Electronic Supplementary Material (ESI) for Green Chemistry.

Machine Learning for CO_2 Conversion Driven by Dielectric Barrier Discharge Plasma and Cs_2TeCl_6 Photocatalyst

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Materials

Cesium chloride (CsCl, 99.9% metals basis, Macklin), Tellurium chloride ($TeCl_4$, 99.5%, Aladdin), Hydrochloric acid (HCl, 37 wt% in water), Ethanol (>99.7%) was purchased from Chongqing Wansheng East Sichuan Chemical Co. LTD. All the chemicals were used without further purification.

Preparation of Cs_2TeCl_6 Perovskites.

First of all, the precursor solution was obtained by dissolving 2 mmol CsCl (0.3367 g) and 1mmol $TeCl_4$ in 5 ml hydrochloric acid according to the stoichiometric ratio, and placed in 25ml polytetrafluoroethylene autoclave. The precursor was heated to 180 ° C within 10 hours and maintained at this temperature for 10 hours, which was then slowly cooled to room temperature within 24 hours. The product was washed with anhydrous ethanol, and centrifuged at 10000 rpm for 5 minutes. Finally, the supernatant was removed and dried at 70 ° C for 4 hours in vacuum, and the Cs_2TeCl_6 microcrystals was obtained.

Characterization

The crystal structure of the as prepared Cs_2TeCl_6 was determined by Cu Ka radiation (MADZU, Japan) powder X-ray diffraction (XRD). The morphology of Cs_2TeCl_6 was determined by scanning electron microscopy (SEM, TM4000Plus II). Plasma experiments were conducted with a plasma generator (CTP-2000, Nanjing Suman Electronics Co., Ltd.). The experimentally obtained gas mixture was analyzed by gas chromatography (GC, Fuli 9790II).

K-fold cross validation

k-fold cross validation is a method that divides all samples equally into k sample subsets, and each time the current subset is used as the validation set while all the remaining samples are used as the training set. The training and evaluation of the model are performed, and finally the average of the k evaluation metrics is taken as the final evaluation metric, and the k value is set to be 5 in this work.

Hyperparameters

In this paper, the hidden layer nodes and the regularization term parameters of the BPANN model are optimized. Where the hidden layer nodes represent the number of neurons in the hidden layer, which determine the complexity of the neural network. Too few hidden layer nodes will result in poor training of the network, while too many will lengthen the training time of the network, and will also result in overfitting when the limited information contained in the training set is not enough to train all the neurons in the hidden layer. The regularization term parameters are also known as the L2 penalty coefficient. When the model performs very well in the training set but poorly in the testing set, this represents model overfitting, and the regularization term parameters serve to prevent overfitting.

Genetic Algorithm

Genetic Algorithm (GA)[1,2] is a stochastic search algorithm that draws on natural genetic mechanisms in the biological world. It imitates the natural evolutionary process and genetically manipulating individuals in a population with a certain structural form to generate a new population that gradually approaches the optimal solution.

The basic Genetic Algorithm consists of the coding initialization, the fitness function, the selection operations, the crossover operations, the mutation operations and the operating parameters. In this study, the hyperparameters in the basic model are encoded as individuals in the Genetic Algorithm through binary, which is due to the genetic operator operates directly on strings of numbers. Then the objective function R^2 is chosen to calculate the fitness value for all individuals generated randomly and based on this fitness value, the better solution is selected. The selected solutions are then reassembled by crossover and mutation operations (Fig. S1) to generate new solutions, and iterations are repeated until the best combination of hyperparameters is found. And the operating parameters contain the coding length, population size, crossover probabilities, mutation probabilities and termination conditions. The model of GA algorithm combined with the BPANN is named GA-BPANN model.

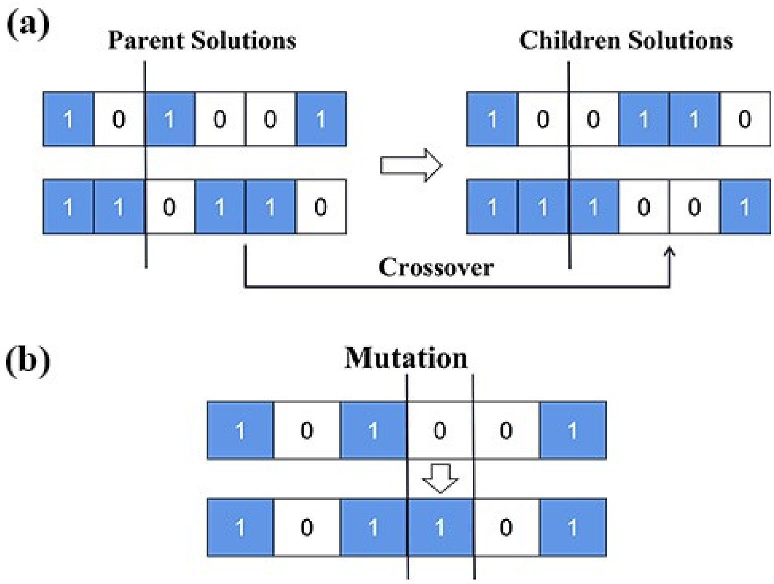

Fig. S1 (a) The crossover operations: chromosomes of two individuals are exchanged after a random exchange of starting points. (b) The mutation operations: mutation operators change the genes in solutions.

Particle Swarm Optimization

The basic idea of the Particle Swarm Optimization (PSO)[3] is to simulate birds in nature and find a path closest to food by competing and cooperating with other birds. When it is used to optimize a neural network, the hyperparameters are the particles, and each particle searches independently in the set hyperparameter area and marks the best location found. Then, the particles are evaluated by the fitness function, and the current particle will compare with the historical individual optimum and population optimum to update its own speed and position,[4] with the following formula:

$$V_i = V_i + C_1 r(P_i - X_i) + C_2 r(G_i - X_i) \quad \text{* MERGEFORMAT (1)}$$

$$X_i = X_i + V_i \quad \text{* MERGEFORMAT (2)}$$

Where V_i is the velocity of the particle, P_i and G_i is the historical best positions of the individual and the population, respectively, r is a random number between the interval (0,1), X_i is the current position of the particle, and both C_1 and C_2 are learning factors.

Before reaching the expected error accuracy or maximum number of iterations, the PSO can be used to iterate repeatedly to find the optimal hyperparameters. The BP neural network model combining PSO algorithm is named as PSO-BPANN model in this study.

Bayesian Optimization

Bayesian Optimization (Bayesian)[5] is an algorithm for automatically adjusting parameters. Its basic idea contains two points: the surrogate function and the acquisition function.

Bayesian optimization is a loop iterative process (Fig. S2) until the target value reaches the desired. First, the prediction of observation points is completed by Gaussian process regression (GPR) as the surrogate function, and the predicted mean value of each point on the objective function and the confidence level corresponding to that point are estimated based on a small number of observation points. In this study, the observation points are hyperparametric samples, and the objective function is the value of the corresponding evaluation index R^2. Then the acquisition function is based on the mean $\mu(x)$ and variance $\sigma(x)$ obtained by GPR, and the point with the global maximum is selected for the next observation, and the iterative results will be closer to the true maximum as the number of observation points increases.[6] The difference between Bayesian optimization and other automatic parameter adjusting algorithms is that the previous evaluation results will be referred to when trying the next set of hyperparameters, which can obtain results quickly and save more time, making it an effective global optimization method. The neural network model obtained by combining Bayesian optimization with BPANN is named as Bayesian-BPANN model in this study.

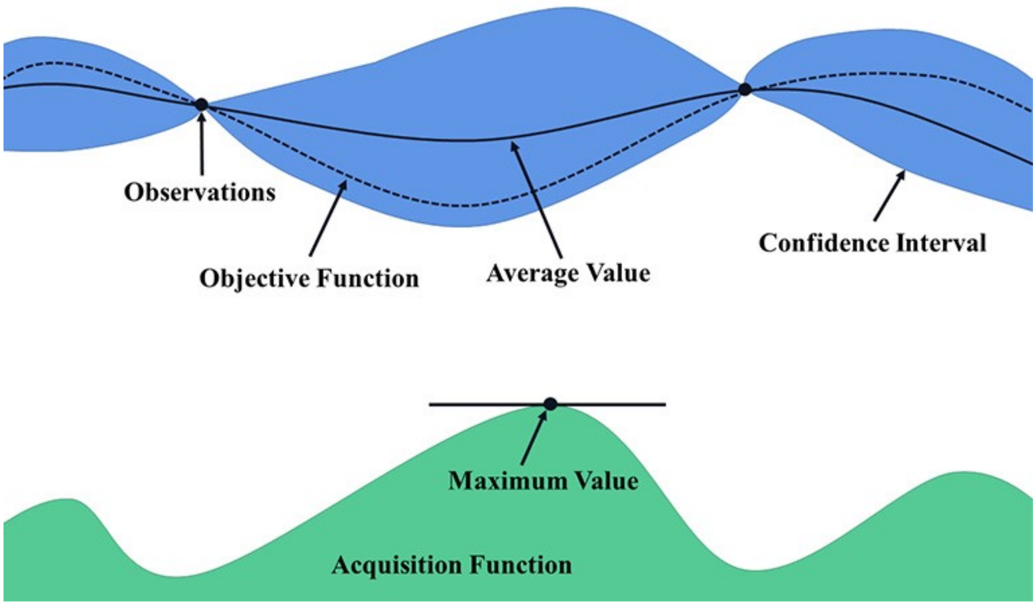

Fig. S2 The basic element of Bayesian optimization: the acquisition function finds the next observation based on the information obtained from the GPR model, thus approaching the maximum R^2 value the fastest.

Training Error Curves

The Fig. S3 shows the training error curves of the four BPANN prediction models, and it can be found that the three optimized models have improved both in terms of convergence rate and prediction performance compared with the basic BPANN model, and the GA-BPANN model holds the best comprehensive performance. This also demonstrates that the three optimized BPANN models can improve some shortcomings of the BP algorithm to a certain extent.

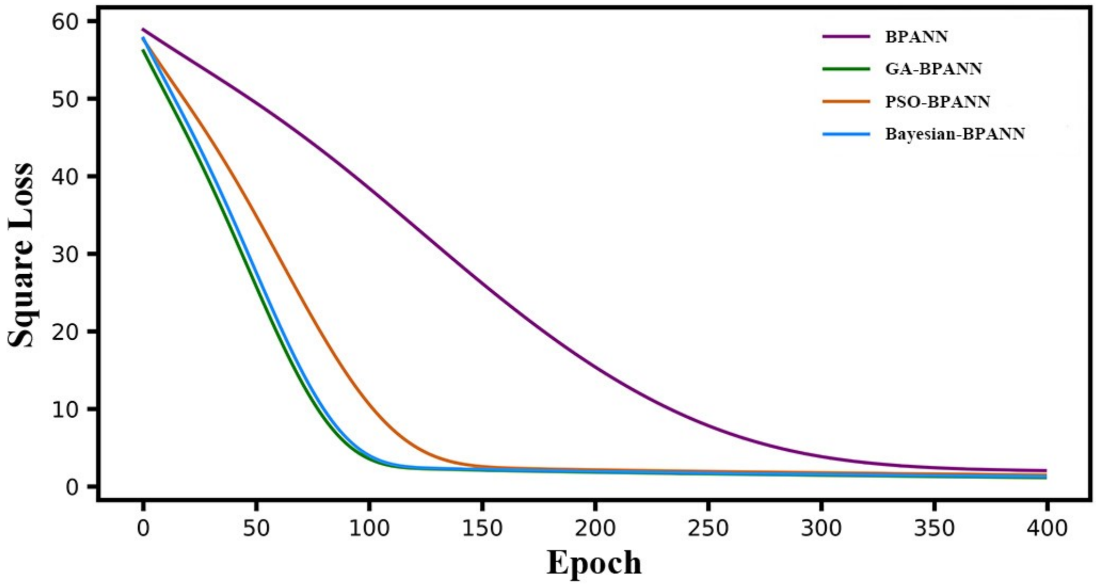

Fig. S3 The training error curves of the four BPANN prediction models.

Table S1: The dataset of ML contains 90 plasma samples

Discharge Power (W)	Gas Flow (sccm)	Catalyst Dose (mg)	CO_2 Conversion Ratio (%)	Energy Efficiency (%)
17.86	20	10	23.40	4.01
18	30	10	20.71	5.25
18.9	40	10	19.85	6.40
16.59	50	10	17.78	8.17
11.97	60	10	12.57	9.64
11.41	70	10	8.80	8.24
21.6	20	10	28.30	4.01
23.5	30	10	23.37	4.53
27.3	40	10	20.40	4.55

24.77	50	10	18.59	5.72
21.28	60	10	16.19	6.98
23.4	70	10	15.45	7.05
41.2	20	10	17.09	1.27
39.62	30	10	16.35	1.88
39.15	40	10	15.64	2.43
33.93	50	10	14.96	3.36
32.21	60	10	14.81	4.22
33.32	70	10	14.19	4.55
54.41	20	10	13.39	0.75
45.68	30	10	14.48	1.44
46.66	40	10	14.92	1.94
43	50	10	12.78	2.26
39.92	60	10	10.68	2.45
43.25	70	10	11.53	2.84
57.33	20	10	13.23	0.70
59.06	30	10	13.25	1.02
57.19	40	10	11.00	1.17
51.38	50	10	10.52	1.56
48.24	60	10	10.20	1.94
62.82	70	10	10.29	1.75
20.31	20	5	17.22	2.59
25.19	30	5	16.68	3.02
18.1	40	5	14.12	4.75
18.04	50	5	13.24	5.59
15.4	60	5	11.16	6.65
15.84	70	5	10.54	7.11
26.77	20	5	18.90	2.16
26.66	30	5	16.90	2.89
21.29	40	5	14.80	4.23
24.75	50	5	14.40	4.43
23.89	60	5	13.20	5.07
26.17	70	5	12.83	5.24
31.72	20	5	13.26	1.27
36.97	30	5	12.46	1.53
39.99	40	5	11.14	1.69
41	50	5	10.65	1.98
36.63	60	5	10.21	2.56
30.57	70	5	9.73	3.40
46.36	20	5	13.69	0.90
45.04	30	5	13.26	1.34
40.24	40	5	11.00	1.66
47.23	50	5	11.20	1.80

56.46	60	5	12.23	1.98
45.02	70	5	10.83	2.57
53.87	20	5	12.05	0.68
70.68	30	5	11.51	0.74
49.17	40	5	9.72	1.20
46.51	50	5	9.24	1.51
51.23	60	5	8.88	1.59
45.33	70	5	8.28	1.95
19.27	20	15	26.80	4.25
19.2	30	15	18.74	4.45
14.86	40	15	14.23	5.83
26.44	50	15	13.60	3.92
24.99	60	15	12.50	4.59
23.48	70	15	11.14	5.07
26.81	20	15	25.08	2.86
32.24	30	15	19.01	2.69
31.07	40	15	17.28	3.39
31.92	50	15	14.66	3.50
28.15	60	15	12.24	3.99
24.41	70	15	9.98	4.37
41.61	20	15	19.67	1.44
40.51	30	15	14.71	1.65
38.37	40	15	13.64	2.16
41.57	50	15	13.50	2.47
42.12	60	15	13.35	2.91
37.7	70	15	12.66	3.58
49.64	20	15	23.11	1.42
45.84	30	15	16.66	1.65
49.24	40	15	13.84	1.71
55.8	50	15	13.35	1.82
51.52	60	15	13.04	2.32
46.43	70	15	12.49	2.87
64.13	20	15	15.35	0.73
55.64	30	15	14.79	1.21
61.52	40	15	14.58	1.44
54.2	50	15	12.71	1.78
58.49	60	15	12.28	1.92
60.04	70	15	9.49	1.68

Table S2: Optimized hyperparameters

Value of the hyper-parameter		
	Hidden nodes	alpha
BPANN	100	0.0001
GA-BPANN	850	0.0681
PSO-BPANN	514	0.0946
Bayesian-BPANN	878	0.1889

Table S3: Performance of neural network models after hyperparameters optimization

	R^2 of Training Set			R^2 of Testing Set		
	Model	CO_2 Conversion Ratio (%)	Energy Efficiency (%)	Model	CO_2 Conversion Ratio (%)	Energy Efficiency (%)
BPANN	0.9595	0.9243	0.9840	0.9455	0.9155	0.9752
GA-BPANN	0.9713	0.9507	0.9870	0.9622	0.9401	0.9838
PSO-BPANN	0.9711	0.9468	0.9899	0.9562	0.9307	0.9818
Bayesian-BPANN	0.9674	0.9436	0.9843	0.9577	0.9335	0.9805

Table S4: Result of neural network model trained for 200 times

	training set	testing set

Average R^2 of BPANN Model	0.9560	0.9467
Average R^2 of GA-BPANN Model	0.9692	0.9632
Average R^2 of PSO-BPANN Model	0.9675	0.9624
Average R^2 of Bayesian-BPANN Model	0.9648	0.9579

Table S5: 10 sets of experimental and predicted results

Discharge Power (W)	27	17	26	25	57	31	40	28	23	15
Gas Flow (sccm)	58	43	41	28	62	29	48	50	58	39
Catalyst Dose (mg)	10	10	8	6	14	8	12	10	8	7
CO_2 Conversion Ratio (%)										
Experimental	17.70	19.68	20.02	15.04	13.48	16.82	14.22	16.61	14.44	16.22
BPANN Predicted	14.88	20.48	16.00	14.40	11.35	16.92	14.23	17.74	13.95	16.50
GA-BPANN Predicted	16.28	19.44	17.53	16.12	11.20	17.11	14.11	17.49	15.07	16.70
Energy Efficiency (%)										
Experimental	5.82	7.58	4.81	2.56	2.24	2.37	2.50	4.48	5.98	6.51
BPANN Predicted	4.15	5.44	2.95	1.07	1.85	2.10	2.73	4.76	5.54	5.32
GA-BPANN Predicted	5.28	6.52	4.02	2.30	1.84	2.18	2.49	4.66	5.59	5.47

Table S6: ML dataset contains 595 plasma samples generated by GA-BPANN model

Discharge Power (W)	Gas Flow (sccm)	Catalyst Dose (mg)	CO_2 Conversion Ratio (%)	Energy Efficiency (%)
11	63	10	11.08962	8.727693
11	47	12	14.51679	7.504844
11	66	8	10.7641	8.380277
11	61	5	9.211145	6.884028
11	41	5	12.53273	5.71089

11	49	7	13.59316	7.321038
11	69	14	5.91753	7.22632
11	25	13	23.48035	5.394102
11	57	14	8.565131	6.82981
11	56	11	12.58168	8.468121
11	33	7	16.9665	5.460984
12	62	5	9.293478	6.704324
12	47	12	14.7949	7.320605
12	33	12	20.32548	6.145131
12	52	12	13.14116	7.60471
12	58	13	9.83826	7.255231
12	43	12	16.0119	7.027293
12	46	5	11.69506	5.879284
12	20	13	26.20108	4.827599
13	21	15	25.17683	4.457213
13	25	5	16.38814	3.664635
13	58	10	13.35891	8.36973
13	36	11	19.6768	6.471836
13	24	8	21.51569	4.360319
13	36	10	19.39605	6.303774
13	24	5	16.61071	3.537825
13	53	5	10.74701	6.093959
14	36	13	18.15974	5.67698
14	70	6	9.445785	6.927539
14	26	12	24.11347	5.112057
14	28	15	21.06063	4.638962
14	35	9	19.59607	5.802177
14	24	7	19.96858	3.904953
14	39	9	18.92759	6.367052
14	70	11	10.58284	7.993219
14	42	9	18.52092	6.761586
14	53	14	10.69869	6.10711
14	44	13	14.75247	6.280944
15	24	7	20.11551	3.730576
15	38	12	18.55146	6.020099
15	58	11	13.58609	7.769984
15	46	9	17.83466	7.076919
15	33	14	19.16201	4.978737
15	27	8	20.60895	4.327022
15	22	5	17.46679	2.959761
15	58	9	14.17174	7.78701
15	39	5	13.9607	4.762423
15	31	6	16.89672	4.299603

15	68	14	7.696613	6.398836
15	56	12	12.82588	7.147816
15	39	7	16.70276	5.470662
15	23	6	18.86697	3.355195
15	67	5	9.418178	6.240154
15	69	14	7.530724	6.43334
15	50	9	16.58018	7.47183
15	40	15	14.12076	5.016027
15	41	14	14.63023	5.441539
15	49	15	10.69343	5.31613
15	54	6	12.29301	6.254633
15	49	7	14.51829	6.473489
15	61	6	11.08687	6.512172
16	46	8	16.86485	6.521532
16	54	9	15.56267	7.465362
16	33	13	20.40984	5.13206
16	45	11	18.04729	6.867429
16	23	14	25.50272	4.270436
16	30	8	19.81623	4.502924
16	27	8	20.76002	4.154542
17	43	10	19.44441	6.521779
17	69	14	8.101161	6.051281
17	28	7	19.14552	3.853732
17	63	15	7.980407	5.326646
17	29	9	21.82694	4.480996
17	26	12	24.88014	4.574901
17	65	6	10.91154	6.187686
17	36	12	19.96095	5.501576
17	27	15	22.38137	4.140559
17	54	15	9.831151	5.085502
17	34	11	21.32631	5.439965
17	52	5	11.75613	5.24297
17	61	11	13.44472	7.375985
17	25	10	24.68291	4.320916
17	40	7	17.00672	5.231766
17	62	8	12.97164	6.990417
18	31	5	15.68065	3.453273
18	37	15	16.20651	4.414122
18	28	12	24.23809	4.589477
18	40	10	20.45573	5.987919
18	56	6	12.56141	5.678719
18	25	15	23.74751	3.903612
18	21	13	27.38891	3.9206

18	70	7	11.15047	6.408945
19	28	10	24.0387	4.332688
19	67	13	10.2468	6.099285
19	22	8	22.92039	3.20038
19	65	8	12.92541	6.556983
19	35	13	19.78438	4.767112
19	28	11	24.35369	4.387989
19	29	10	23.60548	4.433077
19	40	7	17.53112	4.856397
19	52	5	12.2214	4.857736
19	61	12	12.74559	6.442876
19	22	10	26.73426	3.831242
19	60	14	10.35331	5.334304
19	39	14	16.29375	4.669325
19	63	14	9.712073	5.439133
19	48	8	17.02373	6.037627
20	62	6	12.12792	5.46715
20	56	5	11.93523	4.815077
20	50	13	14.3028	5.41246
20	58	8	14.62027	6.260089
20	26	7	19.18499	3.09471
20	28	12	24.6219	4.231218
20	51	13	14.02072	5.433655
20	41	15	14.17119	4.220363
20	58	5	11.72349	4.878998
20	49	9	18.07395	6.332285
20	30	8	20.34681	3.819043
21	45	7	16.75935	4.929273
21	48	14	13.52516	4.704934
21	26	14	24.52805	3.694697
21	62	8	13.94409	6.091654
21	43	12	18.22994	5.369711
21	46	10	19.89744	6.116918
21	39	13	18.08271	4.706716
21	31	13	22.45349	4.157824
21	23	6	17.68606	2.332567
21	58	7	13.98788	5.592605
21	69	13	10.51858	5.772344
21	50	13	14.46223	5.216143
21	33	10	22.94369	4.606539
22	43	8	18.82792	4.906343
22	60	7	13.74334	5.409896
22	37	7	17.70378	4.004391

22	68	5	10.89852	4.703768
22	65	9	14.29421	6.280464
22	48	13	15.23814	4.978055
22	31	14	21.37392	3.812536
23	65	10	15.34774	6.416917
23	46	10	19.98401	5.677044
23	24	15	24.80756	3.164578
23	65	15	9.460085	4.423627
23	58	8	15.06986	5.593693
23	25	9	22.96153	3.211702
23	69	9	13.92628	6.068845
23	34	13	20.7325	4.035899
23	44	5	13.05182	3.601831
23	35	15	17.82841	3.629618
23	67	13	11.3809	5.329434
23	59	11	15.49937	6.069946
23	31	14	21.46124	3.674351
23	56	9	16.36185	5.958801
23	34	7	17.70274	3.512781
23	22	11	26.57242	3.241127
23	34	15	18.44664	3.604153
23	49	9	18.45322	5.63685
23	42	15	14.33533	3.788594
24	25	11	25.05363	3.327952
24	65	7	12.86764	5.016679
24	54	14	12.723	4.28349
24	47	6	14.1866	4.026405
24	38	11	21.44033	4.610277
24	31	13	22.61358	3.717051
24	67	7	12.55272	5.031109
24	43	5	13.01052	3.356442
24	23	15	25.43535	2.992155
24	67	8	13.37795	5.45421
24	69	8	13.13986	5.458515
24	69	12	12.66383	5.584717
24	64	9	14.70069	5.82545
24	33	7	17.52955	3.238803
24	25	6	16.72385	2.142872
25	68	8	13.37518	5.234437
25	49	12	17.07974	4.877682
25	61	15	10.64698	3.901382
25	40	8	18.00059	4.085098
25	28	6	16.12424	2.308063

25	36	10	21.19018	4.195212
25	64	12	13.65247	5.27952
25	27	11	23.92762	3.343608
25	29	14	22.70079	3.325438
25	21	10	25.40835	2.891603
25	41	10	20.44989	4.70336
26	22	9	22.84677	2.575128
26	68	8	13.3434	4.997399
26	41	8	17.5354	4.021783
26	38	15	16.39053	3.258986
26	58	11	16.45882	5.422261
26	60	5	11.08722	3.83213
26	33	5	13.87455	2.290464
26	42	11	19.85661	4.62326
26	57	10	16.76048	5.522358
26	62	7	12.93724	4.514208
26	62	10	15.89214	5.61693
26	60	7	13.21246	4.483977
26	21	15	26.13914	2.645205
27	58	10	16.2814	5.2832
27	50	13	15.61971	4.144471
27	57	15	11.72154	3.531475
27	38	5	13.02794	2.52326
27	42	9	18.53276	4.220071
27	55	9	16.02148	5.015481
27	49	15	13.29809	3.45582
27	63	10	15.65506	5.362063
27	56	12	15.79083	4.640472
27	45	11	18.94722	4.657075
27	21	13	26.23902	2.666117
27	54	11	17.34911	5.066533
27	34	12	20.95778	3.641251
27	65	13	12.93561	4.577883
27	41	12	19.0822	4.221678
28	50	10	17.49453	4.661825
28	68	8	12.96512	4.540458
28	44	6	13.29325	3.102538
28	69	7	11.6681	4.132036
28	49	12	17.00924	4.341906
28	59	8	13.80658	4.448765
28	39	10	19.52874	3.943745
28	46	13	16.50224	3.945359
29	51	14	14.38921	3.530554

29	27	5	13.52196	1.487867
29	62	13	13.87461	4.106646
29	42	10	18.61791	3.971395
29	21	10	23.35833	2.227544
29	68	9	14.00885	4.715419
29	60	15	12.08795	3.427198
29	63	14	12.79793	3.845676
29	42	6	13.26901	2.798381
30	48	14	14.6989	3.348353
30	60	14	13.37788	3.560235
30	32	7	15.43501	2.279055
30	37	7	14.88868	2.683011
30	20	6	15.83459	0.889022
30	37	9	18.0296	3.358786
30	27	10	20.54772	2.51594
30	64	7	11.36029	3.665163
30	68	5	10.12707	3.42948
31	48	14	14.52572	3.205523
31	30	12	20.95118	2.782107
31	45	6	12.22379	2.633223
31	36	12	19.2859	3.201769
31	29	8	17.10892	2.182399
31	48	7	13.44922	3.1755
31	32	14	19.006	2.657412
31	28	15	20.42928	2.334156
31	49	8	14.88024	3.613152
31	31	11	20.21759	2.818117
32	56	5	10.17105	2.841523
32	67	13	13.71455	4.042106
32	24	13	23.25572	2.308838
32	43	5	11.00929	2.156864
32	50	11	16.14775	3.83484
32	32	15	17.98124	2.329635
32	20	14	24.89249	1.975337
32	36	11	19.07448	3.098649
32	67	15	12.29166	3.510038
32	53	14	13.71858	3.146339
32	20	9	20.93652	1.583067
32	70	14	12.8351	3.973117
32	53	9	14.7365	3.772594
33	66	13	13.64792	3.868895
33	67	14	13.01745	3.688657
33	46	11	16.59703	3.478192

33	49	9	15.32535	3.412864
33	64	5	9.902043	2.982144
33	51	11	15.58214	3.67373
33	22	9	19.69612	1.582652
33	60	11	14.38641	3.94047
33	29	14	19.94572	2.274754
33	62	14	13.3212	3.379616
33	51	8	13.83039	3.254842
34	54	15	12.82078	2.757335
34	36	8	15.22202	2.40081
34	68	5	9.576	2.938368
34	49	7	12.40705	2.643887
34	31	14	18.62812	2.203251
34	31	15	17.90699	2.023098
34	43	5	10.5561	1.890403
34	36	11	18.31984	2.779162
34	53	12	15.17035	3.517326
34	52	14	13.56096	2.874363
35	67	10	12.98525	3.679
35	64	11	13.52303	3.724268
35	26	15	20.23878	1.736627
35	34	12	18.76337	2.548424
35	43	8	14.33077	2.681711
35	61	14	13.19083	3.198681
35	40	9	15.78097	2.751458
35	45	5	10.18981	1.8658
35	70	8	11.07455	3.218803
35	48	14	13.8938	2.669724
35	65	8	11.0543	3.09656
35	27	8	16.28206	1.588561
36	55	9	12.62337	2.948577
36	64	8	10.84119	2.954794
36	44	5	10.12835	1.710733
36	31	8	15.37584	1.776967
36	50	11	14.65173	3.092583
36	23	15	21.60301	1.517518
36	47	6	10.88065	2.027353
36	63	7	10.1155	2.742193
36	67	8	10.72835	2.953532
36	24	15	21.03858	1.546927
37	23	10	18.88526	1.32839
37	42	11	15.93221	2.605122
37	51	10	13.70636	2.794096

37	48	5	9.804909	1.822447
37	42	14	14.46679	2.279934
37	43	8	13.68478	2.3756
37	52	8	12.38698	2.540784
37	70	11	13.16514	3.683932
37	69	9	11.67579	3.209382
37	51	15	12.85256	2.383146
37	41	9	14.97837	2.467601
38	64	11	12.68293	3.292441
38	37	11	16.62893	2.243084
38	56	10	12.30582	2.706957
38	31	13	18.36324	1.960974
38	61	14	13.01305	3.024737
38	68	10	12.1758	3.233778
38	68	15	12.28629	3.128426
38	64	8	10.33963	2.669356
38	55	6	10.27183	2.199357
38	44	9	14.35795	2.471029
38	41	6	11.1113	1.690824
39	54	9	11.72734	2.369176
39	58	15	12.44501	2.604418
39	55	14	13.14019	2.640201
39	25	5	12.09002	0.826778
39	63	9	10.80112	2.604315
39	47	8	12.71935	2.219856
39	65	8	10.31614	2.626633
39	50	13	13.98708	2.577893
39	41	8	13.43314	2.090209
39	43	9	14.1865	2.30809
39	20	9	18.00765	0.835327
39	46	6	10.64331	1.71802
40	37	13	16.3834	2.057376
40	23	9	16.57658	0.942551
40	29	15	17.57484	1.340314
40	52	5	9.62901	1.821132
40	45	9	13.52928	2.230876
40	54	15	12.59873	2.340049
40	66	8	10.34047	2.603368
40	48	12	14.10656	2.48573
40	57	14	13.02296	2.69641
40	46	8	12.61604	2.116856
40	54	9	11.38884	2.206794
40	41	15	13.46412	1.707211

40	53	5	9.595031	1.86474
40	64	5	9.172981	2.319874
41	61	11	11.94117	2.770968
41	52	13	13.73675	2.543111
41	32	15	15.93811	1.328622
41	47	5	9.859554	1.552874
41	31	7	13.26755	1.363879
41	24	13	20.81234	1.655919
41	66	6	9.286868	2.31209
41	41	10	14.58408	2.099091
41	24	14	20.82669	1.55013
41	22	14	21.71937	1.529508
42	40	5	10.14338	1.307851
42	22	6	13.44487	0.704951
42	38	13	15.83246	1.991109
42	20	13	22.0745	1.437124
42	22	14	21.5743	1.513471
42	20	11	19.46456	1.011848
42	53	12	13.08816	2.496554
42	27	13	19.43335	1.671765
42	37	15	14.06556	1.389482
42	60	6	9.63008	2.041526
42	46	10	13.20849	2.110594
43	56	10	10.8258	2.002659
43	39	5	10.12618	1.256132
43	29	14	18.05367	1.540887
43	53	14	13.08342	2.292719
43	39	11	14.90194	1.884904
43	20	6	13.68637	0.545173
43	32	7	12.85631	1.366407
43	43	9	13.09279	1.888329
43	40	14	14.30479	1.646677
43	57	8	10.14406	1.854166
43	65	14	12.67808	2.880069
44	57	12	12.44643	2.466698
44	56	15	12.36591	2.222494
44	52	12	12.78393	2.255992
44	62	13	12.65315	2.730075
44	69	12	11.68247	2.870883
44	57	6	10.00194	1.877301
44	30	10	15.18153	1.307831
44	20	5	12.39164	0.441073
44	55	8	10.37779	1.768849

44	53	9	10.4962	1.70806
44	63	12	11.9419	2.688448
44	41	9	13.0984	1.728892
44	58	8	9.974875	1.813991
44	43	5	10.13632	1.334555
44	63	15	12.07351	2.575238
44	42	7	11.49645	1.684192
44	60	14	12.75242	2.627198
45	45	14	13.69115	1.809592
45	20	5	12.26814	0.419799
45	42	12	14.04156	1.858421
45	54	6	10.32553	1.745458
45	53	14	13.03322	2.185054
45	50	7	11.25765	1.752776
45	64	6	9.446463	2.038527
45	21	8	14.91974	0.582438
45	40	14	14.34111	1.606472
46	68	14	12.2476	2.746291
46	40	9	12.79264	1.567156
46	27	9	14.21232	0.908269
46	27	6	12.09237	0.906789
46	68	6	9.559118	2.254244
46	22	9	15.02856	0.547696
46	42	9	12.55244	1.638446
46	37	11	14.65738	1.597676
46	44	10	12.67548	1.727026
46	34	9	13.42552	1.318911
46	67	5	9.23751	2.130092
46	26	15	18.5354	1.22278
46	20	15	21.62668	1.18512
46	35	7	12.09154	1.438043
46	31	14	16.84958	1.518621
47	30	14	17.16504	1.488556
47	62	7	10.13553	2.027695
47	61	13	12.02681	2.382888
47	63	15	11.95026	2.413104
47	25	8	13.88331	0.869616
47	36	5	10.10661	1.076436
47	37	9	12.97657	1.41528
48	38	8	12.04364	1.423881
48	54	10	10.25119	1.685915
48	51	15	12.81683	1.874286
48	34	9	13.13942	1.260478

48	31	12	16.01217	1.4254
48	28	5	10.77909	0.765782
48	70	14	11.75435	2.643663
48	32	8	12.80993	1.22626
48	69	12	10.82262	2.452198
48	62	14	12.29996	2.405064
48	46	14	13.7661	1.827221
48	33	14	16.04497	1.51634
48	54	5	9.812852	1.562862
48	41	9	12.32981	1.516878
49	36	9	12.76969	1.308354
49	54	10	10.16646	1.655066
49	70	8	10.33965	2.318742
49	25	5	11.15477	0.629005
49	62	11	10.44644	2.031831
49	68	12	10.67323	2.343961
49	52	12	12.26201	2.009385
49	45	8	11.29798	1.62088
49	35	6	10.99029	1.213728
49	68	8	10.23781	2.232599
49	34	15	14.83599	1.200811
49	51	12	12.39478	1.987469
49	44	12	13.02356	1.678202
50	57	13	12.08076	2.08245
50	66	12	10.7141	2.230385
50	64	15	11.81612	2.283865
50	41	8	11.52522	1.474642
50	23	10	14.75583	0.590483
50	38	15	14.3173	1.344779
50	35	7	11.70442	1.3149
50	59	13	11.84652	2.125762
50	27	5	10.83545	0.712591
50	54	6	10.56987	1.646147
50	67	5	9.764009	2.158972
50	61	12	11.10988	2.116363
50	64	8	10.18066	2.021324
50	29	9	13.34983	0.962322
50	31	15	15.61713	1.156215
50	50	5	10.09787	1.390735
50	32	15	15.31462	1.168976
50	58	9	10.11203	1.717573
50	35	14	15.13624	1.437148
50	61	5	9.693022	1.818363

50	48	9	10.62737	1.482784
50	68	15	11.49857	2.363516
51	50	6	10.84224	1.529909
51	28	9	13.32865	0.905951
51	29	6	11.53745	0.993745
51	21	12	17.6525	0.847142
51	33	8	12.18648	1.159781
51	36	12	14.25083	1.363573
51	46	7	11.06366	1.601091
51	54	13	12.37412	2.039386
51	59	10	10.18579	1.755068
51	47	10	10.90199	1.414416
51	51	6	10.79881	1.561667
51	54	7	10.75716	1.634543
51	64	5	9.910272	1.992944
51	67	7	10.48959	2.266176
51	70	9	10.30988	2.184924
51	40	10	12.50391	1.333201
51	22	6	12.50448	0.684394
51	35	9	12.57067	1.205335
52	43	10	11.61625	1.317851
52	20	12	17.71526	0.762584
52	29	13	16.22981	1.262959
52	67	5	10.02924	2.178392
52	50	13	12.8754	1.945026
52	69	10	10.31538	2.089864
53	28	15	16.80643	1.119842
53	34	7	11.54982	1.214287
53	52	15	13.16262	1.902109
53	26	9	13.29559	0.801045
53	52	8	10.57957	1.553245
53	39	13	13.88185	1.45608
53	55	5	10.09191	1.531324
53	52	11	10.82895	1.61451
54	26	12	15.53155	0.964106
54	55	14	12.4826	1.958997
54	53	12	11.54894	1.785315
54	22	11	15.12897	0.557232
54	28	9	12.97457	0.889282
54	32	6	11.26882	1.128761
54	45	5	10.39321	1.286647
54	33	11	13.6743	1.054426
55	21	13	17.94781	0.873686

55	66	12	10.53712	1.964313
55	53	14	12.67194	1.937841
55	45	11	11.47276	1.397597
55	23	5	11.21003	0.598971
55	42	12	12.71479	1.452024
55	40	15	14.4619	1.483336
55	40	10	11.86895	1.206926
55	29	13	15.60374	1.123678
55	30	12	14.74184	1.044431
55	44	13	13.31277	1.66387
55	68	6	10.91071	2.397596
55	61	13	11.02826	1.893454
56	61	10	10.58062	1.843989
56	65	5	10.61031	2.112998
56	29	7	11.78226	0.985181
56	60	14	11.58254	1.883997
56	22	12	15.91672	0.664982
56	41	9	11.41451	1.305875
56	53	9	10.48995	1.660786
56	23	11	14.56892	0.587718
56	55	6	11.19012	1.809651
56	44	11	11.53644	1.349588
56	69	10	10.57253	2.123922
56	23	6	12.07528	0.793006
56	53	15	12.97918	1.859324
56	60	12	10.52512	1.83435
56	41	15	14.30229	1.511017
56	35	10	12.54059	1.111386
56	51	12	11.57315	1.670523
56	59	12	10.60899	1.808162
56	51	5	10.46515	1.415702
57	56	14	12.07828	1.903246
57	36	5	10.38269	1.103766
57	62	14	11.20835	1.847951
57	67	12	10.56747	1.937684
57	59	15	12.23731	1.974071
57	59	14	11.63705	1.863897
57	55	9	10.60885	1.735444
57	67	10	10.61248	2.072672
57	51	8	10.80837	1.60785
57	26	5	10.90097	0.756399
57	57	14	11.9312	1.89013
57	62	15	11.82274	1.993774

57	46	15	13.68021	1.691731
58	66	8	10.93586	2.178859
58	36	5	10.43379	1.123785
58	69	11	10.69384	2.06794
58	22	15	18.80034	0.943205
58	33	6	11.07822	1.162181
58	32	8	11.71206	1.02243
58	69	5	10.95723	2.399625
58	46	10	11.06315	1.454635
58	21	5	11.4494	0.598745
58	56	10	10.58552	1.752119
58	59	15	12.14029	1.933982
58	51	10	10.66724	1.618564
58	22	13	16.7844	0.787742
59	65	14	10.60177	1.771126
59	69	9	10.90258	2.215243
59	61	6	11.4334	2.128598
59	62	6	11.41677	2.179655
59	69	10	10.80385	2.152456
59	46	7	10.74209	1.490365
59	38	11	12.22747	1.128548
59	50	10	10.8055	1.616182
60	24	8	12.35919	0.766224
60	53	5	10.84282	1.592054
60	40	13	13.33841	1.401425
60	28	15	15.84343	1.009958
60	39	10	11.73919	1.194761
60	48	15	13.35411	1.727616
60	34	13	13.88575	1.115152
60	32	7	11.29364	1.070554
60	46	12	11.92469	1.535724

Table S7: 4 sets of conditions with attractive results in the predicted dataset

Discharge Power (W)	Gas Flow (sccm)	Catalyst Dose (mg)	CO_2 Conversion Ratio (%)	Energy Efficiency (%)
16	45	11	18.04729	6.867429
17	43	10	19.44441	6.521779
18	40	10	20.45573	5.987919
21	46	10	19.89744	6.116918

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