Response-Surface Constrained Kinetic Analysis of Visible-Light Dye Photodegradation on Nitrogen-Modified TiO_2

Light Skills Synthetic Science Demo

Abstract

This synthetic study demonstrates a reproducible environmental-chemistry workflow for visible-light dye photodegradation. A deterministic generator produced 4968 UV-vis time records across 183 experimental conditions covering catalyst formulation, loading, pH, irradiance, and radical-scavenger perturbations. Pseudo-first-order fits recovered an optimum condition using N-TiO2/H2O2 at 0.50 g L^{-1}, pH 7.0, and 105 mW cm^{-2}, with $k_{obs} = 0.0296$ min^{-1} and an apparent half-life of 23.4 min. The paper is a workflow demonstration only: it does not claim a real photocatalyst discovery.

Honesty boundary. All concentration traces are synthetic and generated by the repository script. The package demonstrates a science-style workflow: data, analysis, figures, references, manuscript, LaTeX source, PDF, and preview.

1 Introduction

Semiconductor photocatalysis is a long-running route for light-driven environmental remediation [1, 2, 3]. A realistic computational demonstration should include time-resolved concentration traces, kinetic fitting, design-factor response surfaces, diagnostics, and mechanistic perturbation. This project uses that structure to showcase Light Skills without inventing experimental evidence.

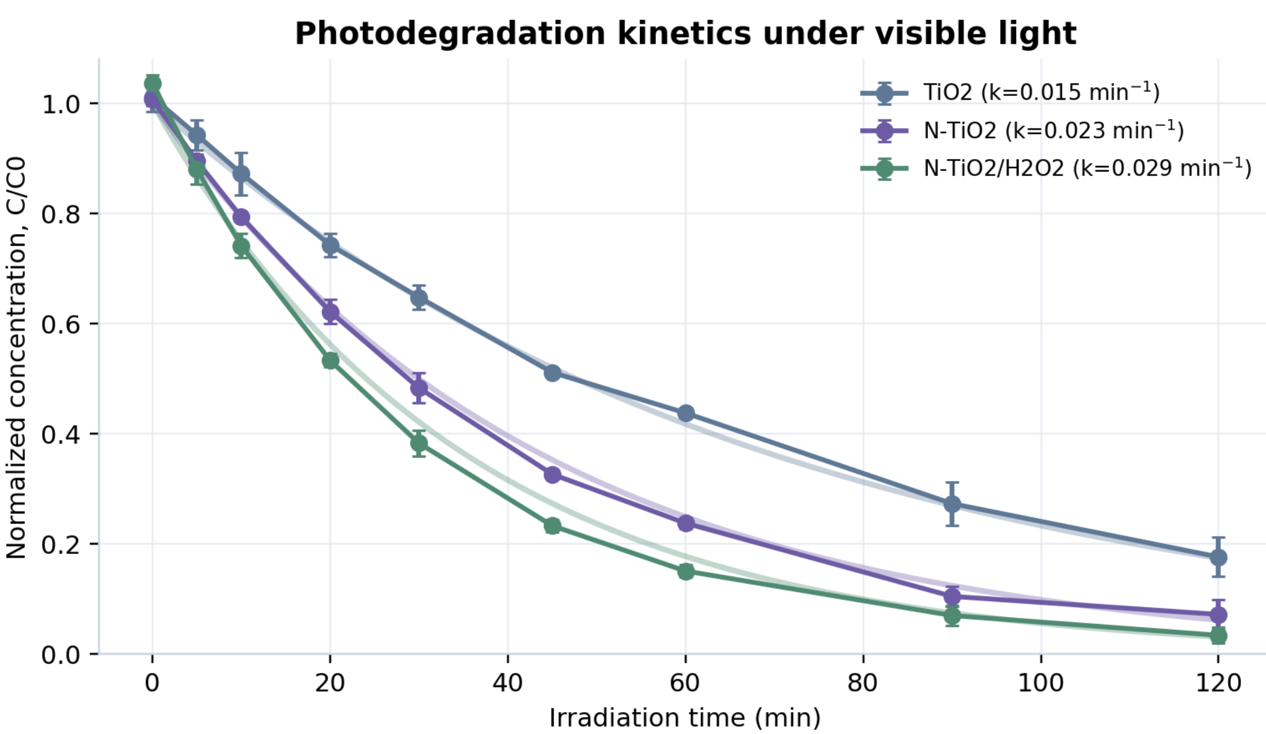

Figure 1: Synthetic visible-light degradation traces at the high-irradiance neutral-pH condition. Markers show replicate means and standard deviations; smooth lines are pseudo-first-order fits.

2 Methods

Synthetic UV-vis absorbance records were generated for three catalyst formulations, five catalyst loadings, four pH levels, three irradiance settings, and a radical-scavenger panel. Rate constants were estimated by fitting

$$\ln(C/C_0) = -k_{\mathrm{obs}}t + b$$

for each condition. The response surface was summarized for N-TiO_2/H_2O_2 at fixed irradiance. Numerical analysis used NumPy, SciPy, and Matplotlib [4, 5, 6].

Table 1: Bootstrap summaries over synthetic no-scavenger design conditions. Values are demonstration outputs, not measured catalyst performance.

Catalyst	Mean k_{obs}	95% CI low	95% CI high	n
N-TiO2/H2O2	0.0235	0.0227	0.0243	60
N-TiO2	0.0182	0.0175	0.0189	60
TiO2	0.0111	0.0107	0.0114	60

3 Results

The response surface selected N-TiO2/H2O2 near neutral pH and intermediate catalyst loading as the fastest simulated condition. The top catalyst-family mean was N-TiO2/H2O2 with mean $k_{\mathrm{obs}} = 0.0235$ min^{-1}. The analysis is intentionally framed as a synthetic benchmark so that the artifact demonstrates a complete science workflow without overstating evidence.

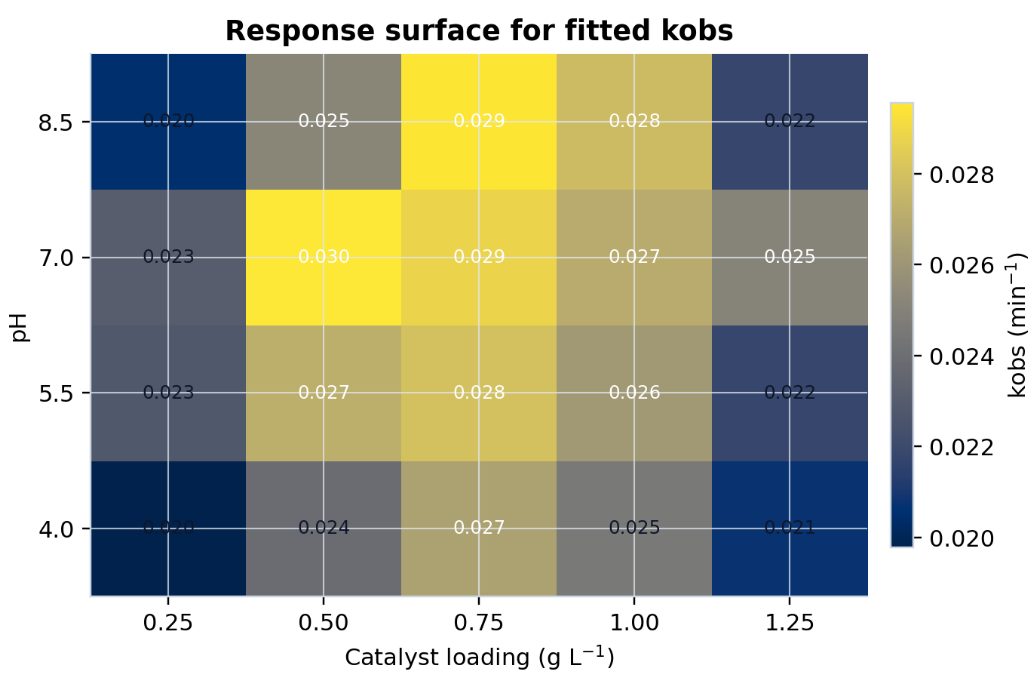

Figure 2: Response surface for fitted k_{obs} under N-TiO_2/H_2O_2 at fixed irradiance. The surface is generated from synthetic data.

4 Mechanistic Perturbation

The radical-scavenger panel is included to mimic a common mechanistic check in photocatalysis papers. In the synthetic generator, IPA causes the strongest activity loss, followed by BQ and EDTA. This ordering is scripted and

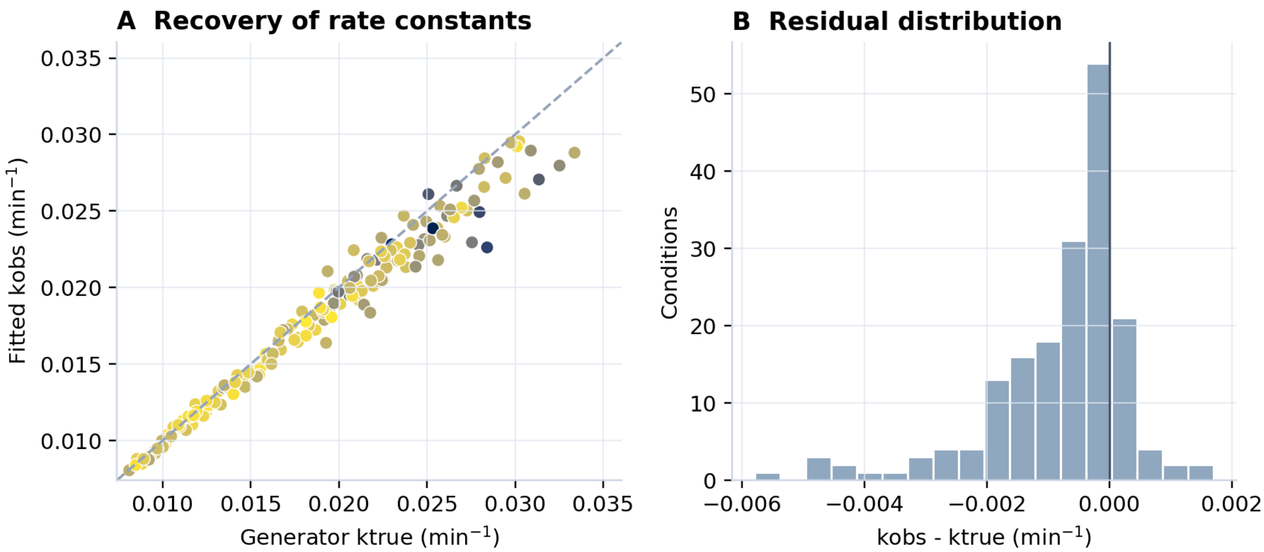

Figure 3: Kinetic fitting diagnostics. Left: fitted vs generator rate constants. Right: residual distribution.

should not be read as real mechanistic evidence.

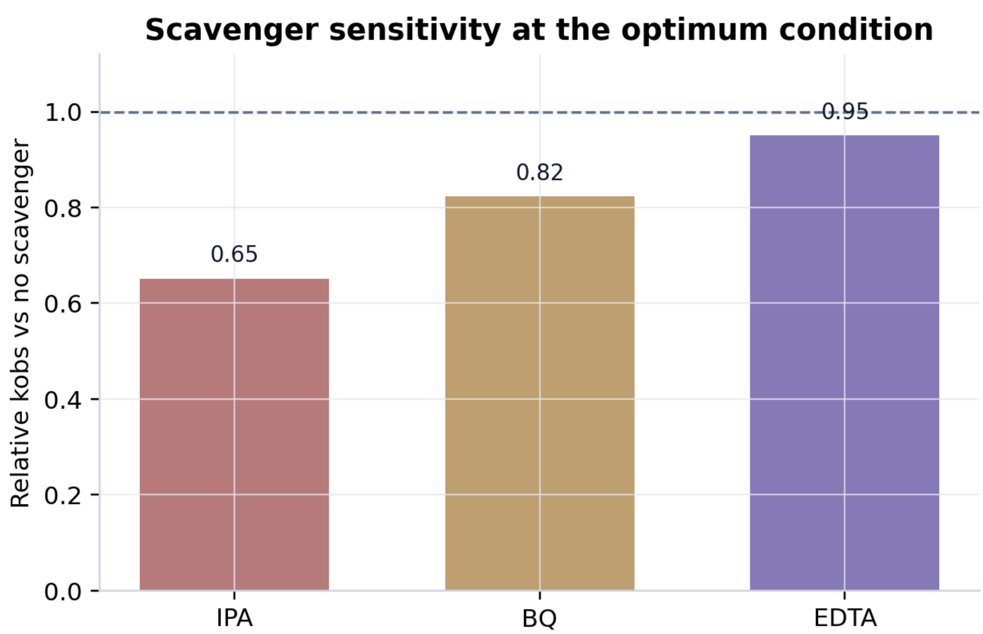

Figure 4: Synthetic scavenger sensitivity under the selected condition. Activity is normalized to the no-scavenger control.

5 Reproducibility and Limitations

Run `python scripts/run_all.py` to regenerate the full project. A real English-journal submission would require actual experiments, instrument calibration metadata, replicate planning, uncertainty analysis, raw spectra, material characterization, and independent domain review. This artifact is a showcase of workflow shape and publication packaging.

References

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