Supporting Information

Fast Microflow Kinetics and Acid Catalyst Deactivation in Glucose Conversion to 5-hydroxymethylfurfural

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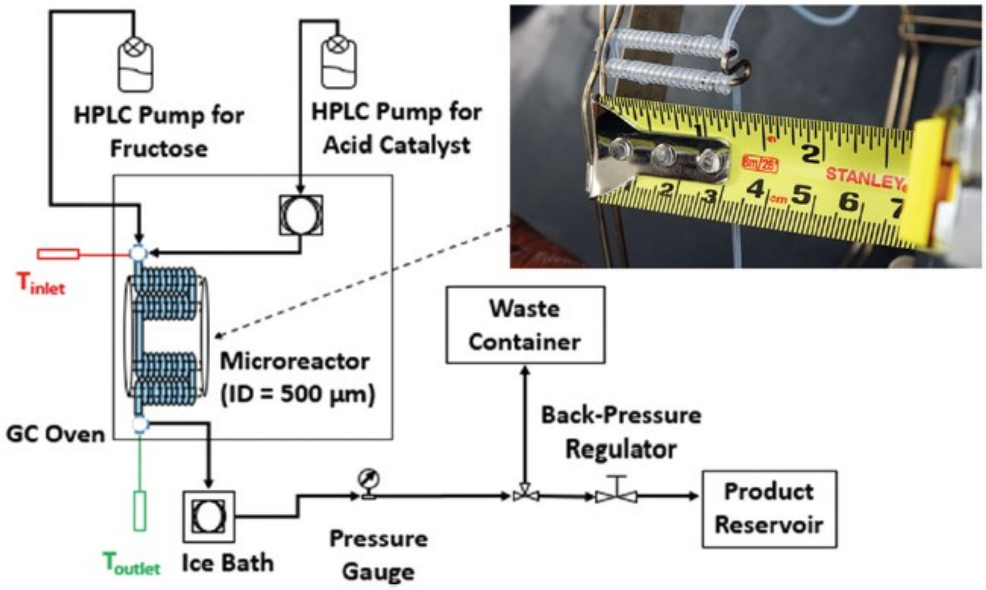
Configuration of the flow microreactor

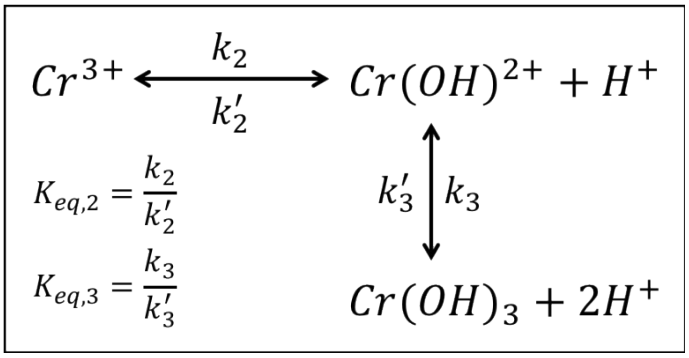


Scheme S1. Schematic overview of the microchannel flow reactor setup. Reprinted with permission from Desir et al.[1] Copyright (2019) Royal society of chemistry.

Proposed reaction network for catalyst speciation model

The proposed reaction network for the catalyst speciation model is shown in Scheme S2. The rate constant of the reverse reactions of R_2 and R_3 are modeled from the equilibrium constant and the forward rate constants. The equilibrium constants of R_2 and R_3 used in this study, obtained from OLI software, are shown in Table S1. The reaction orders are assumed equal to the stoichiometric coefficients for each reactant. The model equation is given by Eqs. (S1), where C_i is the concentration of component i; R_j is the reaction rate of reaction j, $R_j^{'}$ is the reaction rate of reverse reaction j; and α_{ij} is the stoichiometric coefficient of component i in reaction j.

$$\frac{dC_i}{dt} = \sum_j \alpha_{ij}(R_j + R_j^{'}) \tag{S1}$$



Scheme S2. Proposed reaction network for the catalyst speciation model.

Table S1. Equilibrium constant of R_2 and R_3 used in this study.

Temperature [°C]	$K_{eq,2}$ [M]	$K_{eq,3}$ [M]
140	0.0081	0.082
160	0.015	0.23
180	0.026	0.59

Method for calculating the initial glucose reaction rate

The reaction rate of glucose follows first-order kinetics and has the following rate expression as Eq. (S2),

$$r_{glu} = -\frac{dC_{glu}}{dt} \tag{S2}$$

where r_{glu} denotes the rate, and C_{glu} is the glucose concentration at any time. At conversions less than 15%, one can assume that the rate is the initial rate at the inlet of the inlet conditions. Therefore, a linear fit of the glucose concentration vs. time data at <15% conversion is used to obtain the initial glucose reaction rate. A sample caculation is provided in Figure S1.

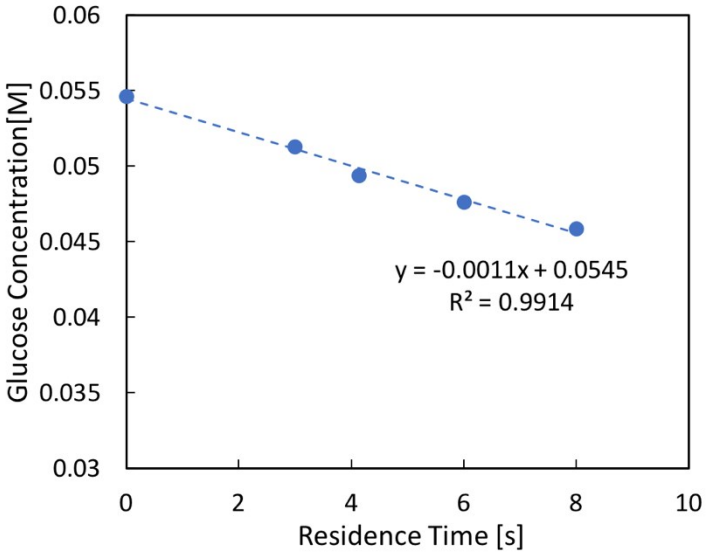


Figure S1. Glucose concentration (C_{glu}) vs. time (t) at 180 °C using a 1.7 mM $CrCl_3$ catalyst which was preheated for 1 mins. A linear fit (dashed line) was used to obtain the initial glucose reaction rate of 11×10^{-4} M/s.

References

1. P. Desir, B. Saha and D. G. Vlachos, *Energy & Environmental Science*, 2019, **12**, 2463-2475.