TableS1 The HOMO, LUMO, $2FED^2_{HOMO}$, $FED^2_{LUMO}+FED^2_{HOMO}$ values of each atom in the IBF molecule

Atom	HOMO	LUMO	$2FED^2_{HOMO}$	$FED^2_{LUMO}+FED^2_{HOMO}$
1(C)	0.08479	0.0723	0.16958	0.1571
2(C)	0.08699	0.0975	0.17398	0.1845
3(C)	0.20979	0.1774	0.41958	0.3872
4(C)	0.07545	0.0795	0.1509	0.1549
5(C)	0.10028	0.0834	0.20056	0.1837
6(C)	0.21114	0.1829	0.42228	0.3940
7(H)	0.0052	0.0064	0.0104	0.0116
8(H)	0.00525	0.0097	0.0105	0.0149
9(H)	0.00454	0.0075	0.00908	0.0120
10(H)	0.00639	0.0085	0.01278	0.0149
11(C)	0.03919	0.0292	0.07838	0.0684
12(C)	0.03225	0.0166	0.0645	0.0489
13(H)	0.00417	0.0042	0.00834	0.0084
14(H)	0.01348	0.0107	0.02696	0.0241
15(C)	0.00616	0.0042	0.01232	0.0104
16(H)	0.00256	0.0013	0.00512	0.0039
17(H)	0.00288	0.0011	0.00576	0.0040
18(H)	0.00075	0.0011	0.0015	0.0018
19(H)	0.00044	0.0007	0.00088	0.0011
20(C)	0.00728	0.0032	0.01456	0.0105
21(H)	0.00074	0.0007	0.00148	0.0014
22(H)	0.00377	0.0025	0.00754	0.0062
23(H)	0.00129	0.0003	0.00258	0.0016
24(C)	0.02836	0.0378	0.05672	0.0662
25(C)	0.02144	0.0207	0.04288	0.0422
26(H)	0.00175	0.0036	0.0035	0.0054
27(H)	0.00492	0.0059	0.00984	0.0109
28(H)	0.0017	0.0017	0.0034	0.0034
29(H)	0.00234	0.0032	0.00468	0.0056
30(C)	0.01447	0.0647	0.02894	0.0792
31(O)	0.01259	0.0375	0.02518	0.0501
32(O)	0.00677	0.0225	0.01354	0.0293
33(H)	0.00087	0.0015	0.00174	0.0023
33(H)	0.00087	0.0015	0.00174	0.0023

Table S2 Atomic charge values in IBF molecules

Atom	Charge value	Atom	Charge value
1(C)	-0.23028	18(H)	0.22927
2(C)	-0.23246	19(H)	0.22461

3(C)	-0.04836	20(C)	-0.68352
4(C)	-0.21835	21(H)	0.22064
5(C)	-0.23233	22(H)	0.2427
6(C)	-0.02998	23(H)	0.23171
7(H)	0.24298	24(C)	-0.35411
8(H)	0.25245	25(C)	-0.67039
9(H)	0.24175	26(H)	0.27345
10(H)	0.24069	27(H)	0.23992
11(C)	-0.46448	28(H)	0.2486
12(C)	-0.23907	29(H)	0.24029
13(H)	0.23453	30(C)	0.94888
14(H)	0.24259	31(O)	-0.68231
15(C)	-0.67661	32(O)	-0.77805
16(H)	0.23618	33(H)	0.51573
17(H)	0.23335		

Table S3 Detection information of IBF and its intermediate products

product	Retention time (min)	Theoretical quality [M-H]	Test quality [M-H]	error (ppm)	Molecular formula
IBF	12.689	205.1234	205.1234	0.00	$C_{18}H_{13}O_2$
P1	11.555	221.1183	221.1185	0.90	$C_{18}H_{13}O_3$
P2	11.502	177.1285	177.1281	2.26	$C_{12}H_{18}O$
P3	8.846	165.0557	165.0552	3.03	$C_9H_{10}O_3$
P4	7.613	149.0972	149.0972	0.00	$C_{10}H_{14}O$
P5	11.040	175.1128	175.1123	2.92	$C_{12}H_{16}O$
P6	8.295	121.0659	121.0660	0.83	$C_8H_{10}O$
P7	9.758	133.0659	133.0658	0.75	$C_9H_{10}O$
P8	8.926	135.0452	135.0452	0.00	$C_8H_8O_2$
P9	4.056	125.0244	125.0241	2.40	$C_6H_6O_3$
P10	9.827	191.1078	191.1076	1.05	$C_{12}H_{16}O_2$
P11	4.522	117.0557	117.0554	2.62	$C_5H_{10}O_3$
P12	8.927	171.0663	171.0667	2.34	$C_8H_{12}O_4$
P13	2.495	72.9931	72.9936	6.85	$C_2H_2O_3$

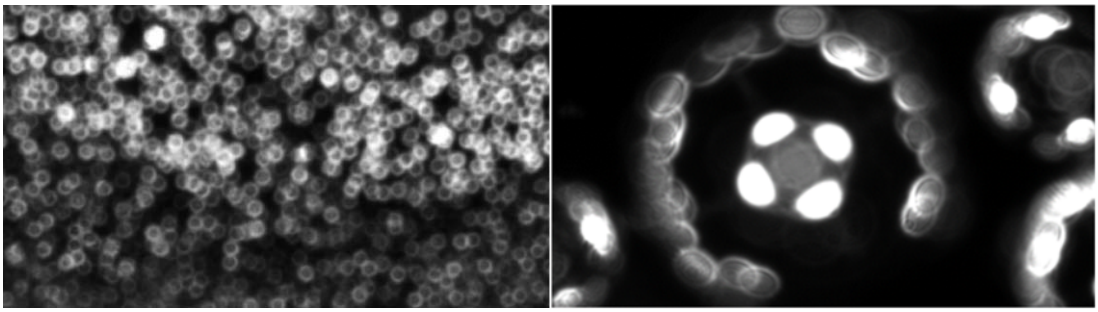

Figure S1 Observation of bubble morphology. (a) Observation of ozone micro-nano bubble morphology; (b) Observation of ordinary ozone bubble morphology

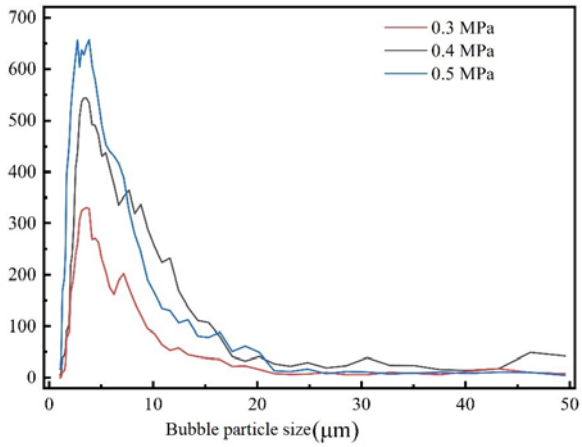

Figure S2 Particle size distribution of ozone micro-nano bubbles

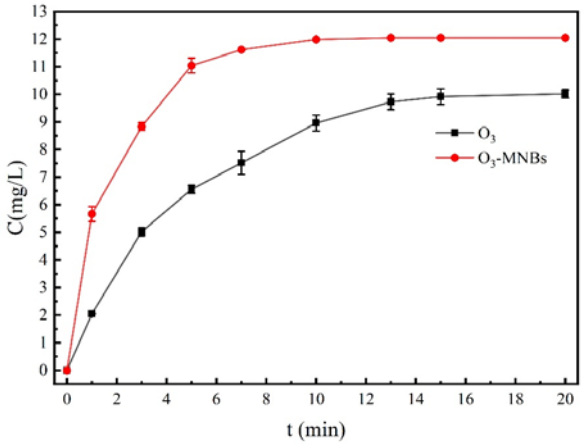

Figure S3 Variations in O_3-MNBs and O_3 concentrations during the two aeration processes

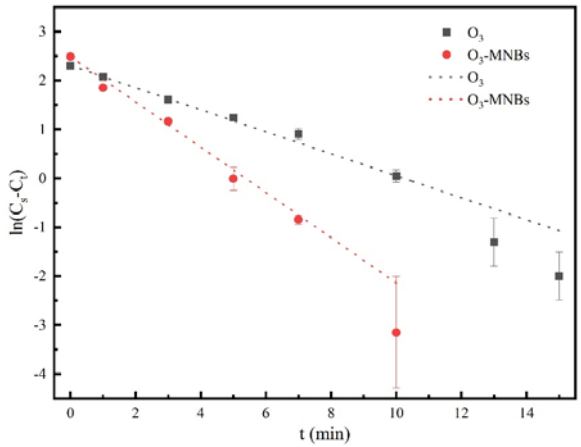

Figure S4 The O_3 mass transfer coefficient in two ozone aeration processes

Equation S1-S2 The O_3 mass transfer coefficient in two ozone aeration processes

$$\frac{d_c}{d_t} = k_z \alpha_t (C_s - C_t) \tag{S1}$$

$$\ln(C_s - C_t) = -k_L \alpha_t t + C \tag{S2}$$

In the equation:

k_L——The mass transfer coefficient of the liquid（m/min）;

α_t——Total specific surface area，$\alpha_t = A_t/V$（m^{-1}）;

A_t——Total surface area for mass transfer（m^2）;

V——The volume of the body of water（m^3）;

$k_L\alpha_t$——The total mass transfer coefficient of the system（min^{-1}）;

C_s——The highest value of the dissolved gas concentration（mg/L）;

C_t——Measured value of dissolved gas concentration（mg/L）.