Supplemental Materials

Accelerate global sensitivity analysis using Artificial Neural Network algorithm: Case studies for combustion kinetic model

Shuang Li[a,b], Bin Yang[b,*], Fei Qi [a,c]

[a] *National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui, 230029, P. R. China*

[b] *Center for Combustion Energy, Department of Thermal Engineering, Tsinghua University, Beijing, 100084, P. R. China*

[c] *Key Laboratory for Power Machinery and Engineering of M. O. E., Shanghai Jiao Tong University, Shanghai 200240, P. R. China*

*Corresponding author

E-mail: byang@tsinghua.edu.cn (Bin Yang).

Table S1

Parameter values of ANN-HDMR in different cases.

Original Sample Size	Number of hidden layer nodes	Maximum number of iteration	Mean square error	Minimum gradient
Sobol' g-function scenario 1				
1024	16	150	1.00E-08	1.00E-10
2048	32	150	1.00E-08	1.00E-10
4096	32	150	1.00E-08	1.00E-10
8192	48	150	1.00E-08	1.00E-10
Sobol' g-function scenario 2				
256	16	100	1.00E-10	1.00E-10
512	16	100	1.00E-10	1.00E-10
1024	16	100	1.00E-10	1.00E-10
Master equation kinetic model				
50	8	100	1.00E-08	1.00E-10
100	16	100	1.00E-08	1.00E-10
200	16	100	1.00E-08	1.00E-10
400	32	100	1.00E-08	1.00E-10
800	32	100	1.00E-08	1.00E-10
1600	32	100	1.00E-08	1.00E-10
3200	32	100	1.00E-08	1.00E-10
6400	32	100	1.00E-08	1.00E-10
12800	32	100	1.00E-08	1.00E-10
Premixed H_2/O_2 ignition model				
512	16	150	1.00E-08	1.00E-10
1024	32	150	1.00E-08	1.00E-10
2048	32	150	1.00E-08	1.00E-10

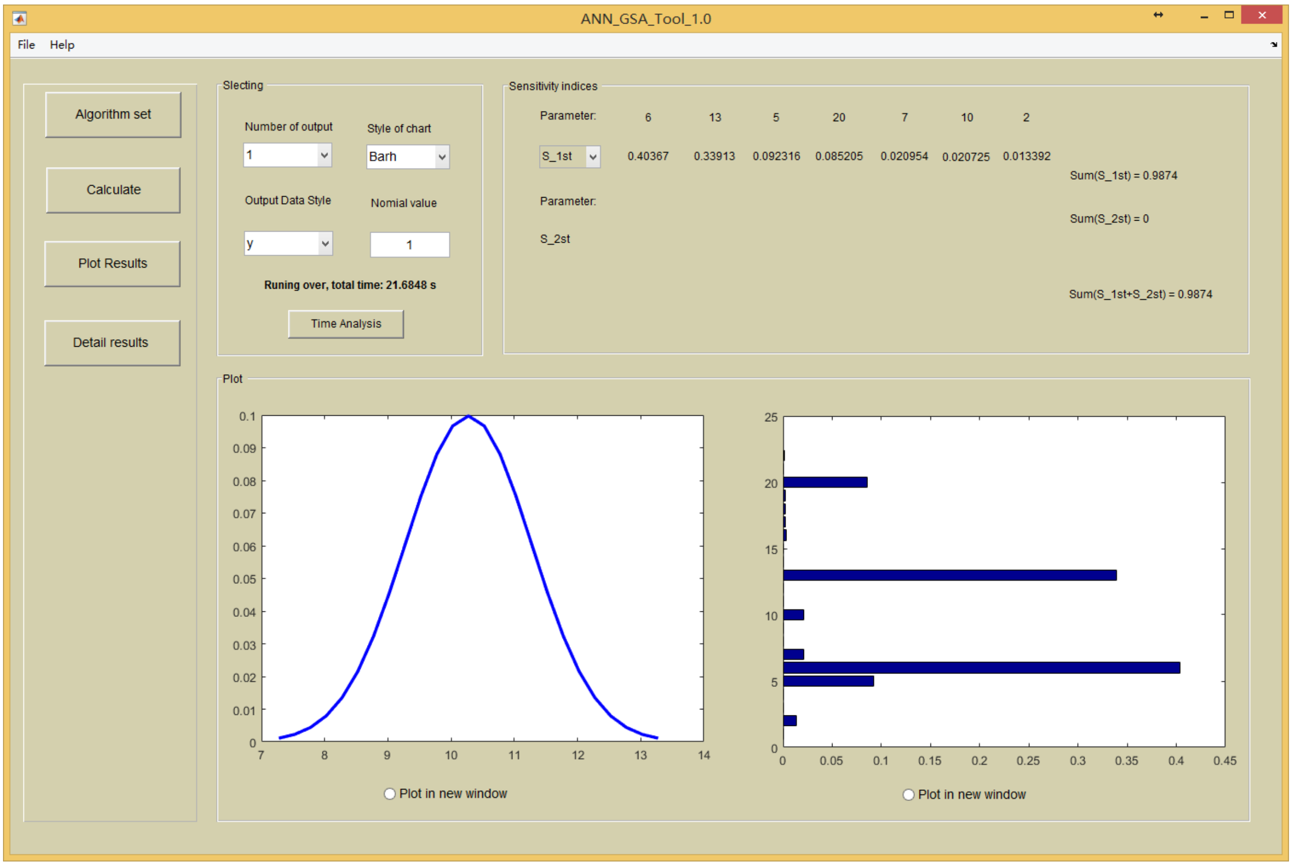


Fig. S1. A screenshot of the main interface of ANN_GSA_Tool.

Global sensitivity analysis was conducted for the case of master equation kinetic model under nine conditions which cover the temperature and pressure ranges in the study [72].

Condition 1: T = 800 K, P = 0.001 atm

Condition 2: T = 800 K, P = 1 atm

Condition 3: T = 800 K, P = high pressure limit (HPL)

Condition 4: T = 1400 K, P = 0.001 atm

Condition 5: T = 1400 K, P = 1 atm

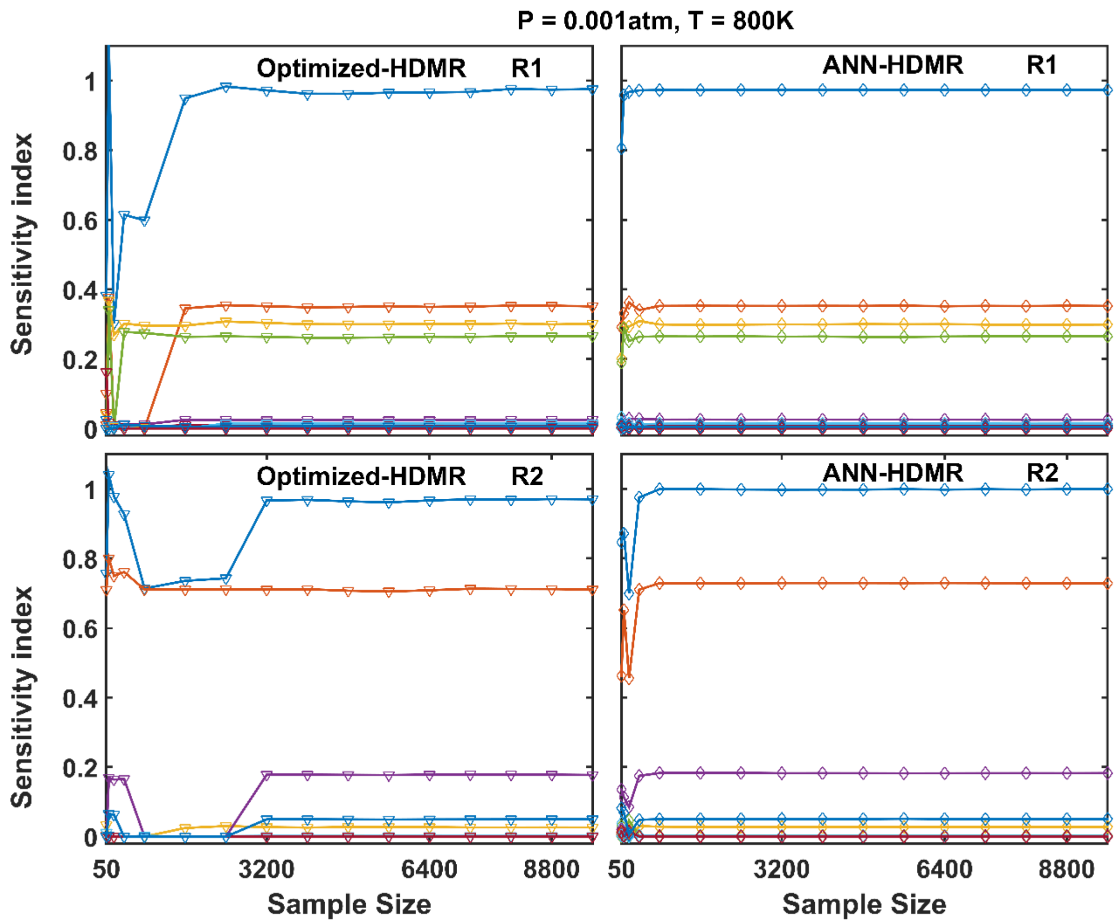
Condition 6: T = 1400 K, P = HPL

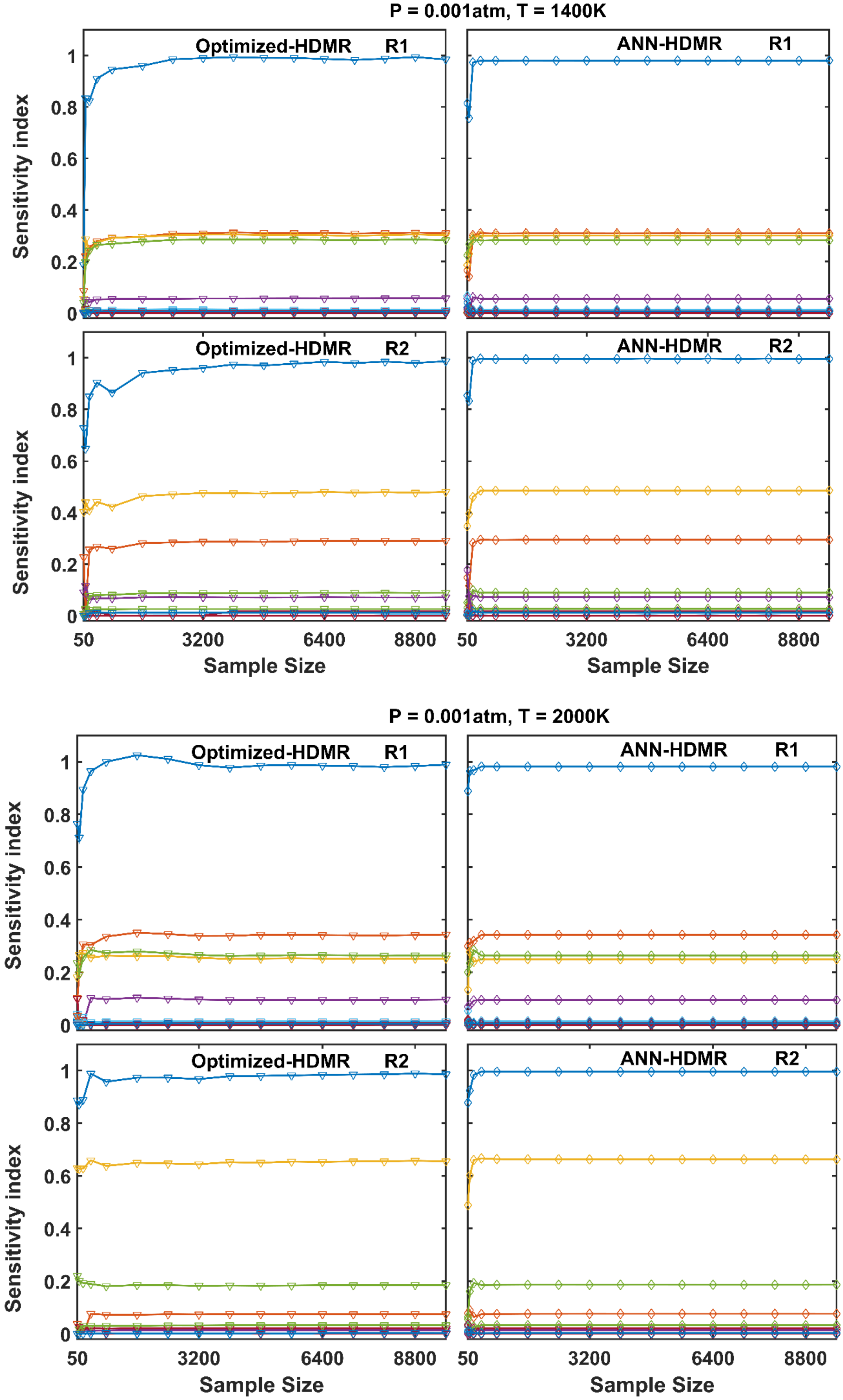
Condition 7: T = 2000 K, P = 0.001 atm

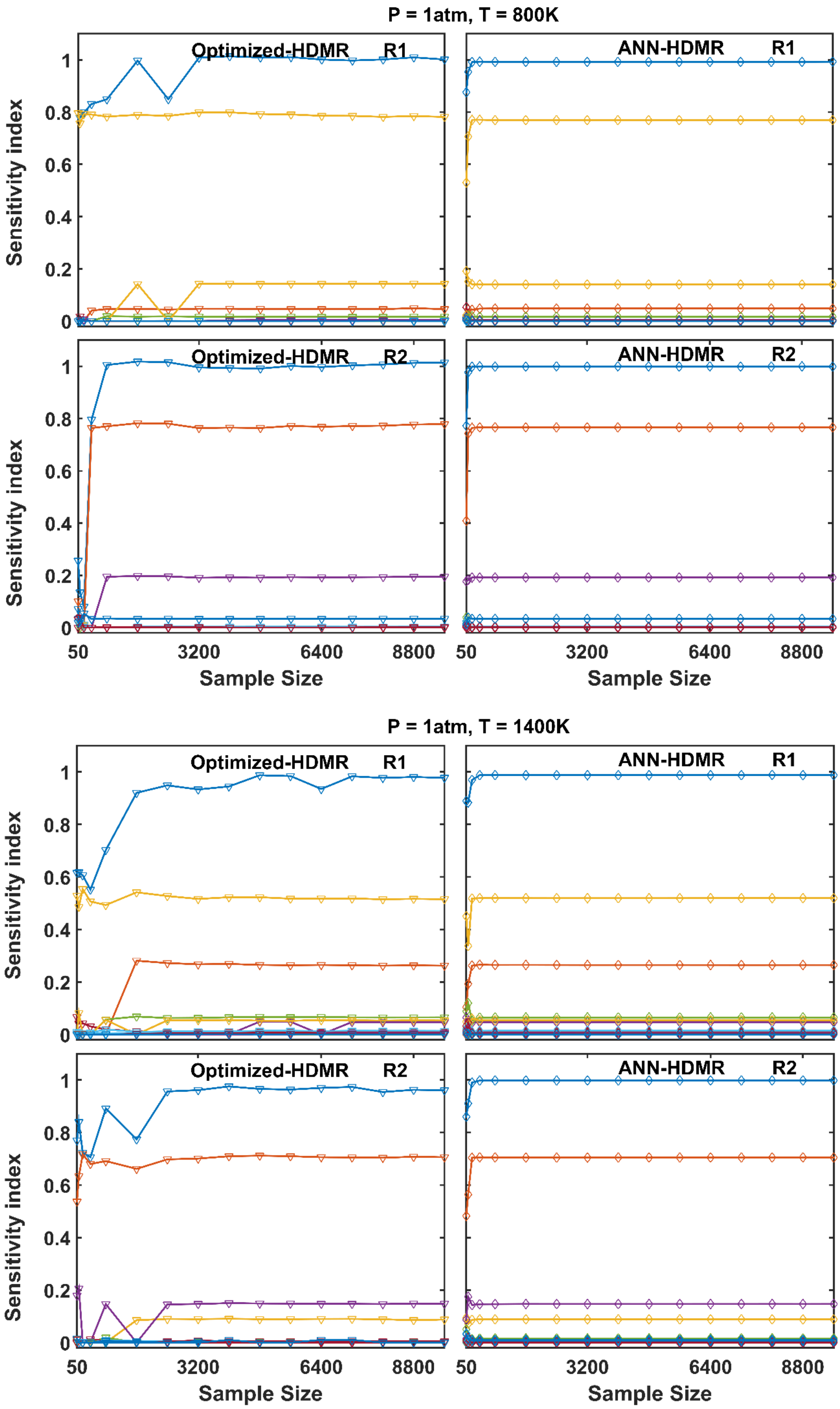
Condition 8: T = 2000 K, P = 1 atm

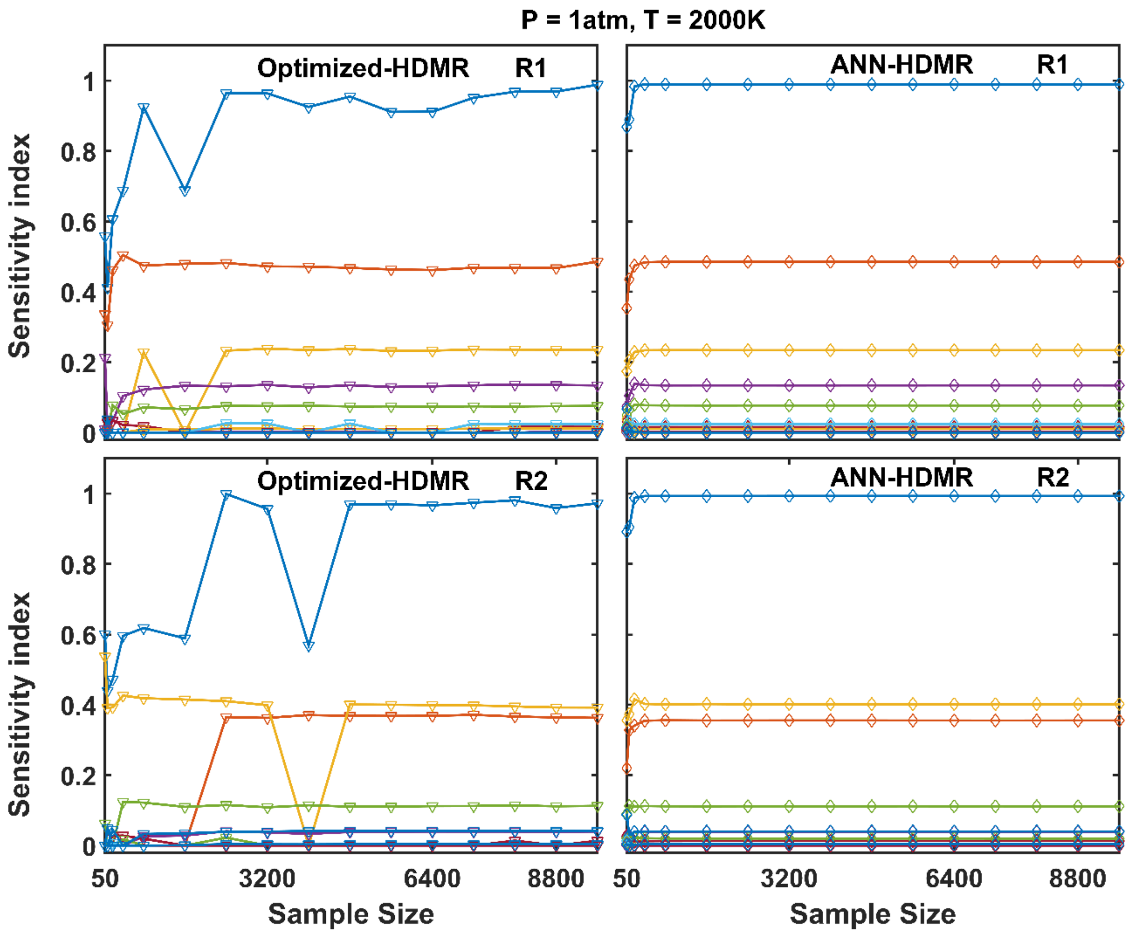
Condition 9: T = 2000 K, P = HPL

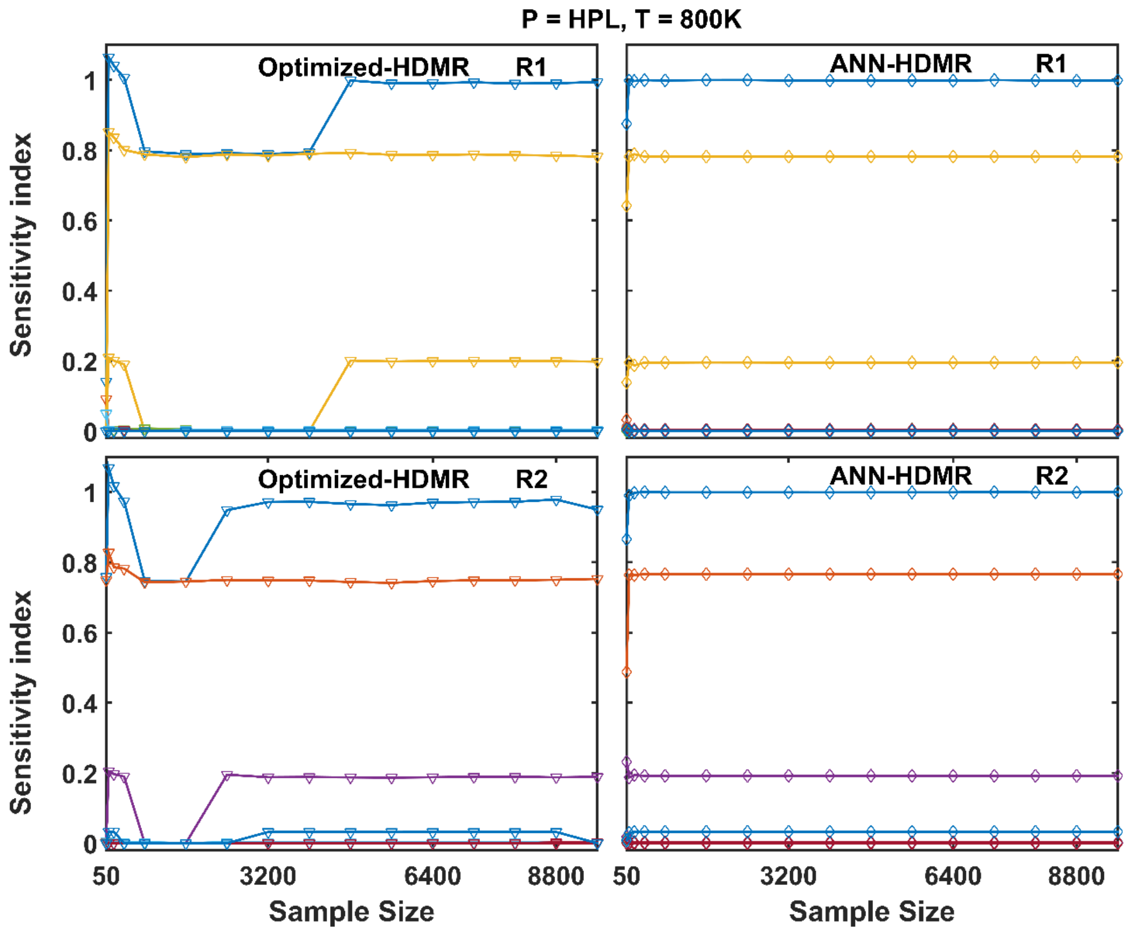
Fig. S2. Shows the first order sensitivity indices of the twenty-two parameters and the sum of the first order sensitivity indices of R1 and R2 versus the original sample sizes using Optimized-HDMR and ANN-HDMR.

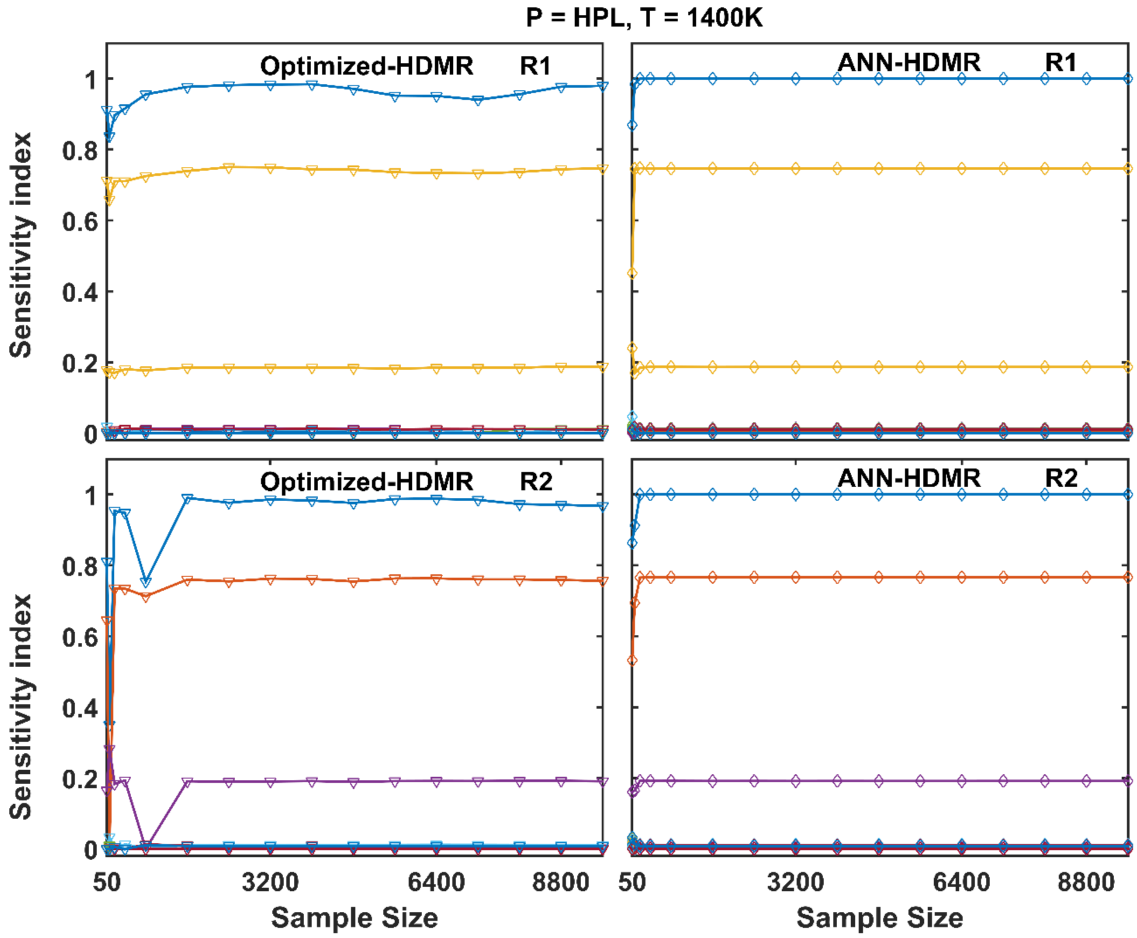



P = 0.001atm, T = 1400K
Optimized-HDMR R1
ANN-HDMR R1
Optimized-HDMR R2
ANN-HDMR R2
Sensitivity index
0
0.2
0.4
0.6
0.8
1
50
3200
6400
8800
Sample Size
P = 0.001atm, T = 2000K
Optimized-HDMR R1
ANN-HDMR R1
Optimized-HDMR R2
ANN-HDMR R2
Sensitivity index
Sample Size


P = 1atm, T = 800K
Optimized-HDMR R1
ANN-HDMR R1
Optimized-HDMR R2
ANN-HDMR R2
Sensitivity index
Sample Size
P = 1atm, T = 1400K
Optimized-HDMR R1
ANN-HDMR R1
Optimized-HDMR R2
ANN-HDMR R2
Sensitivity index
Sample Size


P = 1atm, T = 2000K
Optimized-HDMR R1
ANN-HDMR R1
Optimized-HDMR R2
ANN-HDMR R2
Sensitivity index
Sample Size
0
0.2
0.4
0.6
0.8
1
50
3200
6400
8800


P = HPL, T = 800K
Optimized-HDMR R1
ANN-HDMR R1
Optimized-HDMR R2
ANN-HDMR R2
Sensitivity index
Sample Size
0
0.2
0.4
0.6
0.8
1
50
3200
6400
8800


P = HPL, T = 1400K
Optimized-HDMR R1
ANN-HDMR R1
Optimized-HDMR R2
ANN-HDMR R2
Sensitivity index
Sample Size
0
0.2
0.4
0.6
0.8
1
50
3200
6400
8800

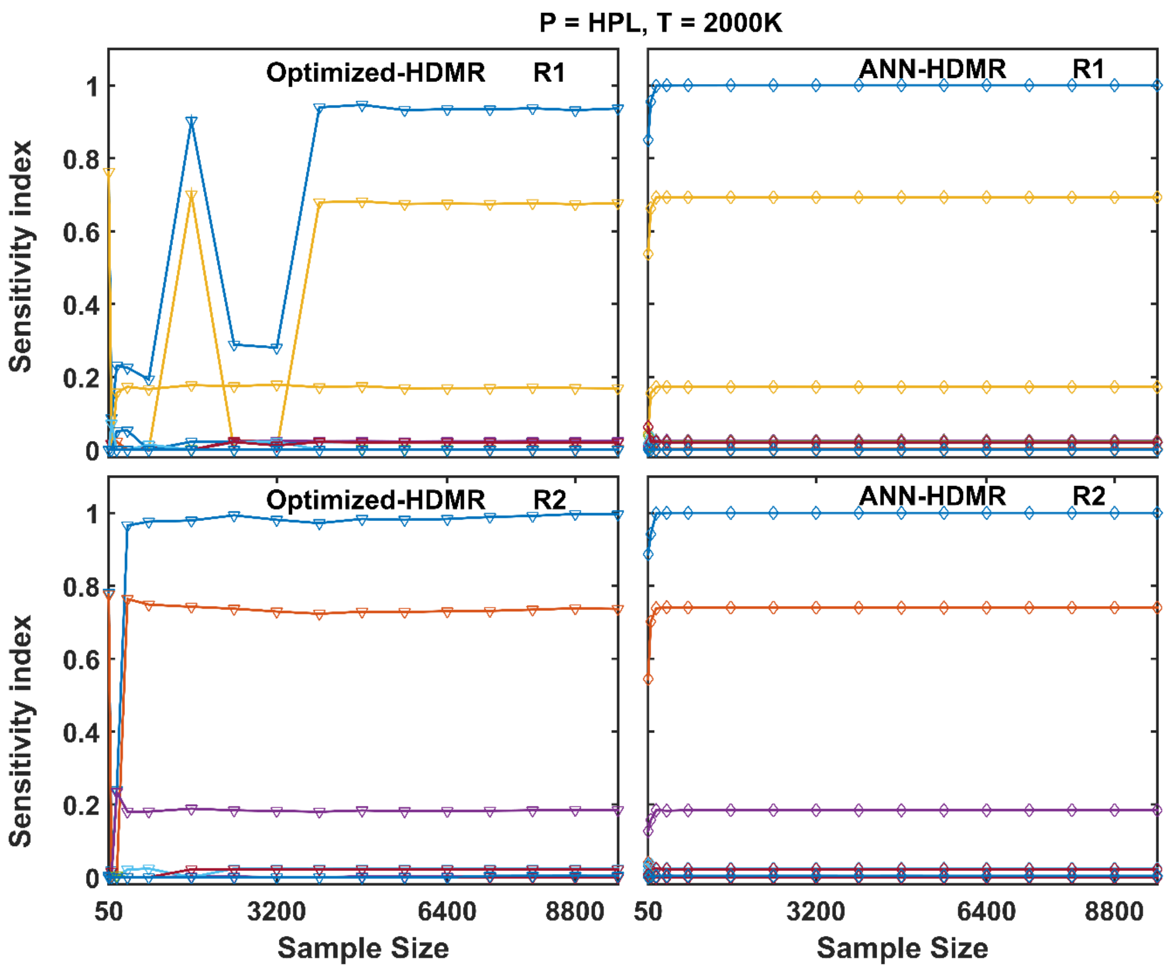

P = HPL, T = 2000K
Optimized-HDMR R1
ANN-HDMR R1
Optimized-HDMR R2
ANN-HDMR R2
Sensitivity index
Sample Size
0
0.2
0.4
0.6
0.8
1
50
3200
6400
8800

Fig. S2. The first order sensitivity indices of the twenty-two parameters and the sum of the first order sensitivity indices of R1 and R2 versus the original sample sizes using Optimized-HDMR and ANN-HDMR under P = 0.001 atm, 1 atm, high pressure limit (HPL), and T = 800 K, 1400 K, 2000 K.

Global sensitivity analysis was conducted for the ignition delay time of H_2/O_2 system under other two conditions which have been studied in the [74].

Condition 1: T = 1000 K, P = 1.07 bar

Condition 2: T = 1000 K, P = 5.62 bar

Fig. S3. Illustrates the important first and second order Sensitivity indices, and the sum of first and second order Sensitivity indices for the ignition delay time of H_2/O_2 system using Optimized-HDMR and ANN-HDMR.

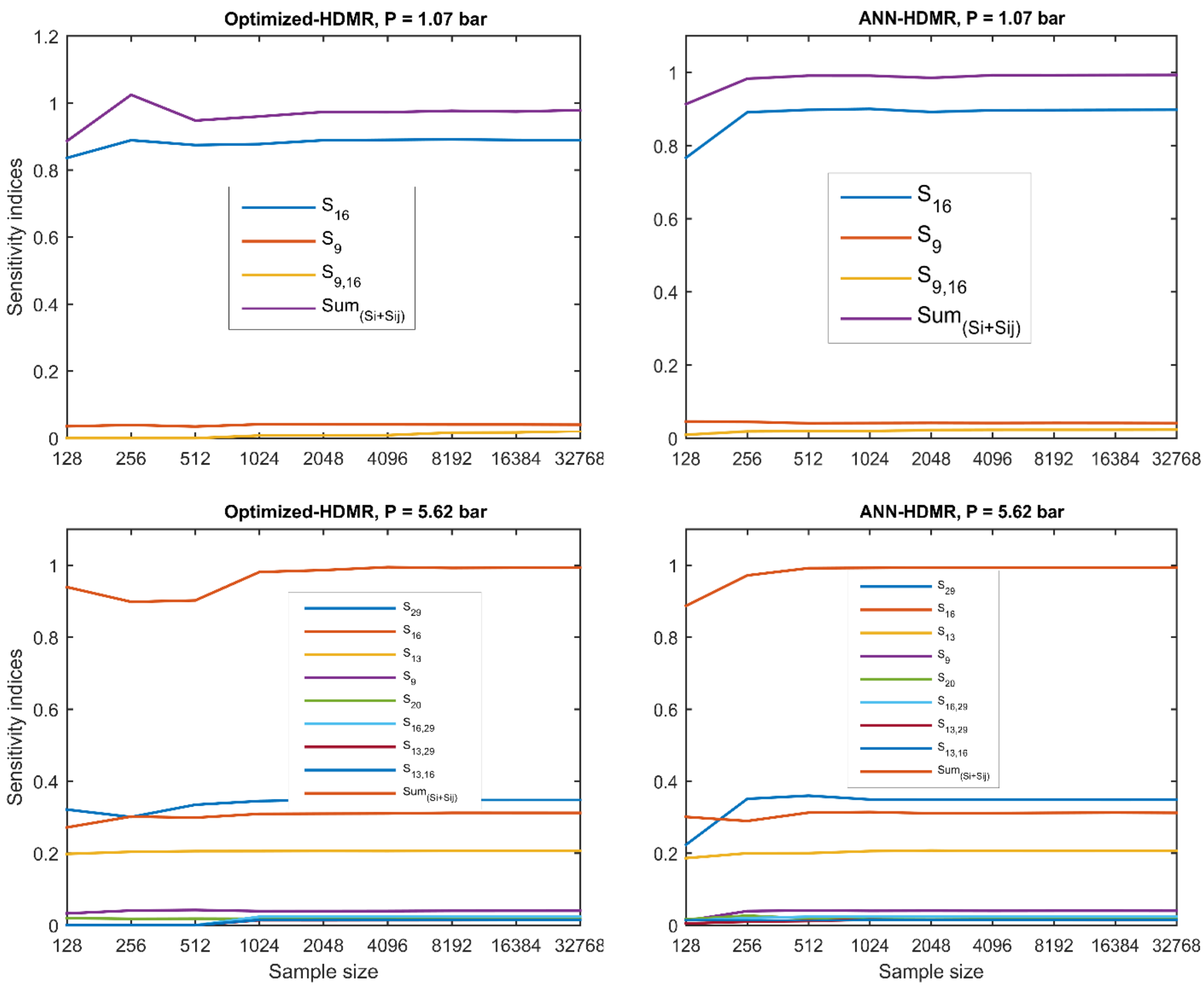


Fig. S3. Important first and second order Sensitivity indices, and the sum of first and second order Sensitivity indices for the ignition delay time of H_2/O_2 system using Optimized-HDMR and ANN-HDMR under (1) P = 1.07 bar, T = 1000 K, (2) P = 5.62 bar, T = 1000 K and stoichiometric mixtures of H_2 and O_2.

Table S2
The reactions and the uncertainty factors (UFs) of methanol combustion kinetic model.

ID	Reaction	UF
1	$H + O_2 <=> O + OH$	1.26
2	$O + H_2 <=> H + OH$	1.58
3	$H_2 + OH <=> H_2O + H$	2
4	$O + H_2O <=> OH + OH$	2.5
5	$H_2 + M <=> H + H + M$	3
6	$H_2 + AR <=> H + H + AR$	3
7	$O + O + M <=> O_2 + M$	2
8	$O + O + AR <=> O_2 + AR$	2
9	$O + H + M <=> OH + M$	5
10	$H + OH + M <=> H_2O + M$	2
11	$H + O_2$ (+ M) <=> HO_2 (+ M) (k∞)	3.16
12	$H + O_2$ (+ M) <=> HO_2 (+ M) (k0)	3.16
13	$HO_2 + H <=> H_2 + O_2$	2
14	$HO_2 + H <=> OH + OH$	2
15	$HO_2 + O <=> O_2 + OH$	3.16
16	$HO_2 + OH <=> H_2O + O_2$	3.16
17	$HO_2 + HO_2 <=> H_2O_2 + O_2$	5
18	$HO_2 + HO_2 <=> H_2O_2 + O_2$	5
19	H_2O_2 (+ M) <=> OH + OH (+ M) (k∞)	3.16
20	H_2O_2 (+ M) <=> OH + OH (+ M) (k0)	2
21	$H_2O_2 + H <=> H_2O + OH$	5
22	$H_2O_2 + H <=> HO_2 + H_2$	5
23	$H_2O_2 + O <=> OH + HO_2$	3
24	$H_2O_2 + OH <=> HO_2 + H_2O$	1.26
25	$H_2O_2 + OH <=> HO_2 + H_2O$	5
26	CO + O (+ M) <=> CO_2 (+ M) (k∞)	2.5
27	CO + O (+ M) <=> CO_2 (+ M) (k0)	2.5
28	$CO + O_2 <=> CO_2 + O$	2
29	$CO + HO_2 <=> CO_2 + OH$	5
30	$CO + OH <=> CO_2 + H$	3.16
31	$HCO + M <=> H + CO + M$	3.16
32	$HCO + O_2 <=> CO + HO_2$	5
33	$HCO + H <=> CO + H_2$	2
34	$HCO + O <=> CO + OH$	2
35	$HCO + OH <=> CO + H_2O$	3
36	$HCO + O <=> CO_2 + H$	3
37	$HCO + HO_2 <=> CO_2 + OH + H$	5
38	$HCO + HCO <=> H_2 + CO + CO$	2
39	$HCO + CH_3 <=> CO + CH_4$	5
40	$HCO + HCO <=> CH_2O + CO$	2
41	$CH_2O + M <=> HCO + H + M$	3.16
42	$CH_2O + M <=> CO + H_2 + M$	3.16
43	$CH_2O + H <=> HCO + H_2$	2

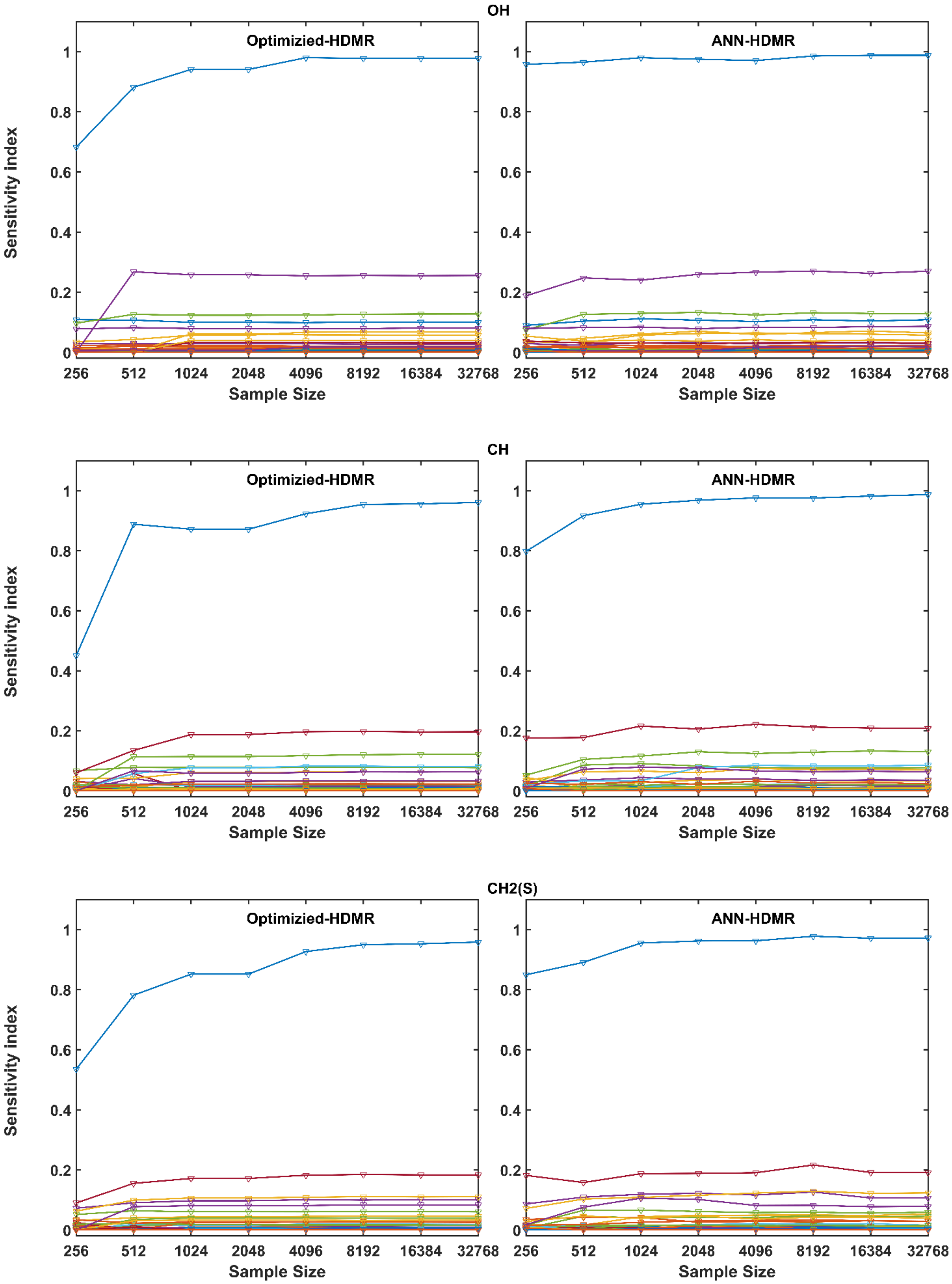
44	$CH_2O + O <=> HCO + OH$	2
45	$CH_2O + OH <=> HCO + H_2O$	5
46	$CH_2O + O_2 <=> HCO + HO_2$	3.16
47	$CH_2O + HO_2 <=> HCO + H_2O_2$	3.16
48	$CH_2O + CH_3 <=> HCO + CH_4$	2
49	$CH_3 + O <=> CH_2O + H$	1.58
50	$CH_3 + O_2 <=> CH_3O + O$	3.16
51	$CH_3 + O_2 <=> CH_2O + OH$	5
52	$CH_3 + HO_2 <=> CH_3O + OH$	3
53	$CH_3 + CH_3$ (+ M) <=> C_2H_6 (+ M) ($k\infty$)	2
54	$CH_3 + CH_3$ (+ M) <=> C_2H_6 (+ M) (k0)	2
55	CH_3 + H (+ M) <=> CH_4 (+ M)	3.16
56	CH_3 + H (+ M) <=> CH_4 (+ M)	3.16
57	$CH_4 + H <=> CH_3 + H_2$	1.58
58	$CH_4 + O <=> CH_3 + OH$	2
59	$CH_4 + OH <=> CH_3 + H_2O$	1.41
60	$CH_3 + HO_2 <=> CH_4 + O_2$	5
61	$CH_4 + HO_2 <=> CH_3 + H_2O_2$	5
62	$CH_2OH + M <=> CH_2O + H + M$	5
63	$CH_2OH + H <=> CH_2O + H_2$	2
64	$CH_2OH + H <=> CH_3 + OH$	2
65	$CH_2OH + O <=> CH_2O + OH$	2
66	$CH_2OH + OH <=> CH_2O + H_2O$	2
67	$CH_2OH + O_2 <=> CH_2O + HO_2$	5
68	$CH_2OH + O_2 <=> CH_2O + HO_2$	5
69	$CH_2OH + HO_2 <=> CH_2O + H_2O_2$	2
70	$CH_2OH + HCO <=> CH_3OH + CO$	5
71	$CH_2OH + HCO <=> CH_2O + CH_2O$	5
72	$2\ CH_2OH <=> CH_3OH + CH_2O$	2
73	$CH_2OH + CH_3O <=> CH_3OH + CH_2O$	2
74	$CH_3O + M <=> CH_2O + H + M$	2
75	$CH_3O + H <=> CH_3 + OH$	5
76	$CH_3O + O <=> CH_2O + OH$	5
77	$CH_3O + OH <=> CH_2O + H_2O$	5
78	$CH_3O + O_2 <=> CH_2O + HO_2$	5
79	$CH_3O + O_2 <=> CH_2O + HO_2$	5
80	$CH_3O + HO_2 <=> CH_2O + H_2O_2$	5
81	$CH_3O + CO <=> CH_3 + CO_2$	5
82	$CH_3O + HCO <=> CH_3OH + CO$	3
83	$2\ CH_3O <=> CH_3OH + CH_2O$	5
84	CH_3OH (+ M) <=> CH_3 + OH (+ M) ($k\infty$)	2
85	CH_3OH (+ M) <=> CH_3 + OH (+ M) (k0)	2
86	CH_3OH (+ M) <=> CH_2(S) + H_2O (+ M) ($k\infty$)	2
87	CH_3OH (+ M) <=> CH_2(S) + H_2O (+ M) (k0)	2
88	CH_3OH (+ M) <=> CH_2OH + H (+ M) ($k\infty$)	5
89	CH_3OH (+ M) <=> CH_2OH + H (+ M) (k0)	5

90	H + CH_3O (+ M) <=> CH_3OH (+ M) ($k\infty$)	3
91	H + CH_3O (+ M) <=> CH_3OH (+ M) (k0)	3
92	CH_2(S) + AR <=> CH_2 + AR	1.6
93	CH_2(S) + H <=> CH + H_2	3
94	CH_2(S) + OH <=> CH_2O + H	3
95	CH_2(S) + H_2 <=> CH_3 + H	3
96	CH_2(S) + CH_3 <=> H + C_2H_4	3
97	CH_2 + CH_2 <=> 2 H + C_2H_2	3
98	CH_2 + H_2 <=> H + CH_3	5
99	CH_2 + CH_3 <=> H + C_2H_4	3
100	CH_2 + H (+ M) <=> CH_3 (+ M) ($k\infty$)	3
101	CH_2 + H (+ M) <=> CH_3 (+ M) (k0)	3
102	CH_2 + OH <=> CH + H_2O	3
103	CH_2 + OH <=> CH_2O + H	3
104	CH_2 + CH_3OH <=> CH_2OH + CH_3	3
105	CH_2 + CH_3OH <=> CH_3O + CH_3	3
106	CH + H_2 <=> H + CH_2	3
107	CH + H_2 (+ M) <=> CH_3 (+ M) ($k\infty$)	2
108	CH + H_2 (+ M) <=> CH_3 (+ M) (k0)	2
109	CH + OH <=> H + HCO	3
110	CH + CH_2 <=> H + C_2H_2	6
111	CH_3OH + H <=> CH_2OH + H_2	4
112	CH_3OH + H <=> CH_3O + H_2	4
113	CH_3OH + O <=> CH_2OH + OH	5
114	CH_3OH + OH <=> CH_3O + H_2O	5
115	CH_3OH + OH <=> CH_2OH + H_2O	5
116	CH_3OH + O_2 <=> CH_2OH + HO_2	2
117	CH_3OH + HCO <=> CH_2OH + CH_2O	5
118	CH_3OH + HO_2 <=> CH_2OH + H_2O_2	2
119	CH_3OH + HO_2 <=> CH_3O + H_2O_2	2
120	CH_3OH + CH_3 <=> CH_2OH + CH_4	3
121	CH_3O + CH_3OH <=> CH_3OH + CH_2OH	5

Table S3

The simulation condition of methanol flame for global sensitivity analysis.

Equivalence ratio	Pressure	Flow rates (SLM)			
	(Torr)	CH_3O	O_2	Ar	Total
0.8	15	0.974	1.826	1.200	4.000


OH
Optimizied-HDMR
ANN-HDMR
CH
Optimizied-HDMR
ANN-HDMR
CH2(S)
Optimizied-HDMR
ANN-HDMR
Sensitivity index
Sample Size
0
0.2
0.4
0.6
0.8
1
256
512
1024
2048
4096
8192
16384
32768

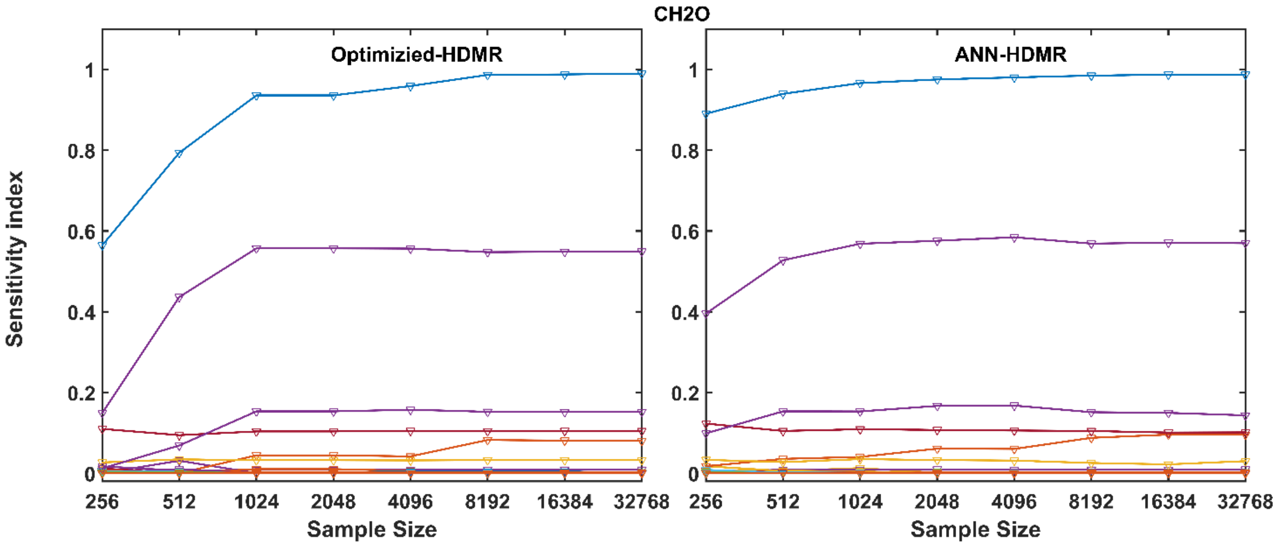


Fig. S4. The first order sensitivity indices and the sum of first and second order sensitivity indices of OH, CH, CH_2(S), CH_2O.