

Supporting Information for

Chemical reaction-transport model of oxidized diethylzinc based on quantum mechanics and computational fluid dynamics approaches

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Geometries Optimized at B3LYP/6-311G(d)

Table S1

Structure: IM1

-2088.1551506 Hartree

0 3

Zn	0.440591	-0.527181	-0.190144
C	1.729902	0.929990	-0.008433
H	1.680995	1.557764	-0.906342
H	1.412130	1.580602	0.815433
C	3.180082	0.475280	0.223780
H	3.869925	1.322110	0.320351
H	3.282975	-0.121131	1.136379
H	3.553280	-0.143460	-0.599007
O	-1.574673	1.768838	-0.821649
H	-2.674399	-0.912541	0.124137
O	-1.493141	2.921017	-0.475886
C	-0.827403	-2.004281	-0.348288
H	-0.336373	-2.929402	-0.023331
H	-1.060261	-2.157981	-1.408869
C	-2.132799	-1.809552	0.441202
H	-2.820599	-2.654732	0.319247
H	-1.951197	-1.703485	1.515957

Table S2

Structure: TS1

-2088.0837547 Hartree

0 3

Zn	0.497572	-0.339560	0.009114
C	1.985624	0.923908	0.010382
H	1.855485	1.586115	-0.852449
H	1.875127	1.567308	0.890156
C	3.384805	0.291962	-0.011164
H	4.176179	1.050592	-0.009534
H	3.561110	-0.349923	0.858077
H	3.543872	-0.328047	-0.899387
O	-1.701096	1.163881	-0.133862
H	-2.173044	0.198414	-0.085747
O	-2.570608	2.111784	0.091263
C	-0.867165	-1.813201	0.022434
H	-0.624188	-2.377454	0.929204
H	-0.601826	-2.427484	-0.844074
C	-2.278503	-1.396781	-0.006511
H	-2.852889	-1.532477	-0.919981
H	-2.861924	-1.440875	0.910276

Table S3

Structure: IM2

-2088.0841882 Hartree

0 3

Zn	0.503426	-0.383902	-0.037 249
C	1.967634	0.907620	-0.059617
H	1.866909	1.505174	-0.972138
H	1.805069	1.608651	0.766308
C	3.375974	0.302483	0.026647
H	4.154476	1.074189	0.009889
H	3.522117	-0.273252	0.946364
H	3.585576	-0.375445	-0.807155
O	-1.651411	1.189112	-0.250779
H	-2.157526	0.309714	-0.170342
O	-2.291681	2.106786	0.450278
C	-0.830067	-1.885052	0.008526
H	-0.568767	-2.423761	0.926317
H	-0.552942	-2.513258	-0.844471
C	-2.247 200	-1.511539	-0.022129
H	-2.823893	-1.624349	-0.935662
H	-2.820381	-1.468137	0.899530

Table S4

Structure: CP

-2088.0724 Hartree

Spin Conversion Point

Zn	0.270790	-0.007678	-0.052795
C	1.925606	1.036560	0.004801
H	1.891330	1.724980	-0.846423
H	1.876915	1.672783	0.894816
C	3.231014	0.233301	-0.006046
H	4.112731	0.884395	0.020062
H	3.307629	-0.437023	0.855884
H	3.324790	-0.389328	-0.901410
O	-1.614833	0.965561	-0.332743
H	-2.268293	0.244809	-0.055497
O	-1.918626	2.156097	0.241325
C	-0.877485	-1.791691	0.027806
H	-0.476797	-2.186332	0.964334
H	-0.450884	-2.291657	-0.8446 94
C	-2.281956	-1.623781	-0.000674
H	-2.840873	-1.705371	-0.926719
H	-2.862527	-1.597463	0.916171

Table S5

Structure: TS2

-2088.0478947 Hartree

0 3

Zn	0.310620	-0.098699	0.030593
C	2.143500	-0.801348	0.070543
H	2.282223	-1.323227	1.024001
H	2.221497	-1.577060	-0.699238
C	3.252928	0.242448	-0.120503
H	4.250630	-0.210854	-0.084843
H	3.174377	0.756911	-1.083750
H	3.229772	1.015892	0.654009
O	-1.536018	-0.924689	-0.000699
H	-2.188428	-0.208515	-0.022500
O	-2.496700	-2.181261	-0.014360
C	-0.713210	1.869823	0.000967
H	-0.156567	2.167167	-0.890587
H	-0.215470	2.166375	0.926910
C	-2.091185	2.105310	-0.043729
H	-2.683742	2.177767	0.861659
H	-2.624232	2.176513	-0.985424

Table S6

Structure: IM3

-2088.1229398 Hartree

0 3

Zn	-1.060903	-0.060194	-0.366407
C	-2.560333	-1.275761	-0.371040
H	-2.703076	-1.631825	-1.396944
H	-2.281190	-2.163370	0.206516
C	-3.873562	-0.687092	0.164783
H	-4.688288	-1.419150	0.131824
H	-3.783632	-0.357222	1.204320
H	-4.200892	0.181092	-0.414947
O	-0.139712	1.574117	-0.333707
H	0.523674	1.816126	0.322582
O	1.033443	-0.286963	-0.494362
C	2.491579	3.446389	0.161917
H	2.652193	4.418774	0.618553
H	1.841342	3.417270	-0.706416
C	3.060626	2.342740	0.638612
H	2.898489	1.374313	0.175594
H	3.713515	2.368309	1.506626

Table S7

Structure: IM4

-2088.1649436 Hartree

0 1

Zn	0.110728	0.761479	0.390764
C	1.964254	0.598594	-0.117766
H	1.991776	0.360891	-1.186224
H	2.443719	1.577460	-0.014502
C	2.748460	-0.458341	0.672108
H	3.785279	-0.534567	0.325443
H	2.786896	-0.229230	1.741614
H	2.305210	-1.453476	0.573515
O	-2.276306	1.389070	-0.279904
H	-3.137177	1.661990	0.057694
O	-1.583538	1.108846	1.000990
C	-0.434704	-2.489125	-0.717786
H	0.216832	-3.213063	-0.237249
H	-0.328896	-2.389457	-1.794163
C	-1.315044	-1.766079	-0.030206
H	-1.982741	-1.053255	-0.502168
H	-1.432125	-1.878487	1.042982

Table S8

Structure: IM5

-2009.5493196 Hartree

0 1

Zn	-0.079120	-0.017705	0.009608
C	1.712747	0.686231	0.018090
H	1.800726	1.395363	-0.811263
H	1.842325	1.276646	0.930706
C	2.816063	-0.378224	-0.081100
H	3.813394	0.075191	-0.074864
H	2.783300	-1.085629	0.753008
H	2.740145	-0.966772	-1.000306
O	-2.542241	0.500140	-0.068821
H	-3.429786	0.125026	-0.074247
O	-1.746071	-0.750764	0.001759

Table S9

Structure: TS3

-2009.4674813 Hartree

0 1

Zn	0.334359	-0.732788	0.158109
C	-1.624205	-0.814778	0.054169
C	-1.913667	0.659907	-0.033925
H	-2.041695	-1.272464	0.951332
H	-1.961535	-1.365338	-0.824543
H	-0.880504	1.302794	0.096064
H	-2.269276	1.001273	-1.006011
H	-2.515387	1.067881	0.779176
O	2.079795	-0.081155	0.266001
O	0.465314	1.203387	0.178497
H	2.464619	0.272223	-0.542359

Table S10

Structure: IM6

-2009.6324133 Hartree

0 1

Zn	0.429818	-0.422676	-0.139659
C	-1.493571	-0.501252	0.054222
C	-1.935442	0.948488	-0.057246
H	-1.747647	-0.916997	1.033023
H	-1.974458	-1.124017	-0.703476
H	-1.052864	2.689795	0.350995
H	-2.209424	1.193816	-1.091193
H	-2.793114	1.182384	0.586257
O	2.201211	-0.456874	-0.355225
O	-0.802841	1.758707	0.343715
H	2.676524	0.357974	-0.180147

Table S11

Structure: TS4

-2009.5953428 Hartree

0 1

Zn	-0.410804	0.595272	-0.011026
C	1.008386	-1.059286	-0.064920
C	2.119256	-0.232269	0.096389
H	0.855663	-1.521291	-1.036814
H	0.689451	-1.654658	0.787153
H	1.577126	2.386620	0.338323
H	2.572611	-0.099000	1.070394
H	2.752778	0.019930	-0.743185
O	-2.205380	0.689326	0.009149
O	1.254125	1.512809	0.086638
H	-2.687746	-0.082606	-0.292877

Table S12

Structure: IM7

-2009.6218768 Hartree

0 1

Zn	-0.259355	0.206256	-0.017983
C	1.448915	-1.610732	-0.548011
C	1.788041	-1.153789	0.659597
H	1.853799	-1.162544	-1.449222
H	0.748797	-2.432076	-0.658542
H	0.352495	2.344197	-0.998493
H	1.371920	-1.592470	1.560368
H	2.476922	-0.322940	0.769684
O	-1.394716	-0.943267	0.735952
O	0.720735	1.487136	-0.778006
H	-2.309978	-0.714752	0.905791

Table S13Structure: Zn(OH)₂**-1930.9983068 Hartree**

0 1

Zn	-0.723842	0.302268	0.075846
O	0.386204	1.668943	0.189316
O	-1.821264	-1.073931	-0.045107
H	-1.930916	-1.626685	0.731380
H	0.279773	2.383824	-0.441642

Table S14

Structure: TS1-1

-1930.8633619 Hartree

0 1

Zn	0.365858	-0.525001	-0.029107
O	0.758338	1.266175	0.010229
O	-1.498238	0.364656	-0.075747
H	-2.151492	0.522460	0.610165
H	-0.603302	1.155816	-0.033484

Table S15

Structure: IM1-1

-1930.8702615 Hartree

0 1

Zn	0.483417	-0.292404	0.004374
O	0.169196	1.478274	0.016149
O	-1.787068	-0.315848	-0.073126
H	-2.570057	-0.402595	0.477726
H	-1.484213	0.631408	-0.064139

Table S16

Structure: ZnO

-1854.4006799 Hartree

0 1

Zn	0.484501	-0.369052	0.004135
O	0.417367	1.418522	0.007797

Table S17Structure: Zn₂(OH)₄**-3862.0775224 Hartree**

0 1

Zn	1.110613	-0.412906	0.208198
O	0.502467	1.394676	0.013256
H	1.002775	2.206172	-0.016524
O	2.616226	-1.363977	0.400512
H	2.528907	-2.316161	0.473379
Zn	-1.390403	1.115503	-0.106231
O	-0.799314	-0.719868	0.090132
H	-1.299059	-1.531841	0.120806
O	-2.922750	2.023246	-0.296793
H	-3.735872	1.515248	-0.316080

Table S18Structure: $\text{Zn}_3(\text{OH})_6$

-5793.1608123 Hartree

0 1

Zn	-2.698720	0.535267	0.014461
O	-1.515907	-0.784314	-0.690275
H	-1.720281	-1.616365	-1.109388
O	-4.434499	0.980084	0.097805
H	-4.667592	1.721427	0.659761
Zn	0.188913	-0.072491	-0.045110
O	-1.024648	1.266612	0.671258
H	-0.823881	2.127891	1.028882
O	1.826690	0.589367	-0.887488
H	1.990095	1.391342	-1.377256
Zn	3.072080	-0.683510	-0.205168
O	1.466138	-1.364061	0.647630
H	1.300349	-2.200142	1.076006
O	4.809224	-1.128514	-0.249112
H	5.093483	-1.832000	0.337417

Table S19**Structure: TS3-1****-5793.1006848 Hartree****0 1**

Zn	-3.246439	-0.734135	0.036217
O	-1.644749	-1.519426	-0.654753
H	1.534740	-2.287156	-1.210082
O	-5.022518	-0.957799	0.074394
H	-5.539822	-0.304200	0.548541
Zn	-0.333801	-0.278300	0.023792
O	-1.931039	0.521324	0.730057
H	-2.035536	1.295195	1.278387
O	3.722382	2.619656	0.618425
H	4.580883	2.775383	0.218899
Zn	2.887936	1.128272	0.089526
O	1.433993	-0.051042	-0.027500
H	2.301692	-0.660395	-0.653649
O	3.460068	-0.501489	-1.015290
H	4.066641	-1.184673	-0.722579

Table S20

Structure: IM3-1

-5793.1091240 Hartree

0 1

Zn	-3.193601	0.098604	-0.049189
O	-1.869493	-1.278491	-0.100378
H	-1.973832	-2.219021	-0.219505
O	-4.964972	0.354026	-0.126329
H	-5.282535	1.257220	-0.071515
Zn	-0.260774	-0.225466	0.086097
O	-1.587355	1.175195	0.141476
H	-1.479230	2.115094	0.265092
O	4.472764	1.426193	-0.123421
H	5.265622	1.001729	-0.459029
Zn	3.056538	0.354119	-0.015862
O	1.492061	-0.487177	0.157210
H	2.551335	-1.812478	-0.042291
O	3.535947	-1.881520	-0.178994
H	3.909724	-2.429367	0.516160

Table S21Structure: Zn₃O₅H₄**-5716.6406833 Hartree**

0 1

Zn	3.171646	-0.096683	-0.000635
O	1.872839	1.308210	-0.067259
H	1.992772	2.253941	-0.095974
O	4.945322	-0.349305	0.036336
H	5.260445	-1.254374	0.070296
Zn	0.242049	0.290139	-0.060953
O	1.547816	-1.150452	0.007002
H	1.422953	-2.095908	0.035964
O	-4.408012	-1.482689	-0.074839
H	-5.256866	-1.038304	-0.122681
Zn	-2.954901	-0.472719	-0.086720
O	-1.513273	0.496224	-0.096548

Table S22

Structure: TS3-2

-5716.6380686 Hartree

0 1

Zn	-2.169941	-0.506891	0.057007
O	-1.603925	1.389645	0.031904
H	-2.133630	2.182922	0.041084
O	-3.851868	-1.117410	0.075743
H	-3.995511	-2.065159	0.083963
Zn	0.239736	1.195356	0.014183
O	-0.301043	-0.767702	0.052389
H	0.178834	-1.591767	-0.017267
O	3.689781	-1.722692	-0.078196
H	4.178709	-2.016249	0.693084
Zn	2.913648	-0.133320	-0.019639
O	2.012036	1.370918	-0.004767

Table S23

Structure: IM3-2

-5716.6394670 Hartree

0 1

Zn	-2.035682	-0.620962	0.025363
O	-1.724491	1.358925	-0.008315
H	-2.358977	2.071433	-0.003800
O	-3.694556	-1.290515	0.050724
H	-3.809688	-2.241921	0.030133
Zn	0.102003	1.425150	-0.016736
O	-0.161725	-0.694739	0.022326
H	0.327337	-1.520020	-0.069147
O	2.603639	-1.962429	-0.083723
H	2.894332	-2.417811	0.709237
Zn	2.363275	-0.198028	-0.019581
O	1.884485	1.506930	-0.013691

Table S24

Structure: TS3-3

-5716.5832213 Hartree

0 1

Zn	1.5011191	-0.957720	-0.349025
O	1.872754	0.919919	-0.410420
H	3.081110	0.297058	-0.126687
O	3.448085	-0.758036	-0.035667
H	4.183734	-0.951035	-0.621730
Zn	0.258537	1.583740	-0.078763
O	-0.281889	-1.291571	-0.266567
H	-0.731302	-2.142165	-0.245367
O	-2.954553	-1.726595	0.208677
H	-3.706906	-1.872470	-0.367918
Zn	-2.091600	-0.142650	0.162929
O	-1.478560	1.545100	0.209768

Table S25

Structure: IM3-3

-5716.5846338 Hartree

0 1

Zn	-1.513338	-0.901599	-0.017335
O	-1.946424	0.913229	0.027573
H	-3.409271	0.082284	-0.264020
O	-3.548882	-0.914600	-0.327482
H	-4.299466	-1.193281	0.203986
Zn	-0.293175	1.580332	0.015415
O	0.250294	-1.344966	0.060065
H	0.659889	-2.213994	0.038724
O	2.991598	-1.728375	-0.073994
H	3.690530	-1.892235	0.561919
Zn	2.077749	-0.173181	-0.011791
O	1.467650	1.518419	0.007214

Table S26Structure: Zn₃O₄H₂**-5640.1052402 Hartree**

0 1

Zn	1.354003	-0.674924	-0.061066
O	2.031270	0.984717	-0.031644
Zn	0.351437	1.692322	-0.008587
O	-0.269845	-1.445454	-0.074568
H	-0.532946	-2.366227	-0.079304
O	-3.116061	-1.688126	0.068627
H	-3.889196	-1.729944	-0.497298
Zn	-2.060278	-0.231869	0.010350
O	-1.393889	1.443250	-0.005470

Table S27

Structure: TS3-4

-5640.0695660 Hartree

0 1

Zn	1.025649	1.387511	0.002465
O	2.387439	0.196480	-0.008924
Zn	1.270068	-1.228293	0.016906
O	-0.749979	1.374952	0.046282
H	-2.120614	1.535275	-0.176874
O	-2.992774	0.868852	-0.278874
H	-3.687803	1.080185	0.348540
Zn	-1.513047	-0.434122	-0.032931
O	-0.401598	-1.867944	0.028064

Table S28

Structure: IM3-4

-5640.0699684 Hartree

0 1

Zn	-0.831950	1.467668	-0.006997
O	-2.297742	0.405785	0.028276
Zn	-1.321975	-1.120495	0.005613
O	0.942096	1.344469	-0.0617148
H	2.513800	1.361262	0.101662
O	3.200808	0.596622	0.155855
H	3.902356	0.716550	-0.488919
Zn	1.491738	-0.500572	-0.005370
O	0.301974	-1.879018	-0.025504

Table S29Structure: Zn₃O₃**-5563.5895128 Hartree****0 1**

Zn	0.740046	1.484117	0.009177
O	2.232023	0.453196	-0.025164
Zn	1.431180	-1.174558	-0.015685
O	-1.069186	1.362501	0.045147
Zn	-1.218430	-0.445113	0.040711
O	-0.207805	-1.950607	0.014201

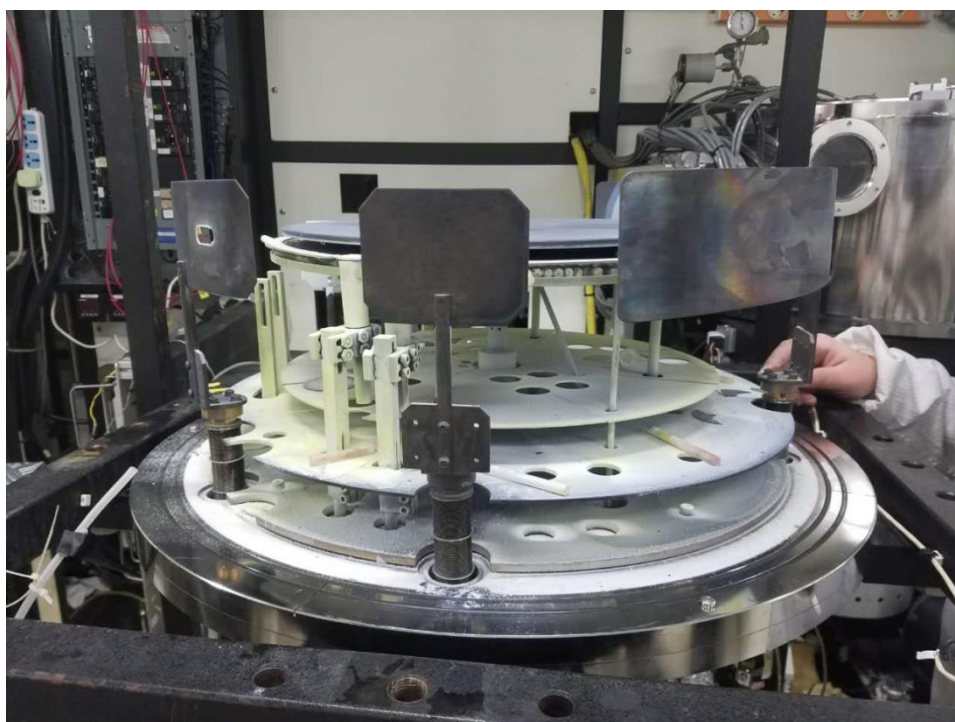
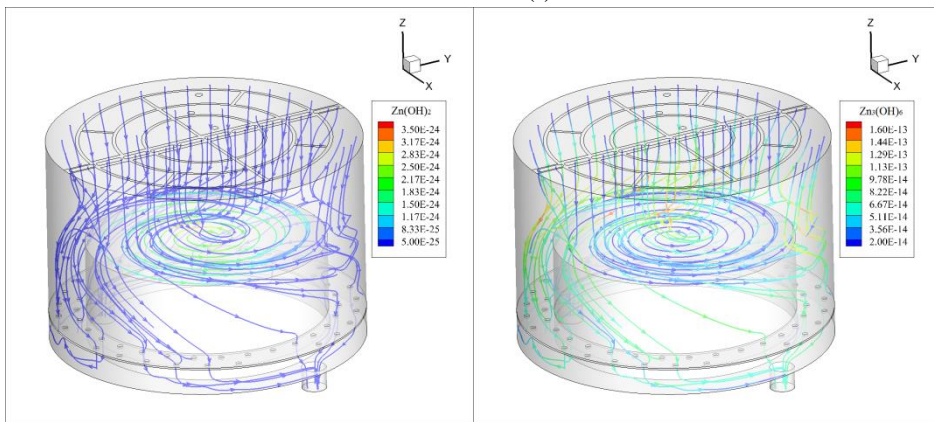
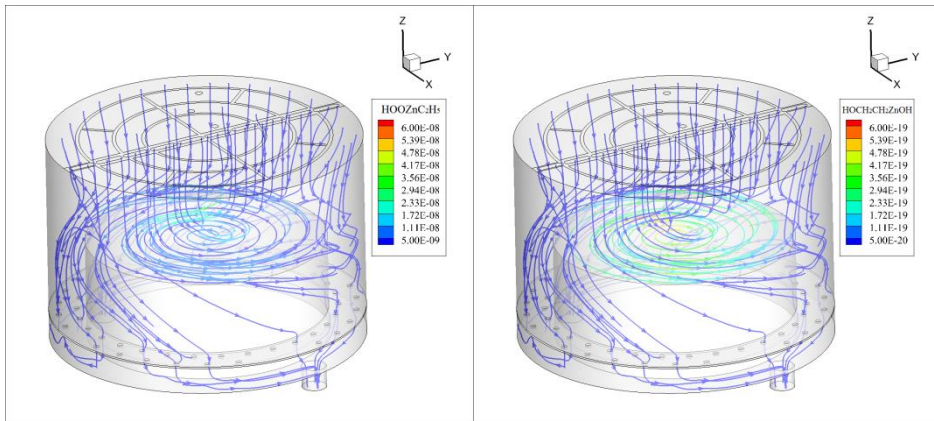
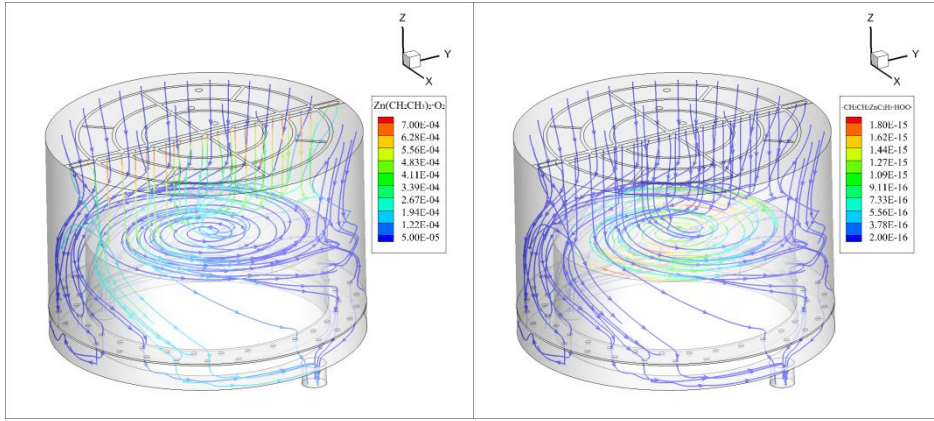
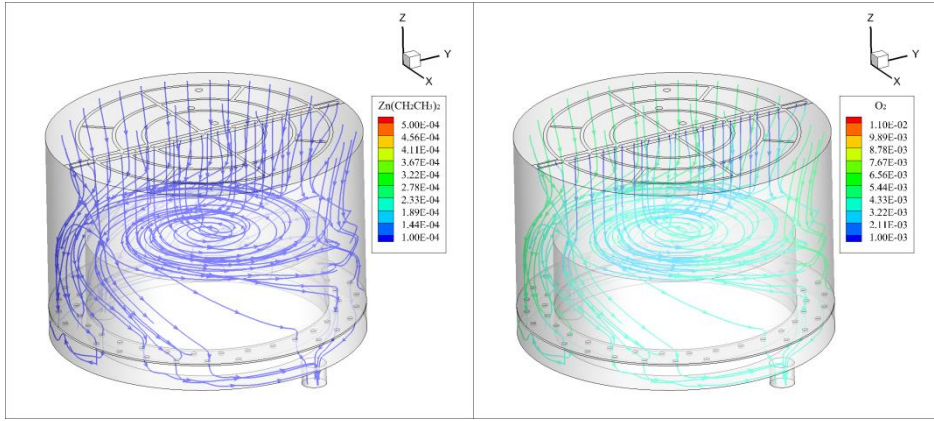


Fig. S1 Solid particles in the MOCVD reaction chamber



(g)

(h)

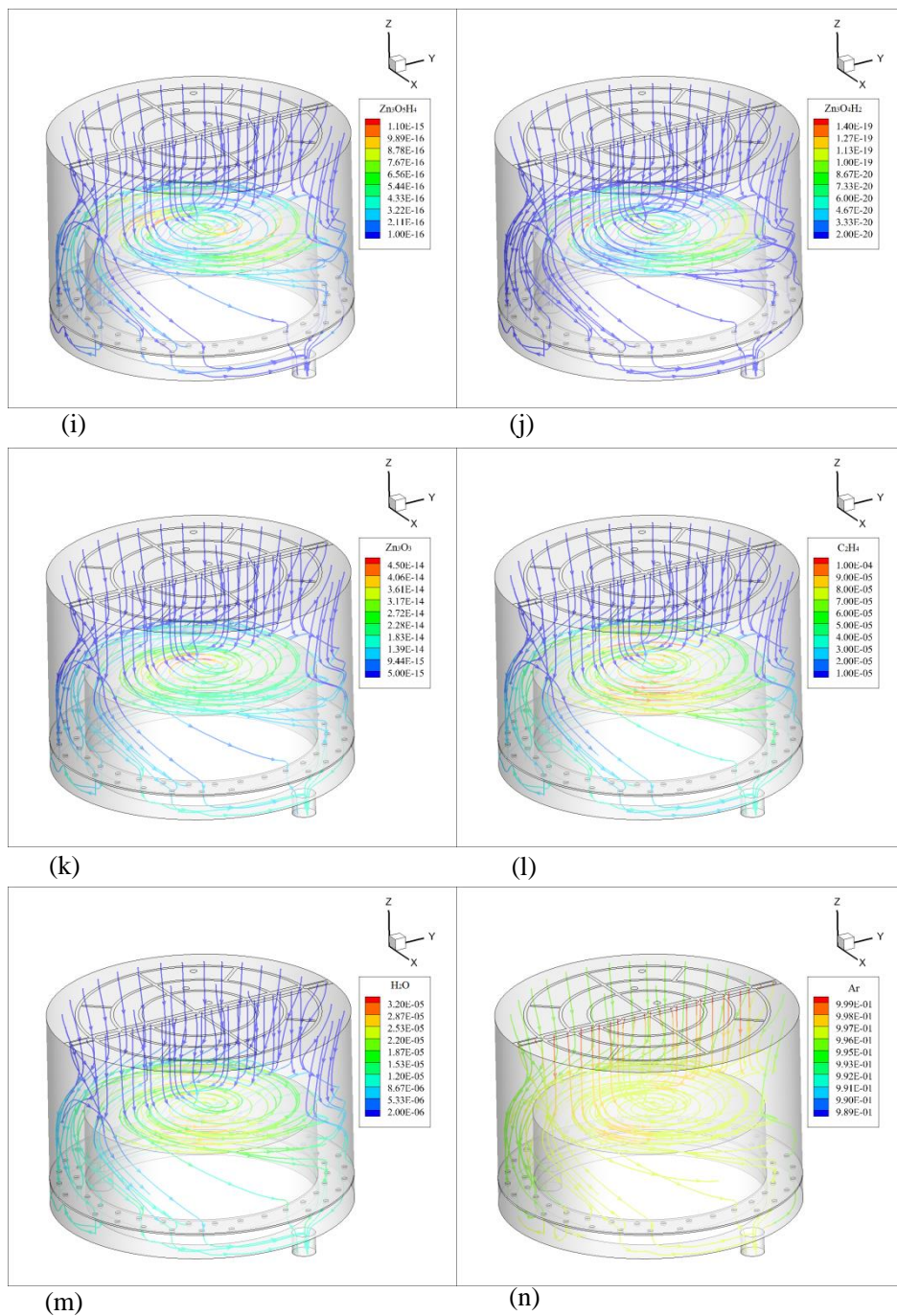
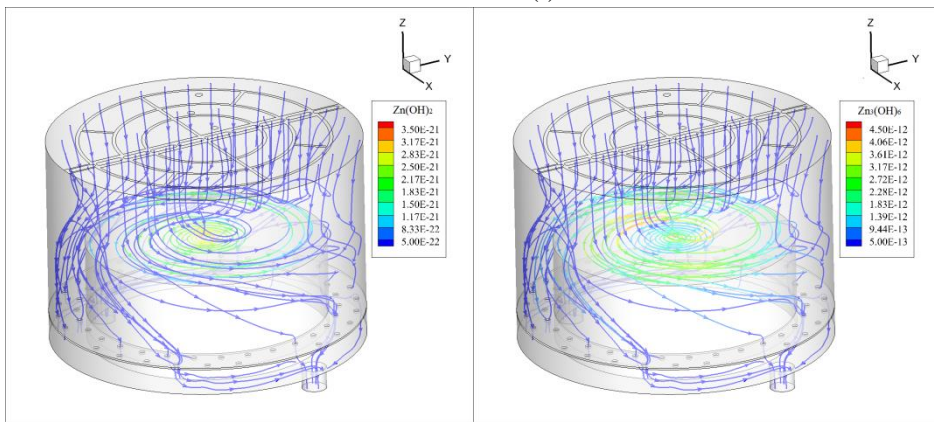
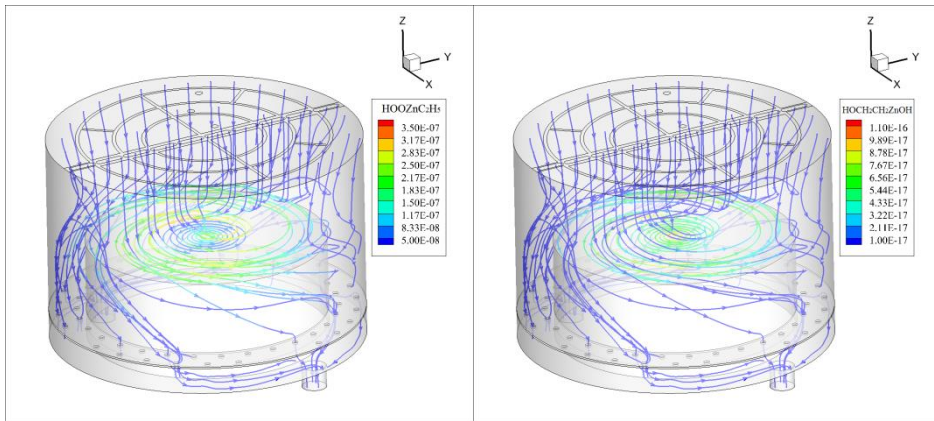
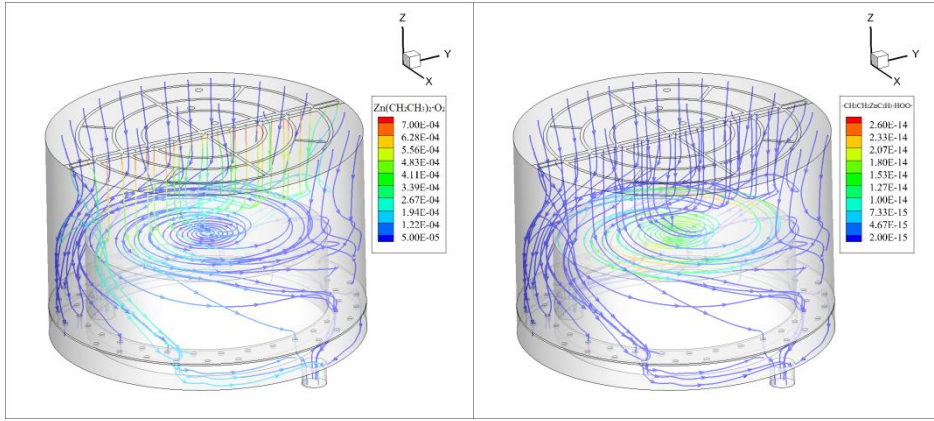
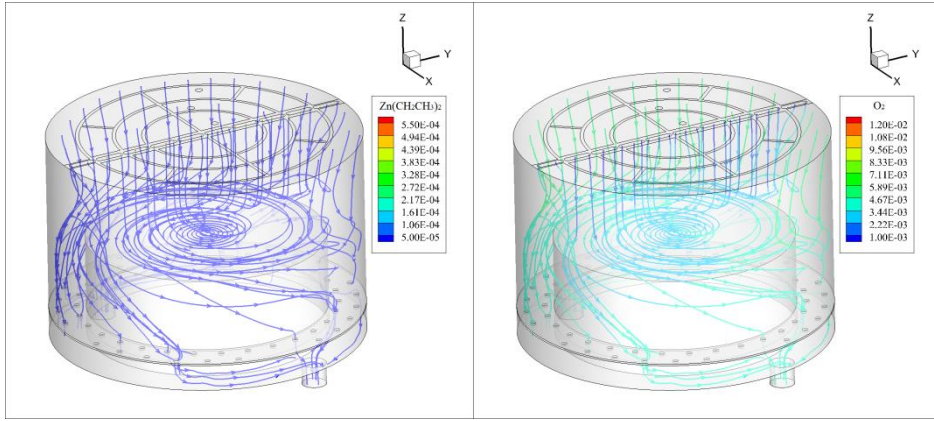


Fig. S2 The flows of the mass fractions of relevant species with the temperature of 773K: (a) $\text{Zn}(\text{CH}_2\text{CH}_3)_2$, (b) O_2 , (c) $\text{Zn}(\text{CH}_2\text{CH}_3)_2 \cdot \text{O}_2$, (d) $\cdot\text{CH}_2\text{CH}_2\text{ZnC}_2\text{H}_5 \cdot \text{HOO}\cdot$, (e) $\text{HOOZnC}_2\text{H}_5$, (f) $\text{HOCH}_2\text{CH}_2\text{ZnOH}$, (g) $\text{Zn}(\text{OH})_2$, (h) $\text{Zn}_3(\text{OH})_6$, (i) $\text{Zn}_3\text{O}_5\text{H}_4$, (j) $\text{Zn}_3\text{O}_4\text{H}_2$, (k) Zn_3O_3 . (l) C_2H_4 , (m) H_2O , (n) Ar



(g)

(h)

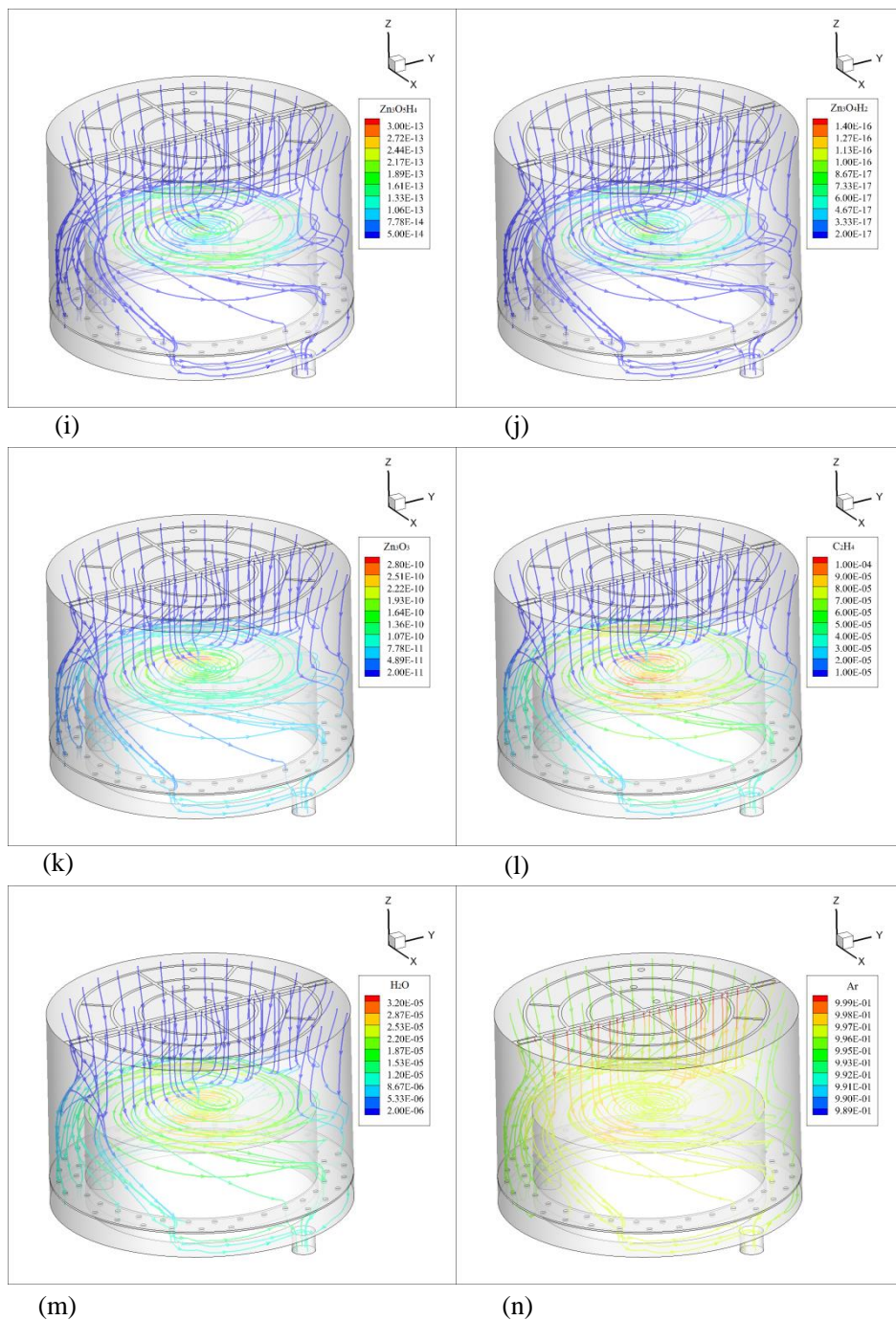
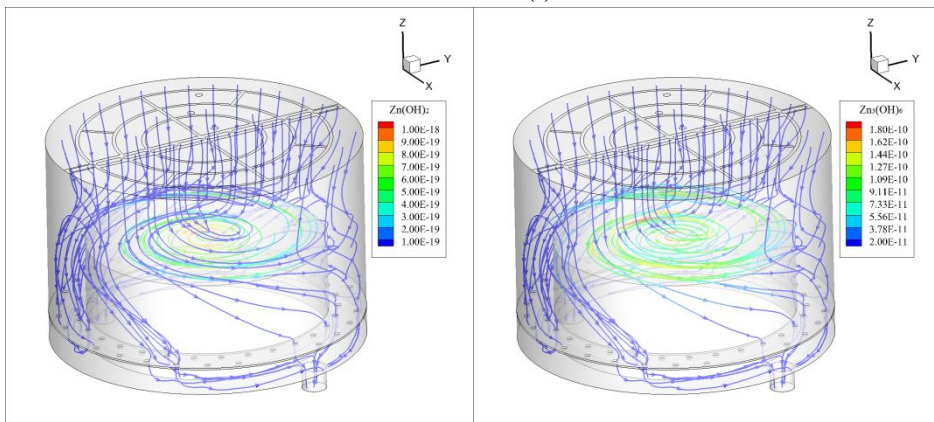
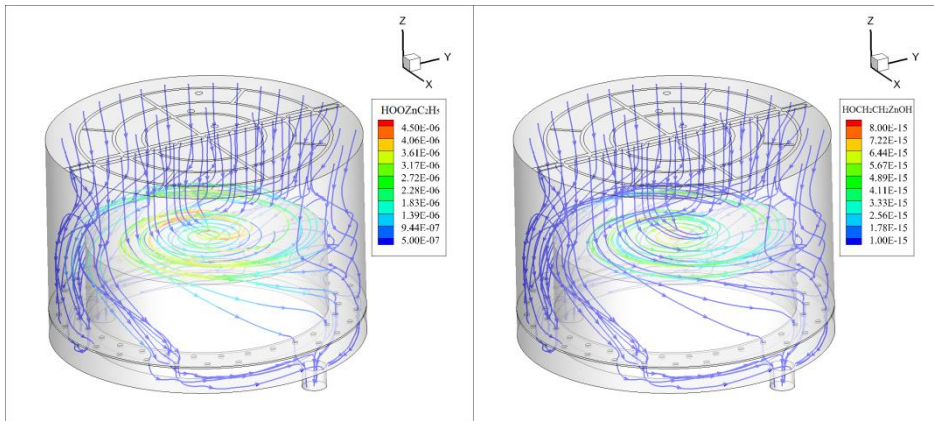
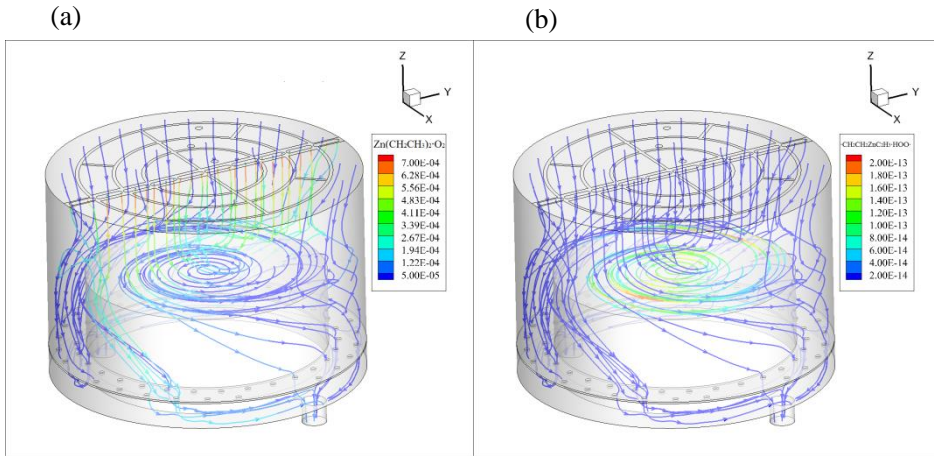
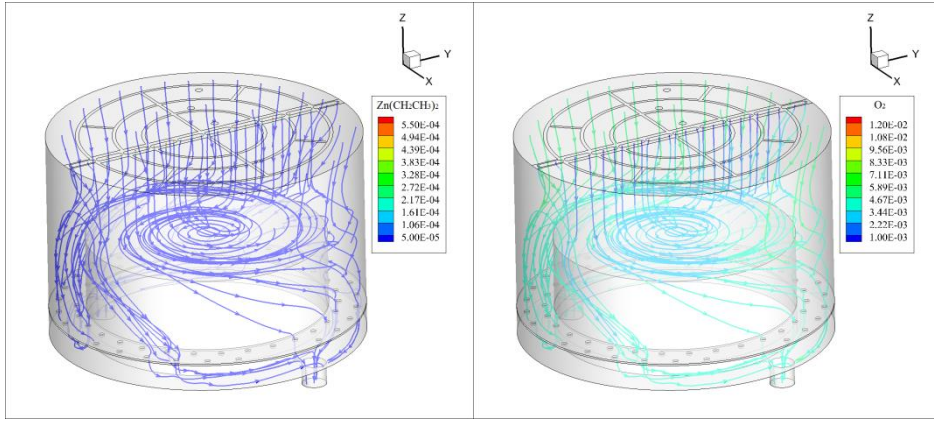


Fig. S3 The flows of the mass fractions of relevant species with the temperature of 873K: (a) $\text{Zn}(\text{CH}_2\text{CH}_3)_2$, (b) O_2 , (c) $\text{Zn}(\text{CH}_2\text{CH}_3)_2 \cdot \text{O}_2$, (d) $\cdot\text{CH}_2\text{CH}_2\text{ZnC}_2\text{H}_5 \cdot \text{HOO}\cdot$, (e) $\text{HOOZnC}_2\text{H}_5$, (f) $\text{HOCH}_2\text{CH}_2\text{ZnOH}$, (g) $\text{Zn}(\text{OH})_2$, (h) $\text{Zn}_3(\text{OH})_6$, (i) $\text{Zn}_3\text{O}_5\text{H}_4$, (j) $\text{Zn}_3\text{O}_4\text{H}_2$, (k) Zn_3O_3 . (l) C_2H_4 , (m) H_2O , (n) Ar



(g)

(h)

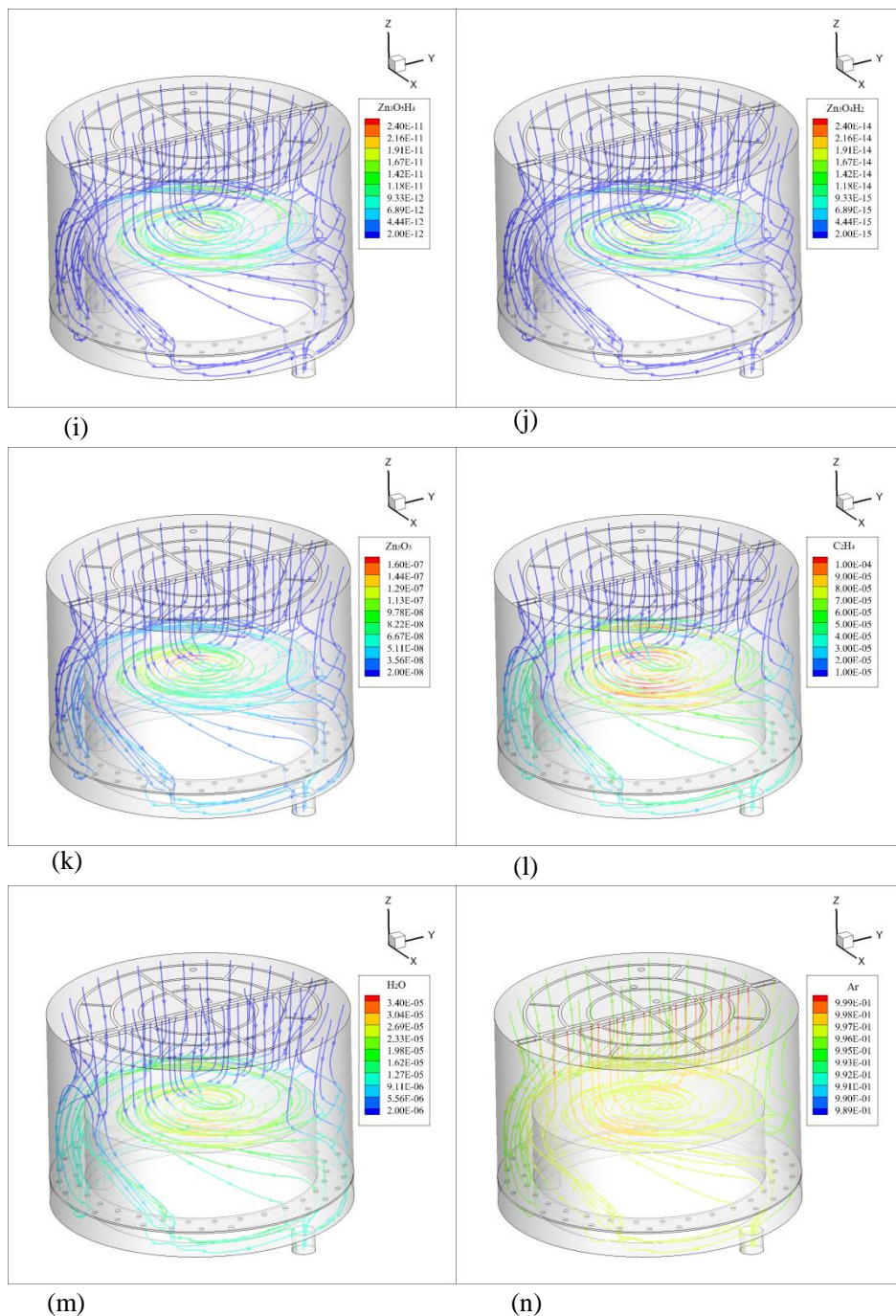
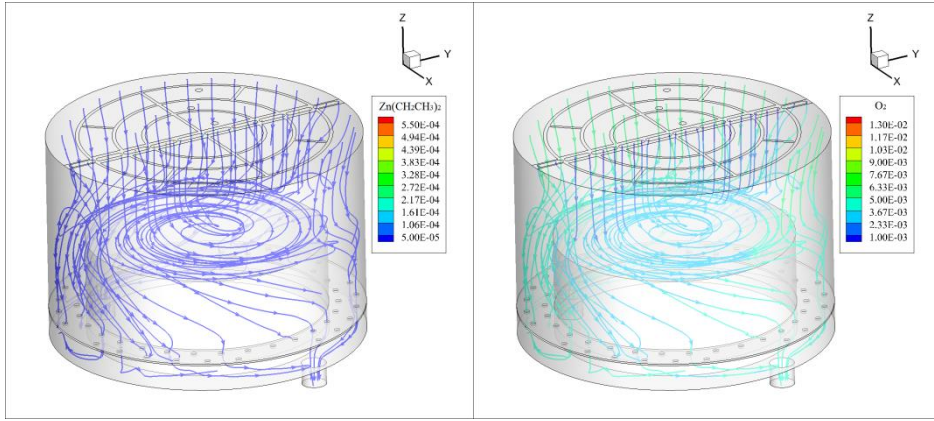
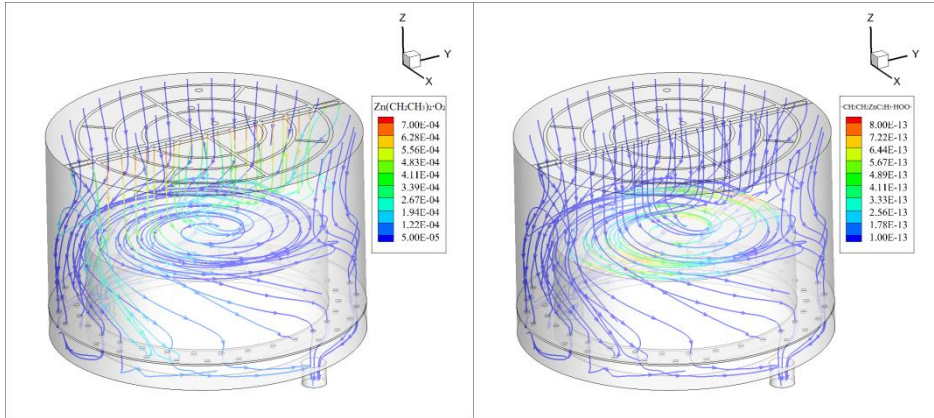


Fig. S4 The flows of the mass fractions of relevant species with the temperature of 973K: (a) $\text{Zn}(\text{CH}_2\text{CH}_3)_2$, (b) O_2 , (c) $\text{Zn}(\text{CH}_2\text{CH}_3)_2 \cdot \text{O}_2$, (d) $\cdot\text{CH}_2\text{CH}_2\text{ZnC}_2\text{H}_5 \cdot \text{HOO}\cdot$, (e) $\text{HOOZnC}_2\text{H}_5$, (f) $\text{HOCH}_2\text{CH}_2\text{ZnOH}$, (g) $\text{Zn}(\text{OH})_2$, (h) $\text{Zn}_3(\text{OH})_6$, (i) $\text{Zn}_3\text{O}_5\text{H}_4$, (j) $\text{Zn}_3\text{O}_4\text{H}_2$, (k) Zn_3O_3 . (l) C_2H_4 , (m) H_2O , (n) Ar



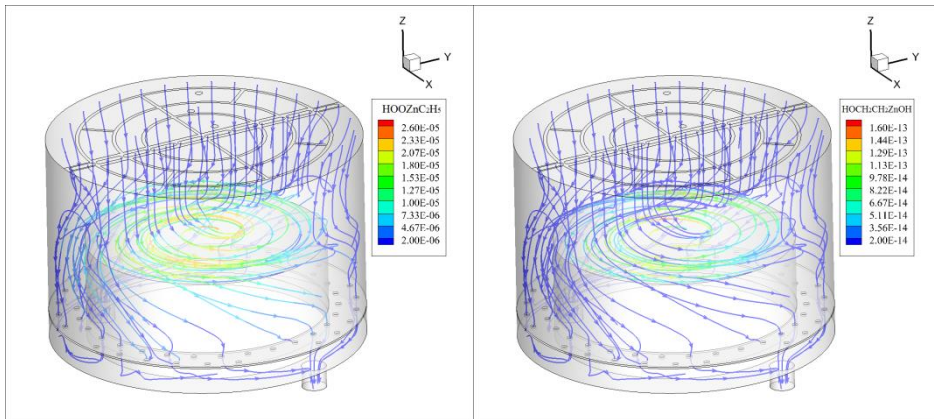
(a)

(b)



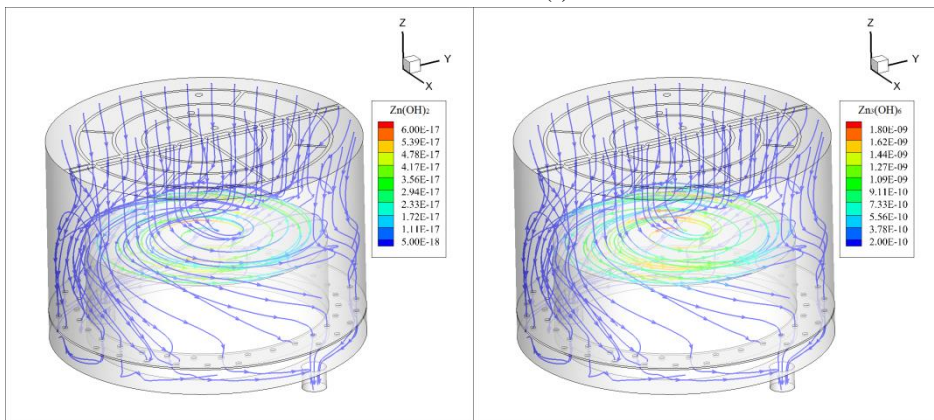
(c)

(d)



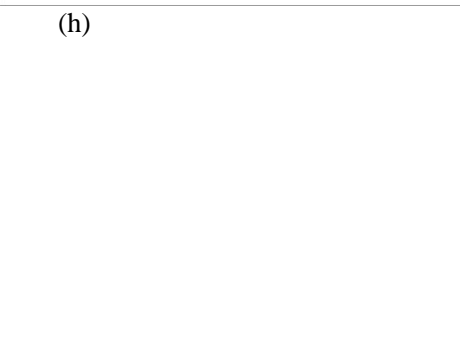
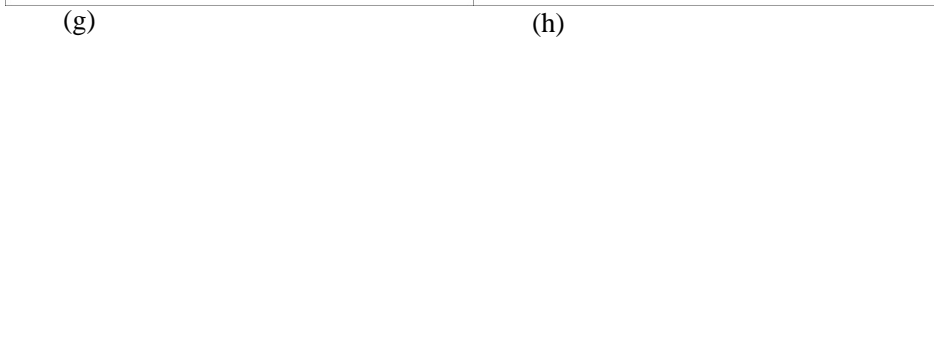
(e)

(f)



(g)

(h)



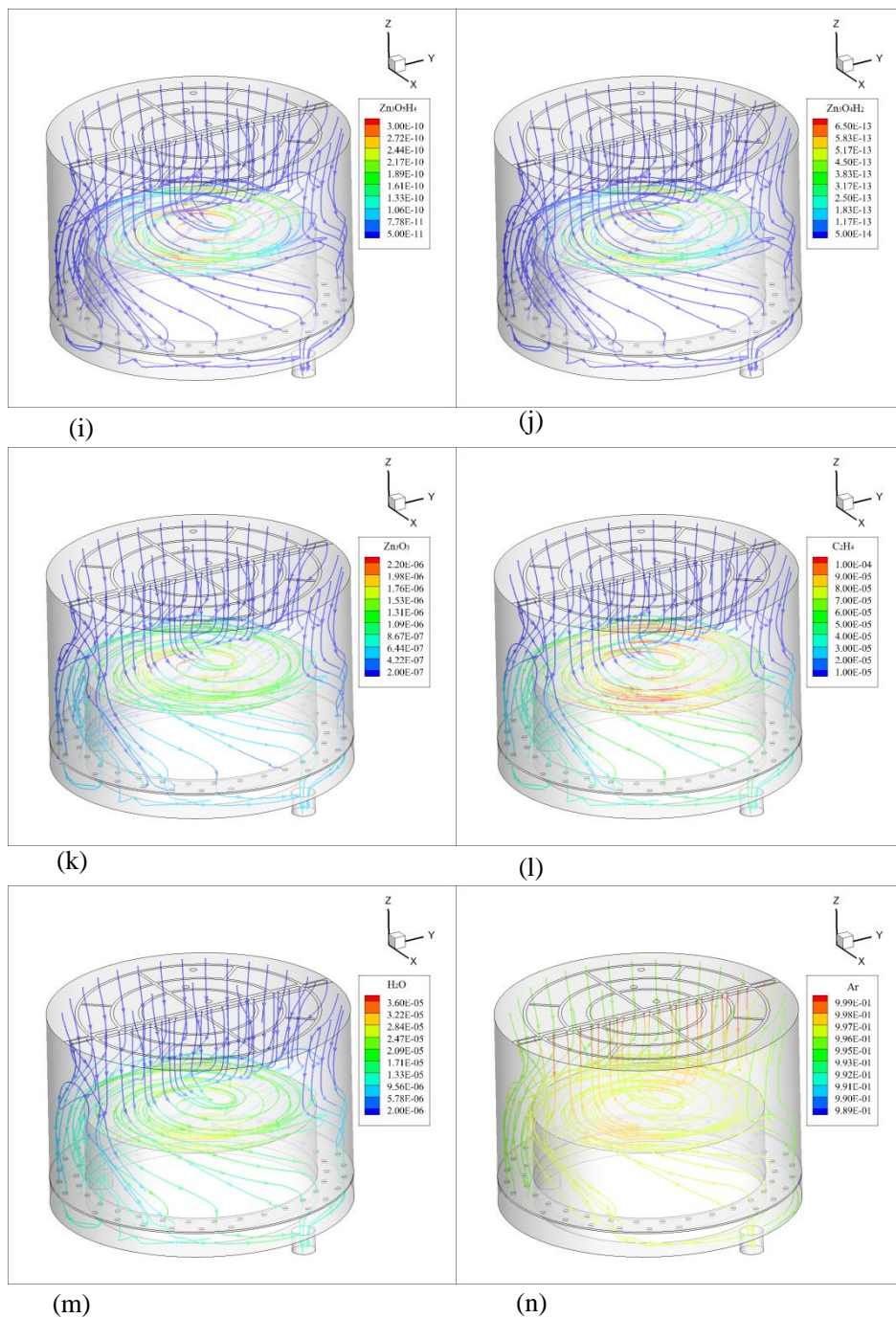


Fig. S5 The flows of the mass fractions of relevant species with the temperature of 1073K: (a) $Zn(CH_2CH_3)_2$, (b) O_2 , (c) $Zn(CH_2CH_3)_2\cdot O_2$, (d) $\cdot CH_2CH_2ZnC_2H_5\cdot HOO\cdot$, (e) $HOOZnC_2H_5$, (f) $HOCH_2CH_2ZnOH$, (g) $Zn(OH)_2$, (h) $Zn_3(OH)_6$, (i) $Zn_3O_5H_4$, (j) $Zn_3O_4H_2$, (k) Zn_3O_3 , (l) C_2H_4 , (m) H_2O , (n) Ar