricity use 2005 to 2010. Anal. Press.
- Lawrence, A., 2019. Is PUE actually going UP? - Uptime Institute Blog [WWW Document]. Uptime Inst.
- Lawrence, A., Ascierio, R., Heslin, K., 2019. Uptime Institute Global Data Center Survey 2019. Uptime Inst. Intell.
- Lei, N., 2020. A robust modeling framework for energy analysis of data centers, in: *ACM International Conference Proceeding Series*. Association for Computing Machinery, New York, NY, USA, pp. 177–180. <https://doi.org/10.1145/3401335.3401648>
- Lei, N., Cheng, Z., Cao, Z., Masanet, E., 2021a. An integrated decision-making framework for sustainable data center operation through intelligent load scheduling. Submitt. to J. Phys. Conf. Ser.
- Lei, N., Masanet, E., 2021. Global Data Center Energy Demand and Strategies to Conserve Energy, in: *Data Center Handbook*, 2nd Edition. WILEY, Palo Alto, CA. <https://doi.org/10.1002/9781119597537.ch2>
- Lei, N., Masanet, E., 2020. Statistical analysis for predicting location-specific data center PUE and its improvement potential. *Energy* 201, 117556. <https://doi.org/10.1016/j.energy.2020.117556>
- Lei, N., Masanet, E., Koomey, J., 2021b. Best practices for analyzing the direct energy use of blockchain technology systems: Review and policy recommendations. *Energy Policy* 156, 112422. <https://doi.org/10.1016/J.ENPOL.2021.112422>
- Lemouari, M., Boumaza, M., Kaabi, A., 2009. Experimental analysis of heat and mass transfer phenomena in a direct contact evaporative cooling tower. *Energy Convers. Manag.* <https://doi.org/10.1016/j.enconman.2009.02.002>
- Li, J., Jurasz, J., Li, H., Tao, W.Q., Duan, Y., Yan, J., 2020. A new indicator for a fair comparison on the energy performance of data centers. *Appl. Energy* 276, 115497. <https://doi.org/10.1016/j.apenergy.2020.115497>
- Masanet, E., Shehabi, A., Lei, N., Smith, S., Koomey, J., 2020a. Recalibrating global data center energy-use estimates: Growth in energy use has slowed owing to efficiency gains that smart policies can help maintain in the near term. *Science* (80-.). <https://doi.org/10.1126/science.aba3758>
- Masanet, E., Shehabi, A., Lei, N., Smith, S., Koomey, J., 2020b. Recalibrating global data center energy-use estimates. *Science* (80-.). 367, 984–986. <https://doi.org/10.1126/science.aba3758>
- McKay, M.D., Beckman, R.J., Conover, W.J., 2000. A comparison of three methods for selecting values of input variables in the analysis of output from a computer code. *Technometrics* 42, 55–61. <https://doi.org/10.1080/00401706.2000.10485979>
- Miller, R., 2012. Too Hot for Humans, But Google Servers Keep Humming [WWW Document]. Data Cent. Knowl.
- Miller, R., 2009. Microsoft's Chiller-less Data Center [WWW Document]. Data Cent. Knowl.

- Morgan, T.P., 2016. A Rare Tour Of Microsoft's Hyperscale Datacenters [WWW Document]. Next Platf.
- Mytton, D., 2021. Data centre water consumption. *npj Clean Water* 2021 41 4, 1–6.
<https://doi.org/10.1038/s41545-021-00101-w>
- Newman, L.H., 2013. Facebook's Data Center Humidity "Challenge" Was Indoor Rain [WWW Document]. GIZMODO.
- Ni, J., Bai, X., 2017. A review of air conditioning energy performance in data centers. *Renew. Sustain. Energy Rev.* <https://doi.org/10.1016/j.rser.2016.09.050>
- Nossent, J., Elsen, P., Bauwens, W., 2011. Sobol' sensitivity analysis of a complex environmental model. *Environ. Model. Softw.* 26, 1515–1525. <https://doi.org/10.1016/j.envsoft.2011.08.010>
- Patankar, S. V., 2010. Airflow and Cooling in a Data Center. *J. Heat Transfer.*
<https://doi.org/10.1115/1.4000703>
- Patterson, D., Gonzalez, J., Le, Q., Liang, C., Munguia, L.-M., Rothchild, D., So, D., Texier, M., Dean, J., 2021. Carbon Emissions and Large Neural Network Training.
- Patterson, M., Azevedo, D., Belady, C., Pouchet, J., 2011. Water usage effectiveness (WUE): a Green Grid data center sustainability metric.
- Ramzy, 2020. Easy Guide to Cooling Tower Efficiency | Linquip [WWW Document]. Linquip Tech News.
- Rasmussen, N., 2011. Calculating Total Cooling Requirements for Data Centers. Schneider Electr.
- Ristic, B., Madani, K., Makuch, Z., 2015. The water footprint of data centers. *Sustain.* 7.
<https://doi.org/10.3390/su70811260>
- Sammeta, H., Ponnusamy, K., Majid, M.A., Dheenathayalan, K., 2011. Effectiveness charts for counter flow corrugated plate heat exchanger. *Simul. Model. Pract. Theory.*
<https://doi.org/10.1016/j.simpat.2010.10.012>
- SATTIRAJU, N., 2020. Secret Cost of Google's Data Centers: Billions of Gallons of Water [WWW Document]. Time. URL <https://time.com/5814276/google-data-centers-water/> (accessed 7.15.21).
- Scaleway, 2021. Environmental leadership [WWW Document]. URL
<https://www.scaleway.com/en/environmental-leadership/> (accessed 7.17.21).
- Schild, P.G., Mysen, M., 2009. Recommendations on Specific Fan Power and Fan System Efficiency. Tech. Note AIVC 65.
- Sharma, P., Pegus, P., Irwin, D., Shenoy, P., Goodhue, J., Culbert, J., 2017. Design and Operational Analysis of a Green Data Center. *IEEE Internet Comput.*
<https://doi.org/10.1109/MIC.2017.2911421>
- Sharma, R., Shah, A., Bash, C., Christian, T., Patel, C., 2009. Water efficiency management in datacenters: Metrics and methodology, in: 2009 IEEE International Symposium on Sustainable Systems and Technology, ISSST '09 in Cooperation with 2009 IEEE International Symposium on Technology and Society, ISTAS. <https://doi.org/10.1109/ISSST.2009.5156773>
- Sharma, R., Shah, A.J., Bash, C., Christian, T., Patel, C., 2008. Water Efficiency Management in Datacenters (Part I): Introducing a water usage metric based on available energy consumption. TR HP Labs.

- Sharma, R., Shih, R., McReynolds, A., Bash, C., Patel, C., Christian, T., 2010. Water Utilization in Data Center Infrastructure, in: Volume 5: Energy Systems Analysis, Thermodynamics and Sustainability; NanoEngineering for Energy; Engineering to Address Climate Change, Parts A and B. ASMEDC, pp. 1413–1419. <https://doi.org/10.1115/IMECE2010-40819>
- Shehabi, A., Smith, S.J., Masanet, E., Koomey, J., 2018. Data center growth in the United States: decoupling the demand for services from electricity use. *Environ. Res. Lett.* 13, 124030. <https://doi.org/10.1088/1748-9326/aaec9c>
- Shehabi, A., Smith, S.J., Sartor, D.A., Brown, R.E., Herrlin, M., Koomey, J.G., Masanet, E.R., Horner, N., Azevedo, I.L., Lintner, W., 2016. United States Data Center Energy Usage Report. Berkeley Lab.
- Siddik, M.A.B., Shehabi, A., Marston, L.T., 2021. The environmental footprint of data centers in the United States. *Environ. Res. Lett.* <https://doi.org/10.1088/1748-9326/abfba1>
- Sobol, I.M., 2001. Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. *Math. Comput. Simul.* 55, 271–280. [https://doi.org/10.1016/S0378-4754\(00\)00270-6](https://doi.org/10.1016/S0378-4754(00)00270-6)
- Squillo, T., 2018. How To Get the Most Energy Efficiency From a Chiller Plant - Facilities Management Insights [WWW Document]. FacilitiesNet.
- Yu, F.W., Chan, K.T., 2007. Part load performance of air-cooled centrifugal chillers with variable speed condenser fan control. *Build. Environ.* 42, 3816–3829. <https://doi.org/10.1016/j.buildenv.2006.11.029>
- Zheng, J., Chien, A.A., Suh, S., 2020. Mitigating Curtailment and Carbon Emissions through Load Migration between Data Centers. *Joule*. <https://doi.org/10.1016/j.joule.2020.08.001>