Supporting Information:

Comparative techno-economic and life-cycle analysis of precious versus non-precious metal electrocatalysts: The case of PEM fuel cell cathodes

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A. Life Cycle Inventory *Pt/C loading*

For the baseline scenario the required amount of catalyst was calculated as follows:

Number of cells used were 380 with an active area of 185 cm² per cell.

The area to be coated is calculated by:

Total area coated with catalyst = $380 \times 185 cm^2 = 70,300 cm^2$

With a loading of 0.125 mg cm⁻² of Pt this gives total amount of Pt loading of:

70,300
$$cm^2 \times 0.125 \frac{mg_{Pt}}{cm^2} = 8.79 g_{Pt}$$

The Pt/C catalyst is made up of 46 wt.% Pt, therefore Pt/C:

$$\frac{8.79 \ g}{0.46 \ wt. \ \%} \approx 20 \ g_{Pt/C}$$

Fe-N-C loading

The total required Fe-N-C for 80 kW PEMFC is based on power density of 290 mW cm⁻² at 0.657 V with loading of 2.5 mg_{FeNC} cm⁻²:

$$\frac{80,000 W \times 0.0025 g cm^{-2}}{0.290 W cm^{-2}} = 690 g_{FeNC}$$

Pt/C Manufacturing calculations

Chloroplatinic acid (CPA) calculations were based on the molar ratios as shown in Equation S1:

$$Pt + 4 HNO_3 + 6 HCl \rightarrow H_2 PtCl_6 + 4 NO_2 + 4H_2O$$
 Eq. S1

Molecular weights were used to calculate the amount of mass required to produce 1.23 kg of CPA.

Table S1. Chloroplatinic acid production inputs.

Inputs	<u>.</u>		
Flow	Amount	Unit	Provider/Category
Hydrochloric acid, without water, in 30%			Market for Hydrochloric acid, APOS, U -
solution state	0.66	kg	RER
Nitric acid, without water, in 50% solution			
state	0.76	kg	Market for nitric acid, APOS, U - RER
Platinum	0.64	kg	Market for platinum, APOS, U - GLO
Outputs			
Chloroplatinic acid	1.23	kg	
Nitrogen dioxide, emission to water	0.55	kg	
			market for wastewater, average - APOS,
Wastewater, average	216	mL	U - Europe without Switzerland

The energy input for CPA production process is ignored in this study as this was considered negligible compared to the total used in the catalyst production process.

Inputs			
Flow	Amount	Unit	Provider
Acetone	768	g	Market for acetone, APOS, U - RER
Carbon black	10	g	Market for carbon black, APOS, U - GLO
Chloroplatinic acid	17.7	g	Table S1
Electricity	4.43	MJ	Market group for electricity, medium voltage, APOS, U - GLO
Ethylene glycol	2.56	kg	Market for ethylene glycol, APOS, U - GLO
Hydrochloric acid, without water, in 30% solution state	318	g	Market for hydrochloric acid, APOS, U - RER
Sodium hydroxide	23	g	Market for sodium hydroxide, APOS, U - RER
Water, deionised	39.7	kg	Market for water, deionised, APOS, U - Europe without Switzerland
Outputs			
Acetone, emission to water	768	g	
Hydrochloric acid, emission to water	318	g	
Pt/C catalyst	20	g	This Table.
Sodium hydroxide, emission to air	23.3	g	
Wastewater, average	39.7	kg	market for wastewater, average - APOS, U - Europe without Switzerland
Ethylene glycol	2.56	kg	

Table S2. Pt/C production inputs for 20 g baseline scenario with provider of LCA data.

Fe-N-C manufacturing inputs

 Table S3. Production process for iron nitrate nonahydrate.

Inputs			
Flow	Amount	Unit	Provider
Iron ore	0.14	g	Market for iron ore, APOS U - GLO
Sodium nitrate	0.46	g	Market for sodium nitrate, APOS U - GLO
Water deionised	0.40	g	Market for deionised water, APOS U - RoW
Outputs			
Iron nitrate nonahydrate	1	g	

Table S4. Production process and estimations for the nicarbazin precursor.

Inputs			
Flow	Amount	Unit	Provider
2-nitroaniline	317	g	Market for 2-nitroaniline, APOS, U - GLO
2-pyridinol	109	g	Market for 2-pyridinol, APOS, U - GLO
Outputs			
Nicarbazin	426	g	

Reaction of HF with silica **Equation S2**:

 $4HF + SiO_2 \rightarrow SiF_4 + 2H_2O$ Eq. S2

Equipment	Power	Duration of usage (h)	Energy (kWh)
	Consumption (kW)		
Planetary ball mill	2.2	1	2.2
Tube furnace	7	3	21
Filtration pump	0.5	4	2
Dry Oven	1	8	8
Tube furnace	7	3	21

Table S5. Energy inputs for 25 g production of Fe-N-C.

Table S6. Production process inputs for Fe-N-C catalyst, 691 g baseline scenario, with provider

of LCA data.

Inputs			
Flow	Amount	Unit	Provider/Category
Silica	1.38	kg	Market for activated silica, APOS, U - GLO
			Market group for electricity, medium voltage, APOS, U -
Electricity	5,393	MJ	GLO
Hydrogen fluoride	2.21	kg	Market for hydrogen fluoride, APOS, U - RER
Iron nitrate			
nonahydrate	0.345	kg	Table S3
Nicarbazin	3.46	kg	Table S4
			market for water, deionised, APOS, U - Europe without
Water deionised	138	kg	Switzerland
Outputs			
Silica	1.38	kg	Market for activated silica, APOS, U - GLO
Fe-N-C Catalyst	691	g	This Table
Hydrogen Fluoride	2.21	kg	Emission to air
Nicarbazin	2.76	kg	Table S4
			market for wastewater, average - APOS, U - Europe
Wastewater, average	138	kg	without Switzerland

B. Global Sensitivity Analysis

Total sensitivity indices (equivalent to first-order effects due to linearity of the process inventories) were calculated through sampling 1,000 scenarios from the joint probability distribution of the uncertain factors (process inputs) using low-discrepancy Sobol sequences, then evaluating the midpoint and end-point impacts using OpenLCA linked to python. Note that the input-to-output ratio in the process inventories were kept constant (equal to those in the nominal case) to preserve the mass balances. These scenarios were passed to the software SobolGSA, where the Sobol sensitivity indices were estimated using the RS-HDMR method. The inputs for the sensitivity analysis of Pt/C and Fe-N-C are shown in **Table S7** and **Table S8**. A sensitivity index higher than 0.05 is considered significant here.¹

Table S7. Uncertain factors according to a triangular distribution in the GSA for the baseline

Pt/C process.

Factor (g)	Carbon	CPA (g)	Electricity (MJ)	Ethylene	Hydrochloric	NaOH	H₂O	
	(g)	black (g)	,		glycol (g)	acid (g)	(g)	(kg)
Lower bound	614	8.0	14.4	3.54	2052	254	18.4	32.0
Mode	768	10.0	18.0	4.43	2565	318	23.0	40.0
Upper bound	921	12.0	21.6	5.32	3078	382	27.6	48.0

Table S8. Uncertain factors according to a triangular distribution in the GSA for the baseline

Fe-N-C process.

Factor	Activated	Electricity	Hydrogen	Iron Nitrate	Nicarbazin	Water
Factor	silica (kg)	(MJ)	fluoride (kg)	Nonahydrate (kg)	(kg)	(kg)
Lower bound	1.11	4312	1.77	0.28	2.77	111
Mode	1.38	5393	2.21	0.35	3.46	138
Upper bound	1.65	6473	2.65	0.42	4.15	165

C. Monetization Factors

Table S9. Monetary valuation factors for the endpoint impacts. Factors for human health and ecosystem quality obtained from Dong *et al.*² Conversion of USD to 2023 values were based on inflation.

Endpoint Impact	Unit	Unit Equivalent Monetary	
		Value Factor (USD 2017 /	factor from 2017
		Unit)	to 2023
Human health	DALY	108,836	
Ecosystem quality	Species Year	13,964,286	1.22
Resources	USD 2013	1.05	

D. TEA Calculations

PRODUCTION COST SUM	IMARY	USD kg _{Pt/C} -1
RAW MATERIALS	Chloroplatinic Acid	13,275
	Acetone	38.4
	Carbon Black	0.75
	Ethylene glycol	136.53
	HCI	2.85
	Sodium Hydroxide	1.40
	Water, deionised	97.31
TOTAL RAW MATERIALS		13552.23
TOTAL UTILITIES	Power	23.46
NET RAW MATERIALS &	UTILITIES	13575.69
	Supervisors 1 Employee 29953 USD	1.50
DIRECT FIXED COSTS	Maintenance, Material & Labour 4.0 % of ISBL	7.79
	Direct Overhead 100 % Labour & Supervision	1.50
TOTAL DIRECT FIXED CO	STS	10.79
ALLOCATED FIXED	General Plant Overhead 50.0 % Direct Fixed Costs	5.39
COSTS	Insurance, Property Tax 0.8 % Total Plant Capital	2.10
TOTAL ALLOCATED FIXE	D COSTS	7.50
TOTAL FIXED COSTS		18.28
TOTAL CASH COST		13593.97
Depreciatio	n 0.10 for ISBL & OPC 0.05 for OSBL	29.46
COST OF PRODUCTION F	ER kg	13623.43
		USD kW ⁻¹
COST OF PRODUCTION F	PER kW	3.41

Table S10. Cost of Production for baseline 20 g Pt/C at 500,000 stacks.

						USD		
PRODUCTION COST SUN	IMARY					kg _{Fe-N-C} -1		
RAW MATERIALS	Iron Nitrate Nonahydrat	e				0.42		
	Nicarbazin					37.00		
	Silica					2.00		
	Hydrogen fluoride	Hydrogen fluoride						
	Water, deionised					8.02		
TOTAL RAW MATERIALS						50.64		
TOTAL UTILITIES	Power					229.81		
NET RAW MATERIALS &	UTILITIES					280.45		
	Supervisors	1	Employee		29,953 U.S. \$	1.50		
	Maintenance, Material	& Labo	ur	4.0	% of ISBL ^a	9.58		
DIRECT FIXED COSTS	Direct Overhead			100	% Labour & Supervision	1.50		
TOTAL DIRECT FIXED CO	STS					12.58		
ALLOCATED FIXED	General Plant Overhead			50.0	% Direct Fixed Costs	6.29		
COSTS	Insurance, Property Tax			0.8	% Total Plant Capital	2.54		
TOTAL ALLOCATED FIXE	COSTS					8.83		
TOTAL FIXED COSTS						21.41		
TOTAL CASH COST						130.22		
Depreciatior		0.10	ISBL & OPC	b	0.05 OSBL ^c	35.80		
COST OF PRODUCTION F	ER kg					337.66		
						USD kW ⁻¹		
COST OF PRODUCTION F	ER kW					2.92		
Inside hattery limits						I		

Table S11. Cost of Production for baseline 691g Fe-N-C at 1,000 PEMFC stacks.

^a Inside battery limits

^bOther project costs

^cOutside battery limits

Production Rate	Cathode Catalyst	Membrane + GDL	Bipolar Plates	Gaskets	Stack + Conditioning	Anode Catalyst	Total Cost
Stacks year-1			L	ISD kW ⁻¹			USD kW ⁻¹
1,000	12.61	33.05	15.65	14.23	3.61	2.55	81.70
10,000	7.76	15.75	5.76	6.78	3.05	1.57	40.66
20,000	6.70	12.60	4.26	5.42	2.89	1.36	33.23
50,000	5.53	9.38	2.86	4.04	2.70	1.12	25.63
100,000	4.77	7.50	2.12	3.23	2.57	0.97	21.16
500,000	3.40	4.47	1.05	1.92	2.28	0.69	13.81
F (%)	86.4	80.0	74.0	80.0	95.0	86.4	-
-r (-)	-0.21	-0.32	-0.43	-0.32	-0.07	-0.21	-
A (-)	4330	24437	25166	10518	482	876	-

Table S12. Cost of 80 kW PEMFC components for F = 86.4% learning curve of Pt/C cathode system, with applied and calculated *F*, *r*, and A values.

Production Rate	Cathode Catalyst	Membrane + GDL	Bipolar Plates	Gaskets	Stack + Conditioning	Anode Catalyst	Total Cost
Stacks year-1			U	SD kW ⁻¹			USD kW ⁻¹
1,000	14.58	33.05	15.65	14.23	3.61	2.55	83.66
10,000	8.97	15.75	5.76	6.78	3.05	1.57	41.87
20,000	7.75	12.60	4.26	5.42	2.89	1.36	34.28
50,000	6.39	9.38	2.86	4.04	2.70	1.12	26.49
100,000	5.52	7.50	2.12	3.23	2.57	0.97	21.90
500,000	3.93	4.47	1.05	1.92	2.28	0.69	14.34
F (%)	86.4	80.0	74.0	80.0	95.0	86.4	-
-r (-)	-0.21	-0.32	-0.43	-0.32	-0.07	-0.21	-
A (-)	5005	24437	25166	10518	482	876	-

Table S13. Cost of 80 kW PEMFC components for learning curve of PtCo/C cathode system, with applied and calculated *F*, *r*, and A values.

Production Rate	Cathode Catalyst	Membrane + GDL	Bipolar Plates	Gaskets	Stack + Conditioning	Anode Catalyst	Total Cost		
Stacks year-1		USD kW ⁻¹							
1,000	2.92	129.69	61.41	55.82	14.18	9.91	273.93		
10,000	1.79	61.80	22.59	26.60	11.95	6.10	130.83		
20,000	1.55	49.44	16.71	21.28	11.36	5.27	105.61		
50,000	1.28	36.81	11.23	15.84	10.61	4.34	80.11		
100,000	1.10	29.45	8.31	12.67	10.08	3.75	65.37		
500,000	0.786	17.54	4.13	7.55	8.95	2.67	41.63		
F (%)	86.4	80.0	74.0	80.0	95.0	86.4	-		
-r (-)	-0.21	-0.32	-0.43	-0.32	-0.07	-0.21	-		
A (-)	1001	95892	98753	41273	1891	3404	-		

Table S14. Cost of 80 kW PEMFC components for F = 86.4% learning curve of Fe-N-C cathode system, with applied and calculated *F*, *r*, and A values.

E. LCA Results

Global Sensitivity Analysis

Material and electricity contribution in global sensitivity analysis for Fe-N-C and Pt/C are provided in **Table S15-Table S16**.

Table S15. Total Sobol sensitivity indices for midpoint global sensitivity analysis of Pt/C baseline.

Midpoint Impact Method	Acetone	Carbon black	СРА	Electricity	Ethylene glycol	HCI	NaOH	H ₂ O
Global warming (kg CO ₂ -Eq)	0.0001	0	0.6346	0.3651	0.0001	0.0001	0	0
Acidification potential (kg SO ₂ -Eq)	0	0	0.9972	0.0027	0	0.0001	0	0
Marine eutrophication (kg N-Eq)	0	0	0.7673	0.2326	0	0.0001	0	0
Freshwater eutrophication (kg P- Eq)	0	0	0.9169	0.083	0	0.0001	0	0
Human toxicity potential (kg 1,4-DCB- Eq)	0	0	0.9793	0.0206	0	0.0001	0	0
Fossil resource scarcity (kg oil-Eq)	0.0002	0	0.7458	0.2537	0.0002	0.0001	0	0
Mineral resource scarcity (kg Cu-Eq)	0	0	0.9998	0.0001	0	0.0001	0	0

 Table S16. Total Sobol sensitivity indices of midpoint global sensitivity analysis of Fe-N-C

 baseline.

Midpoint Impact Method	Activated Silica	Electricity	HF	Iron Nitrate Nonahydrate	Nicarbazin	H ₂ O
Global warming (kg CO ₂ - Eq)	0	0.9994	0.0001	0	0.0001	0
Acidification Potential (kg SO ₂ -Eq)	0.0089	0.6135	0.3668	0	0	0
Marine eutrophication (kg N-Eq)	0	0.4086	0	0.0001	0.5912	0
Freshwater eutrophication (kg P-Eq)	0	0.9998	0.0001	0	0.0001	0
Human toxicity potential (kg 1,4-DCB-Eq)	0	0.0064	0.9936	0	0	0
Fossil resource scarcity (kg oil-Eq)	0	0.9987	0.0002	0	0.0011	0
Mineral resource scarcity (kg Cu-Eq)	0.0002	0.964	0.0244	0.0001	0.0103	0



Figure S1. Scenarios of Fe-N-C (baseline, no HF, 380 g, EU electricity) and Pt/C (baseline, 15 g, 55% and 75% Pt recycling for midpoints categories: (a) Global warming (kg CO₂-eq). (b) Fossil resource scarcity. (c) Marine Eutrophication (kg N-eq). (d) Freshwater eutrophication (kg P-eq) (e) Human Toxicity (kg 1,4-DCB-eq). (f) Acidification potential (kg SO₂-eq). (g) Mineral resource scarcity (kg Cu-eq).

		Fe-N-C					Pt/C			
Midpoint Impact Method	Baseline	No HF	380 g	EU electricity	Muffle furnace	Baseline	75% Pt recycling	55% Pt recycling	15 g	
Global warming (kg CO2-Eq)	1,130	1,120	623	677	319	659	162	363	494	
Fossil resource scarcity (kg oil-Eq)	286	282	157	185	83	213	52	118	160	
Marine eutrophication (kg N-Eq)	0.09	0.09	0.05	0.10	0.06	0.03	0.01	0.02	0.03	
Freshwater eutrophication (kg P-Eq)	0.55	0.55	0.30	0.64	0.15	0.83	0.21	0.46	0.62	
Human toxicity potential (kg 1,4- DCB-Eq)	7,140	856	3,930	7,030	7,138	2,300	571	1,260	1,720	
Acidification Potential (kg SO ₂ - Eq)	8.36	3.79	4.60	7.44	6.58	34.4	8.6	18.9	25.8	
Mineral resource scarcity (kg Cu-Eq)	1.01	0.90	0.56	1.28	0.45	81.9	20.5	45.0	61.4	

Table S17. Midpoint impact results for baseline and varying scenarios.



Figure S2. Midpoint impacts for Fe-N-C for different electricity mix scenarios.

	Fe-N-C							
Midpoint Impact Method	Baseline (Global electricity)	EU electricity	Poland electricity	Sweden electricity				
	1130	677	1520	129				
Global warming (kg CO ₂ -Eq)	286	185	387	34				
oil-Eq)	200	100	567	0.1				
Marine eutrophication (kg N-Eq)	0.09	0.10	0.17	0.06				
Freshwater eutrophication (kg P-Eq)	0.55	0.64	1.93	0.05				
Human toxicity potential (kg 1,4-DCB-Eq)	7140	7030	7380	6590				
Acidification Potential (kg SO ₂ -Eq)	8.36	7.44	12.7	4.11				
 Mineral resource scarcity (kg Cu-Eq)	1.01	1.28	1.17	1.17				

Table S18. Midpoint impact results for baseline (global electricity) and EU, Poland, and Sweden electricity mix for Fe-N-C.

Impact Method Contribution	Fe-N-C	Pt/C
Human Health (10 ⁻³ DALY)	2.01	3.16
Climate Change	1.04	0.62
Human Toxicity	0.47	1.16
Ionising Radiation	0.00	0.00
Ozone Depletion	0.00	0.00
Particulate Matter Formation	0.50	1.38
Photochemical Oxidant Formation	0.00	0.00
Resources (USD 2013)	54.66	59.41
Fossil resources scarcity	54.43	40.47
Mineral resources scarcity	0.23	18.94
Ecosystem Quality (10 ⁻⁵ Species·Year)	0.61	5.65
Freshwater ecotoxicity	0.00	0.02
Freshwater eutrophication	0.04	0.06
Global warming, freshwater ecosystem	0.00	0.00
Global warming, terrestrial ecosystem	0.32	0.18
Land use	0.12	4.56
Marine ecotoxicity	0.00	0.00
Marine eutrophication	0.00	0.00
Ozone formation, terrestrial ecosystem	0.03	0.12
Acidification potential	0.08	0.69
Terrestrial ecotoxicity	0.00	0.00
Water consumption, aquatic ecosystem	0.00	0.00
Water consumption, terrestrial ecosystem	0.01	0.01

Table S19. Midpoint contribution to endpoints for baseline scenario.

Table S20. Total Sobol sensitivity indexes for endpoint global sensitivity analysis of Pt/Cbaseline.

Endpoint Impact Method	Acetone	Carbon black	СРА	Electricity	Ethylene glycol	HCI	NaOH	H ₂ O	
Human health (DALY)	0	0	0.9829	0.0170	0	0.0001	0	0	
Ecosystem quality (species·Year)	0.0008	0	0.7615	0.2370	0.0007	0.0001	0	0	
Resources (USD 2013)	0.0004	0	0.8714	0.1277	0.0004	0.0001	0	0	

Table S21. Total Sobol sensitivity indexes for endpoint global sensitivity analysis of Fe-N-Cbaseline.

Endpoint Impact Method	Activated Silica	Electricity	HF	Iron Nitrate Nonahydrate	Nicarbazin	H₂O
Human health (DALY)	0.0011	0.9428	0.0561	0	0.0034	0
Ecosystem quality (species∙year)	0	0.9954	0.0007	0	0.0039	0
Resources (USD 2013)	0	0.9955	0.0006	0	0.0039	0

			Fe-N-	·С	Pt/C				
Endpoint Impact Method	Baseline	No HF	380 g	EU	Muffle furnace	Baseline	75% Pt	55% Pt	15 g
Human health (10 ⁻³ DALY)	2.01	1.68	1.10	1.49	1.04	3.16	2.37	1.74	0.79
Ecosystem quality (10⁻⁵ species·year)	0.61	0.60	0.34	0.46	0.18	5.65	4.24	3.11	1.41
Resources (USD 2013)	54.7	53.4	30.1	35.3	17.4	59.4	44.6	32.8	14.4

Table S22. Endpoint impact results for baseline and different scenarios.

Table S23. Endpoint impact results for baseline and scenarios considering differentproduction location electricity mix for Fe-N-C.

		Fe-N-C							
Endpoint Impact Metho		Baseline (Global electricity)	EU electricity	Poland electricity	Sweden electricity				
Human he DA	Human health (10 ⁻³ DALY)		1.49	2.72	0.48				
Ecosystem quality (10⁻⁵ species∙year)		0.61	0.46	1.03	0.17				
Resources	(USD 2013)	54.7	35.3	34.7	10.5				



Figure S3. Endpoint scenarios for Fe-N-C for different electricity mix supplies.



Figure S4. Sensitivity analysis on catalyst material feedstock price variance for a.) cathode catalyst material costs for baseline and varying catalyst scenarios and b.) catalyst production cost variance. c.) Electricity price variance on catalyst production cost variance.



Figure S5. Percentage breakdown of 80 kW PEMFC component costs with cathode (a) Fe-N-C. (b) Pt/C.



Figure S6. Different *F* values applied for baseline Fe-N-C based 80 kW PEMFC stack. For F = 74 and 95%, this *F* value is applied to all PEMFC components. F = 86.4% is only applied to the catalysts, with other values found in Table S20.



Figure S7. a.) Learning curve of 80 kW PEMFC stack containing cathode PtCo/C. b.) Corresponding percentage breakdown of component costs.



Figure S8. Different scenarios of Pt consumption over time based on PEMFC electric vehicle (FCEV) production from World Platinum Investment Council (WPIC)³ of lower (11 million FCEV) and upper (15 million FCEV) by 2040. Also, IEA 2050 net zero scenario (equivalent to 2.85 million FCEV)⁴ and 2030 government targets (2.5 million FCEV).⁵ 10% annual Pt consumption limit for deployment of new technology based on ref,⁶ with error representing variation in Pt production between 2017-2023.⁷



Figure S9. Amount of Pt required for PEMFC power at different Pt specific power density (US DOE 2020,⁸ EU 2030 ⁹ and 75% Pt recycling targets¹⁰) as a function of scale. Assumed 80 kW fuel cell electricity vehicle production. IEA 2030 Government targets (vertical dash blue)⁵ and upper limit scenario given by upper 2040 WPIC (vertical dash purple).³ Figure design is inspired from Hubert et al.¹¹

G. Discussion and Literature Comparison



Figure S10. Calculated Global warming impact per kW for assumed Pt loadings in references (Usai *et al.* 2021,¹² Evangelisti et al. 2017,¹³ Miotti et al. 2017,¹⁴ Simons and Bauer 2015¹⁵) and this work.



Figure S11. Reported Pt specific power density and targets over time. Toyota Mirai based on reported reductions,¹⁶ with g_{Pt} kW⁻¹ based on calculations from Gröger et al.¹⁷ Targets reported for EU⁹ and US DOE.^{8,18} Previous literature reports from 1991,¹⁹ 2005,²⁰ and 2016.²¹ The reported values and targets are based on different operation conditions.

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