

# Selective Transformation of Cumene in Electrochemical Batch and Flow Reactors

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Electro-organic synthesis has attracted attention from the viewpoint of sustainability because reactions can proceed well even at ambient conditions [1]. However, in a generic batch reactor, long reaction time is generally required, leading to a poor product selectivity due to side reactions. On the other hand, in a flow reactor, products flow outside the reaction system, which improves the selectivity by suppressing side reactions. Herein, we report selective molecular transformation of cumene in electrochemical batch and flow reactors.

A solution of cumene (**1**) and Et<sub>4</sub>NClO<sub>4</sub> (0.1 M) in MeCN was transferred into the undivided electrochemical reactors equipped with boron-doped diamond (BDD) anode and cathode. A constant current electrolysis was performed at room temperature.

In the batch reactor, **1** was electrochemically converted into cumene hydroperoxide (**2**), acetophenone (**3**), and cumyl alcohol (**4**). The main product was **3**, and the isolated yield was 34% under the optimum condition with the current density ( $j$ ) of 2.1 mA/cm<sup>2</sup> and the amount of charge ( $Q$ ) of 5.0 F (referring to mole of **1**) [2]. On the other hand, in the flow reactor, **4** was obtained as the main product with the GC–MS yield of 44% under the optimum condition:  $j$  of 0.25 mA/cm<sup>2</sup>,  $Q$  of 1.0 F (referring to mole of **1**), and flow rate of 0.375 mL/min (**Table 1**). Obviously, the product selectivity in electro-conversion of cumene can be controlled by changing electrolysis modes. This is especially because an overoxidation of **4** into **3** was suppressed in flow electrolysis.

## References

- [1] A. Wiebe, T. Gieshoff, S. Möhle, E. Rodrigo, M. Zirbes, S. R. Waldvogel, *Angew. Chem. Int. Ed.*, 57 (2018) 5594–5619.  
[2] M. Kitano, T. Saitoh, S. Nishiyama, Y. Einaga, T. Yamamoto, *Beilstein J. Org. Chem.*, 18 (2022) 1154–1158.

**Table 1.** Screening of flow electrolysis conditions.

The reaction scheme shows cumene (1) being converted to cumene hydroperoxide (2), which then further reacts to form acetophenone (3) and cumyl alcohol (4).

Entry <sup>[a]</sup>	$j$ (mA/cm <sup>2</sup> ) <sup>[b]</sup>	$Q$ (F) <sup>[c]</sup>	$v$ (mL/min) <sup>[d]</sup>	Yields (%) <sup>[e]</sup>		
				<b>1</b>	<b>3</b>	<b>4</b>
1	2.0	1.0	3.0	30	n.d.	17
2	2.0	3.0	1.0	14	14	10
3	2.0	5.0	0.6	3	7	6
4	3.0	1.0	4.5	1	3	3
5	1.0	1.0	1.5	trace	3	20
6	0.5	1.0	0.75	52	n.d.	42
7	0.25	1.0	0.375	36	n.d.	44

[a] Reaction conditions: BDD cathode and anode, 5 mM **1**, 0.1 M Et<sub>4</sub>NClO<sub>4</sub>, MeCN (30 mL), undivided flow cell, rt. [b] Current density. [c] Amount of charge (referring to mole of **1**). [d] Flow rate. [e] Determined by GC–MS. n.d.: not detected.