Supplementary Materials

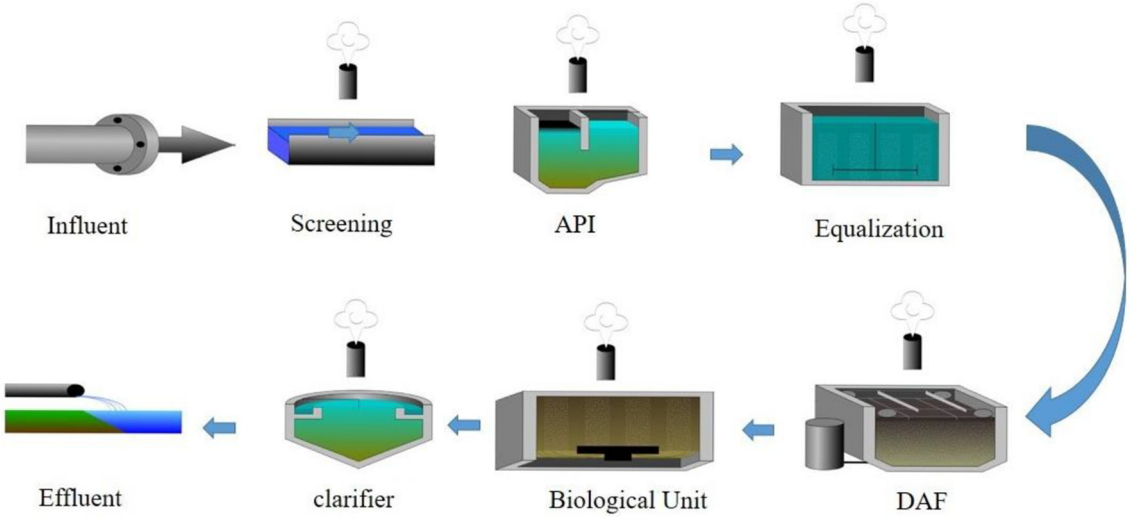

Fig. S1. The general schema of the WWTP of petrochemical company.

Table S1. The Specification of Wastewater Entering the WWTP in the Petrochemical Company

Specification	Value	Specification	Value
Temperature (℃)	33.6±1.1	TCOD (mg/L)	1,319±23
pH	8±1.5	Q_{in} (m^3/h)	200±23
Solved salt (mg/L)	334±16	Benzene (ppm)	187.47±7.3
Oil (mg/L)	41.5±8.2	Toluene (ppm)	23.19±0.4
TSS (mg/L)	227±17	Ethylbenzene (ppm)	30.52±0.5
BOD_5 (mg/L)	967±49	Xylene(ppm)	4.34±0.2

Table S2. Characteristics of the Existing Units in the WWTP

Depth (m)	Volume (m^3)	Unit
6	70	Screen
2.72	510	API
6.3	1860	Equalization
2.15	130	DAF
4.83	5500	Biological treatment
3.5	1580	Clarifier

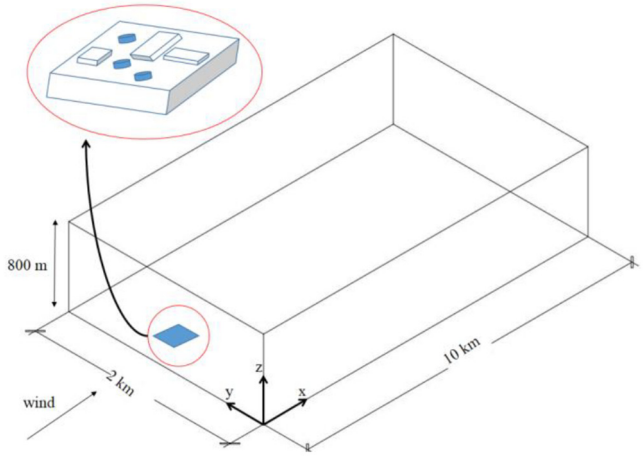

Fig. S2. A schematic representation of space domain along with WWTP location.

Table S3. Properties of BTEX

Compound	1Boiling Point (ºC)	1,2Vapor pressure (mm-Hg)
Benzene	80.1	94.8
Toluene	110.6	28.4
EthylBenzene	136.1	9.6
m-xylene	139.1	8.29
o-xylene	144.5	6.65
p-xylene	138.3	8.84

1. Data is available on the PubChem online database: (https://pubchem.ncbi.nlm.nih.gov/)
2. Vapor pressures are at 25 ºC.

Table S4. Entered and Emitted Values of BTEX to and from the WWTP

Component / Mass flow (g/d)	benzene	toluene	Ethylbenzene	m-Xylene	o-Xylene	p-Xylene	Total
Entering with wastewater	899,870	111,343	146,513	12,673	9,408	11,424	1,179,982
Emission to the air	671,875	79,564	95,842	7,327	6,376	7,443	868,427

Table S5. Reaction List of Reduced Mechanism Generated from Mechanism Reduction Algorithm

Num	Reaction	k*
1	' BENZENE + OH = $RA_{13}O_2$'	5.76E-13
2	' BENZENE + OH = $AROH_{14}$ + HO_2'	6.49E-13
3	' TOLUENE + OH = $RA_{16}O_2$'	4.57E-12
4	' TOLUENE + OH = $AROH_{17}$ + HO_2'	1.01E-12
5	' EBENZ + OH = $RN_{19}O_2$'	7.00E-13
6	' EBENZ + OH = $RA_{19}AO_2$'	6.30E-12
7	' OXYL + OH = $RA_{19}AO_2$'	9.52E-12
8	' OXYL + OH = $RA_{19}CO_2$'	4.08E-12
9	' MXYL + OH = $RA_{19}AO_2$'	1.61E-11
10	' MXYL + OH = $RA_{19}BO_2$'	6.93E-12
11	' PXYL + OH = $RA_{19}BO_2$'	4.29E-12
12	' PXYL + OH = $RA_{19}AO_2$'	1.00E-11
13	' NO + O_3 = NO_2'	1.78E-14
14	' OH + NO_2 = HNO_3'	9.76E-12
15	' NO_2 + hv = NO + O'	0.00892
16	' O_3 + hv = O_{1D}'	3.78E-05
17	' O_{1D} = OH + OH'	31586.4
18	' O_{1D} = O'	5.92E+08
19	' $RA_{19}AO_2$ + NO = $CARB_3$ + $UDCARB_{14}$ + HO_2 + NO_2'	7.73E-12
20	' $RA_{13}O_2$ + NO = $CARB_3$ + $UDCARB_8$ + HO_2 + NO_2'	8.23E-12
21	' HONO + hv = OH + NO'	0.001982
22	' HO_2 + NO = OH + NO_2'	8.49E-12
23	' $C_2H_5O_2$ + NO = CH_3CHO+HO_2+NO_2'	8.70E-12
24	' NO + NO_3 = NO_2 + NO_2'	2.60E-11
25	' OH + O_3 = HO_2'	7.41E-14
26	'OH + NO = HONO'	9.67E-12
27	' HO_2 + NO_2 = HO_2NO_2'	7.42E-13
28	'NO_3 + hv = NO_2 + O'	0.154
29	' $UDCARB_8$ + hv = $C_2H_5O_2$ + HO_2'	1.14E-5
30	' CH_3O_2 + NO = HCHO + HO_2 + NO_2'	7.62E-12
31	' NO_2 + O_3 = NO_3'	3.72E-12
32	' $UDCARB_{14}$ + hv = $RN_{13}O_2$ + HO_2'	9.81E-5
33	' $CARB_3$ + hv = CO + CO + HO_2 + HO_2'	2.78E-5
34	' $RA_{19}AO_2$ + NO = $RA_{19}NO_3$'	1.24E-12
35	' $UDCARB_{14}$ + hv = ANHY + HO_2 + $C_2H_5O_2$'	8.03E-5
36	' $RA_{19}BO_2$ + NO = $CARB_6$ + $UDCARB_{11}$ + HO_2 + NO_2'	7.73E-12
37	' $CARB_6$ + hv = CH_3CO_3 + CO + HO_2'	1.25E-4
38	' $RA_{13}O_2$ + NO = $RA_{13}NO_3$'	7.35E-13
39	' $UDCARB_{11}$ + hv = $RN_{10}O_2$ + HO_2'	9.81E-5
40	' $RN_{10}O_2$ + NO = C_2H_5CHO+HO_2+NO_2'	9.11E-12
41	' CH_3CO_3 + NO = CH_3O_2 + NO_2'	1.97E-11
42	' $RA_{16}O_2$ + NO = $RA_{16}NO_3$'	9.95E-13
43	' $UDCARB_{11}$ + hv = ANHY + HO_2 + CH_3O_2'	8.03E-5
44	' $RA16O_2$ + NO = $CARB_3$ + $UDCARB_{11}$ + HO_2 + NO_2'	5.58E-12
45	' $RA16O_2$ + NO = $CARB_6$ + $UDCARB_8$ + HO_2 + NO_2'	2.39E-12

* The units of rate constants are s^{-1} and $cm^3.molecule^{-1}.s^{-1}$, respectively, for the first and second order reactions

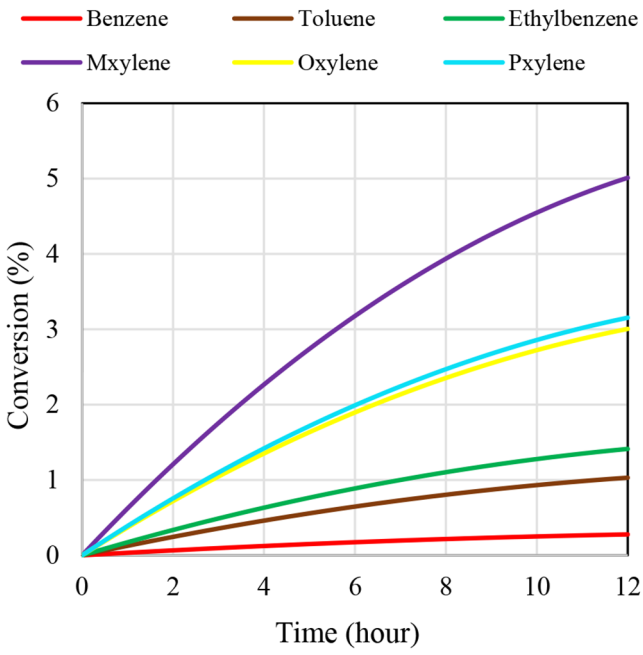

Fig. S3. A comparison of conversion of BTEX compounds for 3D simulation.