Supporting Information

Catalytic Ozonation in Advanced Treatment of Kitchen Wastewater: Multi-scale Simulation and Pilot-scale Study

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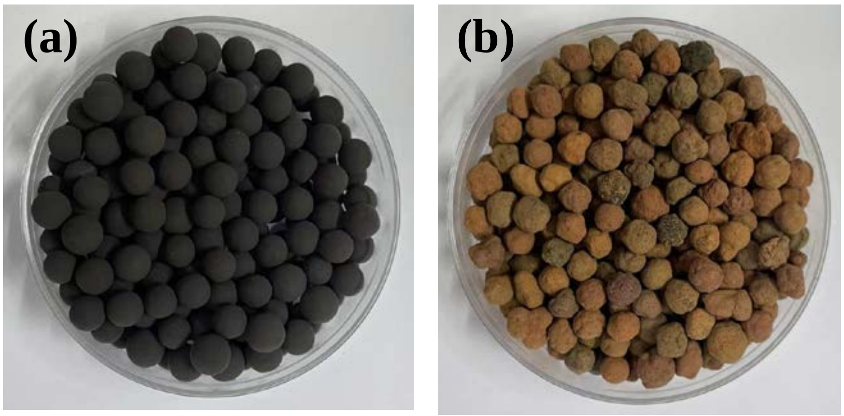

Fig.S1 Physical morphology of (a) Catalysts I and (b) Catalysts II

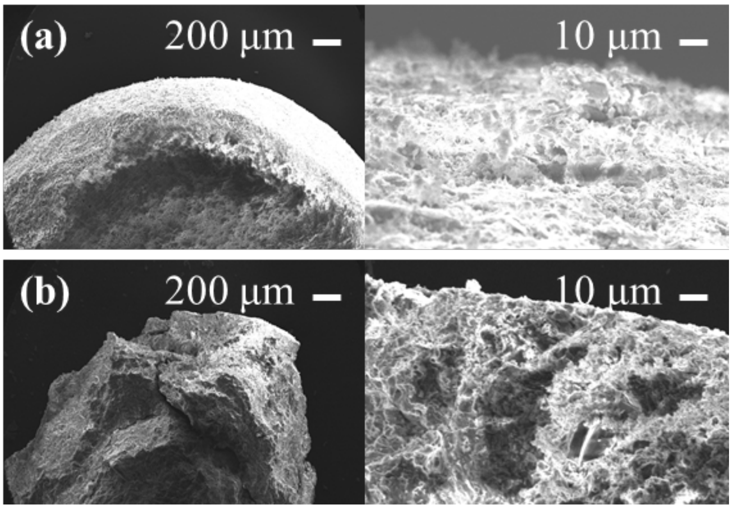

Fig.S2 SEM images for (a) Catalysts I and (b) Catalysts II

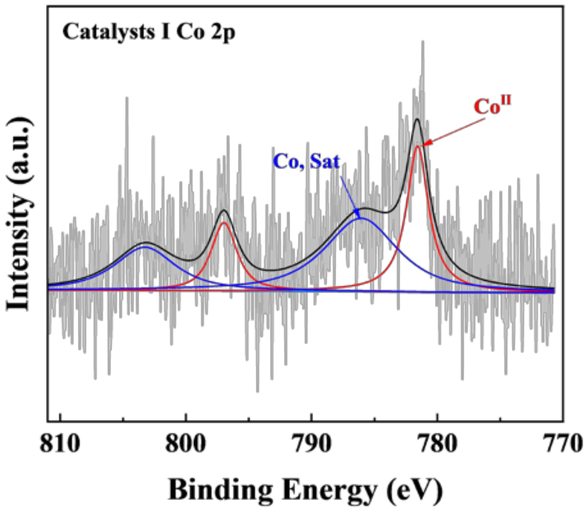

Fig.S3 The high-resolution XPS spectrum of Co 2p for Catalysts I

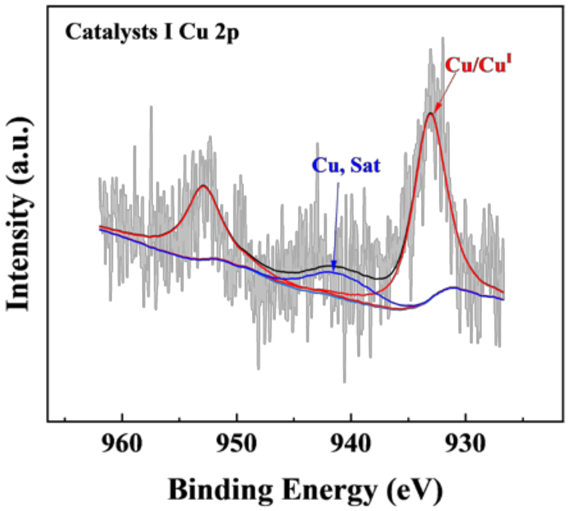

Fig.S4 The high-resolution XPS spectrum of Cu 2p for Catalysts I

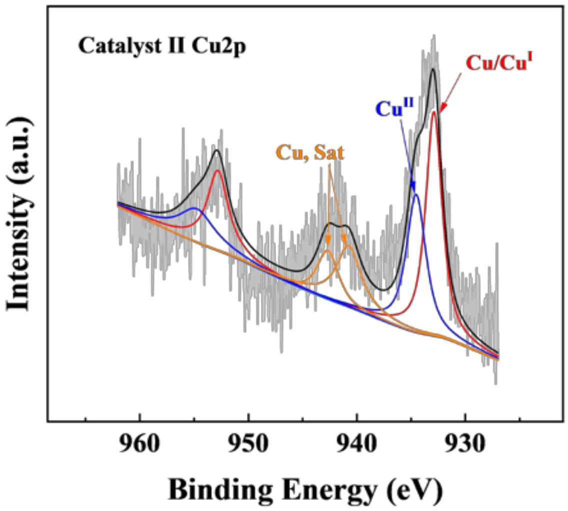

Fig.S5 The high-resolution XPS spectrum of Cu 2p for Catalysts II

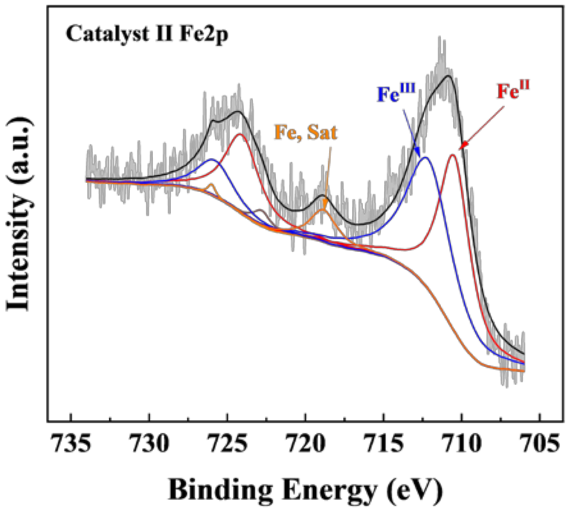

Fig.S6 The high-resolution XPS spectrum of Fe 2p for Catalysts II

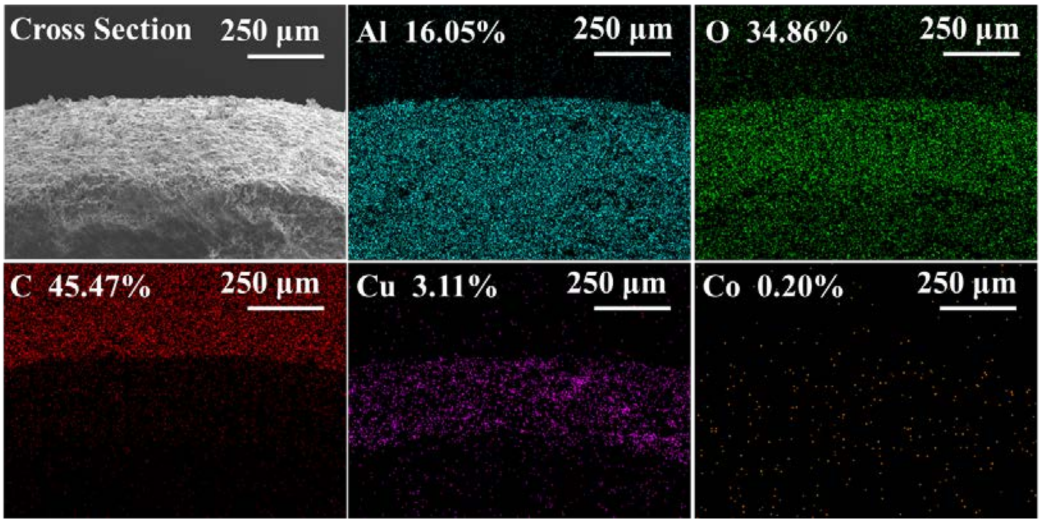

Fig.S7 EDS-mapping analysis for the cross section of Catalysts I

Fig.S7 was EDS-mapping analysis for the cross section of Catalysts I. It was obviously observed that Cu and C were distributed in spherical shell.

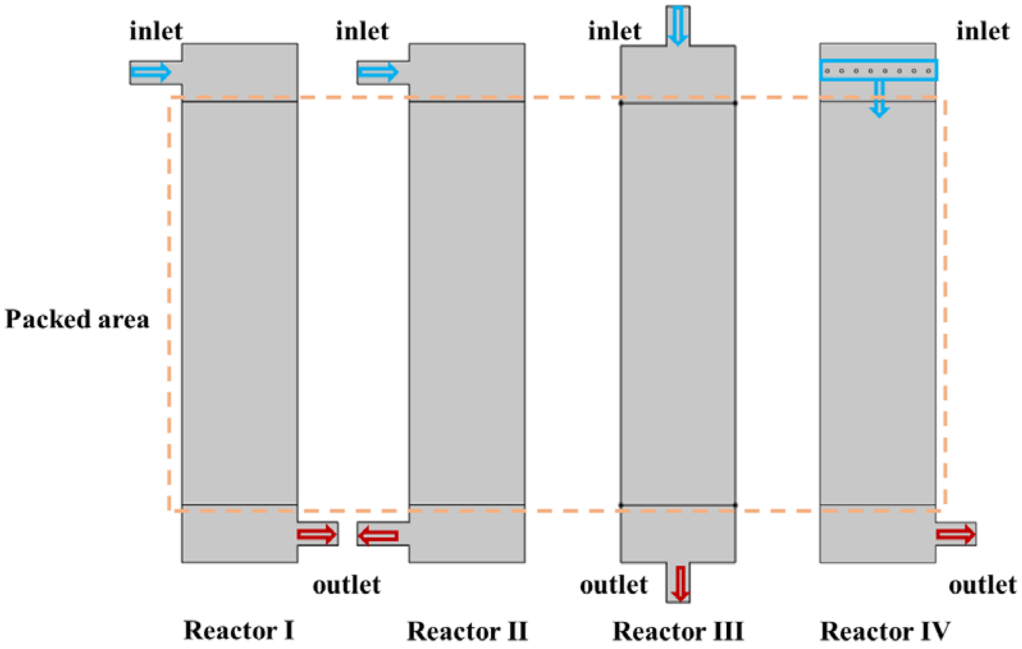

Fig.S8 Four different structures of Reactor I (in and out structure on different sides), Reactor II (in and out structure on the same side), Reactor III (top in and bottom out structure), and Reactor IV (water-distribution structure)

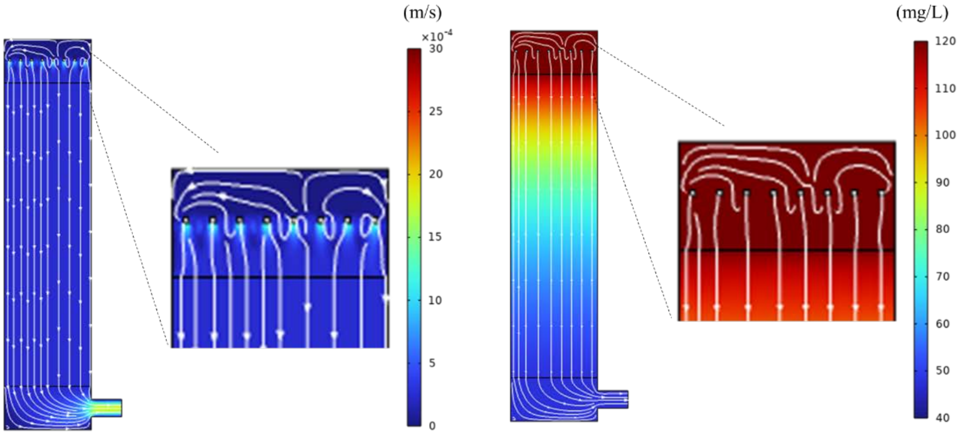

Fig.S9 The enlarged view of (a) velocity and (b) COD distribution details of the Reactor IV

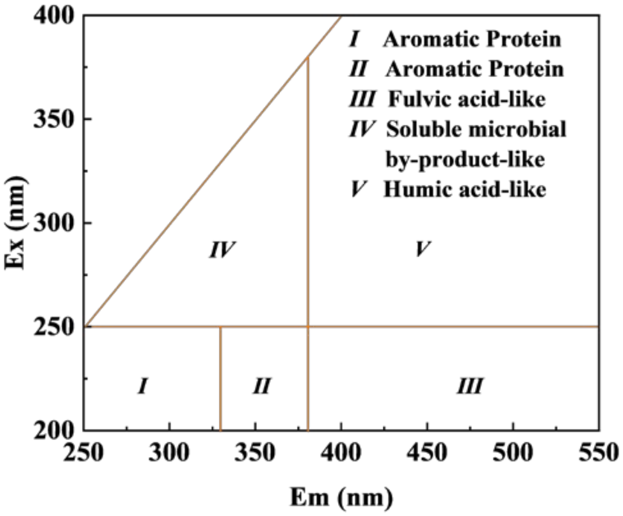

Fig. S10 Schematic diagram of partition for EEM fluorescence spectrum

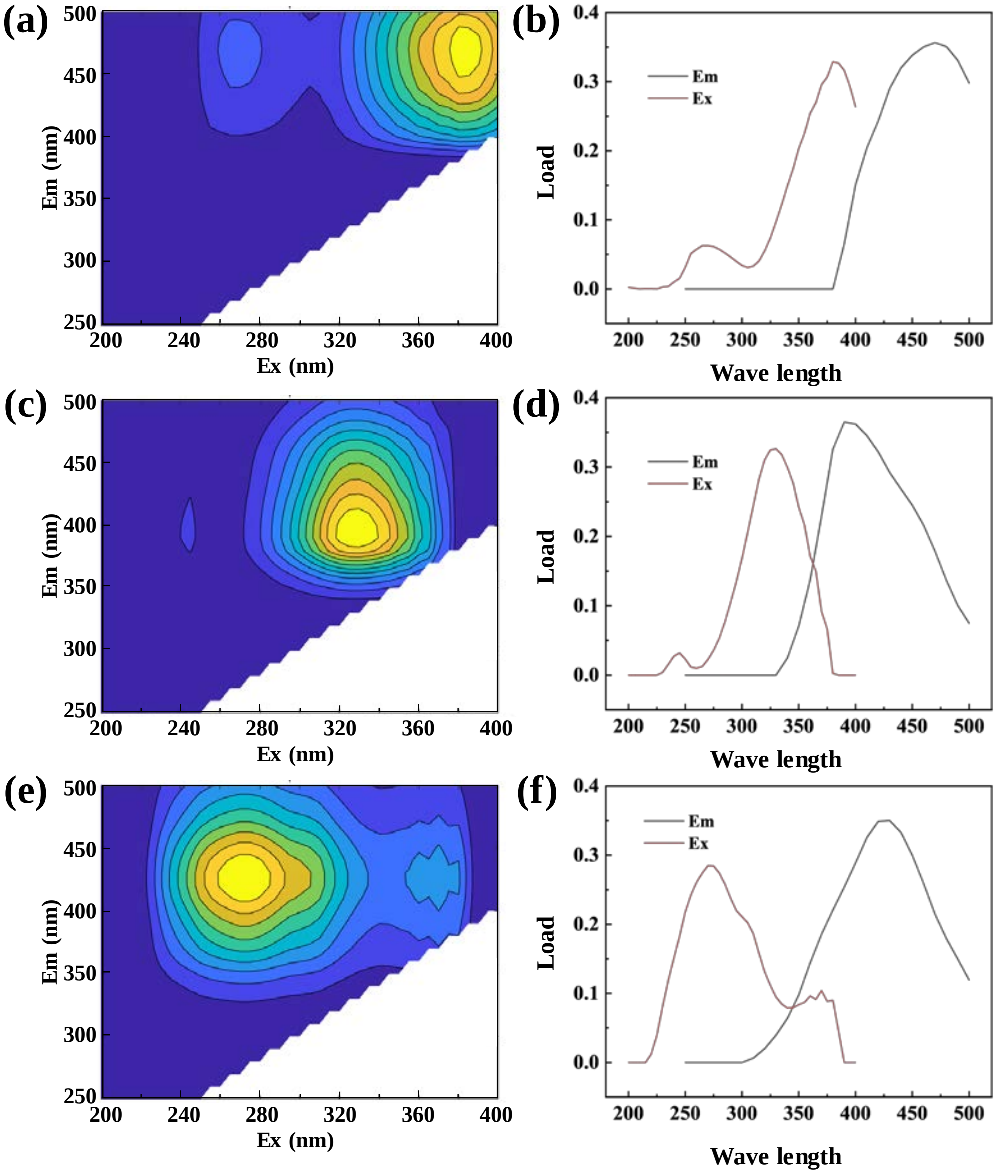

Fig.S11 Parallel factor analysis of EEM for pilot effluent. (a) EEM and (b) load of component 1. (c) EEM and (d) load of component 2. (e) EEM and (f) load of component 3.

The results of PARAFAC analysis were shown in Fig.S11, which illustrated the effluent of O_3/Catalyst I in pilot tests mainly contained three kinds of components. Component 1 (385 nm/470 nm), component 2 (330 nm/400 nm) and component 3 (270 nm/420 nm) were presumably humic acid-like matters.

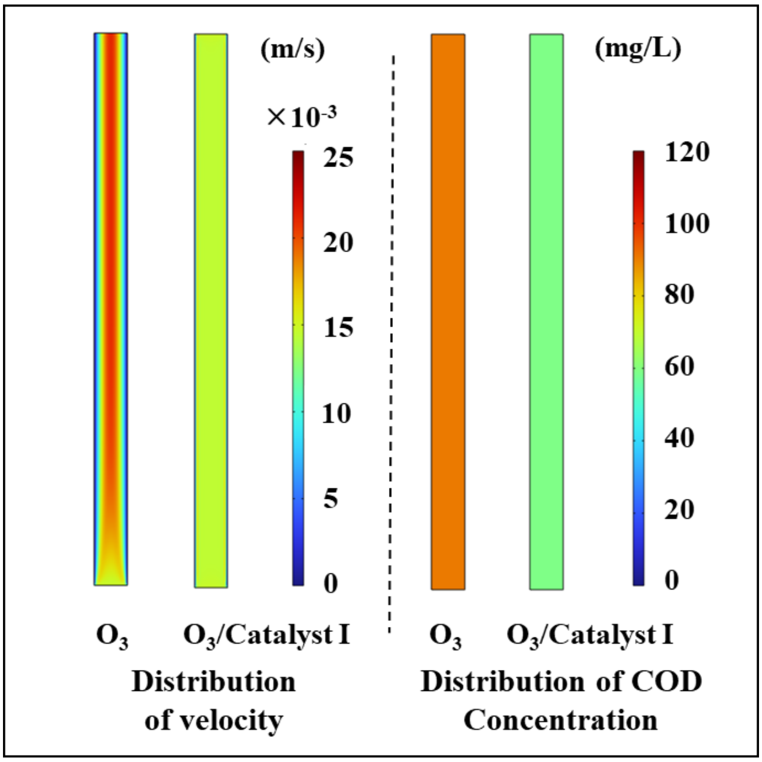

Fig.S12 Distribution of velocity and COD concentration for lab-scale model

Fig.S12 (left) showed the distribution of velocity in O_3 reactor and O_3/Catalyst I reactor. The distribution of velocity in O_3 reactor appeared obvious boundary layer effects. The distribution of velocity in O_3/Catalyst I reactor showed pretty evenly. Fig.S12 (right) showed the distribution of COD concentration in O_3 reactor and O_3/Catalyst I reactor. It illustrated that COD concentration was uniformly distributed and COD was lower in O_3/Catalyst I reactor than O_3 reactor.

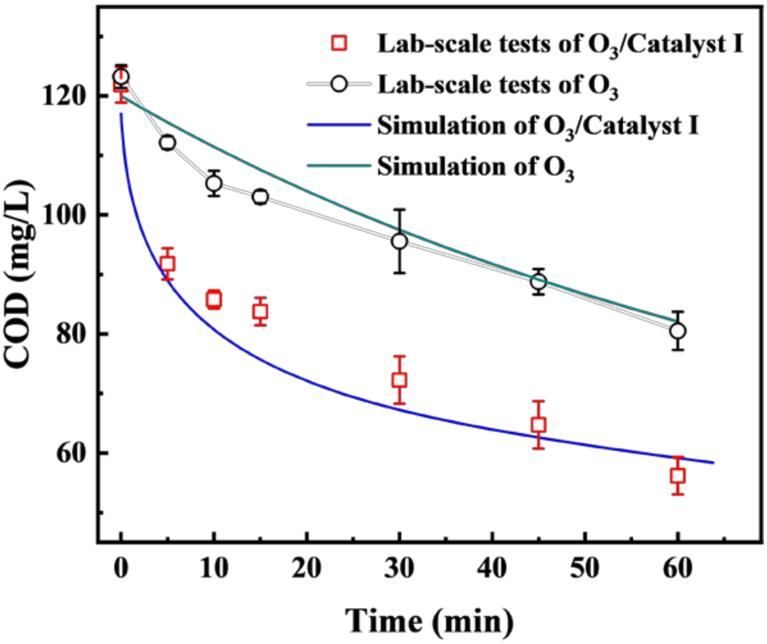

Fig.S13 Results of actual tests and simulation in lab scale

Fig.S13 showed the results of simulation and lab-scale tests, which could prove that this basic model fit well.

Table S1 The parameters of each peak of XPS Co 2p for Catalysts I

Peak species	Binding Energy (eV)	Proportion (%)
Co^{II}	781.57	39.8
Co, Sat	803.26/786.06	60.2

Table S2 The parameters of each peak of XPS Cu 2p for Catalysts I

Peak species	Binding Energy (eV)	Proportion (%)
Cu/Cu^{I}	933.15	88.0
Cu, Sat	941.01	12.0

Table S3 The parameters of each peak of XPS Cu 2p for Catalysts II

Peak species	Binding Energy (eV)	Proportion (%)
Cu/Cu^{I}	932.9	45.5
Cu^{II}	934.54	32.7
Cu, Sat	940.74/ 942.67	21.8

Table S4 The parameters of each peak of XPS Fe 2p for Catalysts II

Peak species	Binding Energy (eV)	Proportion (%)
Fe^{II}	710.46	50.0
Fe^{III}	712.11	43.1
Fe, Sat	722.8/718.83	6.9

Table S5 The chroma and COD for discharge standards and influent/effluent of the pilot reactor

Water quality index	Unit	B level of GB/T 31962-2015	First level of GB 8978-1996	Pilot	
				Influent	Effluent
chroma	Times	64	50	128	8
COD	mg/L	500	60	125±5	60

Table S6 Parameters of multi-scale packed bed reactor model

Expression	Value	Explanation	Source
v_0	0.0025 m/s	Velocity of influent in lab-scale reactor	Measured in lab
V_0	0.014 m/s	Velocity of influent in pilot-scale reactor	Designed in pilot
k^f_1	1.4×10^{-4} L/(mg·min)	Reaction rate constant of O_3/Catalyst I process	Fitted based on lab-scale tests
k^f_2	6.4×10^{-5} L/(mg·min)	Reaction rate constant of O_3 process	Fitted based on lab-scale tests
r_{pe}	2.5 mm	Catalyst particle radius	Measured in lab
r_b	6 mm	Reactor radius of lab-scale reactor	Measured in lab
R_b	0.2 m	Reactor radius of pilot-scale reactor	Designed in pilot
h_b	200 mm	Reactor height of lab-scale reactor	Measured in lab
H_b	1.8 m	Reactor height of pilot-scale reactor	Designed in pilot
ε_b	0.38	porosity of bed	Measured in lab
ε_{pe}	0.4	porosity of catalyst	Measured in lab
κ	1.9826×10^{-8}	Permeability of bed	Calculated from Kozeny-Carman formula

The multi-scale model included three physical fields: chemistry, flow field and material transport. A second-order kinetic reaction for the decomposition of pollutants by ozone oxidation was constructed in the chemical physical field, and the rate constants were obtained by laboratory experiments. The flow field consisted of free flow and porous media flow. The free flow zone was used to describe the water flow in the upper and lower parts of the reactor that were not loaded with catalysts. Porous media flow was used to describe the water flow in the middle of the reactor where the catalysts were loaded. The Kozeny-Carman equation was used to describe the permeability of porous media.

$$\kappa = \frac{d_p^2}{180} \frac{\varepsilon_p^3}{(1-\varepsilon_p)^2}$$

where κ is the permeability of porous media, d_p is the diameter of particle, ε_p is bed porosity, whose value is 0.38.

The material transfer physical field described the movement of reactants in the reactor coupled with chemical reactions and fluid flows. The packed bed model was used to describe the catalyst bed.