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Development and optimisation of a novel magnetic TiO_2 and Carbon Quantum Dots photocatalyst for water remediation

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INTRODUCTION & AIM

The revised EU Urban Wastewater Treatment Directive came into force in 2025 and mandates the implementation of quaternary treatments until 2045 for treatment plants with a load of 150,000 population equivalents or more. These quaternary treatments involve removing micropollutants, such as antibiotics. The application of solar-driven photocatalysis is a possible strategy to address this challenge. However, many photocatalysts in the literature lack efficiency and/or are difficult to implement, recover, and reuse. In this context, experimental designs were applied in this work aiming to:

- Develop a photocatalyst based on TiO_2, Carbon Quantum Dots (CQD) and magnetic nanoparticles (MNP) that allow for after-use separation from water treatment.
- Optimise the photocatalyst for high magnetisation, synthesis yield and removal of amoxicillin (AMX), sulfamethoxazole (SMX) and trimethoprim (TMP).

METHODOLOGY

PHOTOCATALYST PRODUCTION

1) Carbon Quantum Dots (CQD) Synthesis

CQD

CQD were synthesised via a simple hydrothermal treatment using urea as N dopant.

2) TiO_2/CQD Incorporation

TiO_2/CQD

CQD were incorporated onto TiO_2 via a simple sonication.

3) Tested methods for magnetic nanoparticles (MNP) incorporation

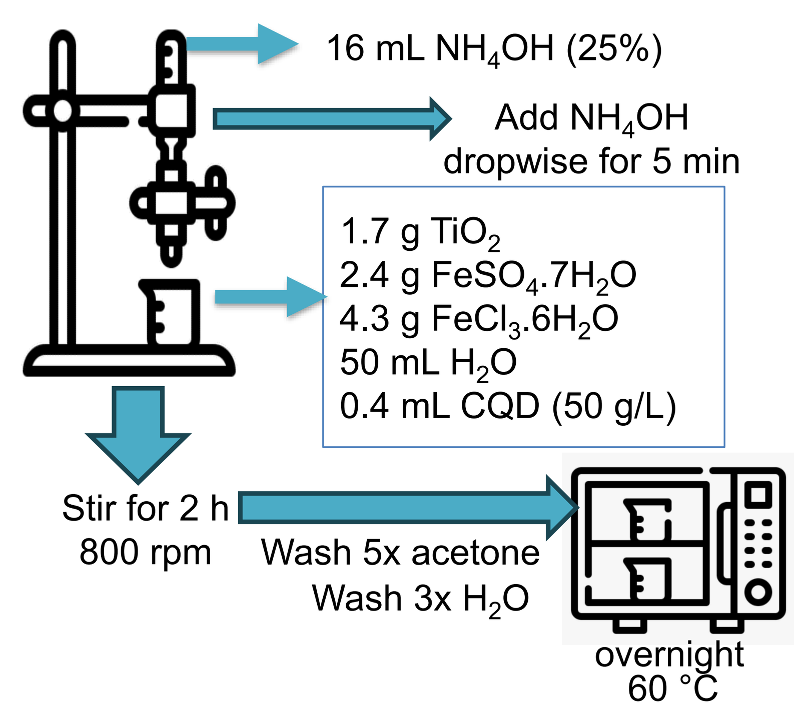
Hydrothermal treatment
- CQD/MNP_h

Functionalisation & coupling via the carbodiimide chemistry
- CQD/MNP_h&TiO_2

Co-precipitation
- MNP
- TiO_2@CQD@MNP
- TiO_2/CQD@MNP
- TiO_2@MNP

4) Selected route for the synthesis of magnetic TiO_2/CQD

The combination of TiO_2, CQD, and MNP was achieved using simple co-precipitation method. Final composite named TiO_2@CQD@MNP.



5) Central composite design (CCD)

6) Full Factorial Design (FFD)

CCD Factors	CCD Coding	Responses	FFD Coding	FFD Factors
Quantity of urea in CQD (g)	x_1	AMX photocatalysis	x_1	$CQD:TiO_2$ ratio
Fe:Ti ratio	x_2	SMX photocatalysis		
		TMP photocatalysis		
Reaction time (min)	x_3	Magnetisation (emu/g)	x_2	Fe:Ti ratio
		Yield (%)		

3 factors varying at 5 levels =17 photocatalysts

2 factors varying at 3 levels = 9 photocatalysts

CCD Level	CCD x_1 (g)	CCD x_2 (mol)	CCD x_3 (min)	FFD Level	FFD x_1 (*w/w*(%))	FFD x_2 (mol)
-1.42	0.49	12	1.7	-1	2	4
-1	1.5	4	3			
0	3	2	5	0	4	2
+1	4.5	1.3	7	+1	6	1.3
+1.42	5.5	1	8.4			

Responses to be fitted to the model (CCD):

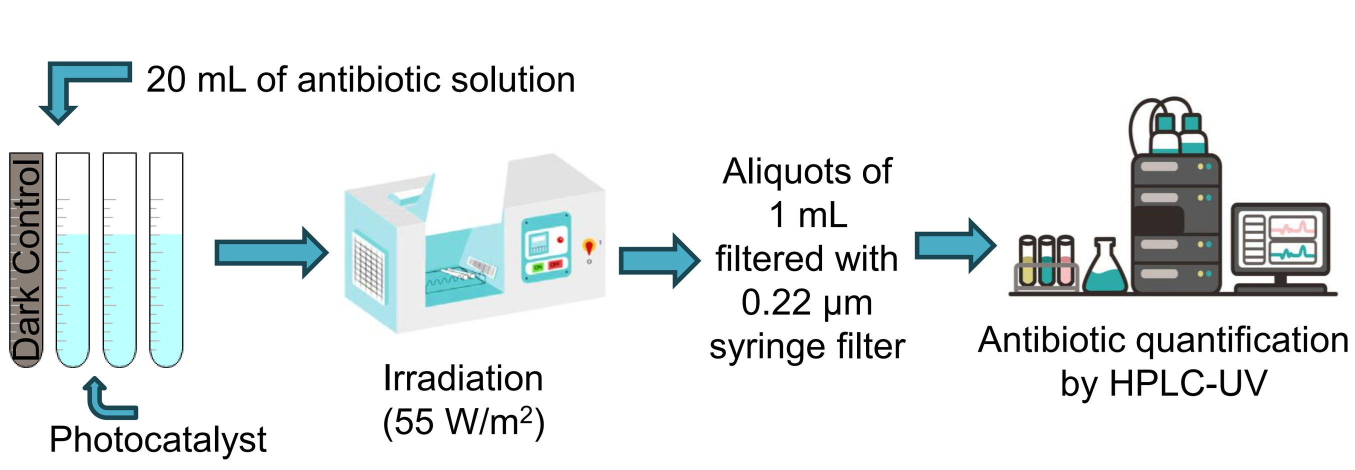
$$Y = k + a.x_1 + b.x_1^2 + c.x_2 + d.x_2^2 + e.x_3 + f.x_3^2 + g.x_1.x_2 + h.x_1.x_3 + i.x_2.x_3$$

Responses to be fitted to the model (FFD):

$$Y = k + a.x_1 + b.x_1^2 + c.x_2 + d.x_2^2 + g.x_1.x_2$$

PHOTOCATALYSIS EXPERIMENTS

The photocatalysts (100 mg/L) were tested in a phosphate buffer (pH 8.0), antibiotic solution. Each solution was irradiated (AMX, 2h; SMX, 1 h; and TMP, 0.5 h for CCD and AMX and TMP, 1 h and SMX 1.5 h) in a solar radiation simulator.



The removal efficiencies of AMX, SMX, and TMP were assessed by measuring the decrease in C/C_0, where C denotes the residual antibiotic concentration after irradiation, and C_0 is the concentration in the corresponding dark control.

RESULTS & DISCUSSION

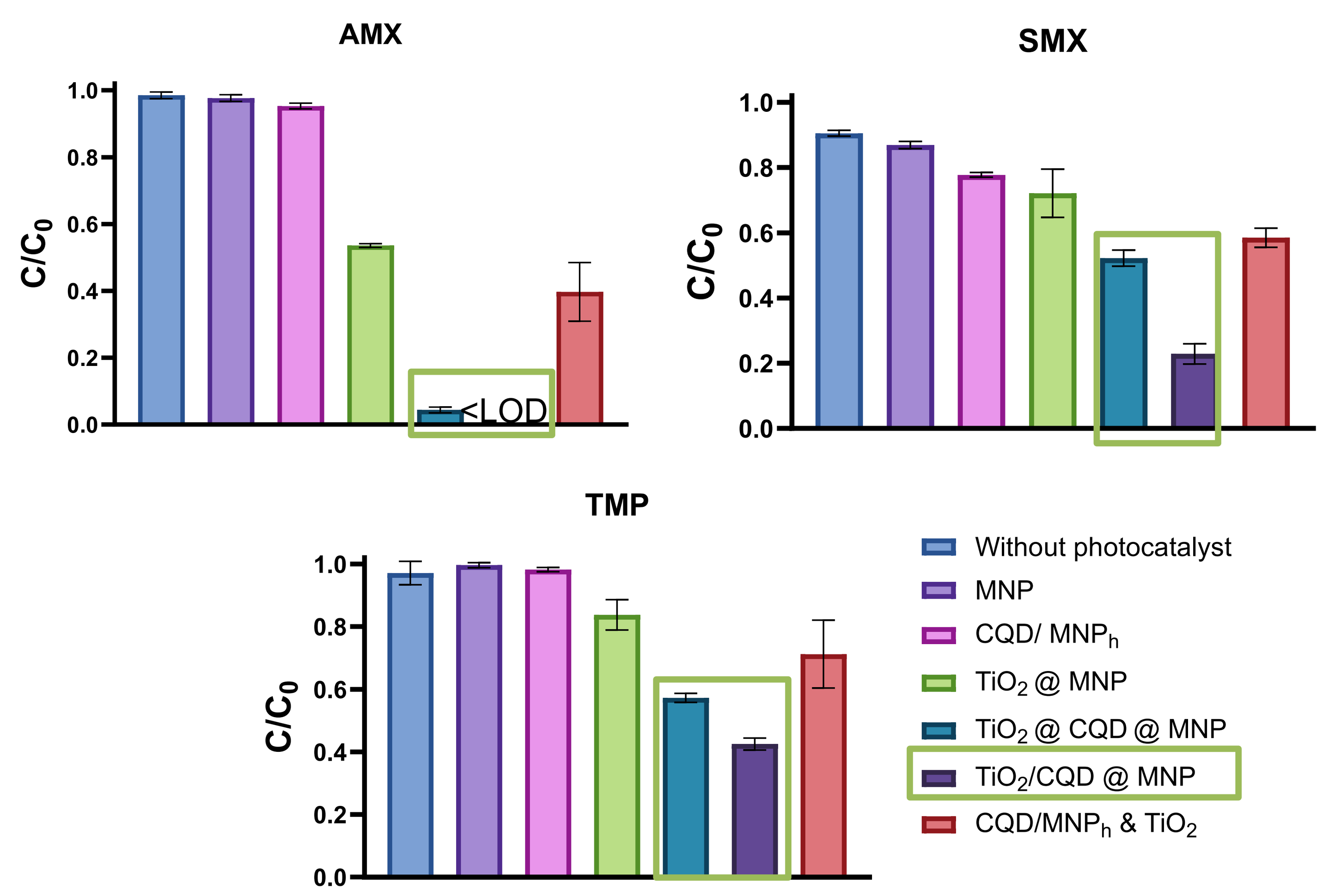


Figure 1. Photodegradation results of the application of different photocatalysts (100 mg/L) for the removal of 10 mg/L AMX, 10 mg/L SMX and 10 mg/L TMP from water using simulated solar irradiation (2 h for AMX, 1 h for SMX and 0.5 h for TMP). (LOD stands for limit of detection.)

The most efficient photocatalyst was identified as TiO_2/CQD@MNP, produced by co-precipitation. However, it required extra steps in its production; therefore, the study continued using **TiO_2@CQD@CQD**.

Table 1. Fitting models of each response of the CCD where factor x_1 is quantity of urea in CQD, factor x_2 is Fe:Ti ratio and factor x_3 is reaction time (min). Y represents the C/C_0 ratio in the photocatalysis experiments, the saturation value in the magnetization response, and the percentage yield in the yield response. When the determination coefficients (R^2) is higher than 0.8 (indicating satisfactory fit) and the lack of fit were higher than 0.05 (no significant) the model was accepted and the response marked in bold.

Response	Best describing model	R^2	R^2 adjusted	Lack of Fit
AMX photocatalysis	$Y= 0.9 + 0.25.x_1 + 0.027.x_1^2 - 0.01.x_2 + 0.03.x_2^2 - 0.06.x_3 + 0.015.x_1.x_3$	0.843	0.748	0.062
SMX photocatalysis	$Y= 0.60 + 0.10.x_1^2 + 0.12.x_2 + 0.06.x_2^2 + 0.04.x_3^2 + 0.05.x_1.x_2$	0.682	0.537	0.780
TMP photocatalysis	$Y=0.74 - 0.04.x_1 + 0.07.x_1^2 + 0.11.x_2 \pm 0.03.x_3 + 0.04.x_3^2$	0.634	0.468	0.434
Magnetisation (emu/g)	$Y= 12 - 1.x_1 + 0.2.x_1^2 + 25.x_2 - 4.0.x_2^2 + 0.1.x_3 - 0.03.x_3^2$	0.967	0.947	0.228
Yield (%)	$Y= 81 + 0.08.x_1^2 - 12.x_2 + 1.9.x_2^2 + 1.0.x_3 - 0.11.x_1.x_3 - 0.3.x_2.x_3$	0.905	0.849	0.153

Factor Analysis

Only Fe:Ti ratio (x_2) significantly affected the responses, as pointed by most of the models.

Table 2. Fitting models of each response of the FFD where factor x_1 is $CQD:TiO_2$ ratio and factor x_2 is Fe:Ti ratio. Note: Y represents the C/C_0 ratio in the photocatalysis experiments, the saturation value in the magnetization response, and the percentage yield in the yield response.

Response	Equation that describes the 3D response surface	R^2
AMX photocatalysis	$Y= -1.82 +5.35X_1 +1.06X_2 -2.46X_1X_2 -2.13X_1^2 -0.11X_2^2 +0.28X_1X_2^2 +1.04X_1^2X_2 -0.12X_1^2X_2^2$	1.00
SMX photocatalysis	$Y= -2.78 +6.62X_1 +2.04X_2 -3.92X_1X_2 -2.59X_1^2 -0.26X_2^2 +0.50X_1X_2^2 +1.54X_1^2X_2 -0.20X_1^2X_2^2$	1.00
TMP photocatalysis	$Y= -3.72 +8.96X_1 +3.23X_2 -4.66X_1X_2 -3.64X_1^2 -0.26X_2^2 +0.56X_1X_2^2 +1.92X_1^2X_2 -9.23X_1^2X_2^2$	1.00
Magnetization (emu/g)	$Y= -10.8 +76.1X_1 +7.37X_2 -14.9X_1X_2 -21.6X_1^2 -0.71X_2^2 +1.32X_1X_2^2 +4.37X_1^2X_2 -0.34X_1^2X_2^2$	1.00
Yield (%)	$Y= 83.2 -29.8X_1 +2.51X_2 +3.78X_1X_2 +11.8X_1^2 -0.54X_2^2 -0.005X_1X_2^2 -3.04X_1^2X_2 +0.17X_1^2X_2^2$	1.00

Desirability Analysis

Optimum synthesis conditions were determined as 4% (w/w) $CQD:TiO_2$ ratio and 1.2:1 Fe:Ti ratio.

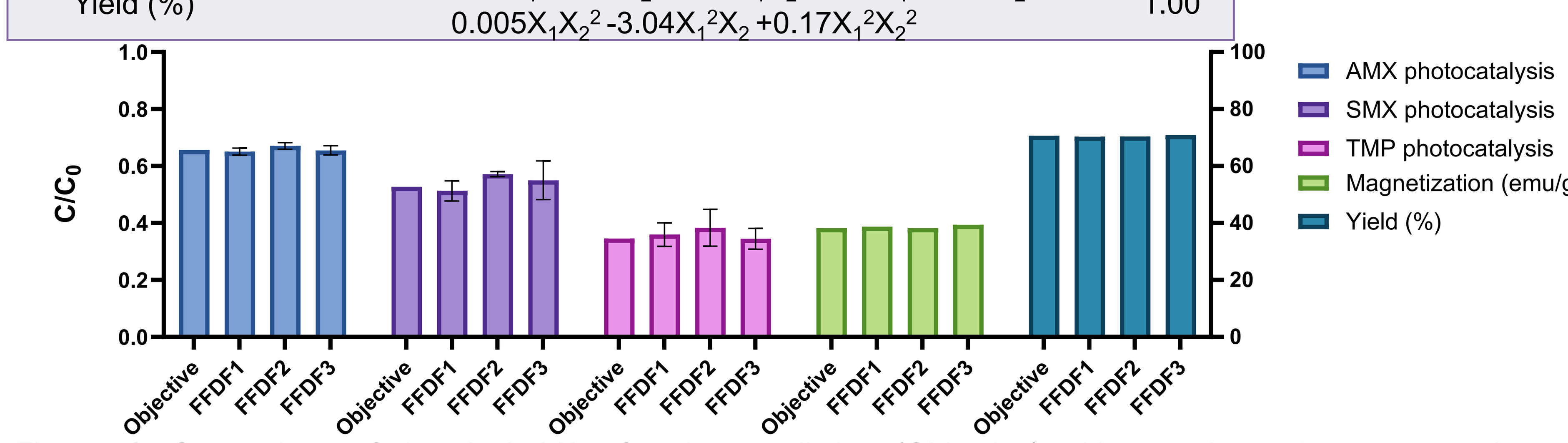


Figure 1. Comparison of the desirability function prediction (Objective) with experimental results on the 5 responses by three batches of photocatalyst (FFDF1, FFDF2 and FFDF3) synthesised according to the determined optimum synthesis conditions.

CONCLUSION

A systematic approach combining different experimental designs (CCD and FFD) was applied to optimise the synthesis of TiO_2@CQD@MNP nanocomposites.

• The optimisation study showed that the Fe:Ti ratio was the most influential factor, and the optimal synthesis conditions were determined as: [Fe:Ti = 1.2:1], [$CQD:TiO_2$ = 4% (*w/w*)].

• Under these conditions, the material exhibited a magnetisation of 38.8±0.6 emu g^{-1}, a yield of 70.5±0.4%, and removal efficiencies of 34 ± 2% (AMX, under 1 h irradiation), 46±5% (SMX, under 1.5 h irradiation), and 64±5% (TMP, under 1 h irradiation).

The results presented demonstrate that the synthesised magnetic TiO_2-carbon quantum dot composites are promising materials for the sustainable and efficient solar-driven removal of antibiotics from water, with potential applications in water treatment systems.

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