

Supplementary Information

Simultaneous determination of enthalpy of mixing and reaction using milli-scale continuous flow calorimetry.

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Picture of the reactor

Figure S1 shows the reactor setup used for the experiments. The liquids are pumped (1 & 2) into the reactor (3). During this process, they are brought to the desired temperature in the preheater (4). The product is then analysed in the FTIR (5).

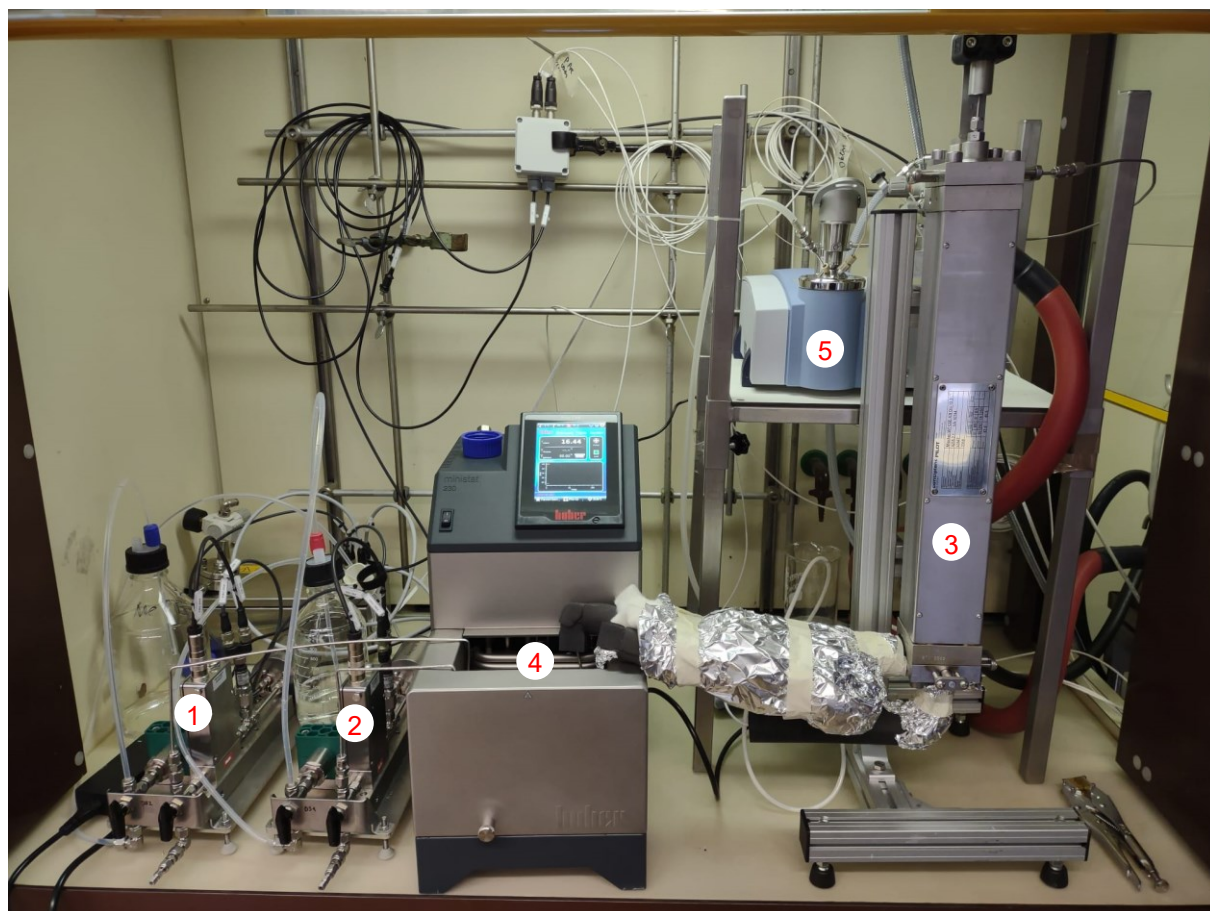


Figure S1 Reactor setup for the experiments.

FTIR Analysis

Figure S2 shows spectra of different concentrations of acetic anhydride (Ac_2O) in acetic acid (AcOH). The analysed signal at approx. 1125 $1/\text{cm}$, characteristic for Ac_2O , is shown at concentrations from 0.32-4.89 mol/l. During the course of the reaction this signal decreases. Both the catalyst HNO_3 and the products (AcOH and H_2O) do not disturb at the wavelength analysed.

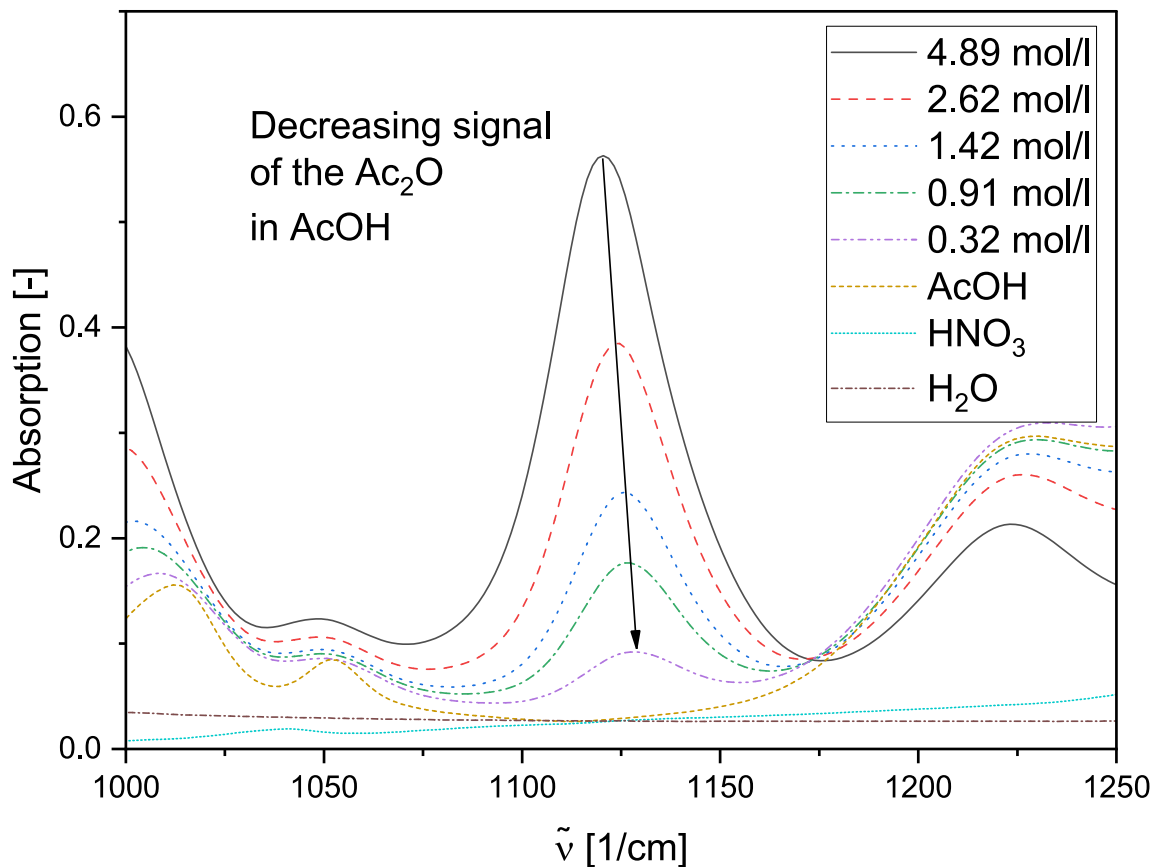


Figure S2 Spectra of different concentrations of acetic anhydride (Ac_2O) in acetic acid (AcOH). The analysed signal at approx. 1125 $1/\text{cm}$ decreases during the hydrolysis reaction.

Ac₂O Calibration

Figure S3 shows the calibration for E1, E2 E3 and E4, it is well reproducible in the measured concentration range.

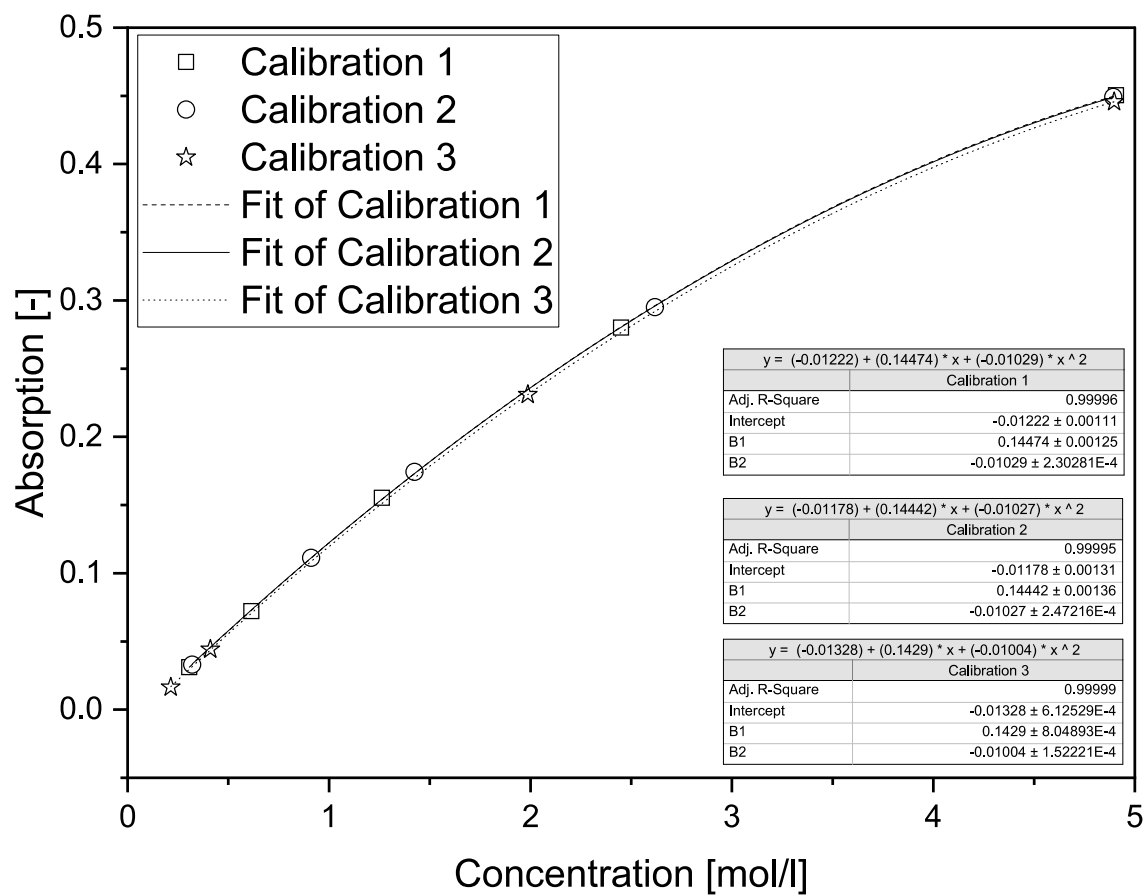


Figure S3 Ac₂O calibration in the concentration range from 0.21-4.91 mol/l.

Substance properties

Table S1 lists the used substance properties applied for the calorimetric calculations.

Table S1 The volume flow $\dot{V}$, viscosity η , density ρ , heat conductivity λ , and the specific heat capacity c_p are listed for each experiment.

$\dot{V}$ [ml/min]	η [Pas]	ρ [kg/m ³]	λ [W/m/K]	c_p [J/kg/K]	exp. series	Literature
18-90	0.001009	1091	0.309	2524	E1	1, 2
18	0.001245	1095	0.261	2464	E2	1, 2
36-72	0.001030	1095	0.300	2476	E2	1, 2
18-72	0.001366	1134	0.242	2482	E3	1, 2
36-72	0.001366	1135	0.242	2483	E4	1, 2

Literature:

1. Yaws CL (2003) Yaws Handbook of Thermodynamic Properties for Hydrocarbons and Chemicals. Knovel / McGraw-Hill, Norwich, New York
2. Bump TR, Sibbitt WL (2002) Heat Transfer Design Data—Aqueous Solutions of Nitric Acid and of Sulfuric Acid. Ind Eng Chem 47:1665–1670. <https://doi.org/10.1021/IE50548A055>