UNESCO-IWRA ONLINE CONFERENCE

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3RD IN THE IWRA ONLINE CONFERENCE SERIES

Emerging Pollutants: Protecting Water Quality for the Health of People and the Environment

Emerging pollutant degradation by UV-AOPs in practical waters: A novel prediction method combining model simulation with portable measurement

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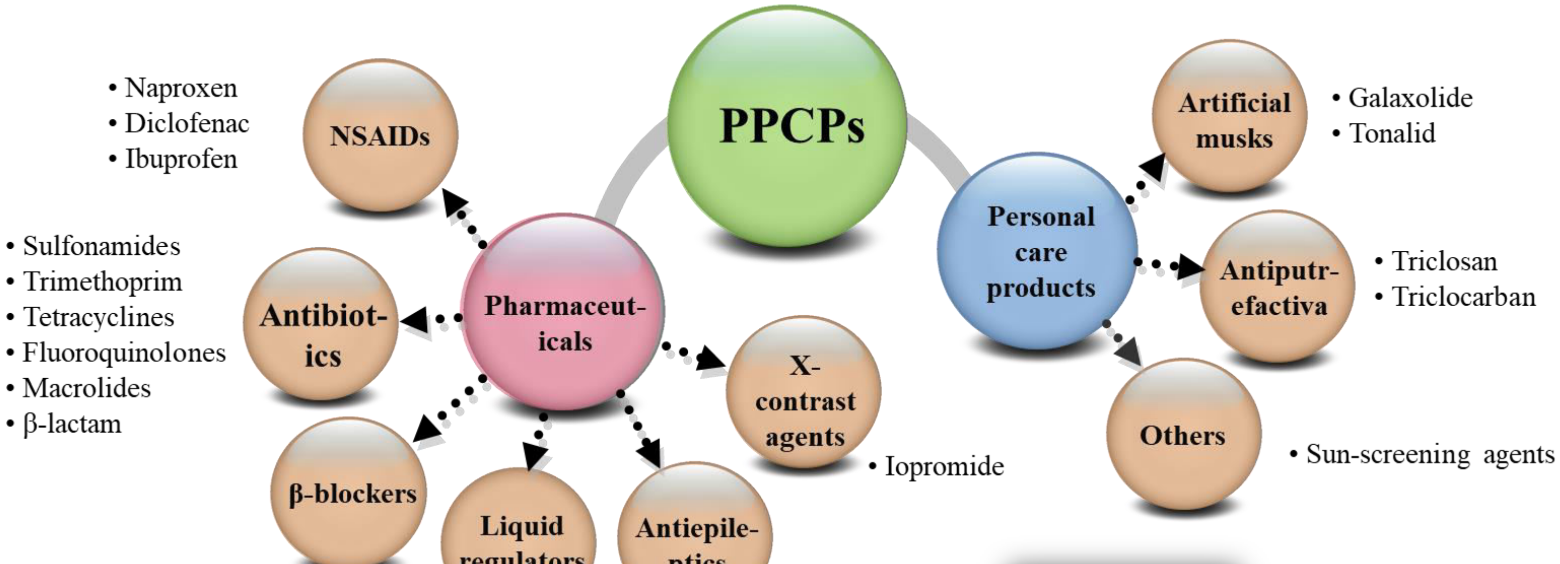
IWRA International Water Resources Association

1. Introduction

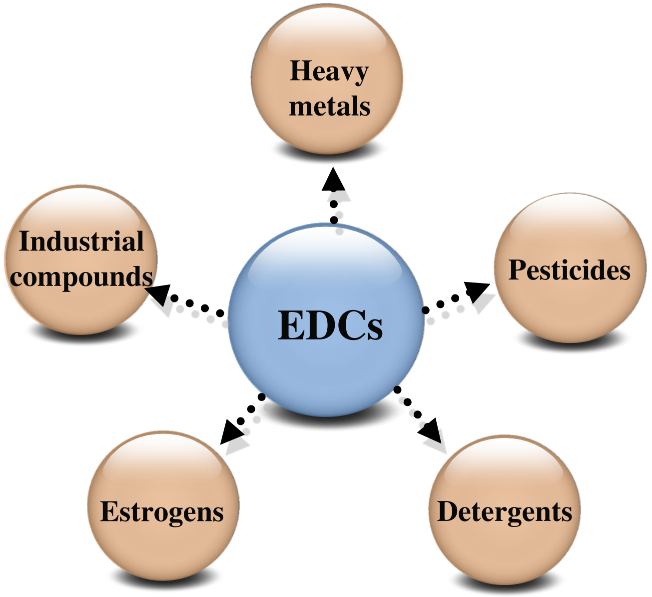
Emerging pollutants (EPs): A key scientific and technical challenge to water safety!

PPCPs: Pharmaceuticals and Personal Care Products



Antibiotic resistant bacteria

EDCs: Endocrine Disrupting Chemicals



Malformation

Feminization

UV-based Advanced Oxidation Processes (UV-AOPs)

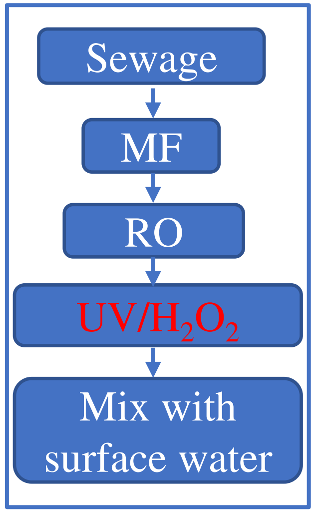
UV-AOPs have been proved highly effective for the removal of EPs in water.

Cornwall drinking water treatment plant in Canada

Andijk drinking water treatment plant in Netherlands

Haidai sewage treatment plant in China

West Basin water recycling plant in America



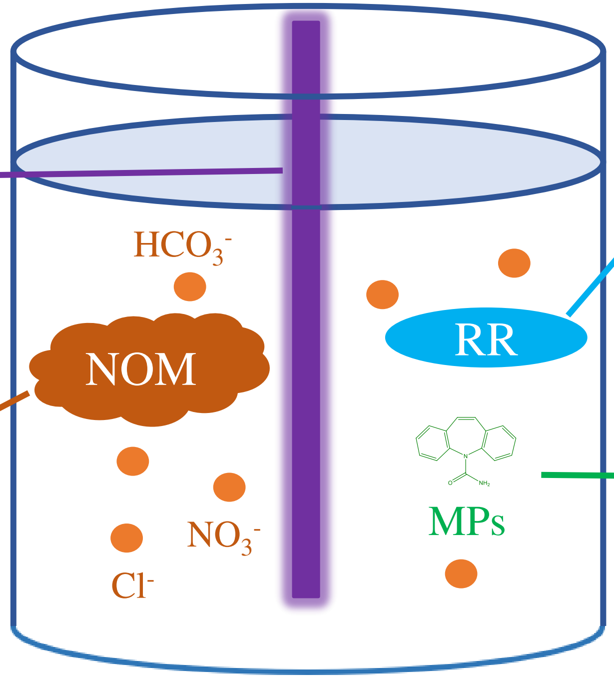
UV-AOPs has been widely used in the advanced treatment of drinking water, sewage and reclaimed water all over the world.

EP Degradation by UV-AOPs

Experimental considerations

- **Various light sources**
  LP, VUV/UV, MP lamps…

- **Various water matrices**
  NOM, Cl^-, HCO_3^-, NO_3^-…



- **Various UV-AOPs**
  UV/H_2O_2, $UV/S_2O_8^{2-}$, UV/Chlorine…

- **Various target emerging pollutants**
  PPCPs, EDCs,….

UV-AOP Performance Evaluation

On-site sampling

Lab-scale experiments

UV-AOP performance evaluation

Current limitations:

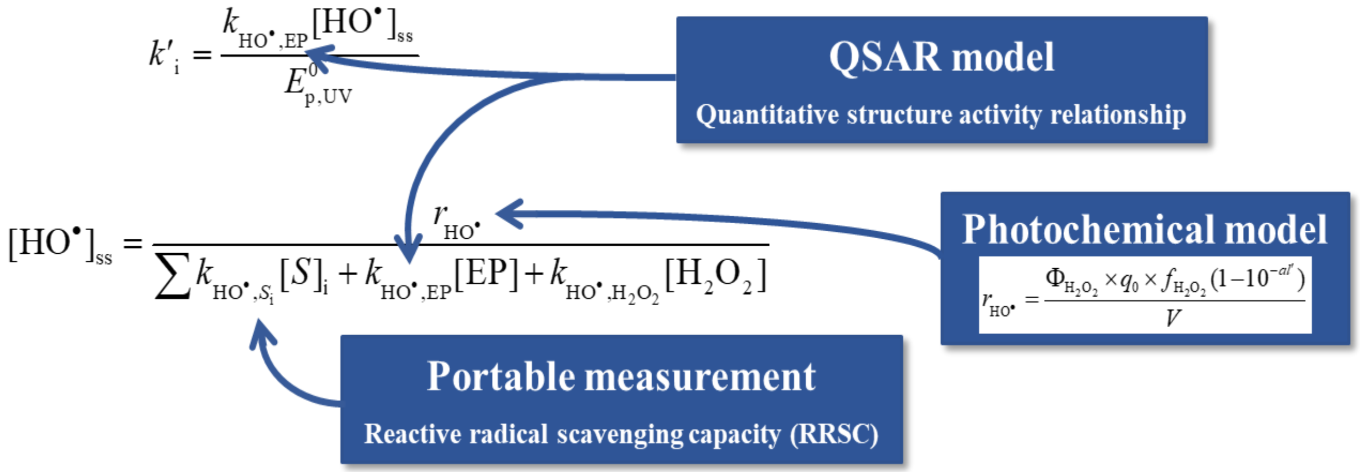
- Heavy workload
  - ✓ Frequent sample transportation
  - ✓ Many lab-scale experiments
  - ✓ Advanced analytical instruments
- High professional requirements
- Time consuming & Expensive!

- It is urgent to develop a rapid & accurate on-site method for UV-AOP performance evaluation for various water matrices.

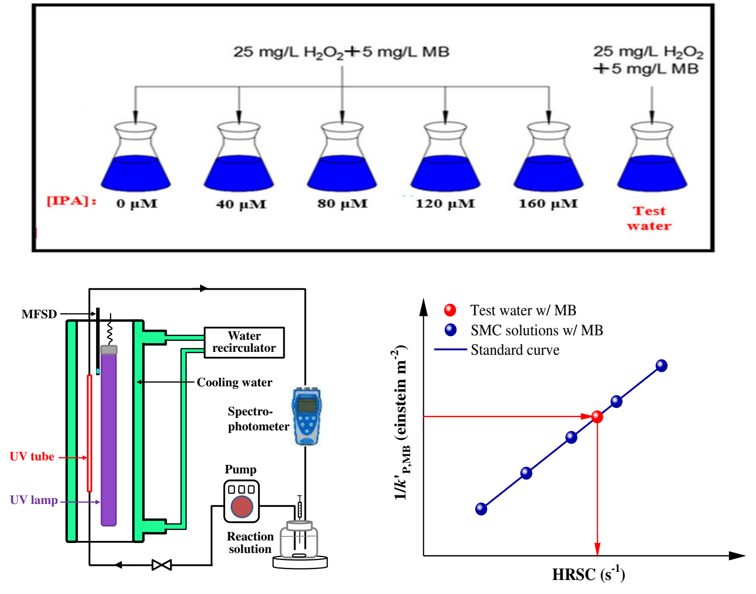
2. Model Simulation & Portable Measurement (MS&PM) Method

- **Model simulation** consisted of steady-state reactive radicals (RR), quantitative structure-activity relationship (QSAR), and photochemical models.
- **Portable measurement** was conducted on a mini-fluidic photoreaction system (MFPS) equipped with a portable spectrophotometer to determine the RR scavenging capacity (RRSC) of a certain water matrix.
- ***k'*$_p$** was predicted and verified.

UV/H_2O_2



Model simulation



Portable measurement w/ MFPS

Test Waters

Plant	Collection point	Sample	pH	UV_{254} (cm^{-1})	DOC (mg L^{-1})
Drinking water treatment plant (Yancheng, Jiangsu)	Raw water	RW1	7.81	0.087	4.096
	Sand-filter eff.	SF	8.01	0.055	3.479
Rural drinking water treatment facility (Changzhou, Jiangsu)	Raw water	RW2	8.86	0.100	5.763
	Ultrafiltration eff.	UF	8.73	0.091	5.306
	Iron coagulation/ultrafiltration eff.	PFS/UF	8.46	0.077	4.775
Municipal wastewater treatment plant (Beijing)	Primary sedimentation eff.	PrS	7.50	0.399	95.29
	Secondary sedimentation eff.	SeS	7.45	0.146	23.90

Drinking water treatment plant

Rural drinking water treatment facility

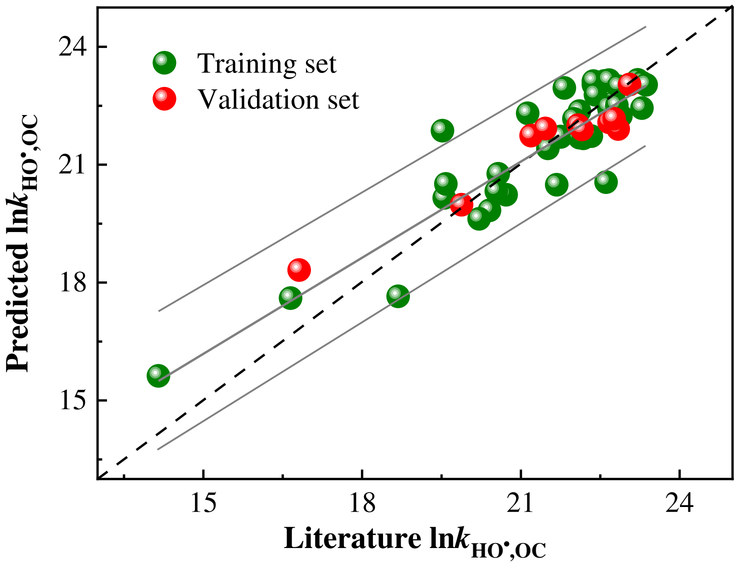
Municipal sewage treatment plant

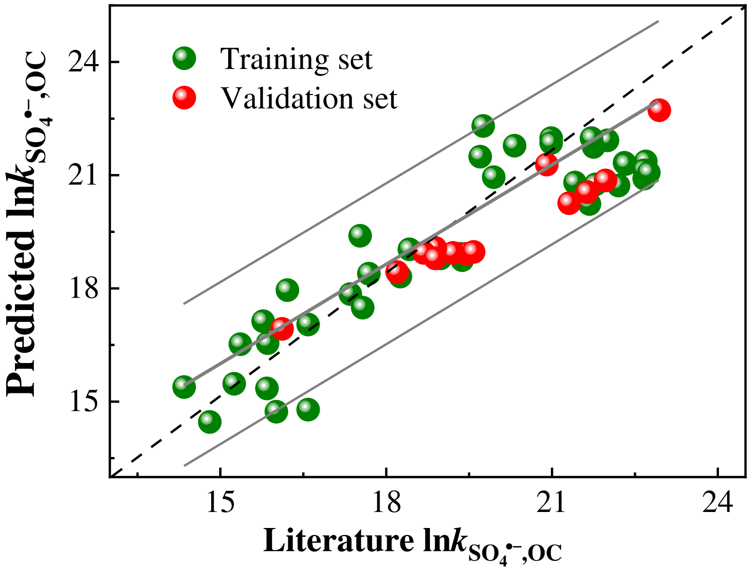
Water samples collected

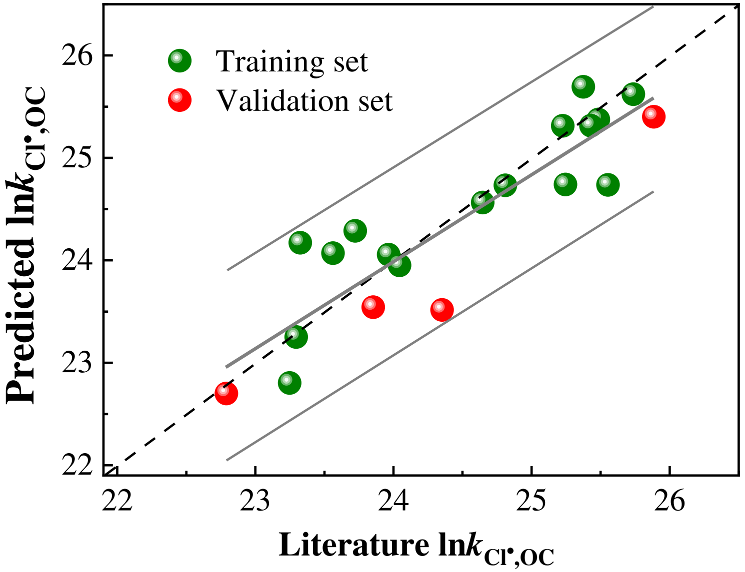
3. Results and Discussion

QSAR model equations

RR	Equation	R^2	Q_{LOO}^2	Q_{Ext}^2
HO•	$\ln k_{HO•,OC} = 27.992 - 2.131 \times (\#O{:}C) + 0.772 \times E_{HOMO}$	0.81	0.74	0.86
SO_4•-	$\ln k_{SO4•-,OC} = 26.335 - 4.103 \times (\#O{:}C) - 0.69 \times \mathrm{HLG}$	0.84	0.83	0.88
Cl•	$\ln k_{Cl•,OC} = 25.001 - 0.487 \times \mathrm{EA} - 0.302 \times \mathrm{DM}$	0.76	0.75	0.79

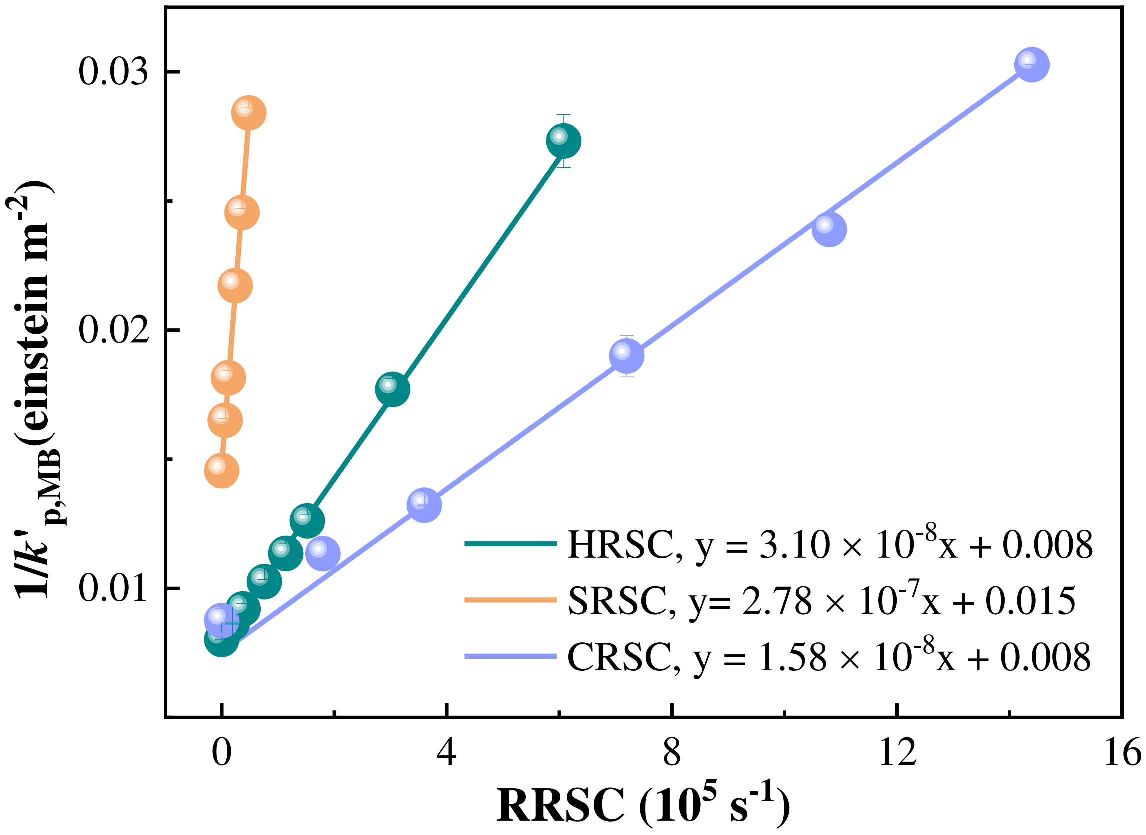




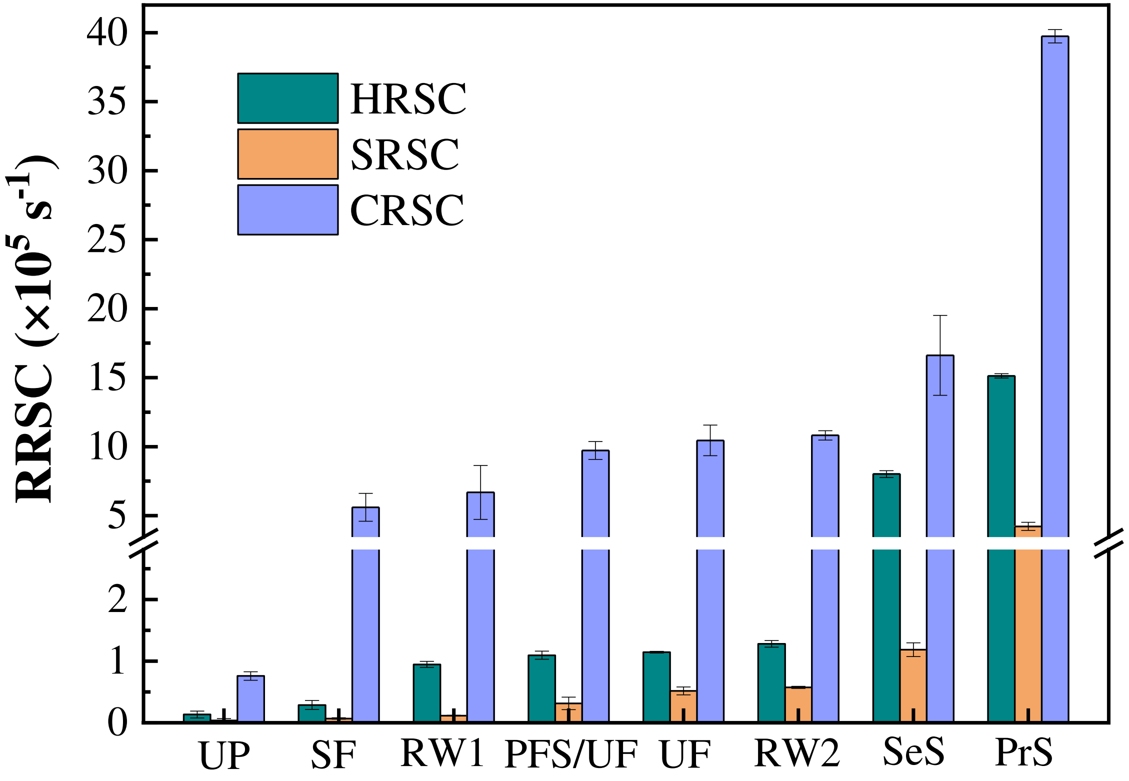


- Internal and external validations proved the QSAR model accuracy.

RRSCs of Test Waters

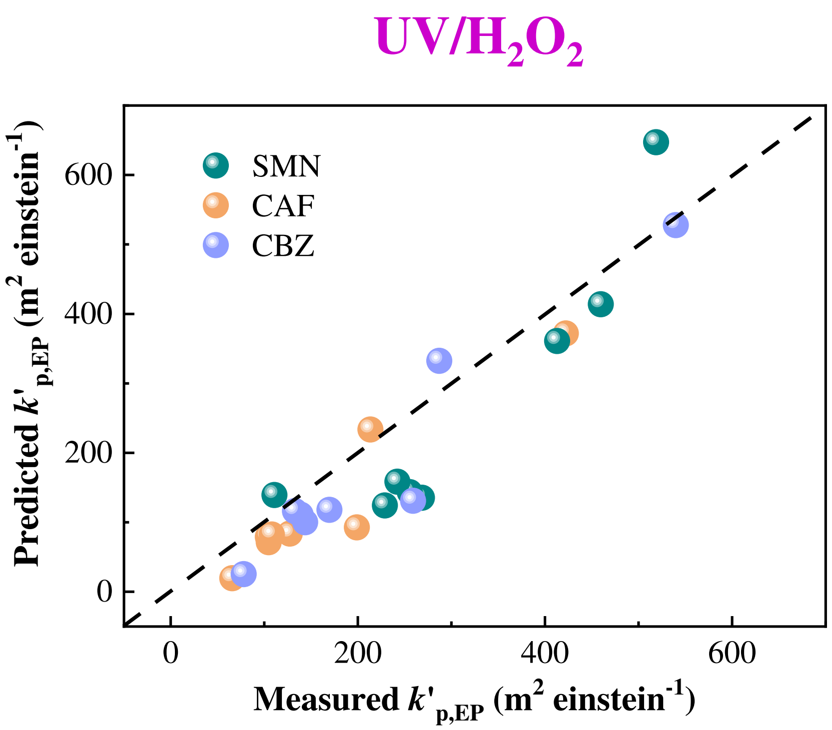


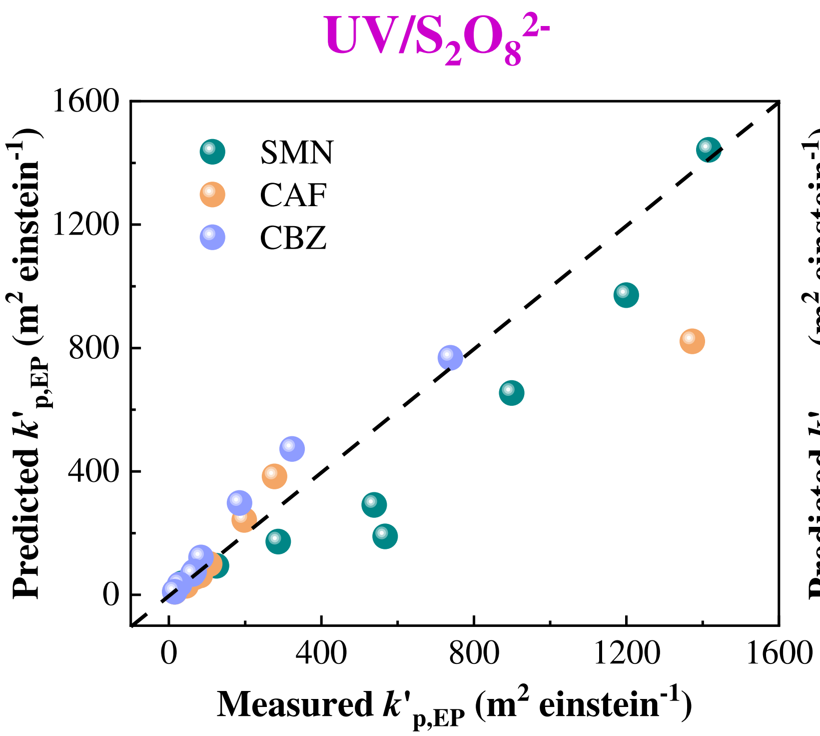
RRSC standard curves

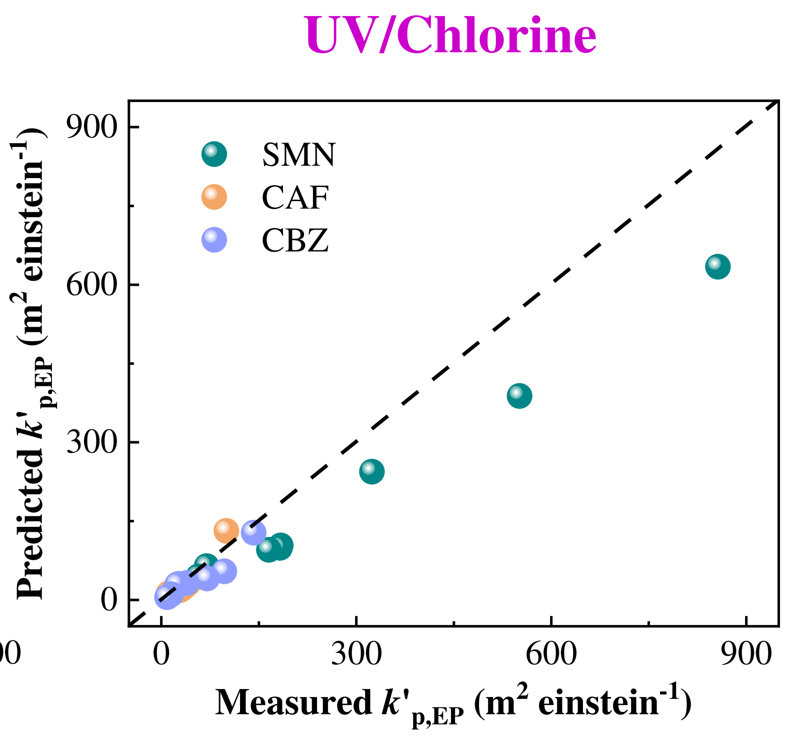


RRSCs of 8 test waters

Predicted vs. Measured k'_p



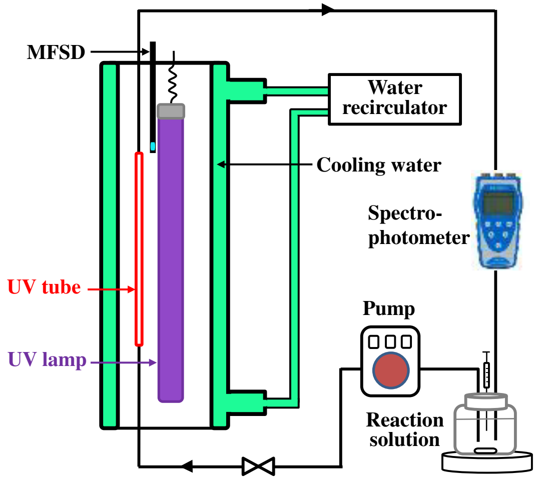




- MS&PM method predicted results agreed quite well with experimental results.

4. Conclusions

- Three kinetic parameters including $k_{RR,EP}$, r_{RR}, k'_{P} were determined by QSAR, photochemical, and steady-state reactive radical models, respectively.
- $\Sigma k_{RR,Si} \cdot [S]_i$ was determined by portable measurement with MFPS.
- An MS&PM method was developed to rapidly evaluate the UV-AOP performance for EP degradation in various water matrices.



PM Device

Software

Water Research, 2022, 221, 118794

Thanks for your attention！

Comments & Questions?

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