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Statistical analysis for predicting location-specific data center PUE and its improvement potential



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ABSTRACT

This paper presents a statistical framework for predictive analysis of data center power usage effectiveness (PUE), with a focus on hyperscale data centers (HDCs). Thermodynamics-based PUE models considering representative economizer choices are proposed, taking climate variables and energy system parameters as inputs for robust PUE predictions. Sobol's method is used to assess total order sensitivity indices of key modeling parameters, suggesting that climate variables and uninterruptible power supply (UPS) efficiencies are the most important parameters. The PUE values of 17 HDCs operated by Google and Facebook were predicted, considering location-specific weather conditions, and uncertainties in energy system parameters and economizer choices. Results were verified using reported PUE values, indicating the model's effectiveness in capturing regional and seasonal PUE variations, and in generating pointestimations for macro-level data center (DC) energy models. Finally, achievable PUE values were computed through differential evolution, identifying minimum practical PUE values that could be obtained with state-of-the-art technologies. The framework can be applied in predictions of locationspecific PUE values, PUE improvement analysis, and PUE target-setting by policy makers.

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1. Introduction

As demand for data center (DC) services grows rapidly, so too has interest in modeling DC energy use at both national [1,2] and global [3-5] levels. Such models are useful for understanding the scale and drivers of DC energy use and for providing visibility to energy planners on potential technology and policy interventions for improving DC energy efficiency moving forward [1,2].

Recent modeling results suggest that, despite rapid growth in demand for DC services, the worldwide energy use of DCs has grown by only around 6% since 2010 [5]. This decoupling of DC energy use and demand for services [6] is partly explained by steady improvements to the energy efficiency and operations of DC information technology (IT) hardware (notably servers).

It is also partly explained by the so-called "hyperscale shift", which describes the increasing share of global DC operations concentrated in large, ultra-efficient hyperscale data centers

(HDCs). For example, Cisco estimates that the share of global

2021 [7], representing a dramatic shift in global DC structure. The efficiency of HDCs is partly explained by their use of efficient power provision and cooling equipment configurations and controls, as well as favorable siting that enables the use of so-called "free cooling". These practices are reflected in low PUE values associated with

servers located in HDCs will rise from 27% in 2016 to over 53% in

HDCs, where PUE is defined as total DC energy use divided by IT energy use [8]. Understanding the future of global DC energy use therefore requires an understanding of HDC energy use; it follows that energy models that can accurately assess the PUE of HDCs may be particularly useful.

Yet in prevailing DC energy models, PUE is typically modelled simplistically [1-4]. Namely, PUE values are often based on a limited number of values reported by various DC operators and industry surveys [9]. Such an approach is inadequate for understanding the future energy use trends of HDCs, since: (1) it is retrospective in nature and not suitable for projections; (2) it cannot explain the underlying factors that determine PUE (e.g., installed equipment and operational decisions) that might be targets of technology and policy interventions; and (3) it cannot

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consider plausible "what if" questions, such as the case when HDCs continue to proliferate and move to locations with less idea "free cooling" conditions, or the case of a warming world where "free cooling" may be less reliable.

This paper proposes a modeling approach for predictive PUE analysis based on thermodynamic models, several of which have been reported in the literature [10-14]. We examine the specific case of HDCs, given their importance for global energy use moving forward and the availability of sufficient equipment, locational, and reported PUE data necessary for model validation. We conduct sensitivity analysis to identify the most important PUE modeling parameters for improving model accuracy and which should be targeted in future data collection efforts, followed by a robust uncertainty analysis to establish plausible uncertainty ranges for use in such models moving forward. Finally, we perform analyses of practical minimum PUE values that may be achieved, which enables policy makers to set PUE targets for incentives or standards. As such, this paper seeks to fill important knowledge gaps related to the use of physics-based PUE models coupled with statistical methods in forward-looking analyses of DC energy use.

2. Previous work

Several previous studies have focused on free cooling technologies, using PUE as a metric for DC energy savings [10,11,14–18]. The most comprehensive study was by Gozcü et al. [10], which applied a thermodynamic model using constant model inputs (e.g. fan power and air flowrate) to estimate PUE and to compare different free cooling methods in 19 cities. Although the previous studies used thermodynamic models to calculate PUE values, their purpose was to compare theoretical PUE reductions under different free cooling assumptions using simplified calculations, as opposed to validating a generalizable model against real-world PUE data. However, the latter is necessary for predicting PUE values in macrolevel energy studies and to location-specific policy decisions [19].

Only two previous studies provided both PUE prediction and model validation [12,20]. Gao [20] developed a 5 hidden layer neural network to predict the PUE of a single Google DC and achieved a mean absolute error of 0.004. However, a significant amount of non-public data is required to train such neural network models (e.g., 2 years of operational data was used in Gao's research), which poses a barrier to broader use by the energy modeling community, whereas the results of a model trained to a specific DC are difficult to generalize to other DCs. Brady et al. [12] carried out a thermodynamic modeling case study to calculate the PUE of one Facebook HDC in Prineville, Oregon, with high accuracy. However, this work was limited to airside economizers at a single DC; its accuracy was not evaluated for other DCs using airside economizers and it did not address waterside economizers. While both studies performed sensitivity analysis, a one-factor-at-a-time approach was used, which can neither assess the relative importance of parameters nor consider important variable interaction effects.

This paper helps to fill the aforementioned knowledge gaps by presenting a statistical framework for predictive analysis of HDC PUE values based on thermodynamics-based models, which further incorporates sensitivity analysis and assessment of location-specific practical minimum PUE values. It differs from previous studies in several ways. First, our predictive PUE modeling includes dynamic interrelationships between key system parameters, for example, how supply water temperature changes with heat exchanger efficiency and differences in supply/return air temperature, for more accurate system simulations. Second, we perform a global sensitivity analysis that considers variable interaction effects, which identifies the most important parameters for reducing

modeling uncertainty. To the best of our knowledge, no previous global sensitivity analyses of HDC PUE models have appeared in the literature. Third, location-specific PUE values were predicted under uncertainty and validated using reported PUE data from 17 HDCs operated by Facebook and Google. Such a multi-location model validation has not appeared in the literature. Fourth, our model framework provides a way to quantify the uncertainty in PUE predictions in light of variance in weather conditions and DC system parameters. Finally, we identified practical minimum PUE values under different weather conditions considering state-of-the-art technologies, which can enable setting of PUE targets [21,22].

3. Research methodology

Fig. 1 depicts our research methodology, which consists of four key components.

First, generalized thermodynamics-based PUE models representing typical HDC infrastructure systems were built to serve the statistical analyses. Second, variance-based sensitivity analysis (Sobol's method) was adopted to identify the most influential parameters for HDC PUE through quantitative parameter ranking. Third, uncertainty quantifications of quarterly and yearly PUE values were performed and compared with the reported values from actual HDCs to validate the proposed PUE models. Fourth, achievable PUE values based on state-of-the-art DC energy system parameters under different weather conditions were computed using the differential evolution optimization method.

3.1. PUE models

We constructed thermodynamics-based PUE models for typical HDC infrastructures, which are based on frameworks that have demonstrated utility in the past [10–14]. Fig. 2 depicts the cooling and power provision systems options available to a typical HDC, upon which the PUE simulations in this paper were based. Three most common free cooling methods used by HDCs were considered: (1) airside economizers combined with adiabatic cooling (AE) [23-25]; (2) waterside economizers that utilize the evaporative cooling capability of cooling towers (WEC) [25-27]; and (3) waterside economizers that utilize seawater for cooling (WES) [28,29]. HDCs typically apply one of these free cooling technologies, and when the chosen economizer cannot provide adequate cooling, a mechanical chiller is used to maintain an acceptable DC indoor thermal environment [30]. The basic features of the PUE models are discussed below. Further details and a link to the modeling code (in Python) can be found in the supplementary information (SI) file.

The PUE models consider all heat generation sources and power consuming components in a DC. Total heat generation and DC power use are expressed by Eq. (1) and Eq. (2)¹:

$$Q^{DC} = p^{IT} + \left(1 - \eta^{UPS}\right)p^{UPS} + \alpha^{PD}p^{PD} + p^{L}$$
(1)

$$p^{DC} = p^{IT} + \left(1 - \eta^{UPS}\right)p^{UPS} + \alpha^{PD}p^{PD} + p^{L} + \sum_{f} p_{f}^{FAN} + \sum_{p} p_{p}^{PUMP} + p^{CH}$$

$$(2)$$

Given outside climate conditions and a specified indoor thermal environment, the PUE models determine the economizer usage

¹ A list of symbols and acronyms is provided at the end of this paper.

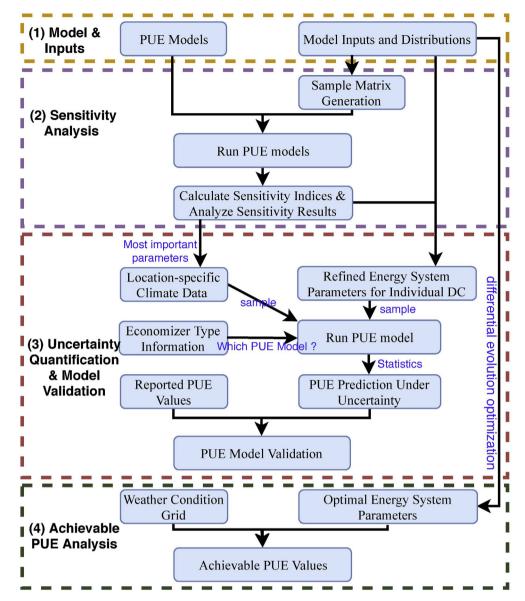


Fig. 1. Flowchart of research design and methodology.

scenario and the amount of additional mechanical cooling that may be required. The AE usage scenario is determined by the enthalpy difference of the supply air and outside air, where outside air prehumidification is applied to take advantage of adiabatic cooling [31,32], but the state of the pre-humidified air has to be constrained by supply air set points.

The WEC and WES economizer usage scenarios are determined by comparing the water temperature that could be delivered by the economizer heat exchanger (T_{WEC} or T_{WES}) and the return facility water temperature (T_{rw}), where the return facility water temperature is used here for a partial economizer use control strategy [13,33]. For HDCs that use waterside economizers, the supply facility water temperature (T_{sw} , $^{\circ}$ C) is set according to the dynamically changing computer room air conditioning (CRAC) supply and return air temperature, described by Eq. (3):

$$T_{sw} = T_{ra} - (T_{ra} - T_{sa}) / \varepsilon = T_{ra} - \Delta T_{air} / \varepsilon$$
(3)

The return facility water temperature $(T_{rw}, {}^{\circ}C)$ is calculated using the temperature difference (ΔT) between the supply and return facility water $(\Delta T_w, {}^{\circ}C)$, whereas the water temperatures that could

be delivered by the WEC and WES economizer heat exchangers are calculated by Eq. (4) and Eq. (5) in the PUE models:

$$T_{WEC} = T_{wb} + AT_{CT} + AT_{EX} \tag{4}$$

$$T_{WFS} = T_{Seq} + AT_{FX} \tag{5}$$

The equipment power consumption parameters in Eq. (2) were calculated based on the related energy and/or mass flows across that equipment, together with the associated equipment parameters (fan/pump pressure and efficiency, chiller efficiencies at different load factors, cooling tower liquid-gas ratio, etc.). The energy flows in the three different PUE models are governed by the quantities of free cooling supplied by the chosen economizer, mechanical cooling supplied by the chiller, and the total heat generated within the HDC, described by Eqs. (6)–(8):

$$Q^{DC} = Q^{AE} + Q^{CH} (6)$$

or

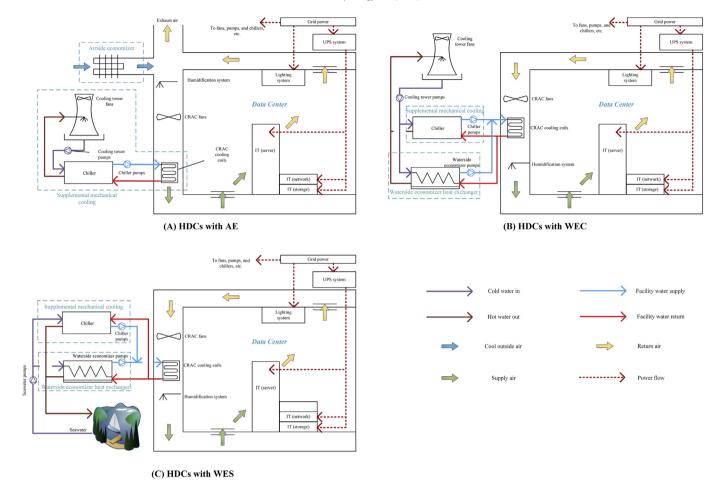


Fig. 2. Energy system diagrams for HDCs with AE/WEC/WES.

$$Q^{DC} = Q^{WEC} + Q^{CH} \tag{7}$$

or

$$Q^{DC} = Q^{WES} + Q^{CH}$$
 (8)

The resulting PUE can be calculated by:

$$PUE = p^{DC} / p^{IT}$$
 (9)

3.2. PUE model input ranges

The PUE models require two major categories of inputs: climate parameters and HDC energy system parameters. The latter category includes equipment specifications, system operational efficiency parameters, and indoor environment set points.

Climate parameters include outdoor dry bulb temperature and relative humidity in the AE and WEC models, and seawater temperature in the WES model. Variations in climate parameters greatly impact energy demand due to their influences on the model's chosen economizer use scenario and chiller efficiency [34]. To quantify these variations for the purpose of sensitivity analysis [35], ranges were chosen as follows: taking into account regional and seasonal variations, ranges for outdoor dry bulb temperature, outdoor relative humidity, and seawater temperature were set at — 10 to $40^{\circ}C$, 0 to 100%, and -2 to $36^{\circ}C$ [36,37], respectively. Uniform probability distributions were chosen for each range [38].

Energy system parameters include uninterruptible power supply (UPS) efficiency, percentage of power loss in power transformation and distribution systems, lighting power to IT power ratio, supply air set points (dry bulb, dew point, and relative humidity), ΔT of supply and return fluids in air and water systems, pressure heads and efficiencies of fans and pumps, approach temperatures of cooling towers and economizer heat exchangers, heat exchanger effectiveness of CRAC cooling coils, liquid-gas ratio of cooling towers, sensible heat ratio in HDC, and chiller efficiency. Ranges for these parameters were determined based on publicly-available HDC information and engineering estimates (Appendix A, Table A.1).

The chiller efficiency, represented as coefficient of performance (COP), is modelled as a function of entering condenser water temperature and partial load factor using regression analysis (SI Eq. (S1)).

3.3. Sensitivity analysis

Sensitivity analysis was used to identify the most important input parameters that affect the resulting PUE values, enabling greater focus on the few parameters for which accurate input data are most important. Variance-based sensitivity analysis was employed, using Sobol's method, which is a global and model independent sensitivity approach to decompose the uncertainty of model outputs attributed to specific model inputs [39]. Global sensitivity analysis is more robust than local sensitivity analysis, because the former considers parameter interactions whereas the latter can only evaluate changes to single variables [35]. The

associated sensitivity evaluations (i.e. quantitative parameter ranking) are expressed by Sobol's first order (S_i) , second order (S_{ij}) , and total order (S_{T_i}) sensitivity indices [40], which are briefly introduced in the SI.

Section (2) of Fig. 1 shows the steps for implementing Sobol's method: generate sample vectors from the ranges and distributions of climate and energy system parameters (Appendix A, Table A.1); run the sample vectors through the PUE model; calculate Sobol's sensitivity indices and analyze the sensitivity results. Furthermore, to assess the accuracy of the sensitivity results, the bootstrap method (with 100 times of sampling with replacement) was used to compute 95% confidence intervals for the sensitivity indices [41].

3.4. PUE uncertainty quantification and model validation

Given variabilities in climate and energy system parameters for HDCs, a non-intrusive uncertainty quantification approach [42] was employed to assess confidence in the outputs of the PUE models. Predicted PUE results were then compared with reported PUE values from 17 different HDCs operated by Facebook and Google to assess PUE model accuracy. Facebook and Google HDCs were chosen because they offer the only publicly-available PUE values with temporal and spatial resolution [43,44], and for which key technical information is available (SI, Table S1).

To reduce parameter uncertainties, conclusions from the sensitivity results were applied. The sensitivity results suggest climate parameters and UPS efficiency are the most important inputs for accurate PUE estimation (Fig. 3). Therefore, locationspecific climate data should be used to reduce uncertainty. As for the UPS efficiency, its uncertainty range used in the sensitivity analysis corresponds to all possible values in HDCs and needs to be refined to a narrower range representing individual cases for more accurate PUE estimation. The UPS efficiency range was set at 96%-99% for Google's HDCs based on data derived from Ref. [45,46]. The UPS efficiency range for Facebook's HDCs could not be established using publicly-available data. The assumed uncertainty ranges for other model inputs are summarized in Appendix A, Table A.1. The uncertainty in PUE model selection (e.g. AE vs. WEC) could be eliminated if information about economizer use has been released by the HDC. If the economizer information for a specific HDC is not available, the uncertainty quantification process needs to be treated as running a hierarchical model that contains each uncertain PUE model as its sub-model, and equal probabilities are assigned to run each sub-model. In this case, the uncertainty of the model result increases due to uncertainty in HDC's actual economizer choice.

Our uncertainty quantification and model validation process is summarized in Section (3) of Fig. 1: refine energy system parameters for individual HDCs based on available information and sensitivity results to reduce data uncertainties; determine whether economizer information is available or a hierarchical model approach should be used to include the uncertainty of economizer choice; gather location-specific weather data with hourly resolution for individual HDCs; draw samples from energy system parameters and probabilistic distributions of hourly weather data and combine them as input vectors (sample vector generation scheme documented in the SI); run the sample vectors through the PUE model developed in section 3.1; compute statistical metrics of model outputs (i.e., mean, variance, and prediction intervals); compare the predicted and reported PUE values for model validation.

3.5. Achievable PUE analysis

Reductions in PUE have long been an efficiency goal of DC operators [47]. We define achievable PUE as the practical minimum PUE value that can be attained within a given set of climate conditions and using state-of-the-art technologies. Identification of achievable PUE values enables DC operators and policy makers to understand available efficiency potentials and to set PUE targets on a location-specific basis [21,22].

We estimate the achievable PUE of HDCs using a given type of economizer by minimizing the objective function of the PUE model subject to the range of the inputs specified in Appendix A, Table A.1 (defined as $X \in \mathbb{R}$). For comparison purposes, we also calculated the maximal PUE value under the same weather conditions and economizer choice by maximizing the objective function while satisfying the constraints of the energy system parameters. That is, for every possible weather condition w (within the same ranges that were used in sensitivity analysis) and a given PUE model denoted as $PUE(\, \cdot\,)$, the following two optimization problems were solved:

$$\min_{\mathbf{X}} PUE(w, \mathbf{X}), \tag{10}$$

and

$$\max_{\mathbf{X}} PUE(\mathbf{w}, \mathbf{X}), \tag{11}$$

subject to:

$$X \in \mathbb{R}$$
 (12)

Due to non-differentiability and discontinuity in the PUE models, a differential evolution approach [48] was used. This stochastic population-based optimization method optimizes an

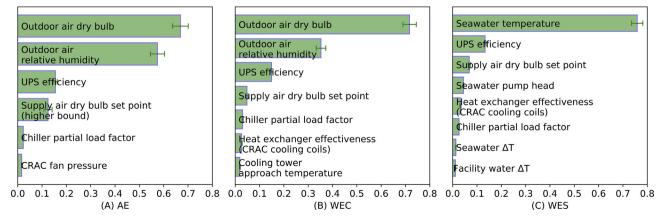


Fig. 3. Sobol's total order sensitivity indices for predicted PUE values using AE/WEC/WES.

objective function by maintaining numerous candidate solutions, and iteratively improves these candidate solutions by creating a trial candidate mutated from existing ones, for which we used the 'best1bin' scheme. For more details relating to this optimization method, readers are referred to Ref. [49].

4 Results and discussions

4.1. Sensitivity results

Results of our sensitivity analysis are summarized in Fig. 3, which plots parameters with Sobol's total order sensitivity indices larger than 0.01. The total order sensitivity index quantifies the total contribution of an input parameter to the variation in predicted PUE value, given the uncertainty distribution of the input parameter and any variance caused by its interactions, of any order, with any other parameters [35]. Further details on the computed Sobol's indices for all parameters can be found in the SI.

In Fig. 3, the error bars represent the 95% confidence intervals obtained from the bootstrapping process. For all three economizer strategies, variance in climate parameters that express the properties of the free cooling medium (i.e., outdoor air dry bulb temperature and relative humidity for AE and WEC, and seawater temperature for WES), emerged as the greatest contributors to variance in predicted PUE values. In all cases, variance in UPS efficiencies and supply air dry bulb set points² were found to be the next largest contributors to variance in predicted PUE values. These results suggest that focusing on reducing uncertainties in these key input parameters is most important for reducing uncertainties in PUE values predicted by the model. Fortunately, climate parameter data are typically available from weather databases in most parts of the world, meaning that most analysts can readily reduce the largest source of uncertainty in location-specific PUE predictions. However, reducing uncertainties related to UPS efficiency and supply air set points requires access to internal, data-center specific practices. This may not be a problem for analysts with access to such data, but it may not be feasible for the broader research community, which would need to rely on improved reporting practices from data center operators to reduce these sources of model uncertainty.

Variance in the remaining parameters in Fig. 3 has a lesser, but still significant, contribution to predicted PUE uncertainty. The chiller partial load factor impacts the chiller COP, which greatly influences energy use when mechanical cooling is required. CRAC fan pressure is important for HDCs with AE, as it relates to the magnitude of the pressure drop required to filter outside air for dust and particle removal, which can offset energy savings from outside air use. Heat exchanger effectiveness and cooling tower approach temperatures both impact the efficiency of waterside economizer systems, contributing to PUE variance. For WES systems, variance in the pump head affects overall pumping energy whereas variance in both seawater ΔT and facility water ΔT affects net heat removal efficiency, which in turn influences PUE.

An interesting observation is that the ΔT of CRAC air, which has been widely accepted as a significant factor influencing energy use of traditional DCs, does not appear in Fig. 3 due to a comparatively low total order index for HDCs. This is because thermal

management of airflow is more efficient in HDCs compared to traditional DCs, thanks to their advanced control systems and better equipment layouts.

Finally, as discussed further in the SI, we can compare the summation of the total order indices $(\sum S_{T_i})$ with the summation of the first order indices $(\sum S_i)$ to assess the extent to which variable interactions influence variability in predicted PUE values of HDCs. These ratios are 2.9:1, 1.9:1, and 1.3:1, for the cases of AE, WED, and WES, respectively, showing that variable interaction effects are evident, particularly for the AE case, justifying the use of total order indices.

4.2. PUE uncertainty quantification and model validation

Fig. 4 presents the uncertainty quantifications for quarterly PUE values of 17 HDCs operated by Google and Facebook, expressed as the mean, 5th, 25th, 75th, and 95th percentiles of the distributions of PUE values predicted by the model. It can be observed that the predicted means lie very close to the reported PUE values for many quarters and HDC locations, suggesting that thermodynamics-based models can reliably predict PUE values in light of inherent uncertainties. Most of the reported values lie within a 50% prediction interval, and nearly all lie within a 90% prediction interval, suggesting reasonable model accuracy. One exception is the Q1 PUE prediction for Google's Netherlands DC, for which the reported value is based on initial DC operations and may thus not be representative of stable operations.

In addition, given the lack of information on economizer use of HDCs in the Netherlands, Singapore, and Chile (o, p, and q), we predicted their PUE values with uncertain economizer use, which indicates that the existence of uncertainty in a HDC's economizer choice will not severely deteriorate the prediction accuracy. This is an important finding for future energy analysts who may seek to predict PUE values with limited technology information.

The figure also shows a regional and seasonal difference in the PUE simulation results, specifically the variation in the shape of the uncertainty ranges. For HDCs a, c, d, e, k, l, n, o, and q, the quarterly uncertainty ranges are narrow and steady across the year due to stable climatic or seawater conditions. HDCs in those locations rarely need to operate a chiller even during their hottest days, which is the major reason for the small uncertainty ranges. For HDCs b, f, g, h, i, j, and m, obvious seasonal PUE variations exist and are well captured by the proposed models. The simulation results display relatively larger uncertainty ranges during the warm quarters, which can be explained by the larger diurnal temperature variations over the summertime. During warmer seasons in those locations, HDCs have higher likelihoods of operating a chiller in the daytime but can still achieve low PUE values taking advantage of colder nocturnal temperatures.

For HDC p, the large quarterly PUE uncertainty ranges across the year are attributable to uncertainties in the indoor environment set points and economizer choice under the special climatic environment of Singapore. According to weather statistics [51], Singapore has a relative humidity greater than 60% and 90% around 98% and 30% of the time in a year and has a wet bulb temperature greater than 18°C and 27°C around 100% and 1.4% of the time in a year. If HDCs use AE under these conditions, the variation in the higher bound set point of supply air relative humidity (uncertain between 60% and 90%) will largely impact whether a chiller would be used for dehumidification. Similarly, if HDCs use WEC under these conditions, the variation in the supply air dry bulb set point (uncertain between $27^{\circ}C$ and $35^{\circ}C$) will determine whether the wet bulb temperature could satisfy the specified supply air temperature, and thus impact the necessity of chiller operation. The uncertainty in chiller operation patterns caused by the variations in set points

² Note: the supply air temperature of typical HDCs with AE is determined by upper and lower bound set points [50]. The higher bound set point determines whether AE can be used or not, and the lower bound set point is applied to prevent disruption by possible freezing outside temperatures [13]. HDCs with waterside economizers (WEC and WES) use only one set point (it could be dynamically adjusted within a range) because the indoor environment has no direct heat exchange with the outside air (more details in the SI).

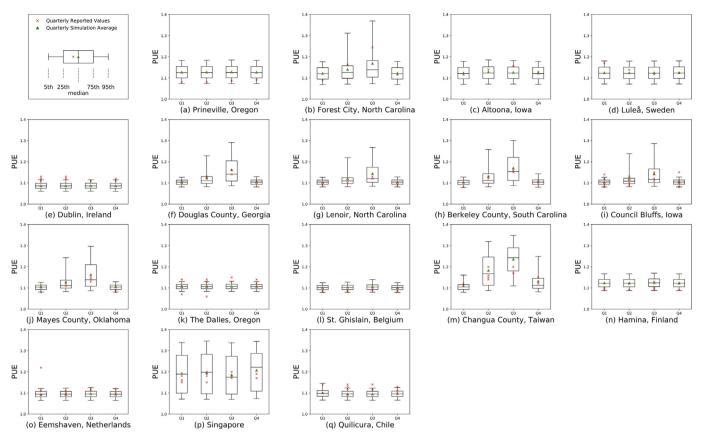


Fig. 4. Location-specific quarterly PUE uncertainty distributions and comparisons to reported values.

increases the uncertainty ranges of the simulation result, which is then slightly enlarged by uncertain economizer choice (SI, Fig. S2). The case of Singapore suggests that variations in the indoor environment set points could lead to wide uncertainty ranges for predicted PUE values under very hot and humid climate conditions.

However, this source of uncertainty could be readily addressed through more publicly-available information on HDC set points, which is not without precedent in the literature [52]. Moreover, it is noted that HDCs a, b, c, and d from Facebook have comparatively wider PUE uncertainty ranges due to larger input ranges of UPS efficiency, reconfirming the importance of UPS efficiency in accurate PUE estimation for individual cases. Uncertainties related to UPS efficiency could also be reduced with greater information sharing by HDCs.

The quarterly uncertainty results above showed good prediction quality verified by HDC quarterly reported values and demonstrated that the PUE model can also reasonably capture regional and seasonal differences in PUE values. However, policy makers and energy analysts may be more inclined to use point-estimations of annual PUE values (mean values) for macro-level DC energy modeling [53]. To assess the accuracy of the model output for point estimations, we present yearly PUE simulation distributions and the simulation averages, with comparison to the yearly reported averages, in Fig. 5. The results show that the model can also generate acceptable annual mean PUE values for point estimations (±4% relative errors at most) even though the uncertainty ranges of the yearly simulation results might be quite large.

4.3. Achievable PUE and related suggestions

Here we present achievable PUE results for HDCs with AE, WEC, and WES under different weather conditions, which are contrasted

against calculated maximal PUE values for the same conditions in Fig. 6. The resulting comparisons quantify the bandwidth of performance that exists between ideal and suboptimal energy management practices for a given weather condition and gives HDCs (whose actual PUE values will fall somewhere in between) and policy makers a useful benchmark to assess current practices and remaining practical PUE reduction potential.

In Fig. 6, non-smoothed lines convey the stochastic nature of the differential evolution algorithm.³ As expected, the results indicate that PUE values of HDCs with AE and WEC generally increase with higher outdoor air dry bulb temperature and relative humidity. Fig. 6 (1) indicates a step change in PUE value at a dry bulb temperature of around 30°C, above which direct adiabatic cooling could not be fully utilized due to the indoor thermal environment restrictions. In Fig. 6 (2), no similar step change occurs because of no such change in operation occurs.

As seen in Fig. 6 (3), in HDCs with WES, lower values of PUE can be maintained until seawater temperature reaches a threshold, beyond which the PUE value increases almost linearly with increasing seawater temperature. These temperature thresholds are mainly determined by the synergy of supply air dry bulb set points and heat exchange efficiencies in both CRAC cooling coils and economizer heat exchangers. The slope of PUE values beyond the threshold is affected by both the chiller COP and the amount seawater pump power use.

To identify how HDCs can make targeted improvements toward practical minimum PUE values, Fig. 7 plots the component-level power use predicted by the model for several weather conditions shown in Fig. 6. The power consumption of all infrastructure

³ Additional descriptions and explanations of Fig. 6 can be found in the SI.

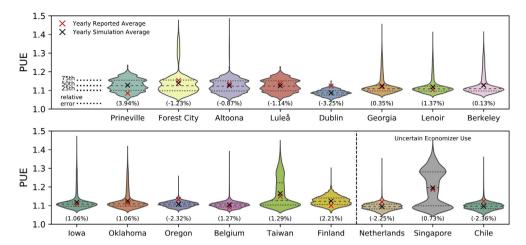


Fig. 5. Location-specific yearly PUE simulations and comparisons with yearly reported averages.

components has been normalized to an IT power of 1 kW for ease of interpretation.

Fig. 7 reveals that most infrastructure power is consumed by the UPS system, CRAC fans, and seawater pumps (WES) under favorable weather conditions (i.e., low temperature and relative humidity), but that power consumption could be more than doubled with the necessary operation of a chiller at higher temperatures and/or relative humidity. Furthermore, the power consumption difference between achievable and maximal PUE values is mostly attributable to the UPS system, CRAC fans, chiller, cooling towers (AE/WEC), and seawater pumps (WES). The comparatively lower UPS power consumption the achievable case is due to its higher UPS efficiency, which is above 99%. However, achieving a 99% UPS efficiency may require running the UPS system in Eco Mode [54] or integrating servers with specialized batteries [46], strategies that may bring tradeoffs such as longer transfer times (which may sacrifice service reliability) or higher capital investments.

Differences in power used by CRAC fans in Fig. 7 (1) is mainly due to the pressure drop difference associated with different outdoor air filtration strategies, while such pressure drop differences in Fig. 7 (2) and (3) are due to different air system layouts. Compared with that of AE, the power used by CRAC fans in the WEC and WES cases could be much lower, suggesting the superiority of waterside economizers in places with poor air quality. Another advantage of the waterside economizer is that it can be combined with server liquid cooling as a more efficient alternative to air-based DC cooling systems [55]. However, HDCs with waterside economizers do not necessarily have lower PUE values than those with AE, especially when the outdoor dry bulb temperature and relative humidity are low and outdoor air quality is acceptable for direct air cooling.

As for the difference in chiller power, this is mainly due to setting the supply air temperature as high as $35^{\circ}C$ in the achievable case, which can maximize economizer use to reduce the chiller power, and partially owing to higher chiller efficiency in the achievable case. The high supply air temperature set point is extremely important to save energy with AE because turning on the chiller requires operation of the whole water system including pumps and cooling towers. Although it seems a high set point is conducive to energy savings, operating servers at higher temperature may consume more IT power due to increased CMOS circuit static power and server fan power [56]. Therefore, a trade-off between IT power use and infrastructure power use must be considered, and it is typically recommended to only apply a high supply air set point when outdoor temperatures are very hot.

Finally, the noticeable difference in power used by cooling

towers in Fig. 7 (1) and (2) could be explained by differences in the cooling tower pump/fan head, pump/fan efficiency, and the liquidgas ratio. The difference in power used by seawater pumps in Fig. 7 (3) is due to the distance and altitude variations between the seawater resource and the HDC location, a critical consideration that will also impact the economics of seawater cooling.

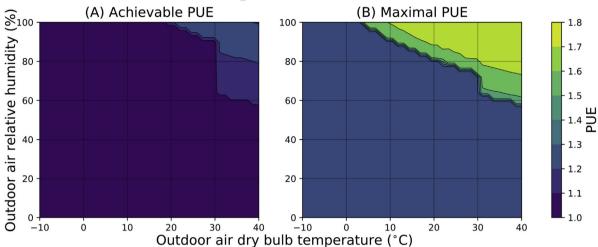
5. Conclusions

This paper demonstrated that, through a combination of thermodynamic modeling and statistical analyses methods, it is possible to predict the PUE values of HDCs using representative free cooling technologies (AE, WEC, and WES) with reasonable accuracy compared to actual reported values, and in consideration of seasonal variations. The use of Sobol's method enabled isolation of the most important modeling parameters, which allows energy analysts to focus on a just few parameters for improved data collection (i.e., climate parameters, UPS efficiency, supply air dry bulb temperature set point) to reduce uncertainty, improving the practical utility of the approach. It was further demonstrated that the approach can be used to identify practical minimum PUE values for HDCs using these free cooling technologies when location-specific climate data are available, and assuming state-of-art technologies and operating practices are employed. Therefore, the methods proposed in this paper can be used to estimate PUE values under different assumptions for locations and technology conditions in regional and global energy systems models that seek to quantify the energy use implications of HDCs in the future. These methods can also be used for setting location-specific targets for achievable PUE values by HDC operators and policy makers, with resolution on specific component-level improvements that can be pursued to such targets. Importantly, our results also demonstrate that there is no "one size fits all" PUE value for HDCs, and that policy makers must take into account local climate conditions and available technology incentives when incentivizing PUE reductions or using policy mechanisms to establish PUE targets.

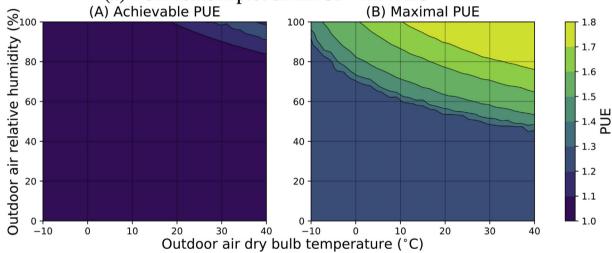
The scope of this study was limited to HDC infrastructure energy analysis with air-cooled IT equipment, given the availability of sufficient equipment, locational, and reported PUE data necessary for model construction and validation. However, the modeling framework could be easily extended to the analysis of non-HDCs using location-specific climate data if sufficient data on installed technologies, control strategies, and energy system parameters are available, as well as reported PUE data for model validation. Such non-HDC analyses should be priorities for future work.

Future model expansions should focus on several important

(1) PUE contour plot of HDCs with AE



(2) PUE contour plot of HDCs with WEC



(3) PUE values of HDCs with WES

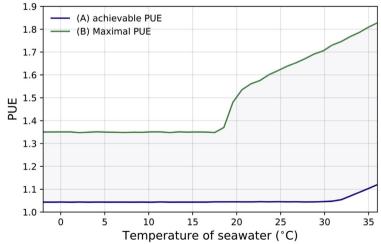


Fig. 6. Achievable and maximal PUE results under different weather conditions (AE/WEC/WES).

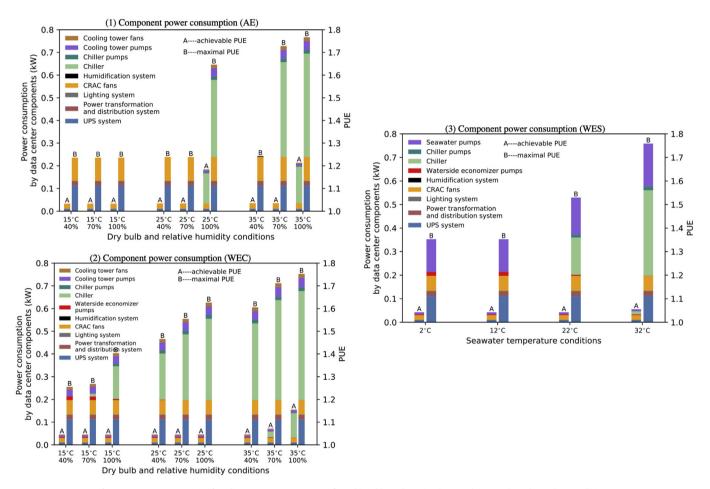


Fig. 7. Power consumption of cooling systems components for achievable and maximal PUE values at selected weather conditions.

HDC technologies and heat configurations, which were beyond the scope of the present study. Liquid cooling is emerging as an important cooling strategy in light of increasing rack-level heat intensities, which may be especially pronounced in deep learning and cryptocurrency mining activities. Liquid cooling can transfer additional heat from IT equipment which cannot be realized by air cooling due to airflow rate constraints. It can also reduce cooling fan power use and lower the temperature of microprocessors with a slight incursion on cooling pump power, thus lead to reduced PUE values and reduced static power losses of CMOS circuits in IT equipment. Liquid-immersion cooling, wherein IT electronics are immersed in electrically compatible fluid, could enable the use of facility water with higher temperatures due to the superior thermal properties of immersion liquids, and thus result in more free cooling hours (and, hence, lower PUE values) across a year in places with less favorable climates. Finally, although the use of DC waste heat recovery does not impact the PUE value of a DC itself, it is gaining momentum recently because it contributes to energy savings by distributing waste heat to nearby facilities that require heating or hot water supply. Incorporating the external benefits of recovered heat into PUE analyses can shed light on system-level energy and resource savings that could accrue at PUE values predicted by the model.

Declaration of competing interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Nuoa Lei: Conceptualization, Methodology, Software, Formal analysis, Investigation, Data curation, Writing - original draft, Visualization. **Eric Masanet:** Conceptualization, Validation, Investigation, Resources, Writing - review & editing, Supervision, Project administration, Funding acquisition.

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CRAC ⊿T

COP

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List of symbols and acronyms

PUE	power usage effectiveness
DC	data center
HDC	hyperscale data center
UPS	uninterruptible power supply
IT	information technology
AE	airside economizer combined with adiabatic cooling
WEC	waterside economizer utilizing the evaporative cooling
	capability of cooling towers
WES	waterside economizer utilizing seawater for cooling

computer room air conditioning

temperature difference

coefficient of performance

Q^{DC}	total heat generation of a DC (kW)
Q^{AE}	free cooling supplied by AE (kW)
Q^{WEC}	free cooling supplied by WEC (kW)
Q ^{WES}	free cooling supplied by WES (kW)
Q^{CH}	mechanical cooling supplied by chiller (kW)
p^{DC}	power used by a DC (kW)
p^{IT}	power used by IT equipment (kW)
p^{UPS}	power across the UPS system (kW)
p^{PD}	power across the power transformation and distribution
r	system (kW)
p^L	power used by lighting system (kW)
p_f^{FAN}	power used by fan type $f(kW)$, including CRAC fans and
•	cooling tower fans
p_p^{PUMP}	power used by pump type $p(kW)$, including chiller
- P	pumps, waterside economizer pumps, seawater pumps,
	cooling tower pumps, and humidification pumps
p^{CH}	power used by chiller (kW)
η^{UPS}	UPS efficiency
α^{PD}	percentage of power loss in power transformation and
	distribution systems (i.e., line and switch loss)
T_{sa}	CRAC supply air temperature (${}^{\circ}C$)
T_{ra}	CRAC return air temperature (${}^{\circ}C$)
ΔT_{air}	temperature difference of supply and return CRAC air
uii	(°C)
T_{rw}	supply temperature of facility water (${}^{\circ}C$)
T_{sw}	return temperature of facility water $({}^{\circ}C)$
ΔT_{w}	temperature difference of facility water (${}^{\circ}C$)
T_{WEC}	water temperature that could be delivered by
20	economizer heat exchanger in WEC (${}^{\circ}C$)
T_{WFS}	water temperature that could be delivered by
***	economizer heat exchanger in WES ($^{\circ}C$)
T_{wb}	wet bulb temperature of outdoor air (° <i>C</i>)
T_{sea}	seawater temperature (${}^{\circ}C$)
AT_{EX}	approach temperature of economizer heat exchanger
LA	(°C)
AT_{CT}	approach temperature of cooling tower (${}^{\circ}C$)
ε	heat exchanger effectiveness of CRAC cooling coils
<i>PUE</i> (•)	PUE model
w	a vector of weather condition

Appendix A. PUE simulation code and input variations

a vector of the energy system parameters

possible ranges of the energy system parameters in

A.1. GitHub link

HDCs

Χ

 \mathbb{R}

The PUE simulation code associated with this article can be found at:

https://github.com/nuoaleon/Data-center-PUE-prediction-tool.

A.2. Model inputs

Table A.1Model input values and ranges

Input variables ^{a b c}	Unit	Variable ranges and data sources		
		AE	WEC	WES
UPS efficiency	%	90-99 [32,45,46]		
Percentage of power loss in power transformation and distribution system	%	0-2 [32,45]		
Lighting power to IT power ratio		0-0.2 [45,57]		
Supply air dry bulb set point (lower bound)		10-18 [50]	_	
Supply air dry bulb set point (higher bound)		27-35 [50,58-60]	_	
Supply air dry bulb set point		_	27-35 [50,58-60]	
Supply air dew point set point (lower bound)		- 12 - -9 [50]	_	
Supply air dew point set point (higher bound)	°C	15-27 [5 0]	_	
Supply air relative humidity set point (lower bound)	%	8-20 [50]	_	
Supply air relative humidity set point (higher bound)		60-90 [50,52]	_	
Sensible heat ratio (SHR)		_	0.95-0.99 [61,62]	
Temperature difference (supply/return CRAC air)	°C	13.9-19.4 [13,52,57]	•	•
Temperature difference (supply/return facility system water)	°C	5-10 [50,55]		
Temperature difference (supply/return cooling tower water)	°C	4-6 [55,57]		_
Temperature difference (supply/return seawater)	°C	_	_	5-10 [55]
Fan pressure (CRAC)		500-1000 [13,63]	400-600 [13,63]	
Fan efficiency (CRAC)	%	65-90 [64-66]	•	•
Fan pressure (cooling tower)	Pa	100-400 [67,68]		_
Fan efficiency (cooling tower)	%	65-90 [64-66]		_
Pump pressure (humidification pump)		6300-7700 [69]		
Pump efficiency (humidification pump)	%	60-80 [70]		
Pump pressure (chiller pump)	kPa	114.9-172.4 [71-75]		
Pump efficiency (chiller pump)	%	60-80 [70]		
Pump pressure (cooling tower)	kPa	166.9-250.4 [72,74-77]		_
Pump efficiency (cooling tower)	%	60-80 [70]		_
Pump pressure (waterside economizer pump)	kPa	_ ,	114.9-172.4	4 [73–76]
Pump efficiency (waterside economizer pump)	%	_	60-80 [70]	
Pump pressure (seawater pump)	kPa	_	_	294-1470 [78,79]
Pump efficiency (seawater pump)	%	_	_	60-80 [70]
Approach temperature (cooling tower)	°C	2.8-6.7 [50]		_ ` '
Approach temperature (economizer heat exchanger)	°C	_	1.7-2.8 [50	1
Chiller partial load factor	%	20-80 [80-82]		•
Liquid-gas ratio (cooling tower)	_	0.2-4 [83-85]		_
COP relative error to regressed value	%	- 11-11 [81]		
Heat exchanger effectiveness (CRAC cooling coils)	%	_	70-90 [86,8]	71

aUniform distributions were used for all energy system parameters in both the sensitivity analysis and uncertainty quantification. bIn the sensitivity analysis, the outdoor dry bulb temperature, outdoor relative humidity, and seawater temperature is uniformly distributed within ranges of -10 to 40° C, 0 to

100%, and -2 to 36°C, respectively. Also, it is assumed that atmospheric pressure uniformly varies within ±10% of standard atmospheric pressure (101.325 kPa). cSources of weather data used in the uncertainty quantification are [51,88,89] (sampling with replacement).

Appendix B. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.energy.2020.117556.

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