Derivation for equations used to calculate adiabatic expansion

The two equations used to convert a pressure profile to volume were:

$$\int_{T_0}^{T_c} \frac{\gamma}{\gamma-1}\frac{dT}{T} = \ln\left(\frac{P_c}{P}\right) \tag{1}$$

$$\int_{T_0}^{T_c} \frac{1}{\gamma-1}\frac{dT}{T} = \ln\left(\frac{V_c}{V}\right) \tag{2}$$

Derivation of Eq(1), starting from adiabatic relationship of pressure and temperature:

$$P^{1-\gamma}T^{\gamma} = constant \tag{S1}$$

$$T^{\gamma}dP^{1-\gamma} + P^{1-\gamma}dT^{\gamma} = 0 \tag{S2}$$

$$(1-\gamma)P^{-\gamma}T^{\gamma}dP + \gamma T^{\gamma-1}P^{1-\gamma}dT = 0 \tag{S3}$$

$$\frac{\gamma}{\gamma-1}\frac{dT}{T} = \frac{dP}{P} \tag{S4}$$

$$\int_{T_0}^{T_c} \frac{\gamma}{\gamma-1}\frac{dT}{T} = ln(\frac{P_c}{P_0}) \tag{S5}$$

Derivation of Eq(2), starting from adiabatic relationship of volume and temperature:

$$TV^{\gamma-1} = constant \tag{S6}$$

$$V^{\gamma-1}dT + TdV^{\gamma-1} = 0 \tag{S7}$$

$$V^{\gamma-1}dT + (\gamma-1)V^{\gamma-2}TdV = 0 \tag{S8}$$

$$\frac{1}{\gamma-1}\frac{dT}{T} = -\frac{dV}{V} \tag{S9}$$

$$\int_{T_0}^{T_c} \frac{1}{\gamma-1}\frac{dT}{T} = -ln(\frac{V_C}{V_0}) = ln(CR) \tag{S10}$$

Volume Profile used in engine-like simulation

Table 1 Pressure and Volume profile for engine-like simulation. Averaged from over 500 CRF RON 100 runs

Crank Angle Degree	time/ms	P/bar	V/cm^3
-146	0	1.08943	9.02700647
-145	0.278241514	1.0877	9.02700647
-144	0.556483027	1.092386	9.008259364
-143	0.834724541	1.100782	8.95695933
-142	1.112966055	1.108882	8.908007308
-141	1.391207568	1.107988	8.913283004
-140	1.669449082	1.113268	8.881688252
-139	1.947690595	1.1058	8.926489622
-138	2.225932109	1.12621	8.805269925
-137	2.504173623	1.12876	8.790345858
-136	2.782415136	1.13881	8.732255179
-135	3.06065665	1.13808	8.736112698
-134	3.338898164	1.146564	8.688048762
-133	3.617139677	1.155816	8.635882342
-132	3.895381191	1.159486	8.61500076
-131	4.173622705	1.169682	8.55900234
-130	4.451864218	1.177792	8.514660291
-129	4.730105732	1.194806	8.423775932
-128	5.008347245	1.205688	8.366912552
-127	5.286588759	1.21604	8.313553785
-126	5.564830273	1.217262	8.306914309
-125	5.843071786	1.232756	8.228954523
-124	6.1213133	1.23934	8.196250759
-123	6.399554814	1.240644	8.189729782
-122	6.677796327	1.257538	8.106721957
-121	6.956037841	1.276934	8.014391597
-120	7.234279354	1.284074	7.981043052
-119	7.512520868	1.302316	7.897305204
-118	7.790762382	1.301502	7.900701244
-117	8.069003895	1.31481	7.840975569
-116	8.347245409	1.334996	7.751901333
-115	8.625486923	1.349028	7.691404437
-114	8.903728436	1.370482	7.600695729
-113	9.18196995	1.377792	7.570581511

-112	9.460211464	1.396168	7.495423352
-111	9.738452977	1.409872	7.44059097
-110	10.01669449	1.415524	7.41859082
-109	10.294936	1.435706	7.340170595
-108	10.57317752	1.455328	7.265339866
-107	10.85141903	1.47905	7.17791268
-106	11.12966055	1.49187	7.131462762
-105	11.40790206	1.511398	7.062250878
-104	11.68614357	1.534844	6.980795137
-103	11.96438509	1.558224	6.901952114
-102	12.2426266	1.56247	6.888127352
-101	12.52086811	1.588484	6.803094414
-100	12.79910963	1.609338	6.736481265
-99	13.07735114	1.63569	6.654707448
-98	13.35559265	1.66416	6.569243197
-97	13.63383417	1.684014	6.51081544
-96	13.91207568	1.719546	6.409369883
-95	14.1903172	1.744802	6.339409942
-94	14.46855871	1.766556	6.280569999
-93	14.74680022	1.780018	6.244669329
-92	15.02504174	1.820184	6.140562682
-91	15.30328325	1.853138	6.058032149
-90	15.58152476	1.876692	6.000847799
-89	15.85976628	1.91037	5.921056481
-88	16.13800779	1.939424	5.853831308
-87	16.4162493	1.982844	5.757056962
-86	16.69449082	2.009306	5.699653589
-85	16.97273233	2.052964	5.607893546
-84	17.25097385	2.092934	5.526994054
-83	17.52921536	2.128466	5.457135213
-82	17.80745687	2.171928	5.374756056
-81	18.08569839	2.205614	5.312443351
-80	18.3639399	2.24642	5.239530571
-79	18.64218141	2.294832	5.155928108
-78	18.92042293	2.337678	5.08438222
-77	19.19866444	2.396576	4.989526664
-76	19.47690595	2.431706	4.934925558
-75	19.75514747	2.482592	4.858253666
-74	20.03338898	2.545192	4.767715906
-73	20.3116305	2.604708	4.68484782

-72	20.58987201	2.658918	4.612399329
-71	20.86811352	2.717922	4.536537807
-70	21.14635504	2.763824	4.479129476
-69	21.42459655	2.84287	4.384538902
-68	21.70283806	2.908116	4.309852942
-67	21.98107958	2.970512	4.240890884
-66	22.25932109	3.055302	4.151478726
-65	22.5375626	3.127258	4.078707016
-64	22.81580412	3.201798	4.006541584
-63	23.09404563	3.278158	3.935477574
-62	23.37228715	3.361708	3.860878957
-61	23.65052866	3.445992	3.788924744
-60	23.92877017	3.546288	3.707170988
-59	24.20701169	3.62738	3.644107048
-58	24.4852532	3.734568	3.56430077
-57	24.76349471	3.829044	3.49705064
-56	25.04173623	3.934034	3.425770192
-55	25.31997774	4.040434	3.356855112
-54	25.59821925	4.152064	3.287933073
-53	25.87646077	4.274852	3.215759922
-52	26.15470228	4.384556	3.15415595
-51	26.4329438	4.527054	3.078215674
-50	26.71118531	4.653012	3.01436924
-49	26.98942682	4.787626	2.949485446
-48	27.26766834	4.93664	2.881143706
-47	27.54590985	5.075034	2.821006296
-46	27.82415136	5.245758	2.750492039
-45	28.10239288	5.39309	2.692927304
-44	28.38063439	5.558838	2.631197689
-43	28.6588759	5.742816	2.566427416
-42	28.93711742	5.901834	2.513389317
-41	29.21535893	6.08472	2.455179085
-40	29.49360045	6.289344	2.393716529
-39	29.77184196	6.47758	2.340234618
-38	30.05008347	6.689356	2.283221445
-37	30.32832499	6.889474	2.232133551
-36	30.6065665	7.11294	2.178071909
-35	30.88480801	7.34082	2.125927479
-34	31.16304953	7.563064	2.077669764
-33	31.44129104	7.812594	2.026533052

-32	31.71953255	8.044444	1.981401964
-31	31.99777407	8.305274	1.93331587
-30	32.27601558	8.56826	1.887406656
-29	32.5542571	8.832666	1.843746591
-28	32.83249861	9.101796	1.801575926
-27	33.11074012	9.380424	1.760212461
-26	33.38898164	9.673522	1.718873556
-25	33.66722315	9.957422	1.680959485
-24	33.94546466	10.244206	1.644458036
-23	34.22370618	10.544044	1.608194712
-22	34.50194769	10.837338	1.574437212
-21	34.7801892	11.138164	1.54145495
-20	35.05843072	11.441478	1.509742713
-19	35.33667223	11.737762	1.480176118
-18	35.61491375	12.03392	1.451864789
-17	35.89315526	12.332824	1.424545279
-16	36.17139677	12.622188	1.399182707
-15	36.44963829	12.916176	1.374426802
-14	36.7278798	13.18124	1.352962589
-13	37.00612131	13.453878	1.331647006
-12	37.28436283	13.710978	1.312223082
-11	37.56260434	13.973236	1.293077368
-10	37.84084585	14.248056	1.273666625
-9	38.11908737	14.528526	1.254545683
-8	38.39732888	14.865098	1.232421748
-7	38.6755704	15.240872	1.208736104
-6	38.95381191	15.646328	1.184330239
-5	39.23205342	16.095414	1.158531565
-4	39.51029494	16.549474	1.133715941
-3	39.78853645	17.043452	1.108062495
-2	40.06677796	17.577048	1.081818843
-1	40.34501948	18.160688	1.054593285
0	40.62326099	18.780256	1.02739547
1	40.9015025	19.442654	1
2	41.17974402	20.144636	0.972691804
3	41.45798553	20.878356	0.945892214
4	41.73622705	21.616876	0.920579148
5	42.01446856	22.388858	0.895677538
6	42.29271007	23.143684	0.872756722
7	42.57095159	23.898986	0.851087252

8	42.8491931	24.62082	0.831494504
9	43.12743461	25.353514	0.81261252
10	43.40567613	26.07706	0.79492147
11	43.68391764	26.79878	0.778086649
12	43.96215915	27.498484	0.762518437
13	44.24040067	28.18878	0.747859043
14	44.51864218	28.91703	0.733038888
15	44.7968837	29.678896	0.718235092
16	45.07512521	30.525724	0.702548947
17	45.35336672	31.370594	0.687642337
18	45.63160824	32.26448	0.672636019
19	45.90984975	33.363348	0.65514059
20	46.18809126	34.4987	0.638132486
21	46.46633278	35.375552	0.62565711
22	46.74457429	36.127512	0.615403009
23	47.0228158	36.503602	0.610400928
24	47.30105732	36.506086	0.61037604
25	47.57929883	36.242912	0.613847154
26	47.85754035	35.640834	0.622004438
27	48.13578186	34.986604	0.63111944
28	48.41402337	34.124242	0.643645486
29	48.69226489	33.27172	0.656577653
30	48.9705064	32.34174	0.67135209
31	49.24874791	31.474578	0.685866414
32	49.52698943	30.484274	0.703285182
33	49.80523094	29.571812	0.720262978
34	50.08347245	28.666502	0.738043735
35	50.36171397	27.793402	0.756189673
36	50.63995548	26.928412	0.7751679
37	50.91819699	26.06616	0.795160224
38	51.19643851	25.230306	0.815735436
39	51.47468002	24.45814	0.835825673
40	51.75292154	23.702396	0.856620912
41	52.03116305	22.97771	0.877652681
42	52.30940456	22.251908	0.899975717
43	52.58764608	21.60323	0.921026197
44	52.86588759	20.946602	0.943503709
45	53.1441291	20.329074	0.965821713
46	53.42237062	19.745032	0.988021508
47	53.70061213	19.145636	1.012061499

48	53.97885364	18.60356	1.034979625
49	54.25709516	18.053592	1.059481865
50	54.53533667	17.534586	1.083841372

Sensitivity analysis for engine-like simulation

Conditions: ϕ = 1, T0 = 400 K, P0 =1.09 bar, adiabatic, effective V(t) defined by RON100 P(t) for pure butane and blends of 2% mol additive in butane. Local sensitivity is taken at T = 925K. For the additive blends, the top 50 most sensitive reactions from pure butane are filtered out to emphasize the effect of the additives. Reactions are drawn in the direction which they proceed at the given time point. Note that the range for the x-axis is not constant between figures.

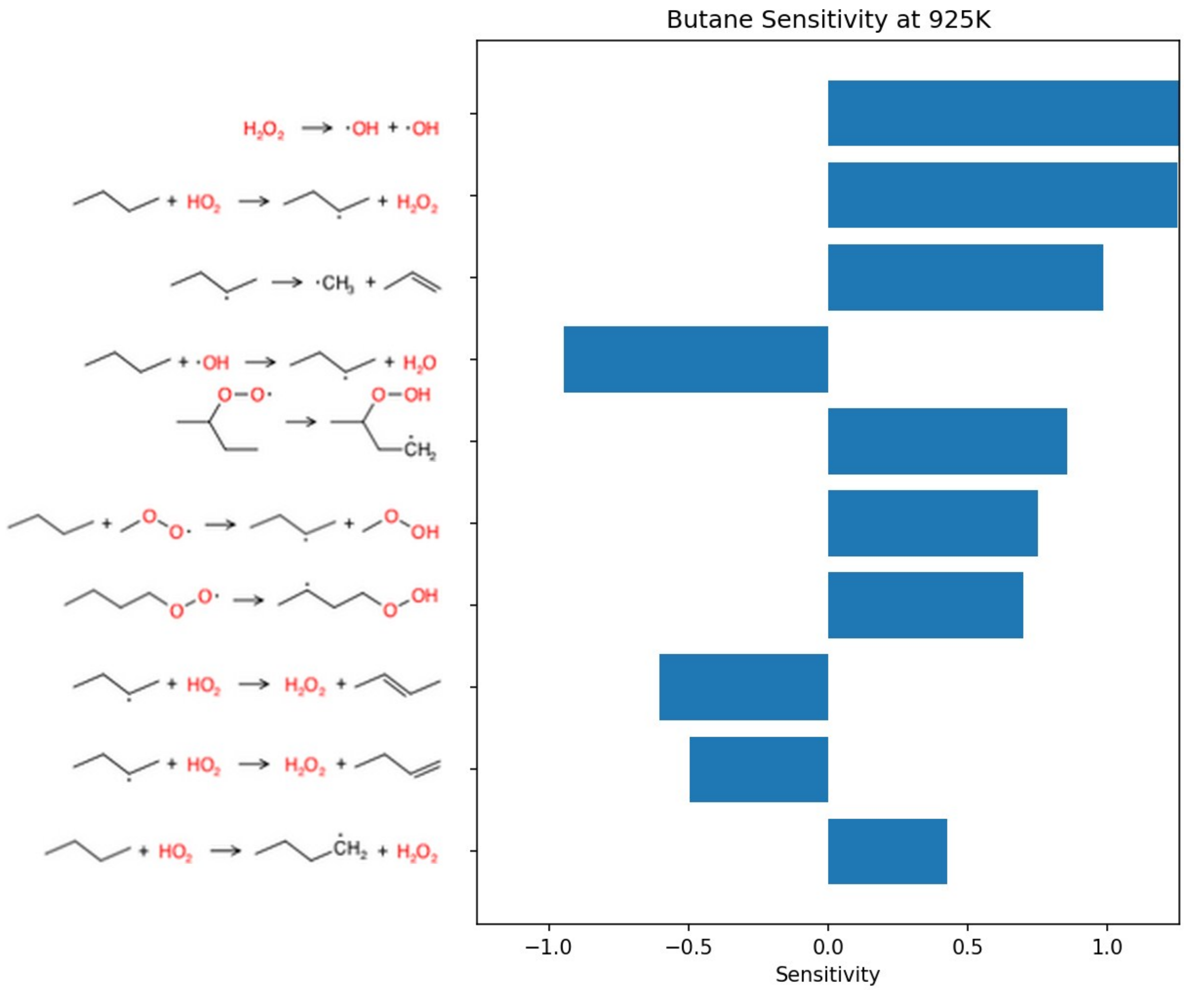

Figure 1 Sensitivity analysis for OH concentration for the engine-like simulation of butane given at t = 4.62 ms and T = 925K.

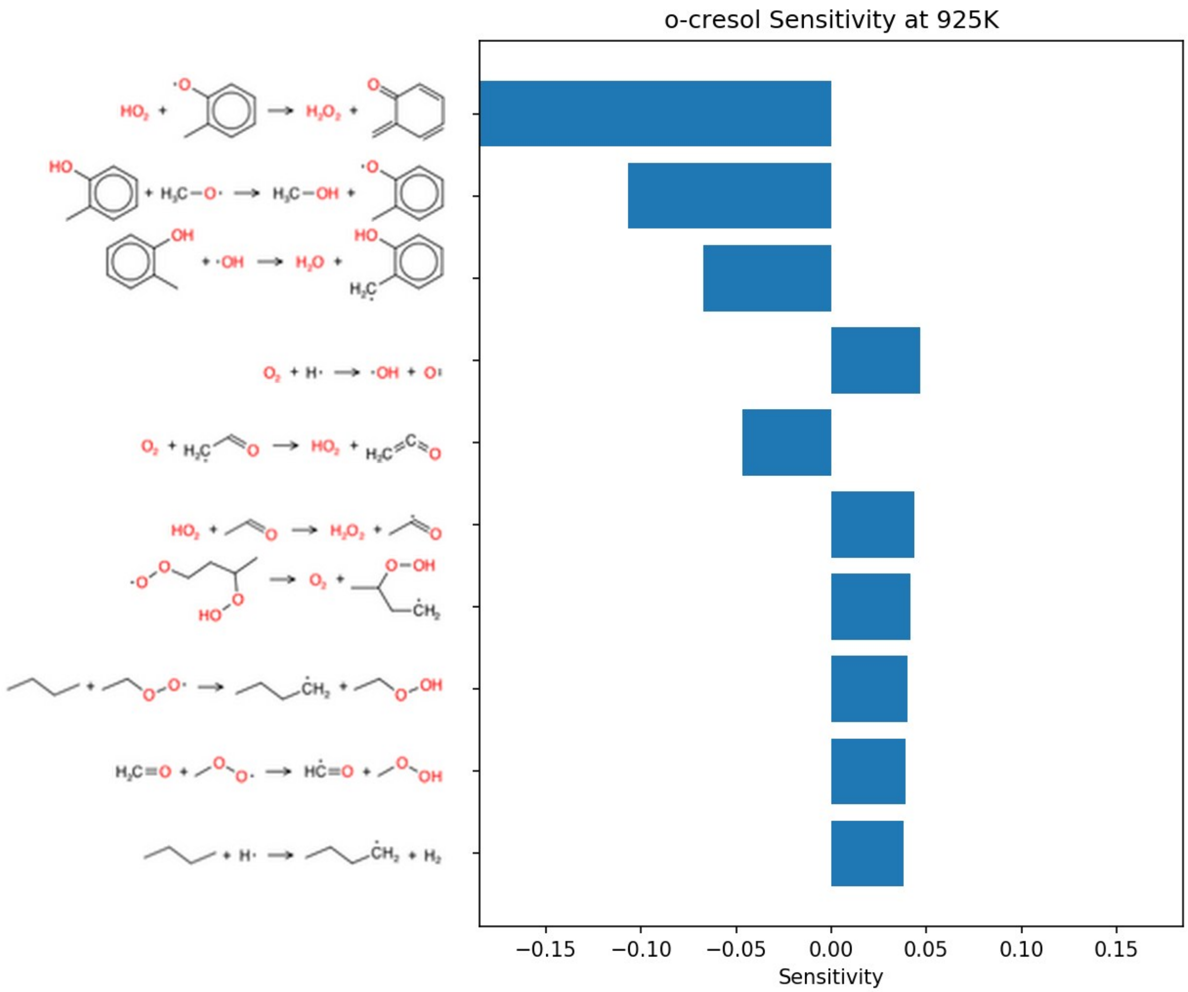

Figure 2. Sensitivity analysis for OH in a 2% mol o-cresol blend in butane for the engine-like simulation given at t = 4.62 ms and T = 925K. The top 50 sensitive reactions of pure butane were filtered out to underscore the reactions involving o-cresol..

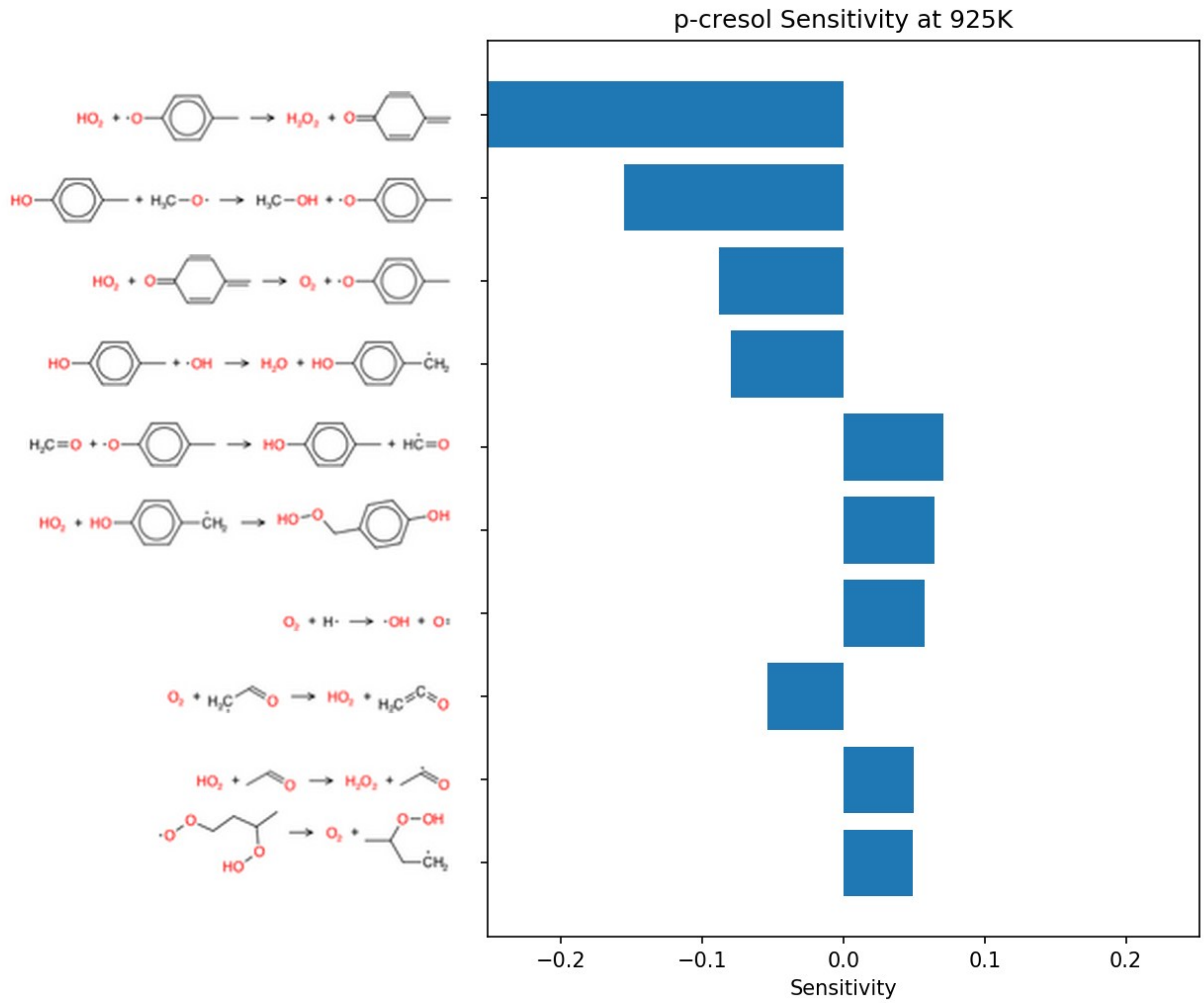

Figure 3 Sensitivity analysis for OH in a 2% mol p-cresol blend in butane for the engine-like simulation given at t = 4.62 ms and T = 925K. The top 50 sensitive reactions of pure butane were filtered out to underscore the reactions involving p-cresoll.

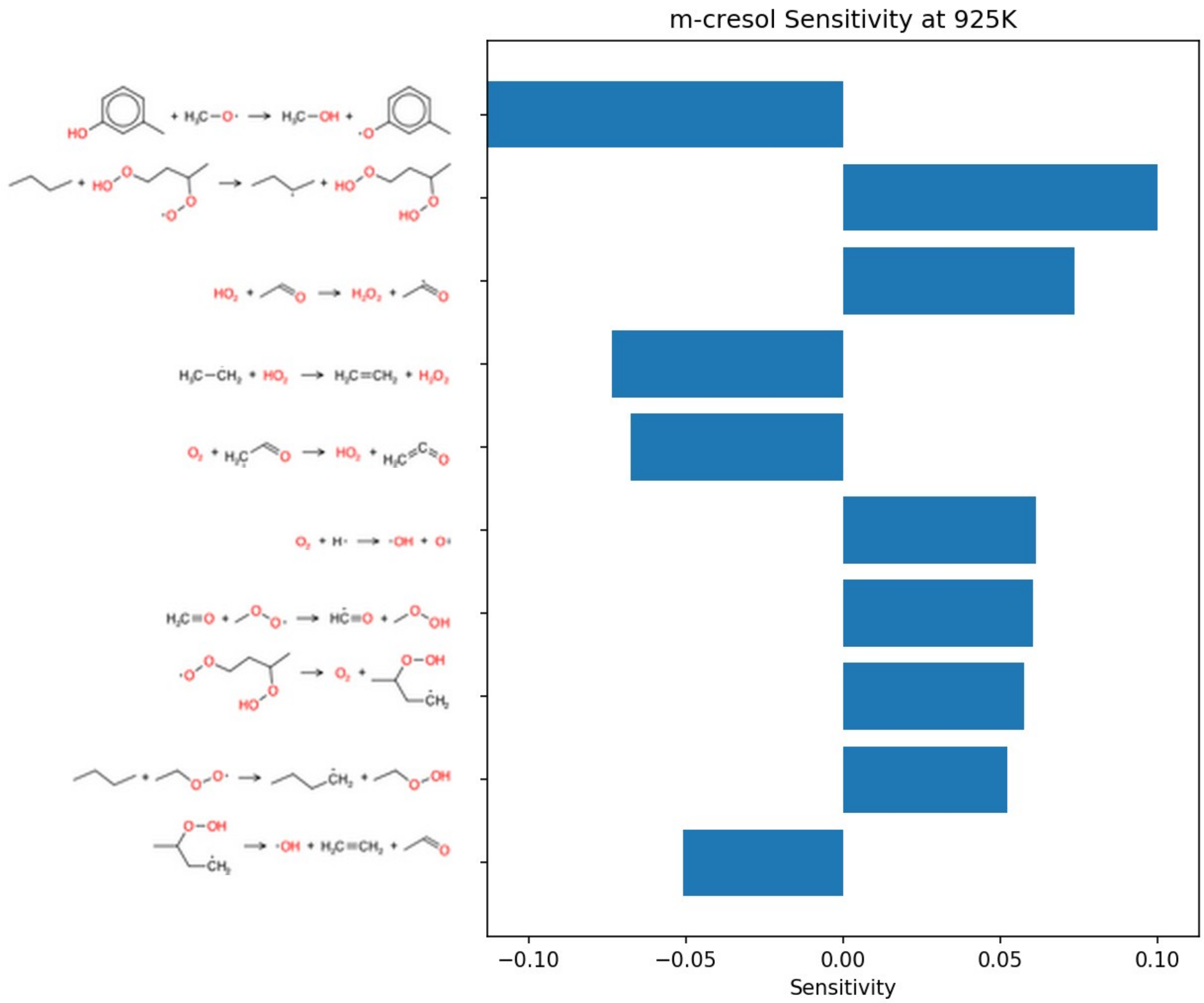

Figure 4 Sensitivity analysis for OH in a 2% mol m-cresol blend in butane for the engine-like simulation given at t = 4.62 ms and T = 925K. The top 50 sensitive reactions of pure butane were filtered out to underscore the reactions involving m-cresoll.

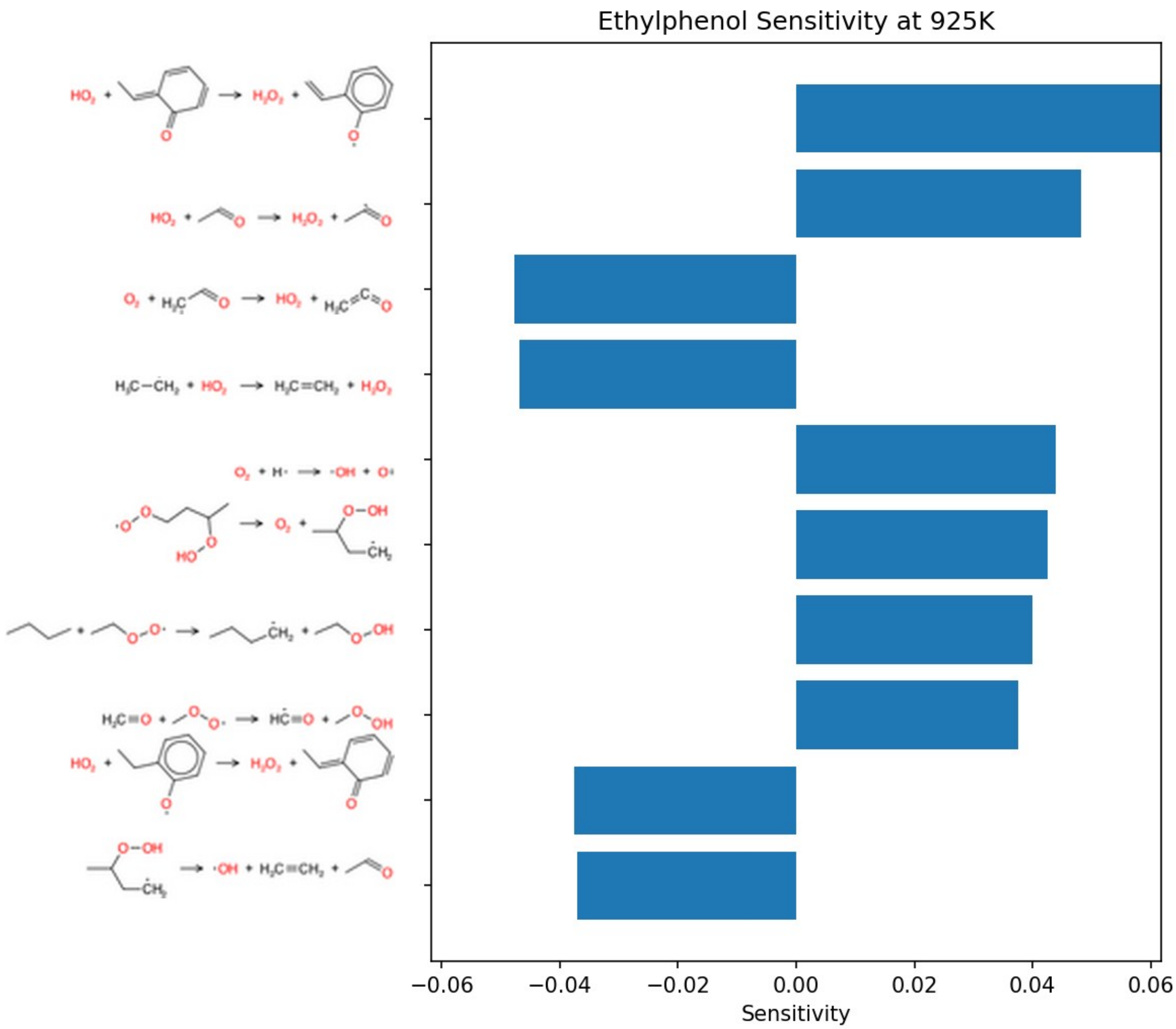

Figure 5 Sensitivity analysis for OH in a 2% mol ethylphenol blend in butane for the engine-like simulation given at t = 4.62 ms and T = 925K. The top 50 sensitive reactions of pure butane were filtered out to underscore the reactions involving ethylphenol..

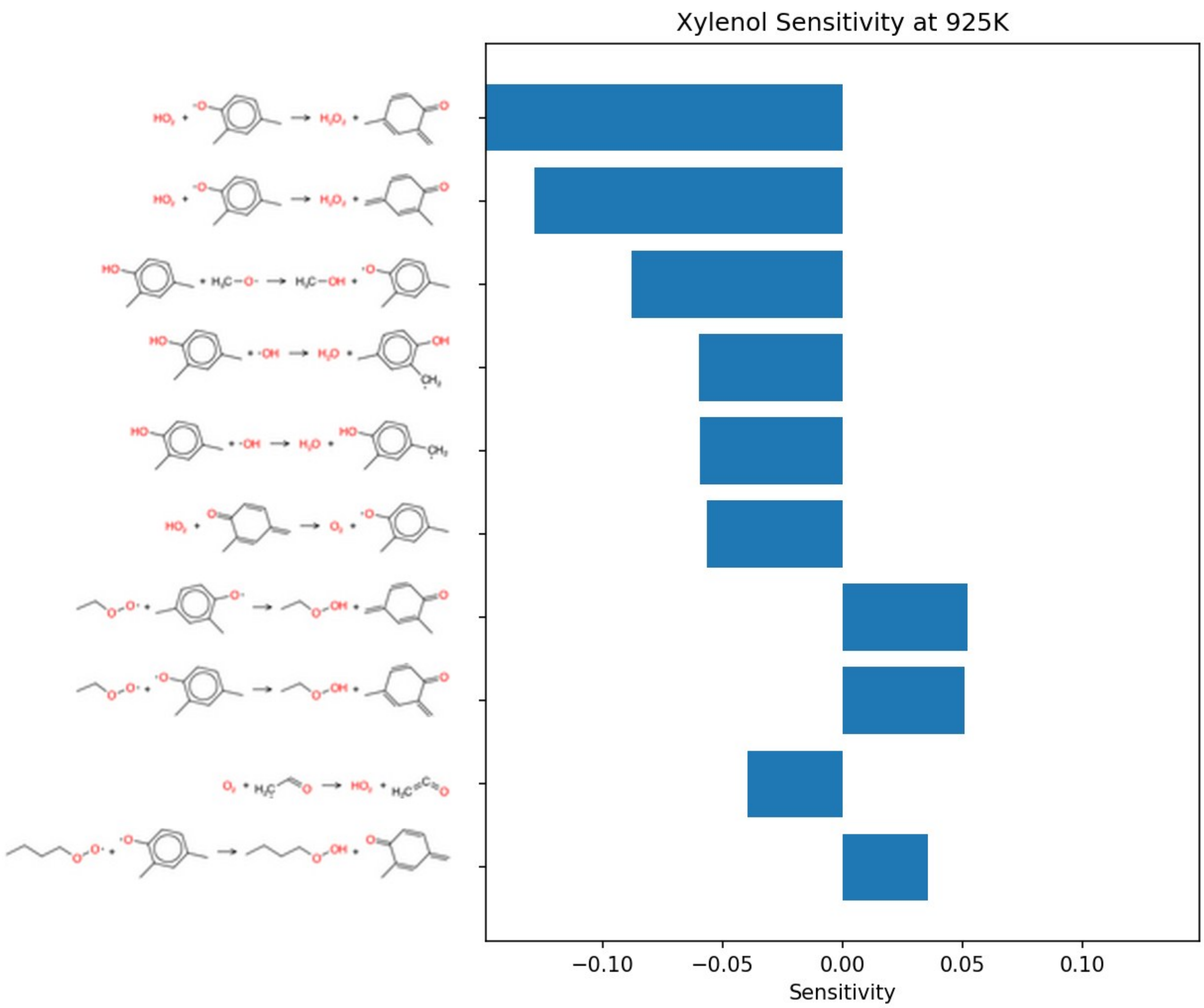

Figure 6 Sensitivity analysis for OH in a 2% mol xylenol blend in butane for the engine-like simulation given at t = 4.62 ms and T = 925K. The top 50 sensitive reactions of pure butane were filtered out to underscore the reactions involving xylenoll.