Investigations on the photocatalytic Methanol Oxidation to yield formaldehyde in a continuous laboratory plant

Supporting Informations

Stubenrauch, Florian[1]; Schörner, Markus[1]; Andreas, Bösmann[2]; Schühle, Patrick[2]; Wasserscheid, Peter[1,2]

[1]Forschungszentrum Jülich GmbH, Helmholtz-Institut Erlangen-Nürnberg for renewable Energy (IEK-11)

[2]Lehrstuhl für chemische Reaktionstechnik, Friedrich-Alexander-Universität Erlangen-Nürnberg

1. Continuous laboratory plant flow chart

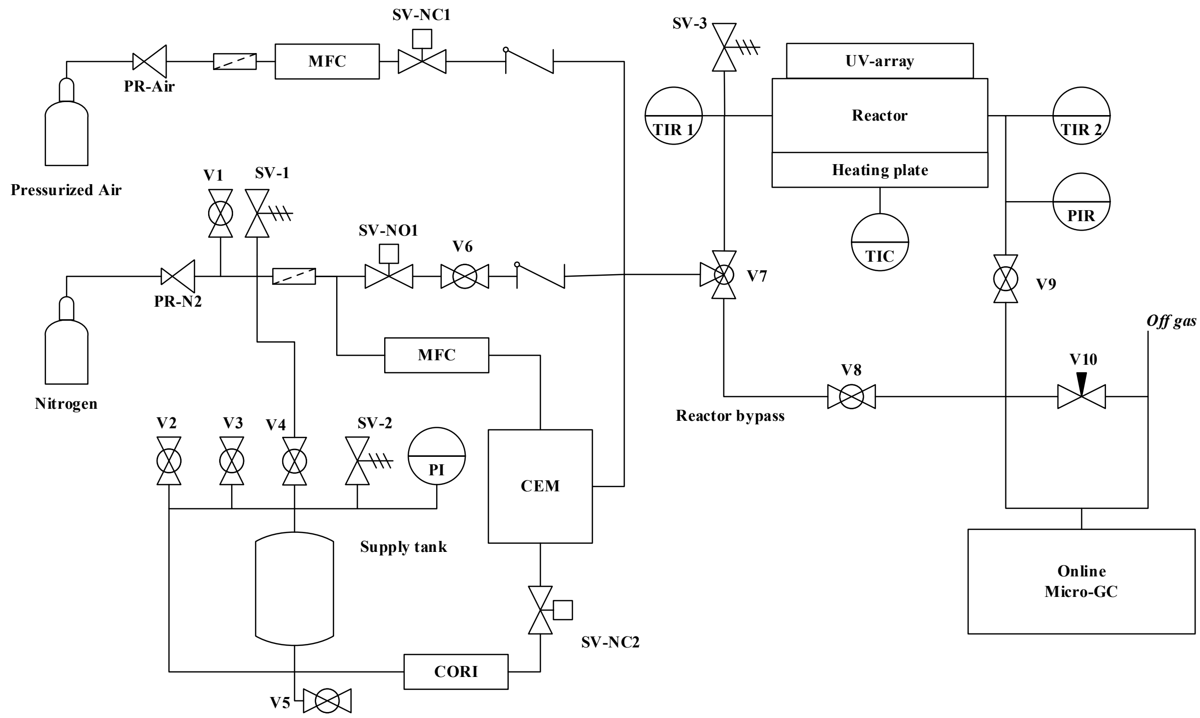

Figure S1: PI-flow diagram of the laboratory plant used in this study.

2. Gas chromatography setup details: Inficon Micro-GC Fusion

Module	*Injector*	*Column*	*Carrier gas*	*Detector*	*Substances*
A	Backflush	Rt-Molsieve 0.25 mm 10 m	Ar	TCD	H_2, O_2, N_2, CO
B	Variable Volume	Rt-U-Bond 0.25 mm 8 m	He	TCD	CO_2, HCHO, H_2O
C	Large Volume	Stabilwax DB 0.25 mm 10 m	He	TCD	DMM, DME, MF, MeOH, HeFal

3. UV-irradiance and local intensity

Tabelle S1: Second degree polynomial fit equation in x and y direction for irradiance in the reactor with determined parameters.

$p20x^2 + p10x + p02y^2 + p01\,y + p11xy + p00$		**Goodness of fit**	
p20	-9.324 E-03	SSE:	601.4
p10	1.442	R^2	0.9531
p02	-4.464 E-02	Adj. R^2	0.9374
p01	3.585	RMSE	6.332
p11	-3.078 E-04		
p00	1.066 E+02		

4. Long term experiment course: Products

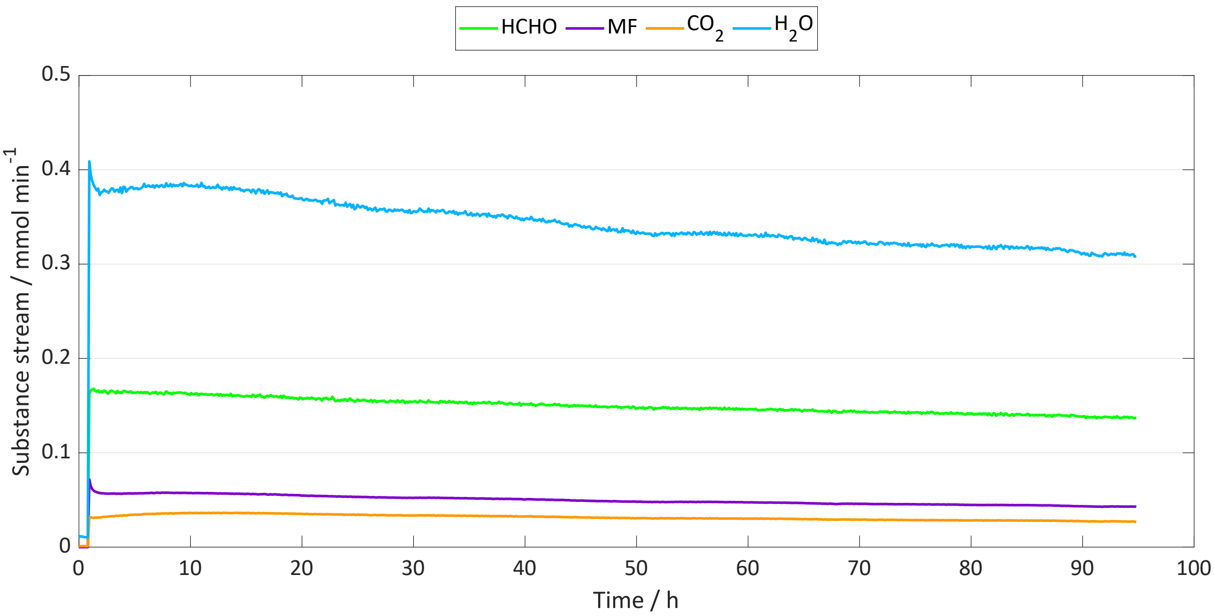

Figure S2: Conversion over time in a standard experiment. $m_{Catalyst}$ = 0.1561 g; $\omega_{Catalyst}$ = 1.1478 mg cm^{-2}; T = 78 °C; τ = 11.8 s; E = 186.8 mW cm^{-2}

5. Conversion of oxygen and product yields at different loadings and irradiations

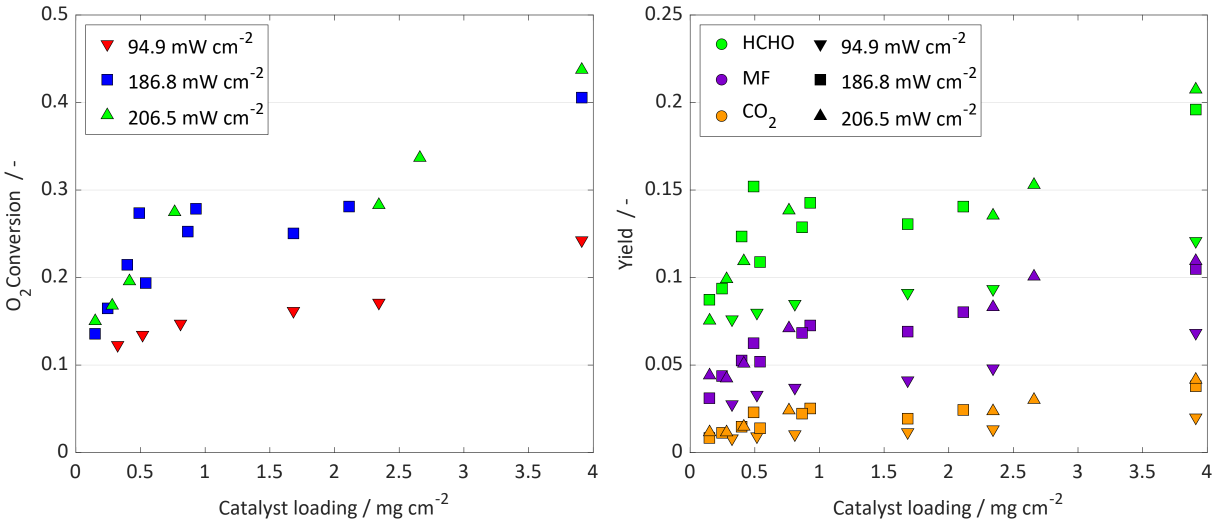

Figure S3: Resulting conversion of O_2 (left) and yields (right) towards HCHO, MF and CO_2 for different catalyst loads on the irradiated area. T = 78 °C, τ = 11.8 s

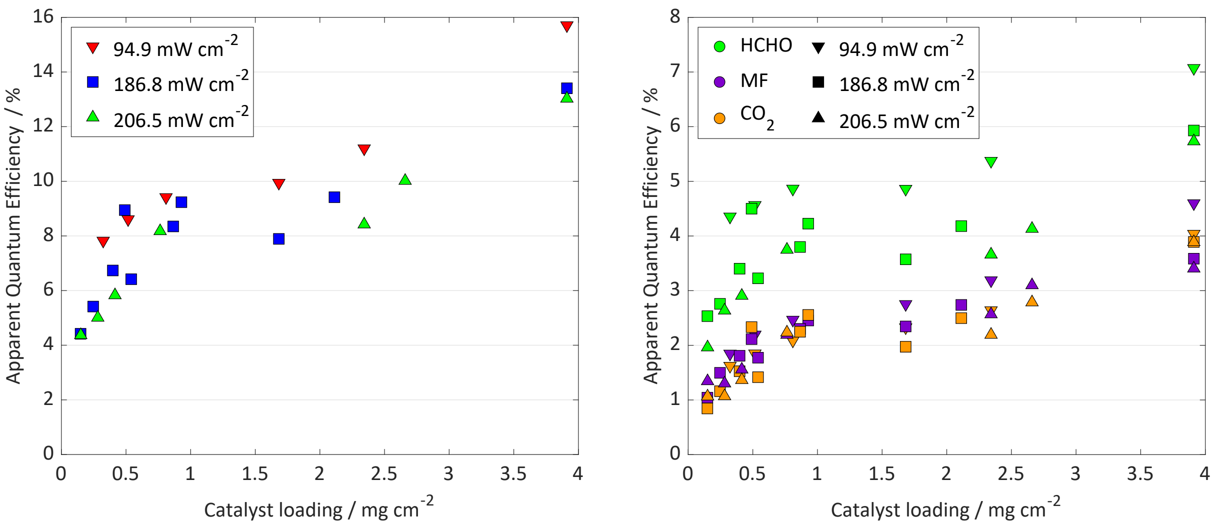

Figure S4: Apparent quantum efficiencies in total (left) and broken down to product species (right). T = 78 °C, τ = 11.8 s

6. Residence Time influence: Yields and AQE

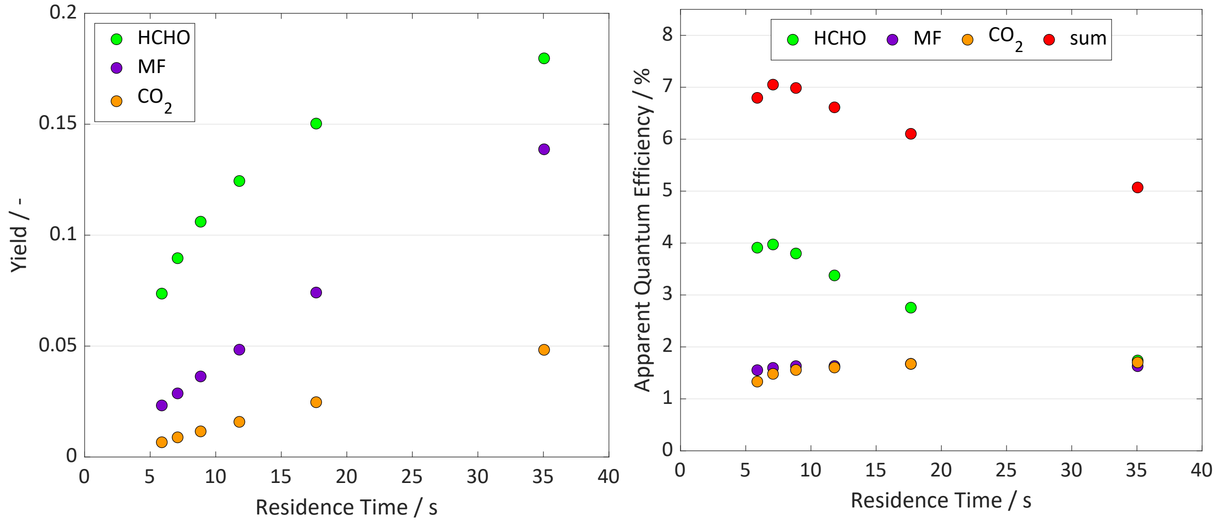

Figure S5: Yield (left) and AQE (right) at different residence times. $m_{Catalyst}$ = 0.0465 g; $\omega_{Catalyst}$ = 0.3419 mg cm^{-2}; T = 78 °C; E = 186.8 mW cm^{-2}

7. Irradiance Influence: Yields and AQE

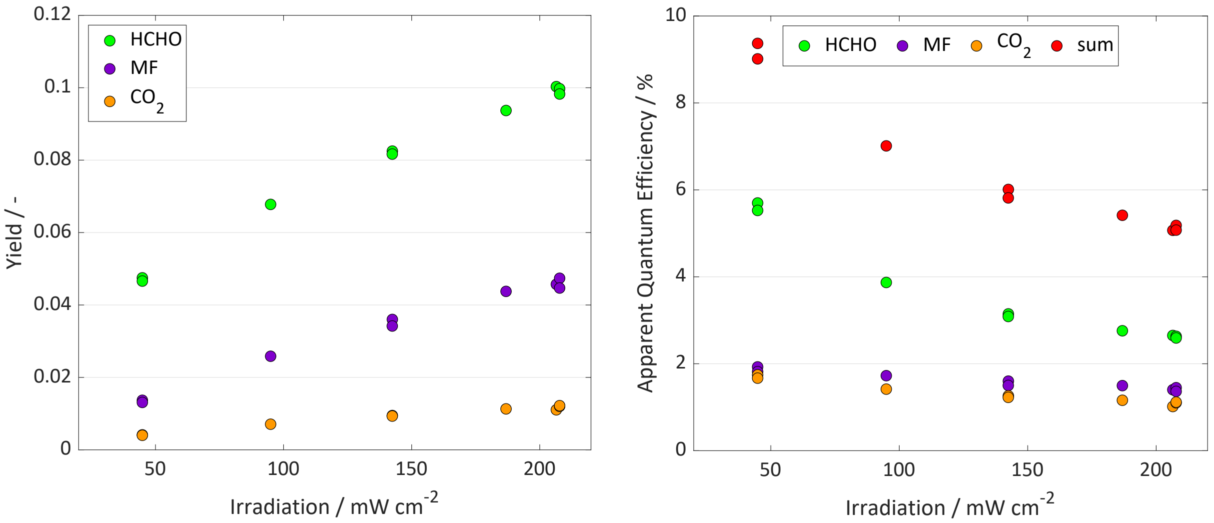

Figure S6: Yields (left) and AQE (right) for different irradiation intensities. $m_{Catalyst}$ = 0.0335 g; ω = 0.2463 mg cm^{-2}; T = 78 °C; τ = 11.8 s

8. Temperature influence: Yields and AQE

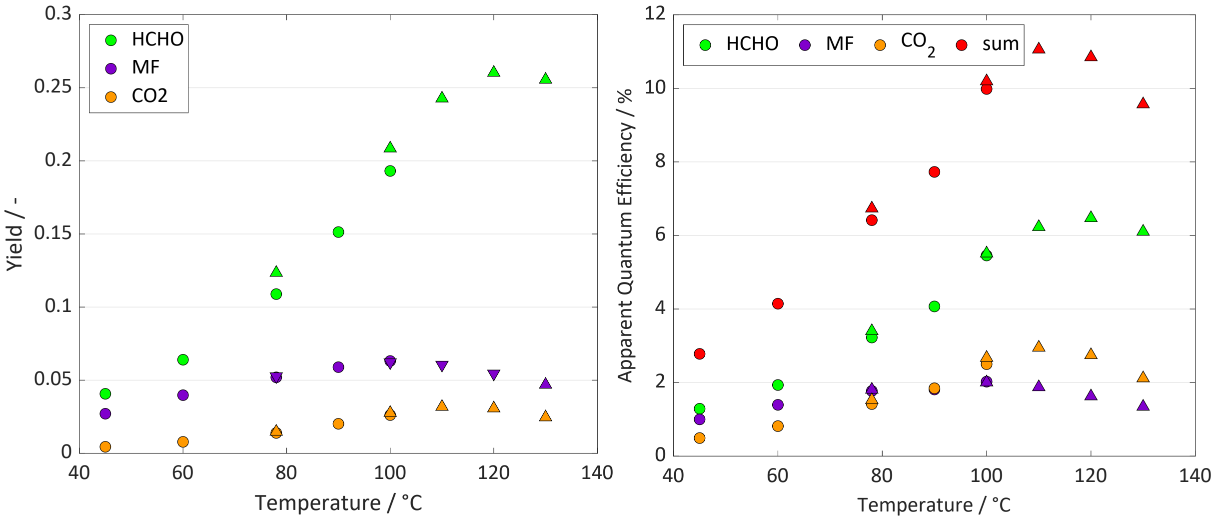

Figure S7: Yield towards product species (left) and AQE for product species and in total at different temperatures. $\boldsymbol{m_{Catalyst} = 0.0735}$ ***g (circles) / 0.0541 g (triangles);*** $\boldsymbol{\omega_{Catalyst} = 0.5404}$ ***mg cm***$\boldsymbol{^{-2}}$ ***/ 0.3978 mg cm***$\boldsymbol{^{-2}}$***;*** $\boldsymbol{\tau = 11.8}$ ***s; E = 186.8 mW cm***$\boldsymbol{^{-2}}$

9. Temperature Variation: Reproduction experiment

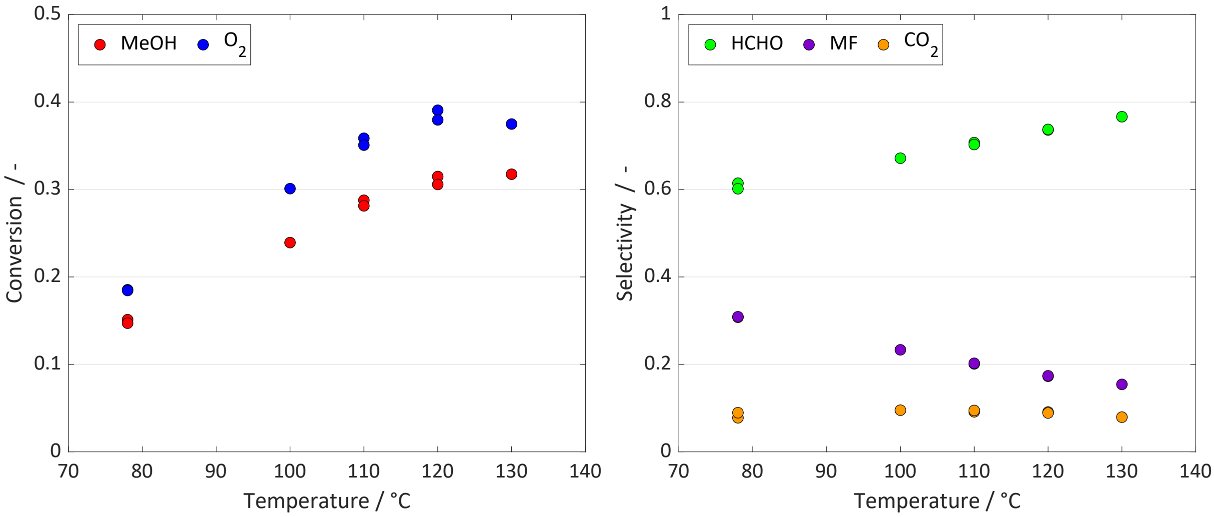

Figure S8: Conversion of MeOH and O_2 and product selectivities for different temperatures. $m_{Catalyst} = 0.0484$ g; $\omega_{Catalyst} = 0.3559$ mg cm^{-2}; $\tau = 11.8$ s; $E = 186.8$ mW cm^{-2}

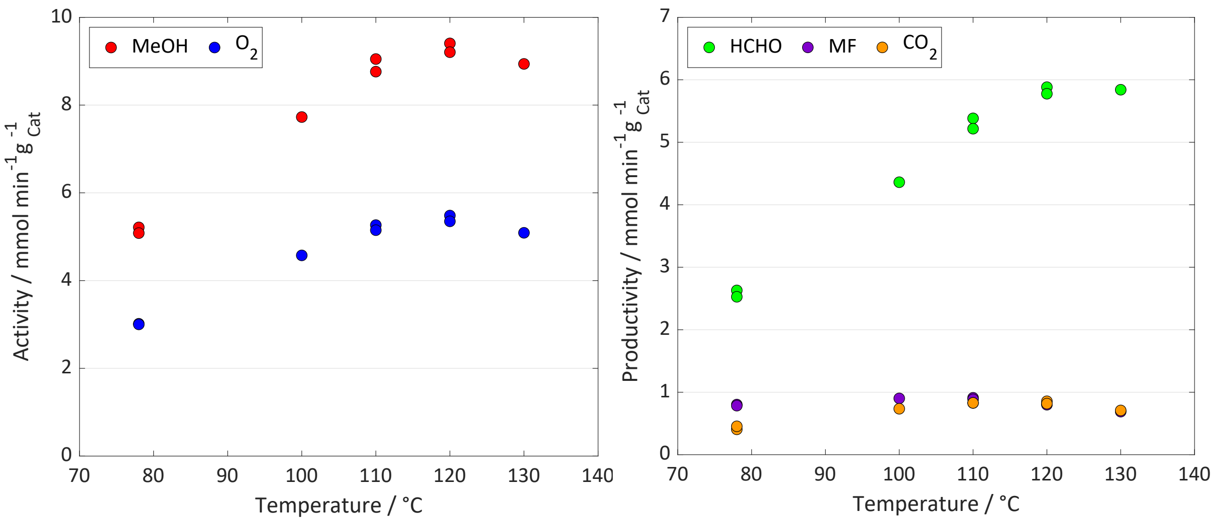

Figure S9: Catalyst activities (MeOH and O_2 consumption rates, left) and productivities (right) for different temperatures. $m_{Catalyst} = 0.0484$ g; $\omega_{Catalyst} = 0.3559$ mg cm^{-2}; $\tau = 11.8$ s; $E = 186.8$ mW cm^{-2}

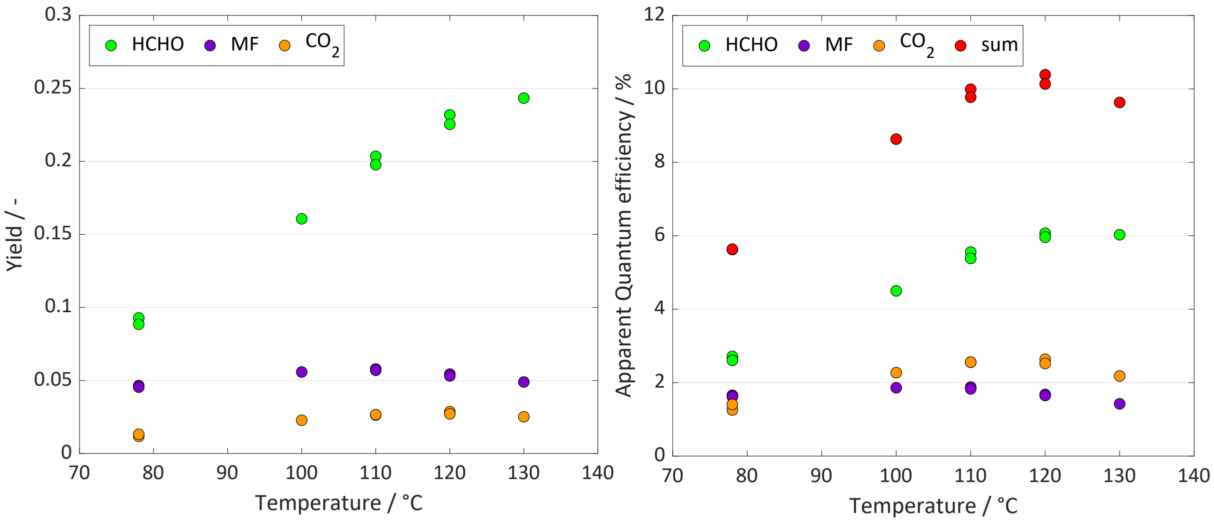

Figure S10: Yield towards products (left) and apparent quantum efficiencies (right) for different temperatures. $m_{Catalyst} = 0.0484$ g; $\omega_{Catalyst} = 0.3559$ mg cm^{-2}; $\tau = 11.8$ s; $E = 186.8$ mW cm^{-2}