PhotoScale: An Automated Continuous-Flow Photoreactor for Data-Driven Photocatalysis

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Abstract

PhotoScale is an automated continuous-flow photoreactor built at ICIQ as a platform for data-driven, autonomous photocatalysis. Optimising a new transformation means searching a high-dimensional space — catalyst loading, chemicals, solvents, photon flux, residence time, temperature — where manual screening limits throughput and reproducibility. PhotoScale embeds sensing, control and logging in the hardware and defines a layered upgrade path: structured logging with quality-control gating, machine-vision kinetics, edge-AI closed-loop optimisation, and an LLM pipeline distilling catalyst knowledge from the literature.

Hardware at a glance

Light source	8 × 450 nm LUXEON LED matrix plates (48 LEDs each)
LED power	Phoenix Contact 48 V / 20 A supply
Dimming	4 PWM channels, 0–100 %, independent on/off
Flow sensing	In-line ultrasonic flow meter
Thermal	Up to 8 temperature sensors + external chiller
Control	Raspberry Pi • 7″ touchscreen • VNC • per-run logs

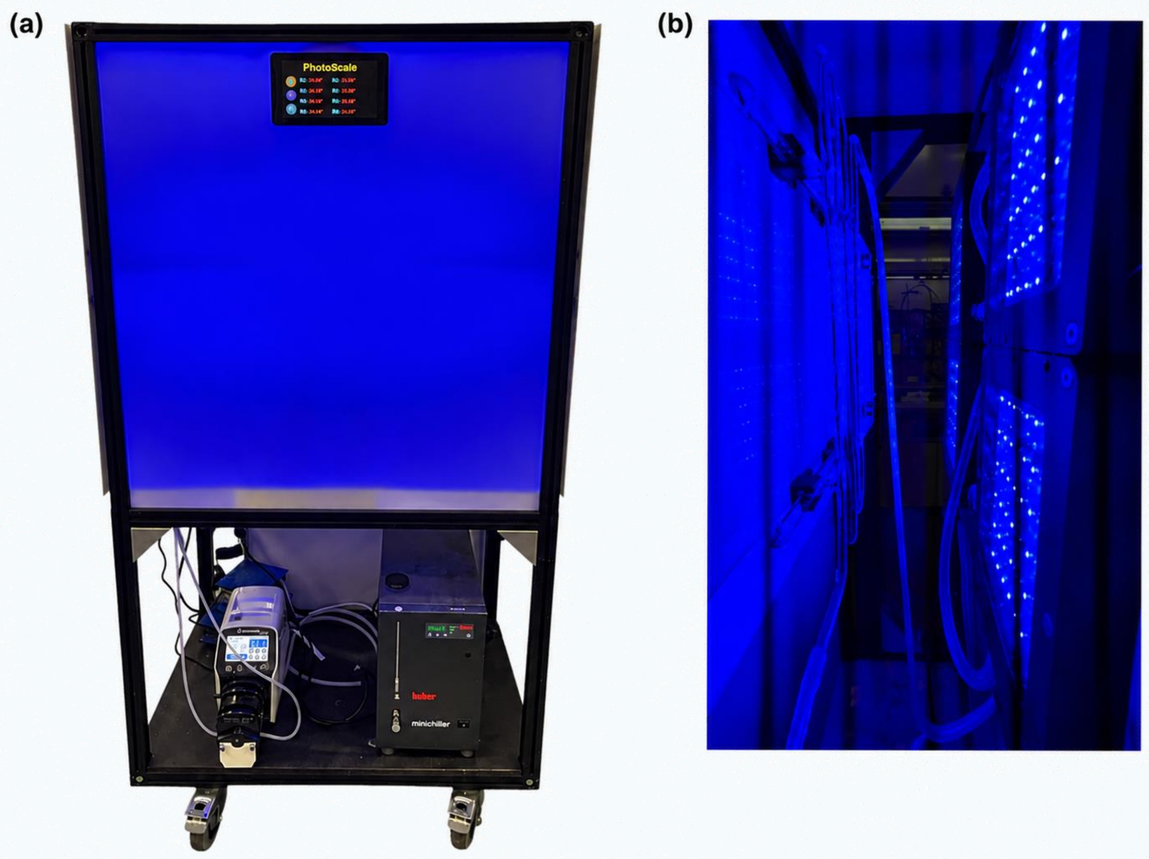


Figure 1. PhotoScale continuous-flow photoreactor: (a) front view with the 7-inch touchscreen displaying per-plate temperatures; (b) internal view of the recirculation tubing between the 450 nm LED matrix plates.



Scheme 1. Representative 450 nm photocatalytic coupling (R¹–H + R²–X → R¹–R²) targeted on the PhotoScale platform.

2. PhotoScale Architecture

- Recirculating flow path: reagent reservoir → peristaltic pump → in-line ultrasonic flow meter → glass tubular reactor.
- Illumination: eight 450 nm LUXEON high-power LED matrix plates (48 LEDs each) surround the reactor, water-cooled by an external chiller.
- Control: Raspberry Pi with full-screen touchscreen app, auto-started at boot as a system service; remote operation and configuration via VNC.
- Four PWM channels set LED intensity 0–100 % (two plates per channel) with independent on/off; temperatures and flow are logged for every run.

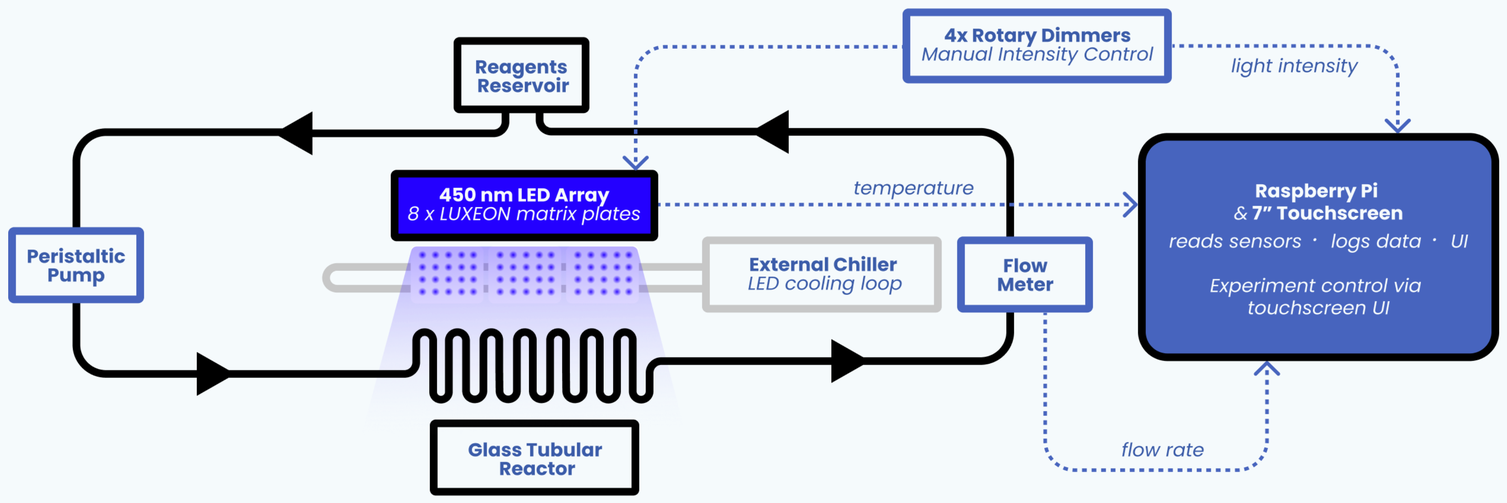


Figure 2. Architecture of the PhotoScale platform: recirculation through a peristaltic pump, in-line ultrasonic flow meter and glass tubular reactor; eight water-cooled 450 nm LED plates driven by four rotary dimmers; a Raspberry Pi reads sensors, logs data and hosts the touchscreen interface.
Scheme 1. Representative 450 nm photocatalytic coupling (R¹–H + R²–X → R¹–R²) targeted on the PhotoScale platform.

3. Current Status & Preliminary Results

- Platform constructed and validated in routine use: touchscreen UI, PWM LED control, eight-channel temperature logging, flowmeter, hotspot and VNC all function, auto-started at boot.
- Standard recirculation runs logged as a reference; software tracked under Git version control.
- Under active development: current & light sensors, the machine-vision pipeline and the edge-AI control loop.
- Every module ships with a simulation mode, so APIs, dashboards and logging progress regardless of hardware availability.

4. Conclusions

- Robust, programmable continuous-flow photoreactor with a transparent, modular path from manual to automated photocatalysis.
- Implemented hardware and logging form a verified baseline; layered monitoring and quality control define how it is enhanced.
- A testbed for autonomous, high-throughput experimentation in Artificial Photosynthesis and catalyst discovery.

References

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