

Supporting information

Enhancement of the liquid-sided mass transfer in a falling film catalytic microreactor by in-channel mixing structures

Evgeny V. Rebrov^{1*}, Thijs Duisters², Patrick Löb³, Jan Meuldijk¹, Volker Hessel²

¹ Queen's University Belfast, Stranmillis Road, BT9 5AG Belfast, UK

² Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, the Netherlands

³ Institut für Mikrotechnik Mainz GmbH, Carl-Zeiss-Str. 18-20, 55129 Mainz, Germany

1. Effect of catalyst concentration on octanal conversion

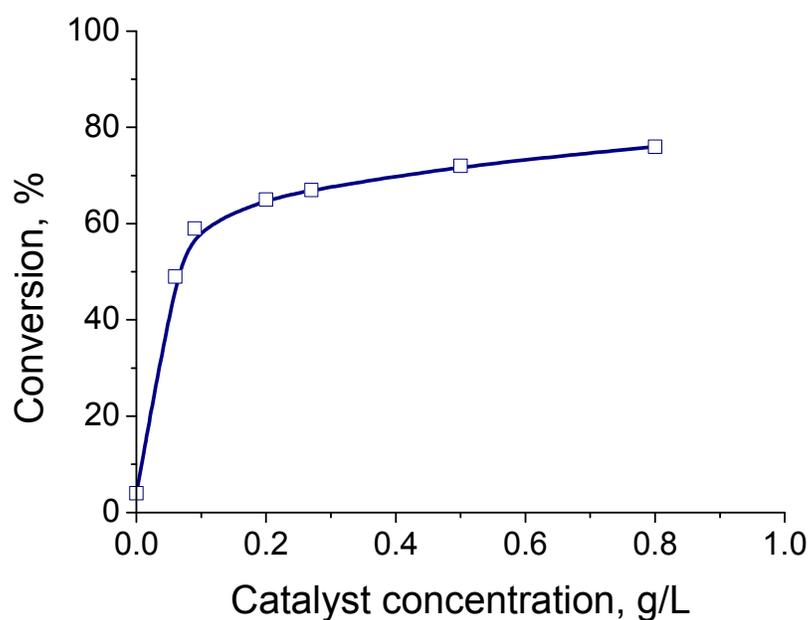


Figure S1. Octanal conversion at 5.0 bar as function of the catalyst concentration. Liquid flow rate: 6.0 ml/min. Gas flow rate: 3.5 ml/min (STP). Liquid residence time: 1.6 s.

2. Temperature distribution in the falling film microreactor

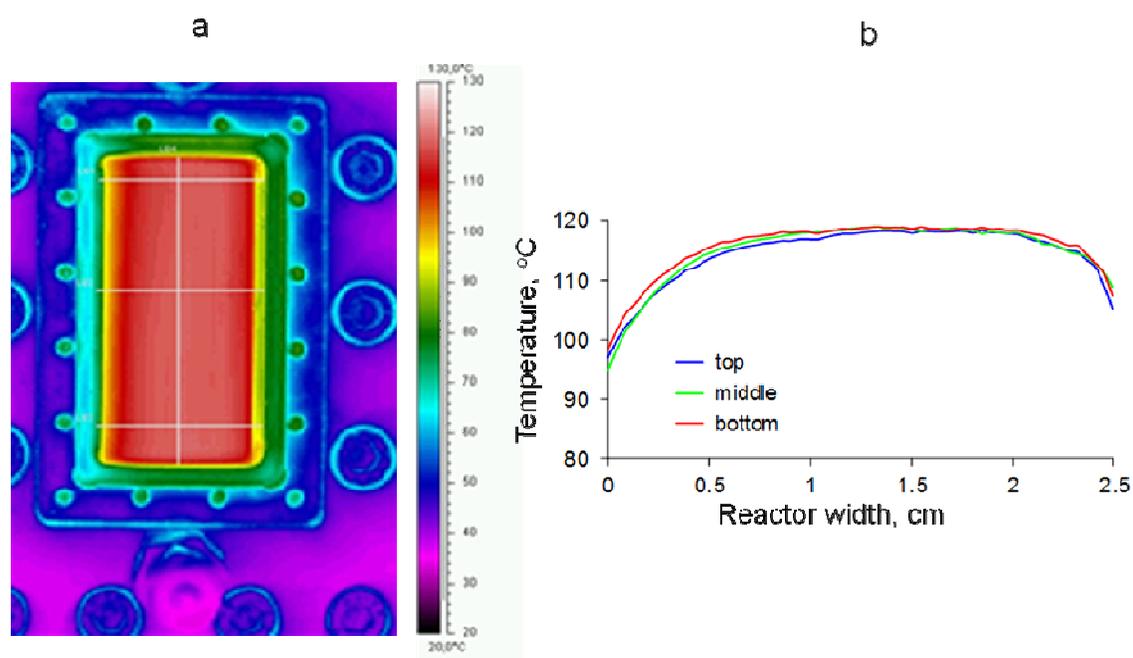


Figure S2. Temperature distribution in the FFMR. (a) 2D map of temperature distribution in the standard reactor plate. (b) Temperature profile in the direction perpendicular to the liquid flow at three positions.

3. Calculation of diffusivities

The diffusivities of octanal and octanoic acid in propionic acid were determined by Wilke-Chang equation:

$$D_{i,j} = n_{WC} \frac{\sqrt{x_j M_j T}}{\mu_j V_i^{0.6}}$$

where $D_{i,j}$ is given in cm^2/s , n is the Wilke-Chang parameter ($n_{WC} = 7.4 \cdot 10^{-8}$), x_j is the association parameter ($x=1$ for octanal and octanoic acid), M_j is the molar mass of propionic acid in g/mol , μ_j is viscosity of solution in cP and V_i is the molar volume of the solute at its normal boiling point in cm^3/mol .

4. Estimation of kinetic parameters

The kinetic parameters were estimated in a capillary microreactor with an internal diameter of 750 μm and a length of 0.05 m. The liquid and gas (oxygen) were mixed in a T-mixer prior to the capillary reactor. The concentration of octanal was changed in the range of 500-1250 mol/m^3 . The flow rates of both gas and liquid were changed in order to keep octanal conversion below 5% (differential reactor approximation). As the reaction progresses, the size of oxygen bubbles reduces along the channel length, however the oxygen concentration in the liquid remains constant. The oxygen conversion was estimated from the mean bubble size taken at the beginning and at the end of the capillary.

Table S1. Octanal and oxygen conversion in a capillary microreactor.

$C_{O_2}^0$, mol/m^3	C_B^0 , mol/m^3	F_L , m^3/s	F_G , m^3/s	Conversion, %		Reaction rate, $\text{mol}/(\text{m}^3 \cdot \text{s})$
				Octanal	O_2	
30	1250	$2.83 \cdot 10^{-9}$	$1.88 \cdot 10^{-9}$	4.7	98	11.8
30	1050	$2.47 \cdot 10^{-9}$	$1.40 \cdot 10^{-9}$	4.5	94	8.3
30	800	$2.12 \cdot 10^{-9}$	$9.27 \cdot 10^{-10}$	4.0	72	4.8
30	500	$1.41 \cdot 10^{-9}$	$6.18 \cdot 10^{-10}$	3.8	48	1.8

Temperature: 291 K. Catalyst concentration: 0.6 g/L. Reactor volume: $2.21 \times 10^{-8} \text{ m}^3$

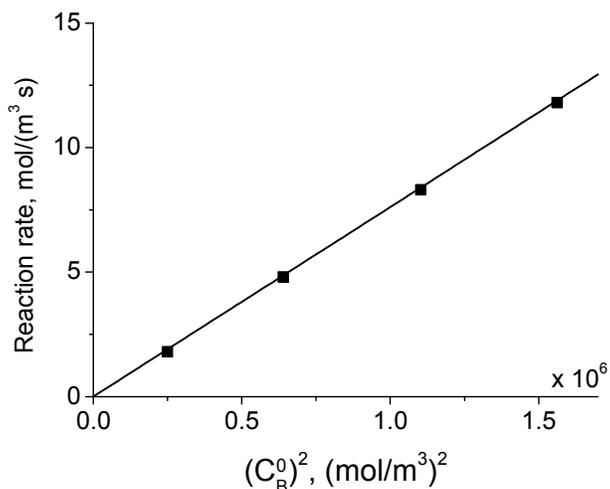


Figure S3. The octanal oxidation reaction rate as a function of the square of the octanal concentration. Reaction conditions are shown in Table S1.

Taking into account the activation energy of 57.3 kJ/mol, the pre-exponential factor of the reaction rate constant is equal to $4910 \text{ m}^6/(\text{mol}^2 \cdot \text{s})$.