Electronic Supplementary Material (ESI) for Reaction Chemistry & Engineering.

Photochlorination of Toluene - The Thin Line Between Intensification and Selectivity. Part 1: Intensification and Effect of Operation Conditions

Supporting Information

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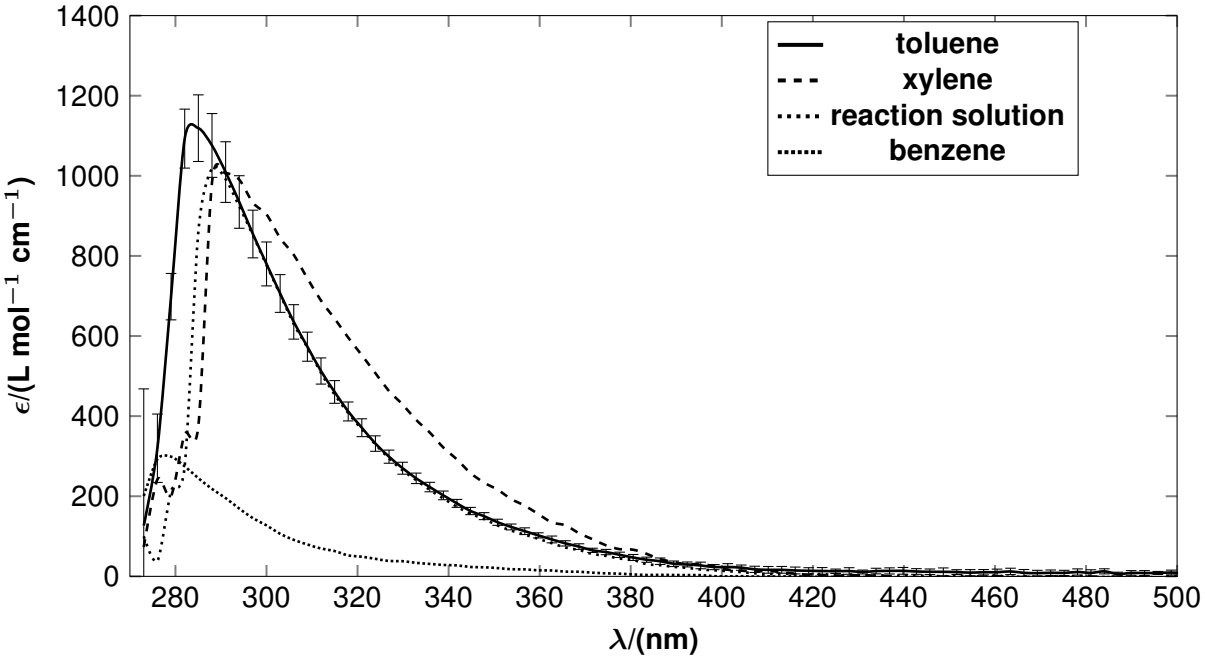

Fig. S1 Absorption spectrum of dissolved chlorine in different solvents.[13]

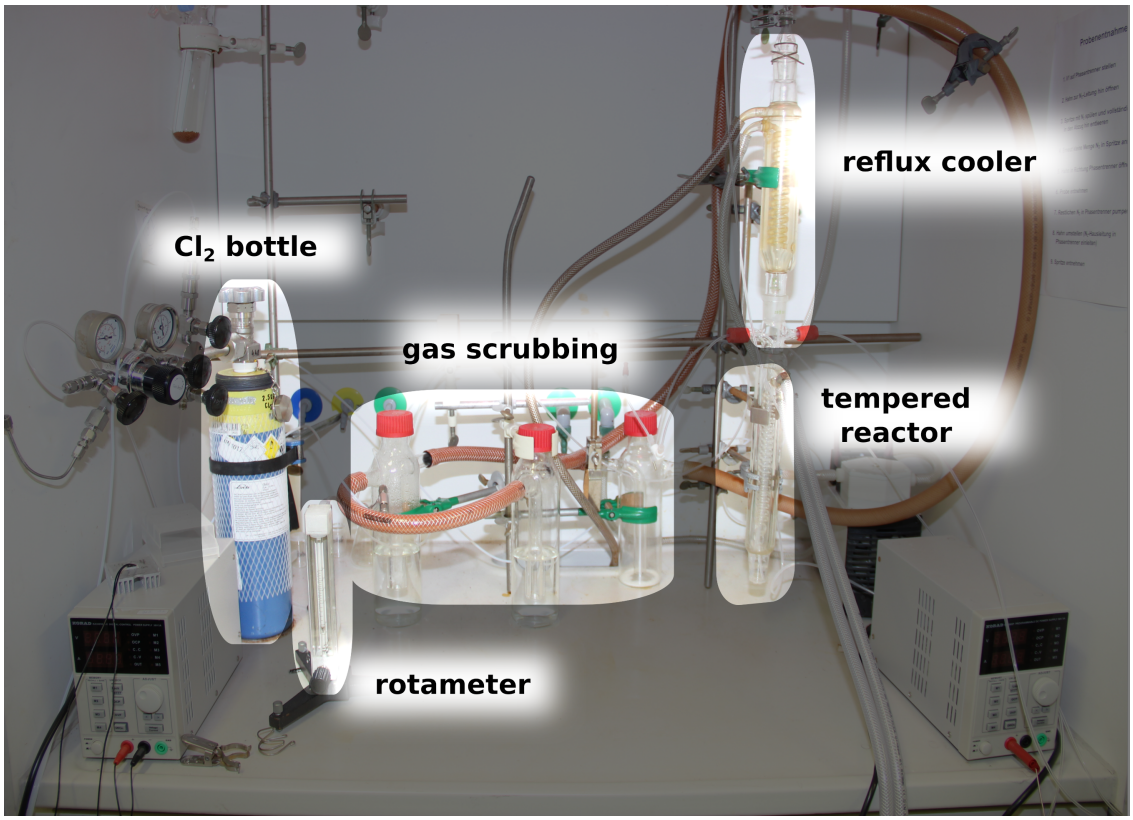

Fig. S2 Picture of the experimental setup for batch reactors.

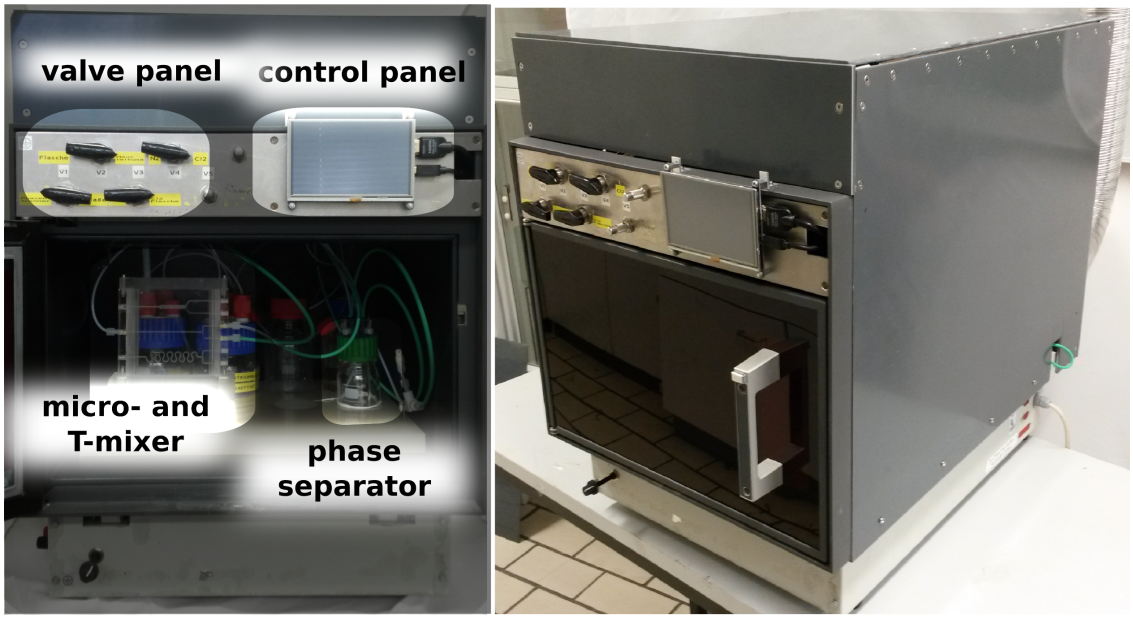

Fig. S3 Picture of the experimental setup for microreactors. The left side shows the inner parts of the setup and the right side shows the external of the box in which the setup was installed. The LED was positioned directly in front of the glass plate of the mixers.

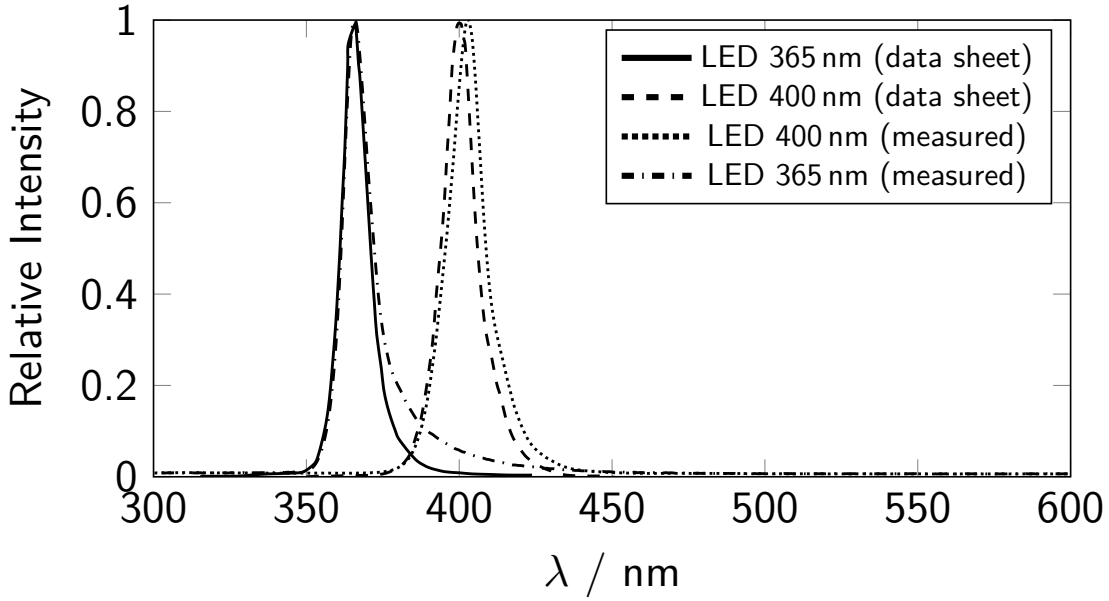

Fig. S4 Emission spectra for the used LEDs according to the data sheet and measured.

Table S1 Experimental conditions used to investigate different aspects of the photochlorination of toluene under high chlorine concentrations. *: 150 W medium pressure mercury vapour lamp (MVL), RT: room temperature, conti: continuous irradiation, P:/x/y: pulsed operation; x - seconds LED switched on; y - seconds LED switched off, IDA: irradiation during absorption; IAA: irradiation after absorption; T-M: T-mixer, M-M: micromixer, n. r.: not relevant (Cl_2 saturated solutions).

reactor type	V_{Tol}/mL	$\dot{V}_{Tol}$/mL min^{-1}	$\dot{V}_{Cl_2}$/mL min^{-1}	Q/mol min^{-1} L^{-1}	light source	I/mA	Irradiation	reac. temp./°C
batch A	100		240	0.107	365 nm LED	600	conti.	RT
batch A	100		240	0.107	365 nm LED	600	P: 2/10	RT
batch A	100		240	0.107	365 nm LED	600	P: 3/30	RT
batch A	100		240	0.107	400 nm LED	600	P: 2/10	RT
batch A	100		240	0.107	400 nm LED	500	conti.	RT
batch A	100		80	0.035	365 nm LED	100	conti.	RT
batch A	100		150	0.067	365 nm LED	100	conti.	RT
batch A	100		240	0.107	365 nm LED	100	conti.	RT
batch B	40		100	0.107	365 nm LED	600	conti.	10
batch B	40		100	0.107	365 nm LED	600	conti.	30
batch B	40		100	0.107	365 nm LED	600	conti.	50
batch B	40		100	0.107	365 nm LED	600	conti.	70
batch B	40		120	0.107	365 nm LED	600	conti.	RT
batch B	40		100	0.107	MVL	*	conti.	RT
batch B	20		90	0.200	365 nm LED	600	conti.	RT
batch B	20		160	0.357	365 nm LED	10	conti.	RT
batch B	20		200	0.446	365 nm LED	600	conti.	RT
microreactor	30	1	10	0.015	365 nm LED	1200	IDA T-M	30
microreactor	30	1	20	0.030	365 nm LED	1200	IDA T-M	30
microreactor	50	2	50	0.045	365 nm LED	1200	IDA T-M	30
microreactor	25	1	25	0.045	365 nm LED	1200	IDA T-M	40
microreactor	25	1	25	0.045	365 nm LED	1200	IDA T-M	70
microreactor	30	1	10	0.015	365 nm LED	1200	IDA M-M	30
microreactor	50	2	50	0.045	365 nm LED	1200	IDA M-M	30
microreactor	25	1	25	0.045	365 nm LED	1200	IDA M-M	40
microreactor	25	1	25	0.045	365 nm LED	1200	IDA M-M	70
microreactor	25	1	25	0.045	365 nm LED	1200	IAA	40
microreactor	25	1	25	0.045	365 nm LED	1200	IAA	50
microreactor	25	1	25	0.045	365 nm LED	1200	IAA	70
microreactor	n. r.	1	20–200	0.9–8.5	365 nm LED	1200	IDA T-M	RT
microreactor	n. r.	1	20–200	0.9–8.5	365 nm LED	1200	IDA M-M	RT