Comparing energy and water use of aqueous and gas-based metalworking fluids

Sarang D. Supekar,[1] Diane J. Graziano,[2] Steven J. Skerlos,[3] Joseph Cresko[4]

[1] Energy Systems Division, Argonne National Laboratory, Lemont, IL, USA

[2] Decision & Infrastructure Sciences Division, Argonne National Laboratory, Lemont, IL, USA

[3] Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI, USA

[4] Advanced Manufacturing Office, U.S. Department of Energy, Washington, DC, USA

Abstract: Gas-based metalworking fluids (MWFs) have been proposed as alternative coolants and lubricants in machining operations to mitigate concerns surrounding water use and pollution, industrial hygiene, occupational health, and performance limitations associated with water-based (aqueous) MWFs that are ubiquitously used in the metals manufacturing industry. This study compares the primary energy and water use associated with the consumptive use, delivery, and disposal of aqueous MWFs with three gas-based MWFs in the literature—minimum quantity lubricant-in-compressed air (MQL), liquid/gaseous N_2, and liquid/supercritical CO_2. The comparison accounts for reported differences in machining performance in peer-reviewed experimental studies across several machining processes and materials. The analysis shows that despite the reported improvement in tool life with N_2 and CO_2-based MWFs, the electricity- and water-intensive separation and purification processes for N_2 and CO_2 lead to their higher primary energy and water use per volume of material machined relative to water-based MWFs. Although MQL is found to have lower primary energy use, significant consumptive water use associated with the vegetable oil commonly used with this MWF leads to higher overall water use than aqueous MWF, which is operated in a recirculative system. Gas-based MWFs thus shift the water use upstream of the manufacturing plant. Primary energy and water use of gas-based MWFs could be reduced by focusing on achieving higher material removal rates and throughput compared to aqueous MWF instead of solely targeting improvements in tool life. Additionally, the consumptive use of CO_2 and N_2 MWFs could be minimized by optimizing their flow rates and delivery to precisely meet the

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cooling and lubrication needs of specific machining processes instead of flooding the tool and workpiece with these gases.

Keywords: cutting fluids, tool life, sustainable manufacturing, water-energy nexus, dry factories, industrial ecology

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Address correspondence to: Sarang D. Supekar, Argonne National Laboratory, 9700 S Cass Ave, Bldg 362, Lemont, IL 60439, USA. *Email:* ssupekar@anl.gov

INTRODUCTION

Aqueous metalworking fluids (MWFs) are typically formulated as complex emulsions of petroleum-based oils in water that provide heat removal, lubrication, and chip evacuation in machining processes. With an estimated global market of about 2.5 million tonnes of concentrate valued at 9 billion USD (Global Market Insights 2018), MWFs are a critical input in metals manufacturing. Aqueous MWFs typically contain additives for emulsion integrity, corrosion protection, biocidal properties, and performance enhancement (Byers 2017). The resulting chemistry of aqueous MWFs, while essential to fulfilling their functional role of cooling and lubrication, also leads to well-documented environmental (Cheng et al. 2005; Skerlos 2013) and occupational health concerns (Calvert et al. 1998; Simpson et al. 2003; Gordon 2004; Mirer 2010; Burton et al. 2012). The procurement, operation, maintenance and disposal of aqueous MWFs can pose significant cost burdens, which could add up to as much as 17% of total production costs (Byers 2017). Further, conventional aqueous MWFs, which operate at pressures ranging from 0.2 – 0.6 MPa, have been known to limit material removal rates when machining recalcitrant materials such as titanium and nickel alloys, necessitating higher pressures up to 30 MPa (Ezugwu 2005; Bermingham et al. 2014). This further increases energy use, costs, and occupational health problems (Heitbrink et al. 2000).

While exploration of alternatives to aqueous MWF has historically been motivated in part to alleviate occupational health and cost concerns created by aqueous MWFs, this study spotlights potential issues related to machining performance and environmental impacts. A comprehensive discussion of the pros and cons of various alternative MWF technologies such as advanced filtration

and recycling, environmentally-adapted lubricants, and tool coatings for machining without MWFs can be found in (Skerlos et al. 2008), (Brinksmeier et al. 2015), and (Goindi and Sarkar 2017).

The alternative MWF technologies analyzed and discussed in paper are based on the principle of "dry" or water-less machining achieved by replacing water with industrial gases as the bulk medium for MWF delivery. Such MWFs are called "gas-based" MWFs in this study. The most extensively studied gas-based MWFs in research and practice, which are the focus of this study, are: (1) atomized oil in compressed air, commonly known as oil-in-air minimum quantity lubrication (MQL MWF); (2) liquid or gaseous nitrogen (N_2 MWF) with or without lubricants; and (3) liquid or supercritical carbon dioxide with or without lubricants (CO_2 MWF). Notwithstanding the different phases that CO_2 or N_2 may exist in the course of being drawn from a reservoir to impingement on the workpiece material, we refer to these MWFs as "gas-based." Additional information on each of these three gas-based MWF systems are provided in section S1 in the supporting information (SI).

Gas-based MWFs have been shown to have a higher penetration into the cutting zone created between the cutting tool and the workpiece. Figure S1 in the supporting information shows the cutting zone geometry in detail. In the case of N_2 and CO_2, rapid expansion from a pressurized state to ambient pressure leads to rapid cooling as a result of the Joule-Thompson effect. Improved access to regions of friction and heat generation through lower surface tension, along with significantly cooler delivery media in the case of N_2 and CO_2 thus creates the potential for more effective heat removal and lubrication despite lower volumetric heat removal capacities as gases compared to aqueous MWFs (Supekar et al. 2012; Wang and Clarens 2013). Indeed, numerous experiments performed over the last two decades to evaluate and compare the functional performance of gas-based MWFs with aqueous MWFs have shown better tool life, cutting forces, and surface finish with gas-based MWFs. Reviews in the MWF literature (Skerlos et al. 2008; Yildiz and Nalbant 2008; Debnath et al. 2014) have qualitatively summarized key results from a few of these studies.

Despite the abundant literature on comparing aqueous and gas-based MWFs, only a handful of studies have attempted to quantify the environmental impacts of gas-based MWFs relative to aqueous MWFs. (Clarens et al. 2008) evaluate the environmental impacts of CO_2, MQL, and aqueous MWFs, and show that CO_2 and MQL MWFs significantly reduce life cycle water use, land use, and acidification impacts at the expense of marginal increases in fossil energy use and global warming potential compared to aqueous MWFs. (Pusavec et al. 2010) conclude in their analysis of N_2 and aqueous MWFs that N_2 MWFs have lower life cycle water use, acidification impacts, and global warming potential than aqueous MWFs, although this comes at the cost of significantly higher fossil energy use from electricity. (Fratila 2010) shows reductions ranging from 15 – 25% in fossil energy use, global warming potential, and acidification when using MQL MWF over aqueous MWF. All three studies, however, treat the functional performance of the MWFs as comparable, and as a result, do not account for how differences reported in the literature between the functional performance afforded by aqueous and gas-based MWFs could affect the environmental impacts.

In this paper, we begin to bridge this gap in the literature by addressing the following research question: how do the energy and water use associated with the production and use of gas-based MWFs compare with aqueous MWFs, when considering reported differences in their functional performance in published experimental studies? The focus on energy and water use emanates from the close coupling between the two in MWF systems – water-based MWF requires considerable energy during their use phase, and gas-based MWFs, while water-less in their use phase, require considerable energy and water in their production phase. We begin by describing the analysis scope and data sources. Next, we describe the screening criteria used to develop a compendium of peer-reviewed experimental studies, and data extraction procedures used to obtain necessary information from those studies for the analysis. Results from the analysis are then discussed in the context of the research question postulated earlier. The paper concludes with a discussion of how the energy and water use of gas-based MWFs could be reduced, paying particular attention to achieving significantly higher machining rates that may be afforded by gas-based MWFs.

METHODS

Goal, scope definition, inventory data, and impact assessment

The goal of the study is to estimate and compare the primary energy use and consumptive water use of aqueous and gas-based MWFs associated with their production, use phase delivery including any treatment needed for their continued use, and disposal. **Error! Reference source not found.** shows the system boundaries used for this analysis. Operation of the machine tool and any subsequent steps such as part cleaning are excluded. Cutting tool production is also excluded from the analysis due to the high variability observed in the tool base material, tool coatings, and geometries within the published literature, quantifying which would necessitate a separate analysis that is outside of the scope of this paper. Unless specified otherwise, relevant unit processes and their inventory data were obtained from the Ecoinvent 3.5 life cycle database (Ecoinvent 2018). Default Ecoinvent unit processes and providers for a given material or process were modified to reflect U.S.-specific datasets, particularly for electricity and heat/steam, wherever such data were available. Where U.S.-specific datasets were unavailable, the global average values were used. Ecospold files for key MWF materials and processes are included in the supplementary material.[1]

Energy use includes primary energy associated with electricity, heat and fuels used in the production, transportation, machine tool delivery, and disposal of the MWF and its principal constituents. It is expressed in MJ of cumulative energy demand based on characterization factors from (Huijbregts et al. 2010), and is calculated for each MWF both in terms of its total annual use and per cm^3 of material machined over a year. Electricity needed for MWF delivery, recycling, and

[1] These data are freely available in the Zenodo repository at hhttps://zenodo.org/record/3565781#.Xg7235XsY2w

disposal is assumed to be supplied by the Midwestern U.S. average (medium-voltage MRO mix in Ecoinvent) considering the large presence of metalworking industries in this region (U.S. Census Bureau 2016). The composition of this electricity mix is approximately 73% non-renewable, 17% nuclear, and 10% renewable primary energy sources (Ecoinvent 2018). Water use is modeled as liters of water depletion based on ReCiPe-E characterization factors from (Huijbregts et al. 2017), and it includes the consumptive use of process water, cooling water, and water for crop irrigation (for vegetable oil), as well as consumptive water embodied in the energy use associated with the production, transportation, delivery, and disposal of the MWFs. Water depletion is similarly calculated for each MWF on an annual basis as well as per cm^3 of material machined over a year.

Cumulative energy demand and water depletion per unit of material machined (referred to as primary energy use and water use hence, unless qualified by "annual" or "embodied") are calculated based on the reported MWF and machining conditions for each experiment examined in this paper. Experimental studies were selected based on the screening criteria outlined in section 0. For each experimental comparison of aqueous and gas-based MWFs from the literature, the annual primary energy and annual water use for the MWFs is divided by the annual throughput afforded by the different MWF systems. Figure S3 in the supporting information explains this process graphically. At various points in this section, we provide ranges for operational parameters of aqueous and gas-based MWFs. These ranges reflect values used for the sensitivity analysis described in section 0, and apply to all experiments. The parameter exceptions are MWF flow rates, delivery pressures, and lubricant concentrations, which apply specifically to a particular reported experiment, and the contributions of those parameters to the energy and water use are thus calculated individually for each experiment.

Aqueous MWFs

Both synthetic and semi-synthetic formulations are considered for aqueous MWF. Formulations typically dilute the MWF concentrate to 5 – 10% v/v. Compositions of the MWF concentrate for semi-synthetic and synthetic MWFs are based on (Byers 2017), and are provided in Table S1 in the supporting information. The concentrate includes the following additives: emulsifier, biocide, corrosion inhibitor, pH buffer, coupler, and extreme pressure lubricant.

Delivery of aqueous MWFs involves pumping the MWF from a sump, assumed in this study to be a stand-alone reservoir with a capacity of 378 liters (100 gallons), to pressures typically ranging from 0.5 – 3 MPa (80 – 435 psig) for conventional delivery and up to 30 MPa (4350 psig) for high-pressure delivery. Aqueous MWFs are periodically treated and recycled in a batch process during which tramp oils, solids, and metal chips are removed using microfiltration, and the MWF is pasteurized before being pumped back into the MWF sump for reuse. The frequency of recycling is assumed to be 1 – 4 times a month as per advised best practices (Byers 2017; Wendt 2018).

The MWF eventually degrades and must be disposed. Different manufacturing facilities handle their spent MWF using a variety of mechanical, chemical, or biological processes based on the type of MWF and contaminants (Byers 2017). In this study, we consider the end-of-life process to be

comprised of separation in a settling tank, followed by ultrafiltration and nanofiltration, disposal of the oil recovered from the filtration processes via hazardous waste incineration, and discharge of the permeate to a wastewater treatment plant (Byers 2017; Hilal et al. 2004). This treatment process was chosen based on its ability to handle both synthetic and semi-synthetic MWFs. The disposal frequency is assumed to be 1 – 4 times a year (Byers 2017; Wendt 2018). Additionally, MWF is lost daily to evaporation and carry-off with machined parts. This daily loss is assumed to be 2 – 10% of the sump capacity (Byers 2017). The consumptive use of aqueous MWFs and associated primary energy and water use thus collectively emanate from the daily MWF loss and periodic disposal. Details and modeling assumptions behind aqueous MWF recycling and disposal processes can be found in section S1.7 in the supporting information. We note that when MWF wastewater is discharged untreated, its high pollutant loadings (BOD, heavy metals, oils and greases, toxic chemical additives) can seriously endanger water supplies and create substantial burdens and risks for wastewater treatment plants.

Gas-based MWFs

N_2 is assumed to be produced via cryogenic air separation (Smith and Klosek 2001), which involves air compression, air cooling and filtration, and distillation (rectification). CO_2 (beverage grade purity ≥ 99.9% v/v) is assumed to be recovered as a byproduct of ethanol production given the abundant merchant CO_2 supply from bioethanol facilities in the Midwest. Energy and water use data for beverage grade CO_2 is obtained from (Supekar and Skerlos 2014). The CO_2 production process involves capture and compression of by-product CO_2 stream, scrubbing (water-wash), desiccant drying, activated charcoal filtration, distillation, and refrigeration (ammonia-based). Transportation of N_2 and CO_2, respectively is assumed using refrigerated and cooled long-haul container trucks. The transportation distance is assumed to be 50 – 800 km. The lubricant, wherever used in gas-based MWFs, is assumed to be soybean oil given its abundant domestic supply.

N_2 and CO_2 MWFs are usually drawn from central cryogenic supply tanks or pressurized dewars at the manufacturing facility. While N_2 is typically pressurized to about 2 – 18 MPa from the industrial gas production facility itself, its pressure is typically regulated down to a lower value before delivery. As such, no further compression is required in the delivery of N_2 MWF. CO_2 is typically pressurized to about 2 MPa at its production source and may be further compressed to a higher pressure for supercritical CO_2 MWF application. Electricity consumed for gas compression would thus depend on the specified final delivery pressure of MQL and CO_2 MWFs. Since gas-based MWF systems are operated in an open-loop configuration where the gas is emitted back to the atmosphere without recovery or pre-treatment, these MWFs are assumed to have no primary energy or water use at their end of life. We note that air handling systems that vent MWF mists (both aqueous and gas-based) away from the operator space are considered part of the machine tool, and thus excluded from the scope of this analysis, as are subsequent part cleaning steps that can be avoided when using gas-based MWFs (see **Error! Reference source not found.**).

Metalworking fluid performance metric

Several machining performance metrics have been considered in the MWF literature including tool life, material removal rate, throughput, surface roughness, cutting forces, residual stresses, and specific cutting energy. Manufacturers, particularly in high-value industries such as automotive, aerospace, and medical devices, are ultimately interested in increasing their throughput (production volume). As such, we use the annual throughput afforded by the two MWFs being compared in a given experiment as an indicator of their relative machining performance.

$$V_{annual} = MRR \times 50 \times 6 \times \left(1440\mu - N_{tc}T_{tc}\right) \quad (1)$$

$$N_{tc} = \left\lfloor \frac{1440\mu}{T_{mc} + T_{tc}} \right\rfloor \quad (2)$$

The annual throughput (V_{annual}) captures the effects of differences in tool life (T_{mc}) and material removal rate (MRR) through equations (1) and (2). Here, N_{tc} is the number of tool changes per day of production, T_{tc} is the average time per tool change assumed as 0.5 – 3 minutes, and μ is the dimensionless machine utilization factor assumed to be 50 – 80%, with which the number of minutes in a 3-shift work day (1440) is multiplied to obtain the effective planned working minutes in a single day of production. We assume 50 working weeks a year, 6 working days a week, and three 8-hour shifts per day. MRR is expressed in cm^3/min and T_{mc} in minutes.

Screening criteria for published studies, data extraction, and paired analysis

After an extensive survey of peer-reviewed journal and conference publications on experimental comparisons of conventional aqueous and gas-based MWFs, a set of 86 experimental MWF comparisons from 29 studies published between 2001 – 2019 was compiled based on the following criteria: (1) tool life and MRR values must be clearly reported, or tool wear progression charts must be provided along with necessary machining parameters from which tool life could be indirectly ascertained as detailed in section S2 in the supporting information; (2) the different MWFs must be applied to the same workpiece material and machining process *within* the study, and identical tool life criterion (e.g. flank wear, rake wear, notch wear) must be applied to both MWFs; and (3) flow rate, pressure, and concentration of lubricant (if applicable) for each MWF evaluated must be clearly specified in the study or referenced from a previously published study. Table S3 in the supporting information lists these studies along with specifics of the MWFs compared and the number of experiments performed within each of these studies.

Tool life with a given MWF varies considerably across studies depending on the process, material, machining conditions, and other confounding factors that may not always be known. To meaningfully compare MWF performance across studies, we compute and analyze the *differences* in tool life, throughput, and energy and water use per unit volume of material machined across studies using an approach called “blocking” or “pairing” (Box et al. 1978). Comparing differences instead of

absolute values of these observed variables significantly reduces the effect of confounding factors across studies, and increases the precision of the comparison, which allows us to detect meaningful differences between the MWFs even if the magnitude of such differences is small relative to the absolute value of the response variables. However, the data collected from the literature is observational, and thus the collective results from experiments cannot be considered as randomized and pooled. While some support exists in the literature for applying "subjective randomization" to non-randomized observational data (Rubin 1974) to allow hypothesis testing (Fisher 1971), others have cautioned against such an approach citing inherent sampling biases and Type I errors in significance tests applied to observational datasets (Greenland 1990; Copas and Li 1997). As such, in this study we simply calculate the differences and ratios of the response variables for each pair of MWFs tested in an experiment, and report the medians, mean, and standard deviations *without* subsequent hypothesis testing. In lieu of significance tests, we graphically plot the differences in energy and water use from the different pairs of MWFs, and supplement the quantitative metrics with a qualitative discussion in the context of the research question.

Sensitivity analysis

For each MWF, the sensitivity S of a given environmental impact variable E (primary energy use and water depletion) is calculated with respect to an increase (S^+) as well as a decrease (S^-) in the value of the a parameter p belonging to the set P_{MWF} of MWF-specific sensitivity parameters listed in **Error! Reference source not found.**. Sensitivity is measured as the ratio of the relative change in the value of the response variable to the relative change in the value of the parameter. The average of the sensitivities in each experiment x across all X_{MWF} experiments for a given MWF is then reported using equation (3). We note here that each input parameter in **Error! Reference source not found.** is found to affect the primary energy use and water depletion in the same direction; that is, if a parameter increases primary energy use, it is also found to increase water depletion, and vice-versa.

Table 1. Values of input parameters used in sensitivity analysis.

Parameter	Low	Nominal	High	Units
Machine tool				
Tool change time	0.5[wb]	1	3[bw]	minutes
Machine utilization factor	50%[bw]	65%	80%[wb]	-
Aqueous MWFs				
Daily make-up (% of sump capacity)	2%[wb]	5%	10%[bw]	-
Sump fluid replacement frequency	1[bw]	2	4[wb]	times per year
Sump fluid treatment frequency	1[wb]	2	4[bw]	times per month
Gas-based MWFs				
N_2/CO_2 transportation distance	50[bw]	100	800[wb]	km

Notes: [bw]Best-case for gas vs. worst-case for aqueous; [wb]Worst-case for gas vs. best-case for aqueous

$$S_{p\in P_{MWF}}^{+} = \frac{\sum_{x\in X_{MWF}} \frac{\left(E_x^{p^{high}} - E_x^{p^{nominal}}\right)/E_x^{p^{nominal}}}{\left(p^{high} - p^{nominal}\right)/p^{nominal}}}{\left|X_{MWF}\right|}$$

$$S_{p\in P_{MWF}}^{-} = \frac{\sum_{x\in X_{MWF}} \frac{\left(E_x^{p^{low}} - E_x^{p^{nominal}}\right)/E_x^{p^{nominal}}}{\left(p^{low} - p^{nominal}\right)/p^{nominal}}}{\left|X_{MWF}\right|} \quad (3)$$

Further, we calculate the differences in primary energy use and water depletion of aqueous and gas-based MWFs under two additional scenarios beyond the scenario that is defined by the nominal values for aqueous and gas-based MWFs in **Error! Reference source not found.**. The first compares the best-case values for gas-based MWFs against worst-case values for aqueous MWF, a scenario referred to in the discussion as "best-worst." The second compares worst-case values for gas-based MWFs against best-case values for aqueous MWF, which is referred to as "worst-best." The purpose of these scenarios is to develop reasonable upper and lower bounds for the differences in energy and water use of aqueous and gas-based MWFs considering uncertainties in input parameters.

RESULTS and discussion

Tool life and throughput

Tool life and MRR are shown in **Error! Reference source not found.**a for all the paired experiments comparing aqueous and gas-based MWFs in Table S3 in the supporting information. The data shows that experiments generally report an increase in tool life with gas-based MWFs compared to aqueous MWFs in 87% of the experiments – 100% of the experiments with CO_2, 80% of the experiments with MQL, and 89% of the experiments with N_2. In several cases, gas-based MWFs increased tool life by an order of magnitude. We also find that tool life for both gas-based and aqueous MWFs decreases with increasing MRR, which can be ascribed to increased heat generation and related tool wear mechanisms.

Increase in tool life is anticipated to decrease tool costs and minimize unproductive machine down time. However, as shown in **Error! Reference source not found.**b, the reported improvements in tool life do not necessarily translate to improvement in the corresponding annual throughput calculated using equation (1). This is because most (> 90%) experiments were setup to compare tool life keeping the MRR constant in accordance with the conventional practice of comparing MWFs under identical machining conditions (De Chiffre and Belluco 2000).

Error! Reference source not found.a plots the algebraic relationship in equation (1) graphically. It shows that increasing tool life has a marginally diminishing effect on throughput regardless of the MRR. The most pronounced improvements in throughput for a given MRR would be observed when tool life is improved from a few minutes to several minutes or tens of minutes, as shown by points P1 and P2 in **Error! Reference source not found.**a. An identical tool life improvement from P3 to P4 would yield a negligible throughput improvement. This is because throughput gains depend on reduction in down time from fewer tool changes due to improved tool life. Based on equation (2), the rate of tool changes (and down time for tool changes) diminishes approximately quadratically with increasing tool life.

Throughput, however, increases linearly with MRR, though a higher MRR may affect tool life as shown by P3 and P5 in **Error! Reference source not found.**a. Thus, increasing MRR (typically through higher cutting speeds) without compromising much on tool life, if at all, presents another avenue to increase throughput. We find some evidence for this approach in the published literature examined in this study as shown in **Error! Reference source not found.**b, in which throughput improvements are most pronounced (darker circles) either when tool life was increased by several minutes using gas-based MWFs from an aqueous MWF baseline of about 3 – 7 minutes, or by increasing the MRR (circle size). As discussed later in section 0, increasing the throughput can meaningfully reduce the energy and water use of gas-based MWFs per unit of material machined.

Primary energy and water use per unit volume of material machined

The embodied energy and embodied water for each major component of aqueous and gas-based MWFs are shown in Table S3 in the supporting information. The ranges of reported values of flow

rates, lubricant concentrations, and delivery pressures; and calculated values for annual primary energy and water use, and primary energy and water use per unit volume of material machined for all four MWFs are shown in **Error! Reference source not found.**. **Error! Reference source not found.** shows results from *paired comparisons* of primary energy use and water use for aqueous and gas-based MWFs from different experiments, normalized by volume of material machined annually as well as total primary energy use and water use associated with the two MWFs over a year of operation.

The analysis finds that the primary energy and water use of N_2 and CO_2 MWFs are higher in most experiments than aqueous MWF. MQL's primary energy use is found to be lower than aqueous MWF in most experiments, although MQL is found to have a higher water use than aqueous MWF. The magnitude of primary energy and water use values and their differences between MWFs vary considerably across experiments as shown in **Error! Reference source not found.** and **Error! Reference source not found.**a. Given this considerable spread, it is helpful to examine the *ratio* of the primary energy and water use of the MWFs corresponding to differences shown in **Error! Reference source not found.**. These ratios, shown in **Error! Reference source not found.**, indicate that the primary energy use of CO_2, MQL, and N_2 MWFs calculated in this analysis can be 0.5 – 50, 0.1 – 0.8, and 8 – 47 times that of aqueous MWF. The water use of CO_2, MQL, and N_2 MWFs similarly can be 0.6 – 18, 0.4 – 2.6, and 5 – 16 times that of aqueous MWF. All ranges indicate first and ninth deciles. The observed spread in primary energy use and water use values closely follows the spread in flow rates for CO_2 and N_2 MWFs, and oil concentration for MQL due to the high sensitivity of the energy and water impacts to these parameters, as discussed in the subsequent paragraphs.

Table 1. Ranges of reported MWF parameters in the literature, and calculated primary energy use and water use on an annual and per unit volume of material machined basis.

	Aqueous		**CO_2**	**MQL**	**N_2**
	Conv.	Hi-Pr.			
Flow rate (kg/min)					
Median	10.0	17.6	0.7	0.1	0.6
1st decile	4.6	9.0	0.04	0.1	0.6
9th decile	42.0	43.0	2.7	0.4	0.7
Lubricant conc. (% w/w)					
Median	4.3%	6.7%	0.1%	0.2%	0%
1st decile	4.3%	4.3%	0.0%	0.1%	0%
9th decile	6.0%	6.7%	3.7%	1.3%	0%

Delivery pressure (MPa)					
Median	0.6	5.0	13.0	0.5	1.5
1st decile	0.1	5.0	2.0	0.4	0.7
9th decile	0.6	10.0	14.0	0.8	2.4
Annual primary energy use (GJ)					
Median	34	228	482	16	1140
1st decile	24	96	35	5	939
9th decile	59	384	1933	28	1274
Annual water use (m^3)					
Median	21	79	113	38	315
1st decile	20	38	14	11	260
9th decile	29	122	403	55	352
Primary energy use per unit volume of material machined (MJ/cm^3)					
Median	0.018	0.030	0.125	0.016	0.324
1st decile	0.003	0.018	0.010	0.002	0.094
9th decile	0.630	0.081	2.126	0.563	0.828
Water use per unit volume of material machined (L/cm^3)					
Median	0.015	0.010	0.027	0.034	0.089
1st decile	0.002	0.007	0.003	0.002	0.026
9th decile	0.313	0.026	0.464	1.194	0.229

For N_2 and CO_2 MWFs, higher primary energy and water use compared to aqueous MWF (values shown in Table S4 in the supporting information) is due to substantial upstream production impacts of N_2 and CO_2 impacts owing to the energy-intensive processes involved in their separation and purification. Unlike aqueous MWF, gas-based MWFs operate in an open-loop without recovery or recirculation. The use of the energy-intensive N_2 and CO_2 gases as MWFs is therefore entirely consumptive. With MQL, which is also entirely consumptive, vegetable oil is the largest contributor to the higher water use compared to aqueous MWF. Thus, despite the observed increases in tool life with gas-based MWFs over aqueous MWFs, the corresponding increases in throughput are not high enough to reduce the water use for all three gas-based MWFs, and primary energy use for N_2

and CO_2 MWFs. This conclusion holds true even when comparing results for the best-case parameters for gas-based MWFs against the worst-case parameters for aqueous MWF ("best-worst" scenario described in section 0), although the distributions shown in **Error! Reference source not found.** shift to the left. That is, differences and ratios between gas-based MWF and aqueous MWF primary energy and water use become smaller, as shown in Figure S5 in the supporting information.

Results of the sensitivity analysis are shown in **Error! Reference source not found.**. They indicate that tool change time and machine utilization factor have the largest impact on primary energy and water use of aqueous MWFs, although they do not affect the primary energy and water use of gas-based MWFs. This is because both these parameters affect the production time of the machine tool, and since gas-based MWFs operate in an open loop, any changes in the production time affects the throughput and annual primary energy/water use in the same proportion. Aqueous MWF on the other hand has a fixed consumptive use component from daily evaporative losses and periodic filtration that is practically unaffected by production time, and therefore a decrease in production time would lead to higher primary energy and water use for aqueous MWF than in the nominal scenario. Primary energy and water use of aqueous MWF is also sensitive to the daily MWF make-up and MWF filtration frequency during maintenance, which are parameters that contribute most to the consumptive use. Gas transportation distance has a larger impact on the primary energy and water use of CO_2 MWF than N_2 MWF, since production of N_2 comprises a larger proportion of the total MWF impact than CO_2.

Opportunities to reduce the primary energy and water use of gas-based MWFs

We identify two main approaches for reducing the primary energy and water use of gas-based MWFs within our analysis scope. The first applies particularly to CO_2 and N_2 MWFs, and involves increasing cutting speeds to achieve significantly higher MRRs than those allowed by aqueous MWF by exploiting the potential of these gases to deliver more effective cooling and lubrication as discussed section 0. Increasing the MRR without significantly compromising on tool life and dynamic stability of the machining process can lead to substantial increases in throughput as discussed in section 0. This in turn would reduce the primary energy and water use per unit of material machined. To break even with the primary energy and water use per unit of material machined with aqueous MWF, CO_2 and N_2 MWFs would have to increase their throughput by the ratios shown in **Error! Reference source not found.**, assuming flow rates and delivery pressures remain unchanged. For instance, a roughly 25% improvement in MRR with CO_2 MWF over aqueous MWF in (Sadik et al. 2016) while maintaining MWF flow rates/pressures would lead to identical primary energy use per unit of material machined for both MWFs. In other work such as (Stephenson et al. 2014), however, nearly 6-fold increases in MRR would be needed for CO_2 MWF to equal aqueous MWF in its primary energy use. Experimental exploration of whether such leaps in throughput via increased MRR may be possible by modifying machining parameters or tool geometries is scant in the literature, and this presents a significant opportunity for future work to understand the potential of gas-based MWFs.

The second approach involves the optimization of the delivery of gas-based MWFs to precisely meet the needs of specific processes in which they are used. In particular, CO_2 and N_2 MWFs reported in

the literature are largely delivered by flooding the tool-workpiece interface with the gas without consideration for how much gas is in fact needed to achieve effective cooling and lubrication. (Skerlos et al. 2008), (Sadik et al. 2016), and (Bermingham et al. 2012) show that higher gas flow rates yield diminishing returns in terms of tool life improvement beyond a certain point. The direction and point of application of gas-based MWFs is also critical to their performance (Marksberry and Jawahir 2008), and care must be taken to not starve the tool-workpiece interface, which may result in catastrophic tool failure and/or workpiece damage due to sub-optimal nozzle placement, direction, or geometry.

Understanding how consumptive flows of the energy-intensive CO_2 and N_2 gases can be minimized while improving machining throughput compared to aqueous MWFs also presents a significant research opportunity. This includes exploring through-tool delivery of the gases (Sorbo and Dionne 2014; Tahri et al. 2017). Another delivery optimization strategy for CO_2 and N_2 MWFs is to increase their delivery pressure. Both CO_2 and N_2 rely on the Joule-Thompson effect for providing a jet of low-temperature gas to cool the tool-workpiece interface. Given that compression energy during the use phase contributes to less than 2% of the total embodied primary energy of N_2 and CO_2 MWFs, expanding the gases from a higher pressure may facilitate higher heat removal and higher tool life, as shown by (Mulyana et al. 2017) and (Supekar et al. 2012).

System expansion to include a few factors not included in this analysis could also reduce the primary energy and water use of gas-based MWFs. Cutting tools in particular are quite resource-intensive to produce. (Gutowski et al. 2006) estimate the embodied energy of tungsten carbide to be about 400 MJ/kg. Turning and indexable milling inserts typically weigh about 5 grams and have 3 to 4 cutting edges, while a typical half-inch drill weighs about 100 grams and has 2 to 4 flutes. For almost all turning experiments analyzed in this paper where gas-based MWFs improved tool life over aqueous MWF, difference in the annual embodied energy in tools using the 400 MJ/kg value would be 2 – 3 orders of magnitude smaller than the difference in annual primary energy use of the MWFs. For milling, the difference in annual embodied energy of tools could approximately be 5 – 40% of the difference in annual MWF primary energy use. For drilling, the difference in annual embodied energy of tools can be 1 – 2 orders of magnitude higher than the difference in annual MWF primary energy use. Thus, the inclusion of the cutting tool life cycle in the system boundaries may thus meaningfully affect the comparative results for net primary energy use of aqueous and gas-based MWFs depending on the process.

When production quantities are fixed, higher MRR and/or improved tool life with gas-based MWFs may not lead to higher throughput, but it may lead to fewer machine tools needed for achieving the production target. Since the energy consumption of machine tools is significantly higher than energy use of MWFs (Kara and Li 2011), this approach can also considerably reduce the net primary energy use per unit of machined material. Chips and finished parts machined with gas-based MWFs are also largely free of substantial oily residues seen with aqueous MWF materials, and this can further reduce costs primary energy and water use associated with post-machining cleaning.

Finally, we note that although gas-based MWFs shift water use upstream of the manufacturing facility to thermoelectric power use (> 80% of U.S. generation) for gas separation and purification electricity use steps in the case of N_2 and CO_2 and irrigation in the case of vegetable oil used in MQL, the environmental implications of water consumption in a factory (direct use) and water consumption upstream (indirect use) may be quite different. Aside from differences in types and levels of pollutant loadings associated with thermoelectric power generation and process water use, differences in potential water stress that may be created by direct and indirect water use in the context of metals manufacturing (Rao et al. 2019) are worth considering when comparing the relative environmental merits of gas-based and aqueous MWFs. It is also worth considering that as the share of renewables in electricity supply increases, the indirect consumptive water use from electricity use (Macknick et al. 2012) for CO_2 and N_2 MWFs may further decrease in relation to aqueous MWFs.

Comparison of primary energy and water use results with other published work

We discuss the noteworthy differences and similarities between the results from this analysis with other MWF environmental studies and provide possible explanations. As with this analysis, the annual energy use for CO_2 MWF is reported to be higher than aqueous MWF in (Clarens et al. 2008), although the difference is considerably larger in this analysis. Annual water use for CO_2 MWF in (Clarens et al. 2008) is reported to be lower than aqueous MWF, whereas this analysis finds a considerable increase in water use as shown in **Error! Reference source not found.**. In addition to inclusion of tool life considerations, two additional reasons could potentially underlie this difference. One is that this study uses a market-based allocation for industrial CO_2 gas compared to the economic allocation adopted in (Clarens et al. 2008), and therefore includes additional purification steps for CO_2 gas that are water-intensive and electricity-intensive (the latter indirectly increases water use). The other reason is that the CO_2 flow rates assumed in (Clarens et al. 2008) are from a pilot bench-scale setup that has lower flow rates than those reported in other studies.

While (Fratila 2010) reports a decrease in fossil energy use when using MQL over aqueous MWF, the magnitude of this decrease is again found to be much higher in this analysis. Compared to the average flow rate of about 20 kg/min calculated from all aqueous-MQL comparison studies analyzed here, (Fratila 2010) in fact assumes a much higher aqueous MWF flow rate of 100 kg/min. Given that they also consider that aqueous MWF needs a higher cutting power than MQL in their analysis, and that aqueous MWF needs additional energy during subsequent cleaning steps (which MQL does not), the energy use impacts of aqueous MWF in this study are expected to be higher than the reported values in their work. One explanation could be that they only consider 0.6 minutes of machining time in their analysis and exclude consumptive MWF losses.

Results for N_2 MWF impacts relative to aqueous MWF in this analysis are vastly different from those reported by (Pusavec et al. 2010), who claim a reduction in energy and water use with N_2 MWF compared to aqueous MWF. However, a significant shortcoming in their analysis is that electricity use is treated as a separate impact category, and the contributions of this electricity to upstream

non-renewable energy depletion and water depletion are excluded. This omission likely underlies the significant skew of their environmental impacts in favor of N_2 MWF.

Conclusions and outlook

Gas-based MWFs can substitute the use of aqueous MWFs in machine tools and eliminate occupational health concerns associated with exposure to harmful microbes in these systems. Experimental evidence from over two dozen published experimental studies spanning several machining processes and materials shows that gas-based MWFs can improve tool life. However, the analysis presented in this paper shows that gas-based MWFs do not reduce overall water use, and instead move the water burdens upstream to the processes involved in the production of the industrial gases in the case of N_2 and CO_2, and to vegetable oil production in cases where it is used as a lubricant. For N_2 and CO_2 MWFs, we also see a considerable increase in overall primary energy use.

Several potentially useful experimental studies were excluded from this analysis because they did not meet the screening criteria – most commonly due to missing flow rate and pressure data for aqueous and/or gas-based MWFs analyzed in the studies. We recommend that future experimental studies comparing MWF performance should clearly report MWF flow rates, pressures, and lubricant concentrations (where applicable) to allow better contextualization of reported differences in machining performance. To this point, we also find that reporting tool life with different MWFs under a specified tool failure criterion (see Figure S2b in the supporting information) provides better practical insights than experiments reporting tool wear after a fixed machining period. Finally, the experiments analyzed in this study were all observational and thus we caution against universally applying the conclusions surrounding tool life, throughput, and primary energy and water use to a randomly chosen material/ process/machining condition combination unless evidenced by experiments. Any comparisons between the relative performance of the three gas-based MWFs analyzed should also be avoided since the method used here is not designed or equipped to allow such comparisons.

Opportunities for reducing the primary energy and water use of gas-based MWFs include strategically optimizing gas delivery to minimize flow rates and achieving higher material removal rates without significantly compromising tool life – both of which require additional experimental investigation and research to develop a comprehensive understanding of the true productivity potential of gas-based MWFs. Building on their occupational health benefits, such optimized operation of gas-based MWFs that reduces primary energy and water use and MWF system costs holds a promising prospect of gas-based MWFs becoming a sustainable substitute to aqueous MWFs in “dry” (water-less) metal fabrication factories.

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SUPPORTING INFORMATION

This supporting information provides (1) descriptions and relevant details for aqueous and gas-based metalworking fluids (MWFs) on which energy and water use calculations in the paper are based; (2) details of data extraction procedures used to obtain tool life, material removal rate, and MWF parameters from the published literature; and (3) supplementary results for different uncertainty scenarios and a public URL to raw data files used to create figures in the paper, as well as Ecospold and Excel® files for key MWF materials and unit processes.[2]

Figure 1 | a. System boundary used to calculate the primary energy and water use per unit volume of material machined using aqueous and gas-based metalworking fluids. Dashed lines indicate batch flows that only to apply to aqueous metalworking fluids. Overview of the processes used to make b. liquid CO2 and c. liquid N2

[2] These data are freely available in the Zenodo repository at hhttps://zenodo.org/record/3565781#.Xg7235XsY2w

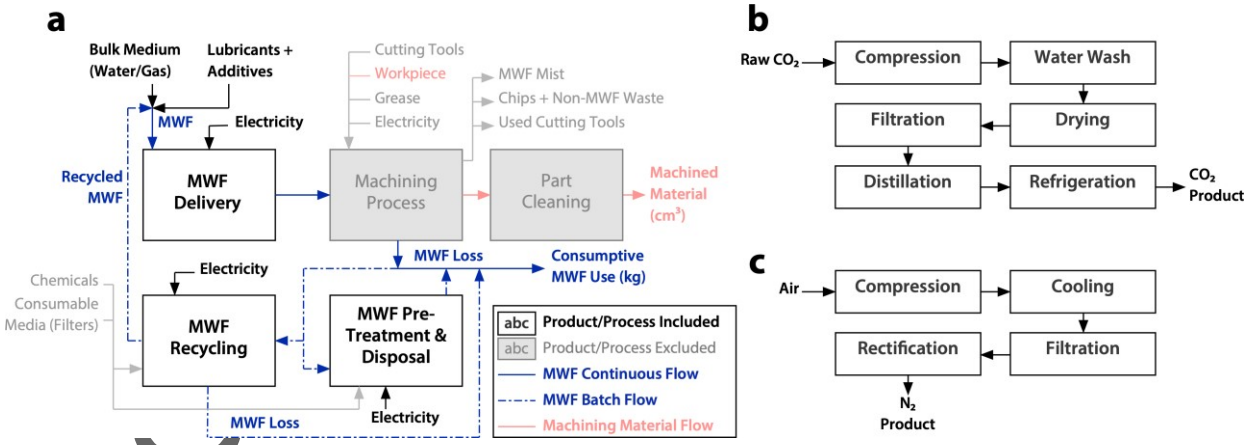

Figure 2 | a. Reported tool life and material removal rates for aqueous and gas-based MWFs in the literature; each pair of points connected by the gray lines represent a paired comparison within an experiment. b. Calculated annual throughput corresponding to the tool life and material removal rates for paired data points in panel a. Underlying data used to create this figure can be found in the data repository (Supekar, Graziano, Skerlos, & Cresko, 2019) using this link

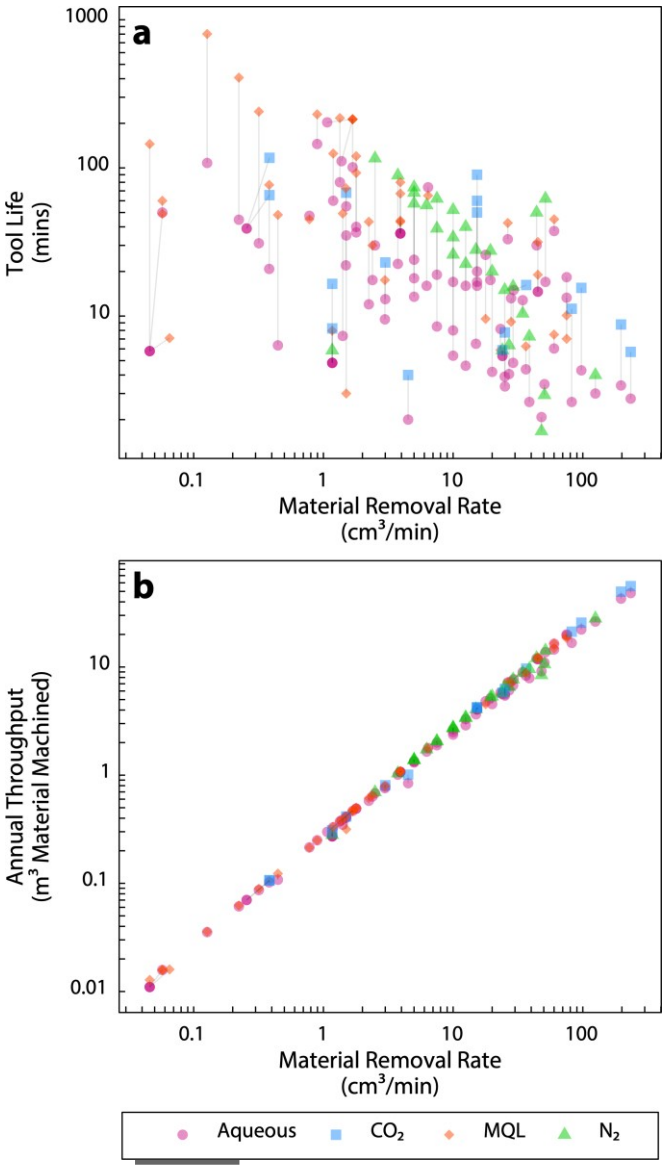

Figure 3 | a. Graphical representation of the algebraic relationship between annual throughput, tool life and material removal rate based on equation (1) assuming tool change time as 1 minute. b. Reported increases in tool life with gas-based MWFs in the literature, shown as a function of the corresponding aqueous MWF tool life and increase in material removal rate within a given experiment

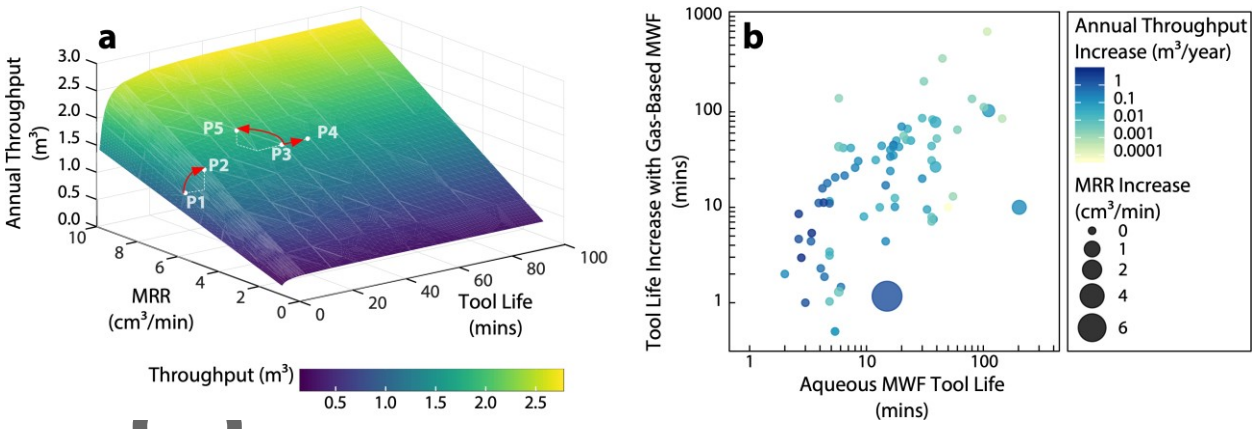

Figure 4 | Primary energy use and water use associated with the production, delivery, and disposal of MWFs expressed a. per unit volume of material machined over a year, and b. on an annual basis. Underlying data used to create this figure can be found in the data repository (Supekar et al., 2019) using this link

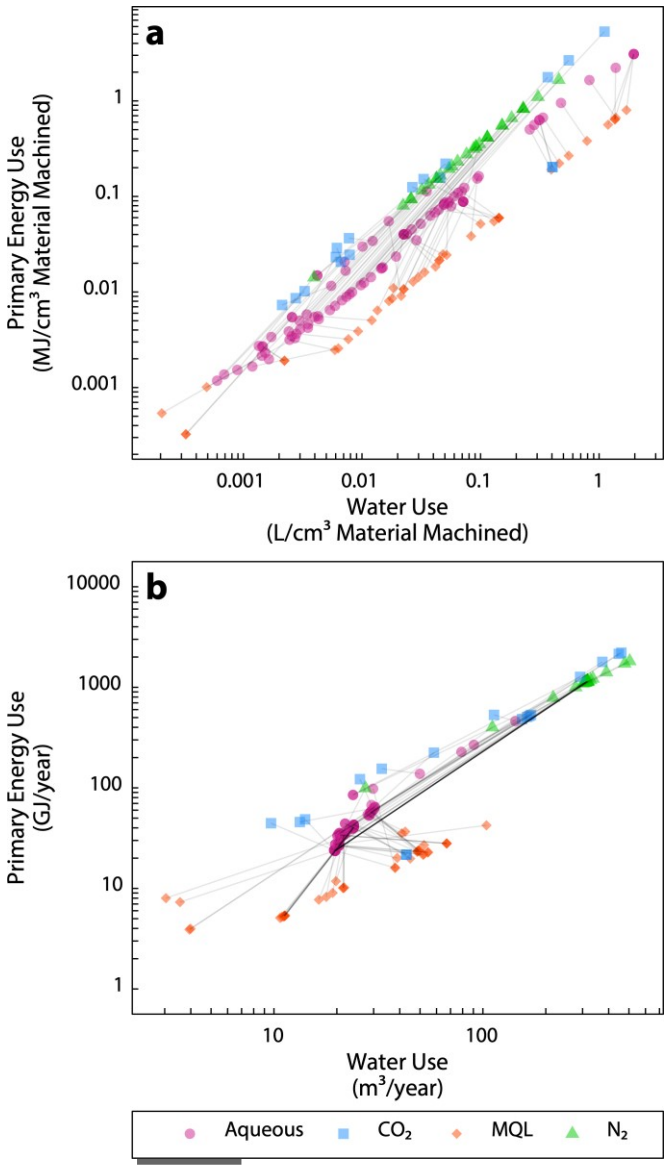

Figure 5 | Differences in a. primary energy use and b. water use per unit of material machined using gas-based and aqueous MWFs based on reported MWF conditions and machining parameters in the experimental literature. Ratios of c. primary energy use and d. water use corresponding to the differences in paired data shown in a–b, where a ratio of 1 indicates that the primary energy or water use for the gas-based MWF is equal to that of the aqueous MWF in a given paired experiment.

Blue dots represent the differences and ratios in primary energy and water use in individual experiments on which the histograms in the figure are based. Underlying data used to create this figure can be found in the data repository (Supekar et al., 2019) using this link

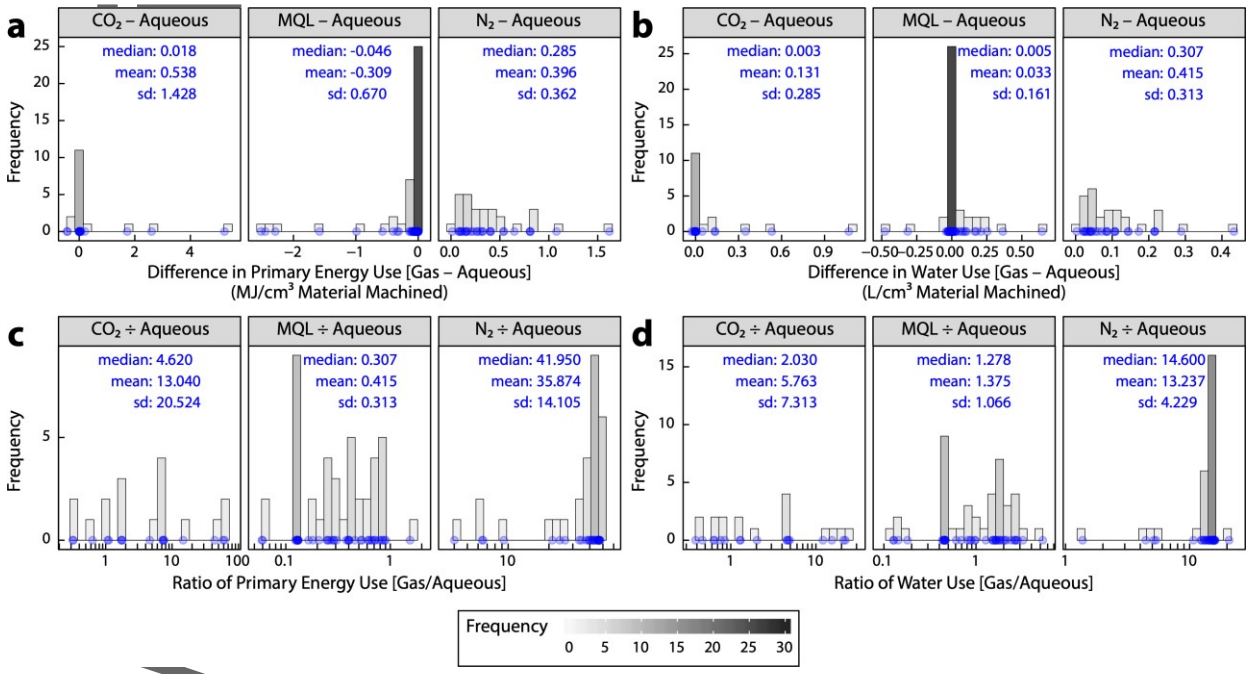

Figure 6 | Sensitivity of energy and water use per unit volume of material machined to MWF and machine tool parameters listed in Error! Reference source not found.