Supplemental Materials

Accelerate global sensitivity analysis using Artificial Neural Network algorithm:

Case studies for combustion kinetic model

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OH, CH, CH ₂ (S), CH ₂ O14

Table S1Parameter values of ANN-HDMR in different cases.

Sobol' g-function scenario 1					
Original Sample	Number of hidden	Maximum number	Mean square	Minimum	
Size	layer nodes	of iteration	error	gradient	
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 e	quation 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	

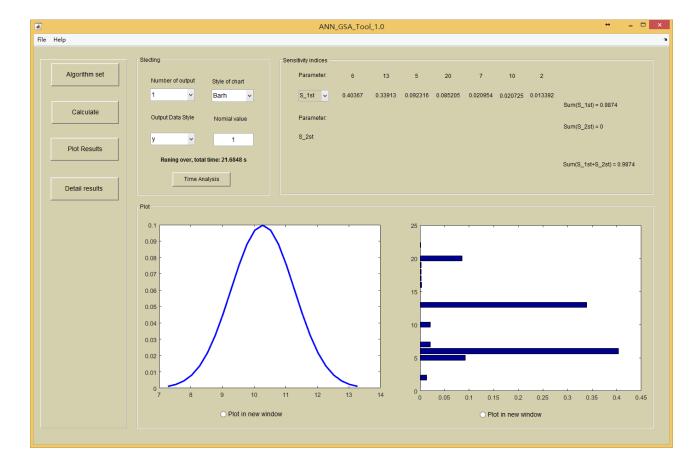


Fig. S1. A screenshot of the main interface of ANN_GSA_Tool.

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

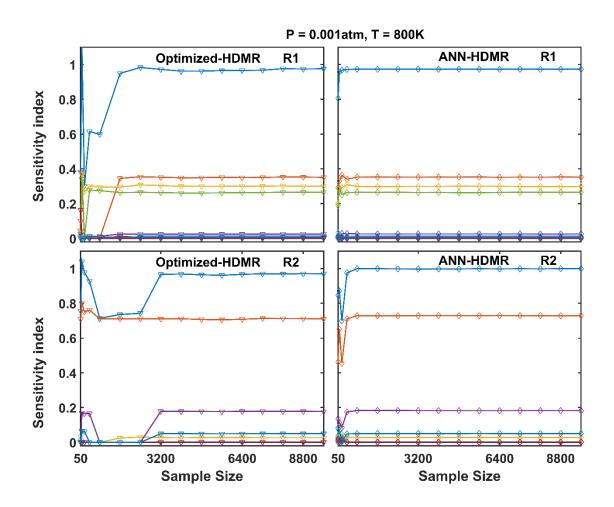
Condition 6: T = 1400 K, P = HPL

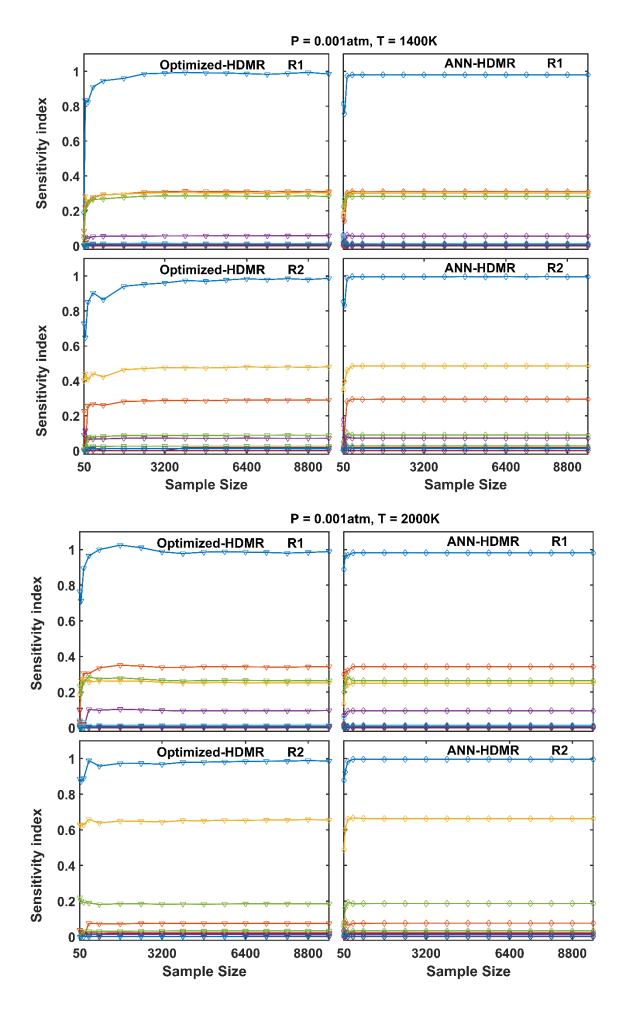
Condition 7: T = 2000 K, P = 0.001 atm

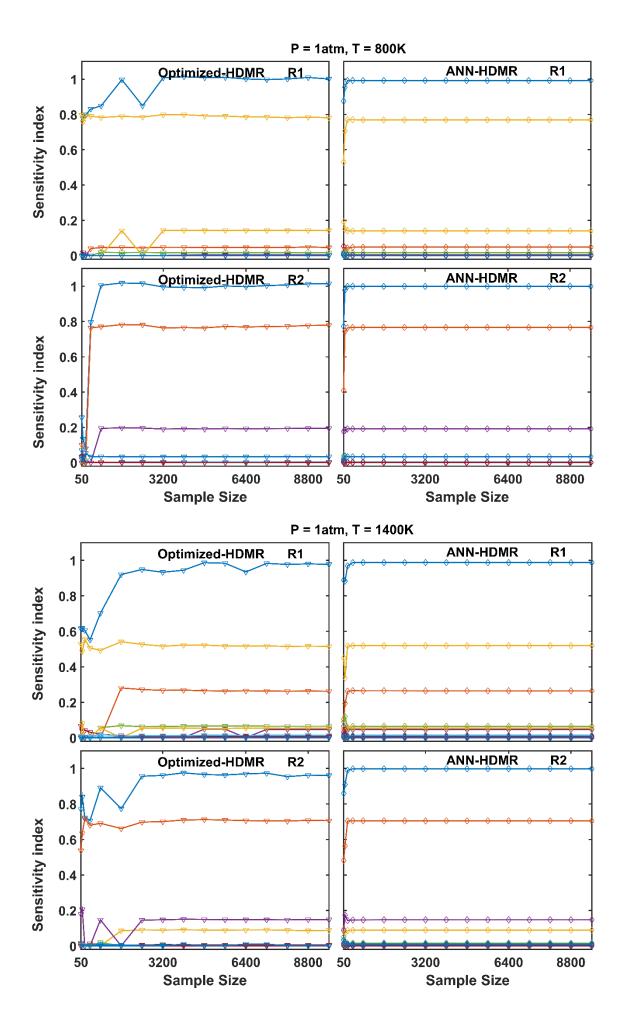
Condition 8: T = 2000 K, P = 1 atm

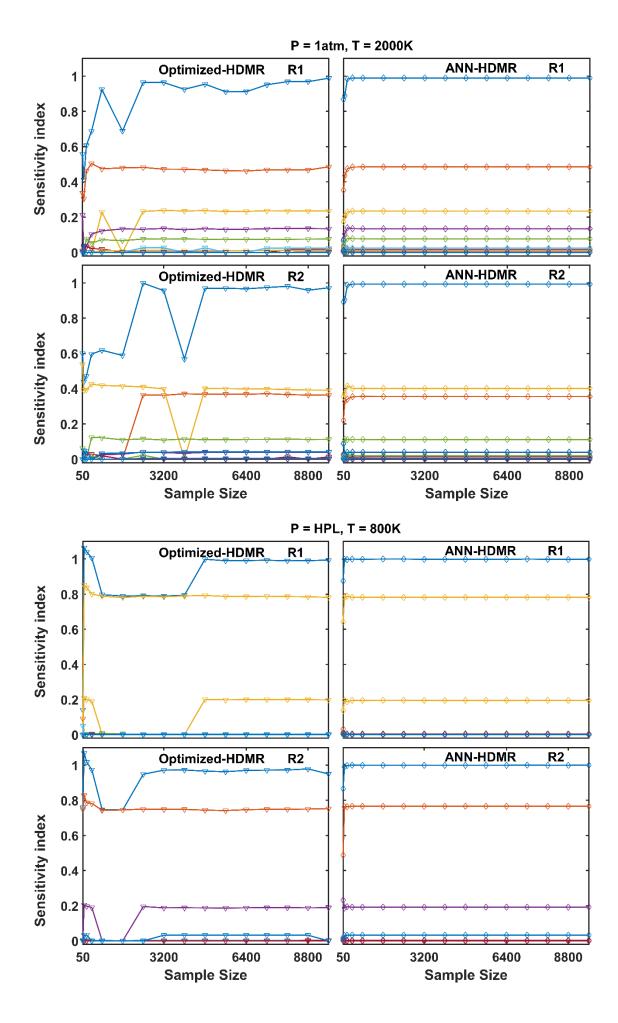
Condition 9: T = 2000 K, P = HPL

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.









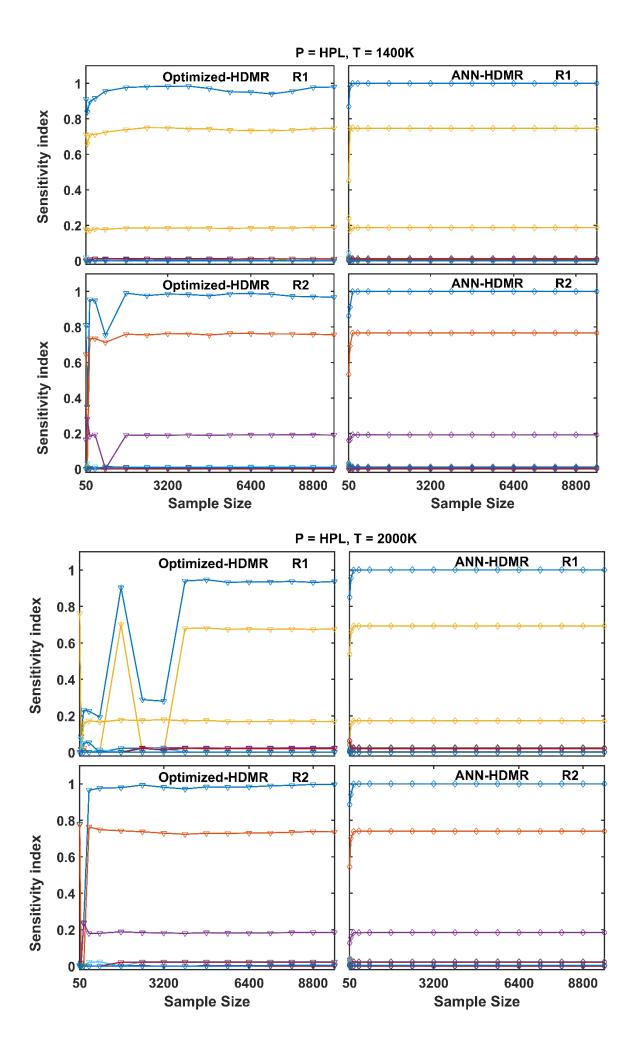


Fig. S2. The first order sensitivity indices of the twenty-two parameters and the sum of the first order sensitivity indices of R1 and R2 versus the original sample sizes using Optimized-HDMR and ANN-HDMR under P = 0.001 atm, 1 atm, high pressure limit (HPL), and T = 800 K, 1400 K, 2000 K.

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 H₂/O₂ system using Optimized-HDMR and ANN-HDMR.

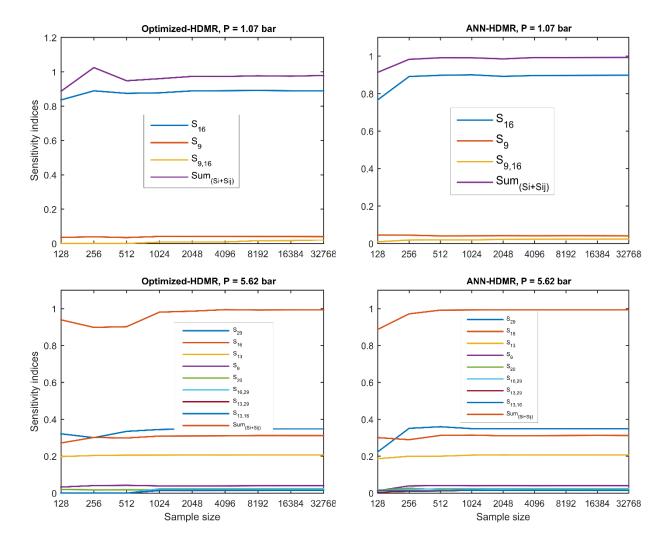


Fig. S3. Important first and second order Sensitivity indices, and the sum of first and second order Sensitivity indices for the ignition delay time of H_2/O_2 system using Optimized-HDMR and ANN-HDMR under (1) P = 1.07 bar, T = 1000 K, (2) P = 5.62 bar, T = 1000 K and stoichiometric mixtures of H_2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

 $\begin{tabular}{ll} \textbf{Table S2} \\ \textbf{The reactions and the uncertainty factors (UFs) of methanol combustion kinetic model.} \\ \end{tabular}$

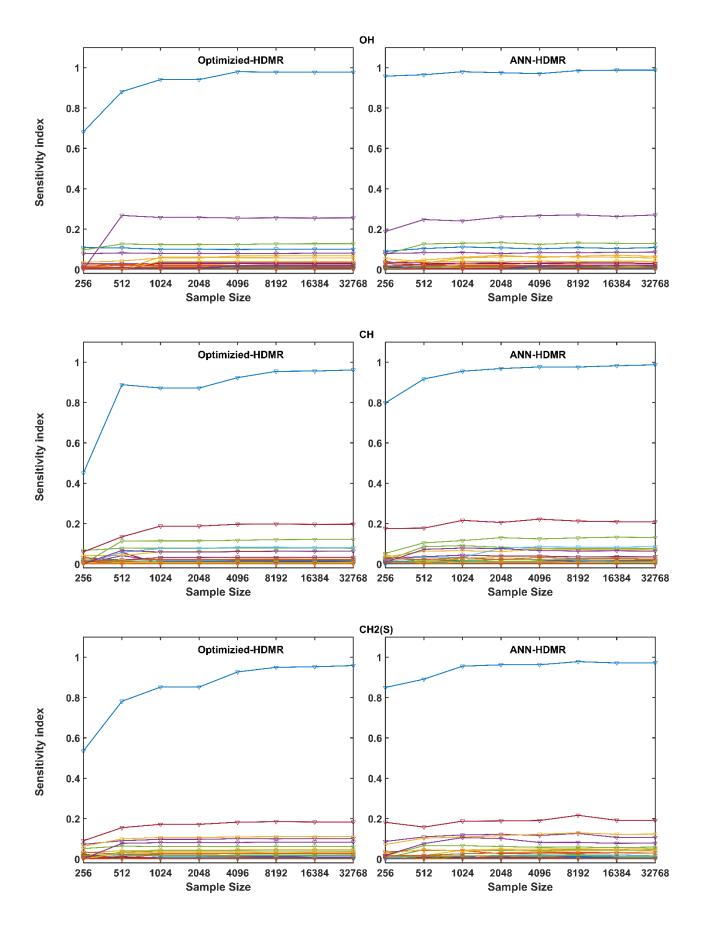
ID	Reaction	UF
1	$H + O_2 \ll O + OH$	1.26
2	$O + H_2 \ll H + OH$	1.58
3	$H_2 + OH <=> H_2O + H$	2
4	$O + H_2O \ll OH + OH$	2.5
5	$H_2 + M \le H + H + M$	3
6	$H_2 + AR <=> H + H + AR$	3
7	$O + O + M \ll O_2 + M$	2
8	$O + O + AR <=> O_2 + AR$	2
9	$O + H + M \ll OH + M$	5
10	$H + OH + M \Longleftrightarrow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

44	$CH_2O + O \iff HCO + OH$	2
45	$CH_2O + OH <=> HCO + H_2O$	5
46	$CH_2O + O_2 \le HCO + HO_2$	3.16
47	CH2O + HO2 <=> HCO + H2O2	3.16
48	$CH_2O + CH_3 \ll HCO + CH_4$	2
49	$CH_3 + O \ll CH_2O + H$	1.58
50	$CH_3 + O_2 <=> CH_3O + O$	3.16
51	$CH_3 + O_2 <=> CH_2O + OH$	5
52	$CH_3 + HO_2 \le CH_3O + OH$	3
53	$CH_3 + CH_3 (+ M) \le C_2H_6 (+ M) (k\infty)$	2
54	$CH_3 + CH_3 (+ M) \le C_2H_6 (+ M) (k0)$	2
55	$CH_3 + H (+ M) \le CH_4 (+ M)$	3.16
56	$CH_3 + H (+ M) \le CH_4 (+ M)$	3.16
57	$CH_4 + H \le CH_3 + H_2$	1.58
58	$CH_4 + O \ll CH_3 + OH$	2
59	$CH_4 + OH <=> CH_3 + H_2O$	1.41
60	$CH_3 + HO_2 \le CH_4 + O_2$	5
61	$CH_4 + HO_2 <=> CH_3 + H_2O_2$	5
62	$CH_2OH + M \leq > CH_2O + H + M$	5
63	$CH_2OH + H \leq > CH_2O + H_2$	2
64	$CH_2OH + H \leq > CH_3 + OH$	2
65	$CH_2OH + O \ll CH_2O + OH$	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	$CH_2OH + HCO \ll CH_3OH + CO$	5
71	$CH_2OH + HCO \ll CH_2O + CH_2O$	5
72	$2 \text{ CH}_2\text{OH} \Longleftrightarrow \text{CH}_3\text{OH} + \text{CH}_2\text{O}$	2
73	$CH_2OH + CH_3O \Longleftrightarrow CH_3OH + CH_2O$	2
74	$CH_3O + M \Longleftrightarrow CH_2O + H + M$	2
75	$CH_3O + H <=> CH_3 + OH$	5
76	$CH_3O + O \iff CH_2O + OH$	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	$CH_3O + HCO \Longleftrightarrow CH_3OH + CO$	3
83	$2 \text{ CH}_3\text{O} \iff \text{CH}_3\text{OH} + \text{CH}_2\text{O}$	5
84	$CH_3OH (+ M) \ll CH_3 + OH (+ M) (k\infty)$	2
85	$CH_3OH (+ M) <=> CH_3 + OH (+ M) (k0)$	2
86	$CH_3OH (+ M) \le CH_2(S) + H_2O (+ M) (k\infty)$	2
87	$CH_3OH (+ M) \le CH_2(S) + H_2O (+ M) (k0)$	2
88	$CH_3OH (+ M) \ll CH_2OH + H (+ M) (k\infty)$	5
89	$CH_3OH (+ M) <=> CH_2OH + H (+ M) (k0)$	5

$\begin{array}{llllllllllllllllllllllllllllllllllll$			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	90	$H + CH_3O (+ M) \ll CH_3OH (+ M) (k\infty)$	3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	91	$H + CH_3O (+ M) \le CH_3OH (+ M) (k0)$	3
$\begin{array}{llllllllllllllllllllllllllllllllllll$	92	$CH_2(S) + AR <=> CH_2 + AR$	1.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	93	$CH_2(S) + H <=> CH + H_2$	3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	94	$CH_2(S) + OH \ll CH_2O + H$	3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	95	$CH_2(S) + H_2 <=> CH_3 + H$	3
$\begin{array}{llll} 98 & CH_2 + H_2 <=> H + CH_3 \\ 99 & CH_2 + CH_3 <=> H + C_2H_4 \\ 31 \\ 100 & CH_2 + H (+ M) <=> CH_3 (+ M) (k\infty) \\ 31 \\ 101 & CH_2 + H (+ M) <=> CH_3 (+ M) (k0) \\ 31 \\ 102 & CH_2 + OH <=> CH + H_2O \\ 31 \\ 103 & CH_2 + OH <=> CH_2O + H \\ 31 \\ 104 & CH_2 + CH_3OH <=> CH_2OH + CH_3 \\ 31 \\ 105 & CH_2 + CH_3OH <=> CH_3O + CH_3 \\ 31 \\ 106 & CH + H_2 <=> H + CH_2 \\ 31 \\ 107 & CH + H_2 (+ M) <=> CH_3 (+ M) (k\infty) \\ 31 \\ 108 & CH + H_2 (+ M) <=> CH_3 (+ M) (k0) \\ 31 \\ 109 & CH + OH <=> H + HCO \\ 31 \\ 110 & CH + CH_2 <=> H + C_2H_2 \\ 41 \\ 111 & CH_3OH + H <=> CH_2OH + H_2 \\ 41 \\ 112 & CH_3OH + CH_2 <=> CH_2OH + CH_2 \\ 41 \\ 113 & CH_3OH + OH <=> CH_2OH + OH \\ 51 \\ 114 & CH_3OH + OH <=> CH_2OH + H_2O \\ 51 \\ 115 & CH_3OH + OH <=> CH_2OH + H_2O \\ 51 \\ 116 & CH_3OH + COH_2 <=> CH_2OH + CH_2O \\ 51 \\ 117 & CH_3OH + COH_2 <=> CH_2OH + CH_2O \\ 51 \\ 118 & CH_3OH + COH_2 <=> CH_2OH + CH_2O \\ 51 \\ 119 & CH_3OH + COH_2 <=> CH_2OH + CH_2O \\ 51 \\ 110 & CH_3OH + COH_2 <=> CH_2OH + CH_2O \\ 51 \\ 111 & CH_3OH + COH_2 <=> CH_2OH + CH_2O \\ 51 \\ 112 & CH_3OH + COH_2 <=> CH_2OH + CH_2O \\ 51 \\ 113 & CH_3OH + COH_2 <=> CH_2OH + CH_2O \\ 51 \\ 114 & CH_3OH + COH_2 <=> CH_2OH + CH_2O \\ 51 \\ 115 & CH_3OH + COH_2 <=> CH_2OH + CH_2O \\ 51 \\ 116 & CH_3OH + COH_2 <=> CH_2OH + CH_2O \\ 51 \\ 117 & CH_3OH + COH_2 <=> CH_2OH + CH_2O \\ 51 \\ 118 & CH_3OH + CH_3 <=> CH_2OH + CH_4 \\ 31 \\ 120 & CH_3OH + CH_3 <=> CH_2OH + CH_4 \\ 31 \\ 130 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 31 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 32 \\ 140 & CH_2 + CH_3OH + CH_4 \\ 33 \\ 140 & CH_2 + CH_3OH + CH_4$	96	$CH_2(S) + CH_3 <=> H + C_2H_4$	3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	97	$CH_2 + CH_2 \iff 2 H + C_2H_2$	3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	98	$CH_2 + H_2 <=> H + CH_3$	5
$\begin{array}{lllll} 101 & CH_2 + H (+ M) <=> CH_3 (+ M) (k0) & 3 \\ 102 & CH_2 + OH <=> CH + H_2O & 3 \\ 103 & CH_2 + OH <=> CH_2O + H & 3 \\ 104 & CH_2 + CH_3OH <=> CH_2OH + CH_3 & 3 \\ 105 & CH_2 + CH_3OH <=> CH_3O + CH_3 & 3 \\ 106 & CH + H_2 <=> H + CH_2 & 3 \\ 107 & CH + H_2 (+ M) <=> CH_3 (+ M) (k\infty) & 2 \\ 108 & CH + H_2 (+ M) <=> CH_3 (+ M) (k0) & 2 \\ 109 & CH + OH <=> H + HCO & 3 \\ 110 & CH + CH_2 <=> H + C_2H_2 & 6 \\ 111 & CH_3OH + H <=> CH_2OH + H_2 & 4 \\ 112 & CH_3OH + H <=> CH_2OH + OH & 5 \\ 114 & CH_3OH + OH <=> CH_2OH + OH & 5 \\ 115 & CH_3OH + OH <=> CH_2OH + H_2O & 5 \\ 115 & CH_3OH + OH <=> CH_2OH + H_2O & 5 \\ 116 & CH_3OH + OH <=> CH_2OH + HO_2 & 2 \\ 117 & CH_3OH + HC <=> CH_2OH + CH_2O & 5 \\ 118 & CH_3OH + OH <=> CH_2OH + CH_2O & 5 \\ 118 & CH_3OH + OH <=> CH_2OH + CH_2O & 5 \\ 118 & CH_3OH + HCO <=> CH_2OH + CH_2O & 5 \\ 118 & CH_3OH + HO_2 <=> CH_2OH + CH_2O & 5 \\ 118 & CH_3OH + HO_2 <=> CH_2OH + CH_2O & 2 \\ 119 & CH_3OH + CH_3 <=> CH_2OH + CH_4 & 3 \\ \end{array}$	99	$CH_2 + CH_3 \iff H + C_2H_4$	3
$\begin{array}{llllllllllllllllllllllllllllllllllll$	100	$CH_2 + H (+ M) <=> CH_3 (+ M) (k\infty)$	3
$\begin{array}{lllll} 103 & CH_2 + OH <=> CH_2O + H & 3 \\ 104 & CH_2 + CH_3OH <=> CH_2OH + CH_3 & 3 \\ 105 & CH_2 + CH_3OH <=> CH_3O + CH_3 & 3 \\ 106 & CH + H_2 <=> H + CH_2 & 3 \\ 107 & CH + H_2 (+ M) <=> CH_3 (+ M) (k\infty) & 2 \\ 108 & CH + H_2 (+ M) <=> CH_3 (+ M) (k0) & 2 \\ 109 & CH + OH <=> H + HCO & 3 \\ 110 & CH + CH_2 <=> H + C_2H_2 & 6 \\ 111 & CH_3OH + H <=> CH_2OH + H_2 & 4 \\ 112 & CH_3OH + H <=> CH_3O + H_2 & 4 \\ 113 & CH_3OH + OH <=> CH_2OH + OH & 5 \\ 114 & CH_3OH + OH <=> CH_2OH + H_2O & 5 \\ 115 & CH_3OH + OH <=> CH_2OH + H_2O & 5 \\ 116 & CH_3OH + OH <=> CH_2OH + H_2O & 5 \\ 116 & CH_3OH + OH <=> CH_2OH + H_2O & 5 \\ 116 & CH_3OH + OH <=> CH_2OH + CH_2O & 5 \\ 117 & CH_3OH + HCO <=> CH_2OH + CH_2O & 5 \\ 118 & CH_3OH + HO_2 <=> CH_2OH + CH_2O & 5 \\ 118 & CH_3OH + HO_2 <=> CH_2OH + CH_2O & 2 \\ 119 & CH_3OH + HO_2 <=> CH_2OH + H_2O_2 & 2 \\ 119 & CH_3OH + CH_3 <=> CH_2OH + CH_4 & 3 \\ \end{array}$	101	$CH_2 + H (+ M) <=> CH_3 (+ M) (k0)$	3
$\begin{array}{llll} 104 & CH_2 + CH_3OH <=> CH_2OH + CH_3 \\ 105 & CH_2 + CH_3OH <=> CH_3O + CH_3 \\ 106 & CH + H_2 <=> H + CH_2 \\ 107 & CH + H_2 (+ M) <=> CH_3 (+ M) (k\infty) \\ 108 & CH + H_2 (+ M) <=> CH_3 (+ M) (k0) \\ 109 & CH + OH <=> H + HCO \\ 110 & CH + CH_2 <=> H + C_2H_2 \\ 111 & CH_3OH + H <=> CH_2OH + H_2 \\ 112 & CH_3OH + H <=> CH_2OH + OH \\ 113 & CH_3OH + OH <=> CH_2OH + OH \\ 114 & CH_3OH + OH <=> CH_2OH + OH \\ 15 & CH_3OH + OH <=> CH_2OH + H_2O \\ 115 & CH_3OH + OH <=> CH_2OH + H_2O \\ 116 & CH_3OH + OH <=> CH_2OH + HO_2 \\ 117 & CH_3OH + HCO <=> CH_2OH + CH_2O \\ 118 & CH_3OH + HCO <=> CH_2OH + CH_2O \\ 119 & CH_3OH + HO_2 <=> CH_2OH + CH_2O \\ 119 & CH_3OH + HO_2 <=> CH_2OH + CH_2O \\ 119 & CH_3OH + HO_2 <=> CH_2OH + CH_2O \\ 120 & CH_3OH + CH_3 <=> CH_2OH + CH_4 \\ 3 & 3 & 3 & 3 & 3 & 3 \\ 3 & 3 & 3 & 3$	102	$CH_2 + OH <=> CH + H_2O$	3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	103	$CH_2 + OH <=> CH_2O + H$	3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	104	$CH_2 + CH_3OH <=> CH_2OH + CH_3$	3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	105	$CH_2 + CH_3OH <=> CH_3O + CH_3$	3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	106	$CH + H_2 <=> H + CH_2$	3
$\begin{array}{llll} 109 & \text{CH} + \text{OH} <=> \text{H} + \text{HCO} & 3 \\ 110 & \text{CH} + \text{CH}_2 <=> \text{H} + \text{C}_2\text{H}_2 & 6 \\ 111 & \text{CH}_3\text{OH} + \text{H} <=> \text{CH}_2\text{OH} + \text{H}_2 & 4 \\ 112 & \text{CH}_3\text{OH} + \text{H} <=> \text{CH}_3\text{O} + \text{H}_2 & 4 \\ 113 & \text{CH}_3\text{OH} + \text{O} <=> \text{CH}_2\text{OH} + \text{OH} & 5 \\ 114 & \text{CH}_3\text{OH} + \text{OH} <=> \text{CH}_3\text{O} + \text{H}_2\text{O} & 5 \\ 115 & \text{CH}_3\text{OH} + \text{OH} <=> \text{CH}_2\text{OH} + \text{H}_2\text{O} & 5 \\ 116 & \text{CH}_3\text{OH} + \text{OH} <=> \text{CH}_2\text{OH} + \text{HO}_2 & 2 \\ 117 & \text{CH}_3\text{OH} + \text{HCO} <=> \text{CH}_2\text{OH} + \text{CH}_2\text{O} & 5 \\ 118 & \text{CH}_3\text{OH} + \text{HCO} <=> \text{CH}_2\text{OH} + \text{CH}_2\text{O} & 2 \\ 119 & \text{CH}_3\text{OH} + \text{HO}_2 <=> \text{CH}_2\text{OH} + \text{H}_2\text{O}_2 & 2 \\ 120 & \text{CH}_3\text{OH} + \text{CH}_3 <=> \text{CH}_2\text{OH} + \text{CH}_4 & 3 \\ \end{array}$	107	$CH + H_2 (+ M) <=> CH_3 (+ M) (k\infty)$	2
$\begin{array}{llll} 110 & CH + CH_2 <=> H + C_2H_2 & 6 \\ 111 & CH_3OH + H <=> CH_2OH + H_2 & 4 \\ 112 & CH_3OH + H <=> CH_3O + H_2 & 4 \\ 113 & CH_3OH + O <=> CH_2OH + OH & 5 \\ 114 & CH_3OH + OH <=> CH_3O + H_2O & 5 \\ 115 & CH_3OH + OH <=> CH_2OH + H_2O & 5 \\ 116 & CH_3OH + O_2 <=> CH_2OH + HO_2 & 2 \\ 117 & CH_3OH + HCO <=> CH_2OH + CH_2O & 5 \\ 118 & CH_3OH + HO_2 <=> CH_2OH + CH_2O & 5 \\ 119 & CH_3OH + HO_2 <=> CH_2OH + H_2O_2 & 2 \\ 119 & CH_3OH + HO_2 <=> CH_3OH + H_2O_2 & 2 \\ 120 & CH_3OH + CH_3 <=> CH_2OH + CH_4 & 3 \\ \end{array}$	108	$CH + H_2 (+ M) <=> CH_3 (+ M) (k0)$	2
$\begin{array}{llll} 111 & CH_3OH + H <=> CH_2OH + H_2 & 4 \\ 112 & CH_3OH + H <=> CH_3O + H_2 & 4 \\ 113 & CH_3OH + O <=> CH_2OH + OH & 5 \\ 114 & CH_3OH + OH <=> CH_3O + H_2O & 5 \\ 115 & CH_3OH + OH <=> CH_2OH + H_2O & 5 \\ 116 & CH_3OH + O_2 <=> CH_2OH + HO_2 & 2 \\ 117 & CH_3OH + HCO <=> CH_2OH + CH_2O & 5 \\ 118 & CH_3OH + HO_2 <=> CH_2OH + CH_2O & 5 \\ 119 & CH_3OH + HO_2 <=> CH_2OH + H_2O_2 & 2 \\ 119 & CH_3OH + HO_2 <=> CH_2OH + CH_2O & 2 \\ 120 & CH_3OH + CH_3 <=> CH_2OH + CH_4 & 3 \\ \end{array}$	109	$CH + OH \ll H + HCO$	3
$\begin{array}{llll} 112 & CH_3OH + H <=> CH_3O + H_2 & 4 \\ 113 & CH_3OH + O <=> CH_2OH + OH & 5 \\ 114 & CH_3OH + OH <=> CH_3O + H_2O & 5 \\ 115 & CH_3OH + OH <=> CH_2OH + H_2O & 5 \\ 116 & CH_3OH + O_2 <=> CH_2OH + HO_2 & 2 \\ 117 & CH_3OH + HCO <=> CH_2OH + CH_2O & 5 \\ 118 & CH_3OH + HO_2 <=> CH_2OH + H_2O_2 & 2 \\ 119 & CH_3OH + HO_2 <=> CH_2OH + H_2O_2 & 2 \\ 120 & CH_3OH + CH_3 <=> CH_2OH + CH_4 & 3 \\ \end{array}$	110	$CH + CH_2 \ll H + C_2H_2$	6
$\begin{array}{llll} 113 & CH_3OH + O <=> CH_2OH + OH & 5 \\ 114 & CH_3OH + OH <=> CH_3O + H_2O & 5 \\ 115 & CH_3OH + OH <=> CH_2OH + H_2O & 5 \\ 116 & CH_3OH + O_2 <=> CH_2OH + HO_2 & 2 \\ 117 & CH_3OH + HCO <=> CH_2OH + CH_2O & 5 \\ 118 & CH_3OH + HO_2 <=> CH_2OH + H_2O_2 & 2 \\ 119 & CH_3OH + HO_2 <=> CH_2OH + H_2O_2 & 2 \\ 120 & CH_3OH + CH_3 <=> CH_2OH + CH_4 & 3 \\ \end{array}$	111	$CH_3OH + H \Longleftrightarrow CH_2OH + H_2$	4
$\begin{array}{lll} 114 & CH_3OH + OH <=> CH_3O + H_2O & 5 \\ 115 & CH_3OH + OH <=> CH_2OH + H_2O & 5 \\ 116 & CH_3OH + O_2 <=> CH_2OH + HO_2 & 2 \\ 117 & CH_3OH + HCO <=> CH_2OH + CH_2O & 5 \\ 118 & CH_3OH + HO_2 <=> CH_2OH + H_2O_2 & 2 \\ 119 & CH_3OH + HO_2 <=> CH_3O + H_2O_2 & 2 \\ 120 & CH_3OH + CH_3 <=> CH_2OH + CH_4 & 3 \\ \end{array}$	112	$CH_3OH + H \le CH_3O + H_2$	4
$\begin{array}{lll} 115 & CH_3OH + OH <=> CH_2OH + H_2O & 5 \\ 116 & CH_3OH + O_2 <=> CH_2OH + HO_2 & 2 \\ 117 & CH_3OH + HCO <=> CH_2OH + CH_2O & 5 \\ 118 & CH_3OH + HO_2 <=> CH_2OH + H_2O_2 & 2 \\ 119 & CH_3OH + HO_2 <=> CH_3O + H_2O_2 & 2 \\ 120 & CH_3OH + CH_3 <=> CH_2OH + CH_4 & 3 \\ \end{array}$	113	$CH_3OH + O \iff CH_2OH + OH$	5
$ \begin{array}{llll} 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 \\ \end{array} $	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
119 $CH_3OH + HO_2 \le CH_3O + H_2O_2$ 2 120 $CH_3OH + CH_3 \le CH_2OH + CH_4$ 3	117	$CH_3OH + HCO \iff CH_2OH + CH_2O$	5
120 $CH_3OH + CH_3 \le CH_2OH + CH_4$ 3	118	$CH_3OH + HO_2 <=> CH_2OH + H_2O_2$	2
	119	$CH_3OH + HO_2 <=> CH_3O + H_2O_2$	2
121 $CH_3O + CH_3OH <=> CH_3OH + CH_2OH$ 5	120	$CH_3OH + CH_3 \ll CH_2OH + CH_4$	3
	121	$CH_3O + CH_3OH <=> CH_3OH + CH_2OH$	5

 $\begin{tabular}{ll} \textbf{Table S3} \\ \textbf{The simulation condition of methanol flame for global sensitivity analysis.} \\ \end{tabular}$

Equivalance notic	Pressure	Flow rates (SLM)			
Equivalence ratio	(Torr)	CH ₃ O	O_2	Ar	Total
0.8	15	0.974	1.826	1.200	4.000



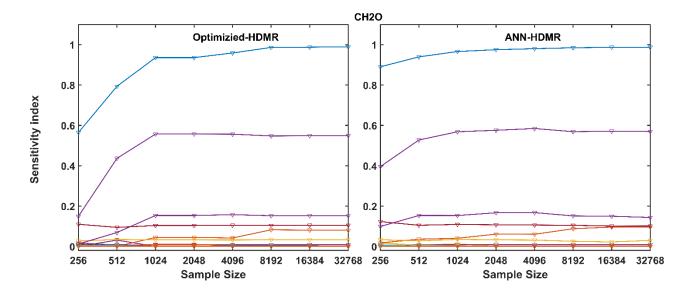


Fig. S4. The first order sensitivity indices and the sum of first and second order sensitivity indices of OH, CH, CH₂(S), CH₂O.