Supplementary Material

Tert-butyl hydroperoxide decomposition as a descriptor for liquid-phase hydrocarbon oxidation over transition metal oxide-based catalysts: a screening study

Julia Büker,[a] Jingqi Shang,[b] Steven Angel,[c] Eko Budiyanto,[d] Harun Tüysüz,[d] Hartmut Wiggers,[c] Christof Schulz,[c] Marcus Grünewald,[b] Baoxiang Peng,[*a,e] and Martin Muhler[*a,e]

[a] Laboratory of Industrial Chemistry, Ruhr University Bochum, Universitätsstr. 150, 44780 Bochum, Germany;
[b] Lehrstuhl für Fluidverfahrenstechnik, Ruhr University Bochum, Universitätsstr. 150, 44780 Bochum, Germany;
[c] EMPI, Institute for Energy and Materials Processes – Reactive Fluids and CENIDE, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, Carl-Benz-Straße 199, 47057 Duisburg, Germany; [d] Department of Heterogeneous Catalysis, Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany; [e] Max Planck Institute for Chemical Energy Conversion, Stiftstraße 34-36, 45470 Mülheim an der Ruhr, Germany
Email: baoxiang.peng@techem.rub.de martin.muhler@ruhr-uni-bochum.de

Table of Contents

Figure S1. Volumetric gas measurement set-up (GASMESS-5) commercially available from MesSen Nord GmbH to record the evolved or consumed gas volume as a function of time.

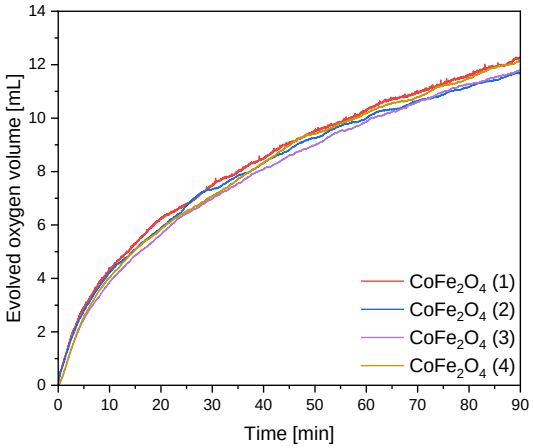

Figure S2. Evolved O_2 volume as a function of time for repeated TBHP decomposition experiments under identical reaction conditions over a commercial $CoFe_2O_4$ catalyst to verify the reproducibility of the volumetric set-up. Reaction conditions: 50 mg catalyst, 20 mL acetonitrile, 500 µL TBHP, 60 °C, 700 rpm.

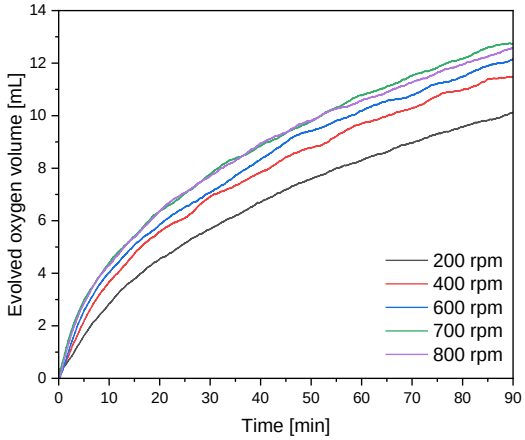

Figure S3. Evolved O_2 volume as a function of time for TBHP decomposition experiments at different stirring speeds. Reaction conditions: 50 mg commercial $CoFe_2O_4$, 20 mL acetonitrile, 500 µL TBHP, 60 °C, 200/400/600/700/800 rpm.

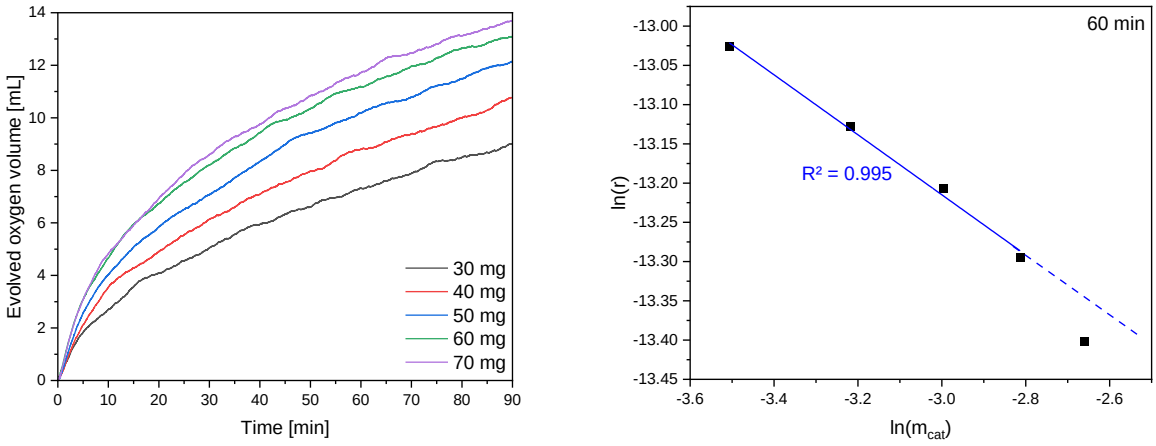

Figure S4. Evolved O_2 volume as a function of time for TBHP decomposition experiments using different catalyst amounts (left) and the corresponding linearized plot of the reaction rate as a function of the catalyst amount after 60 min (right). Reaction conditions: 30/40/50/60/70 mg commercial $CoFe_2O_4$, 20 mL acetonitrile, 500 µL TBHP, 60 °C, 700 rpm.

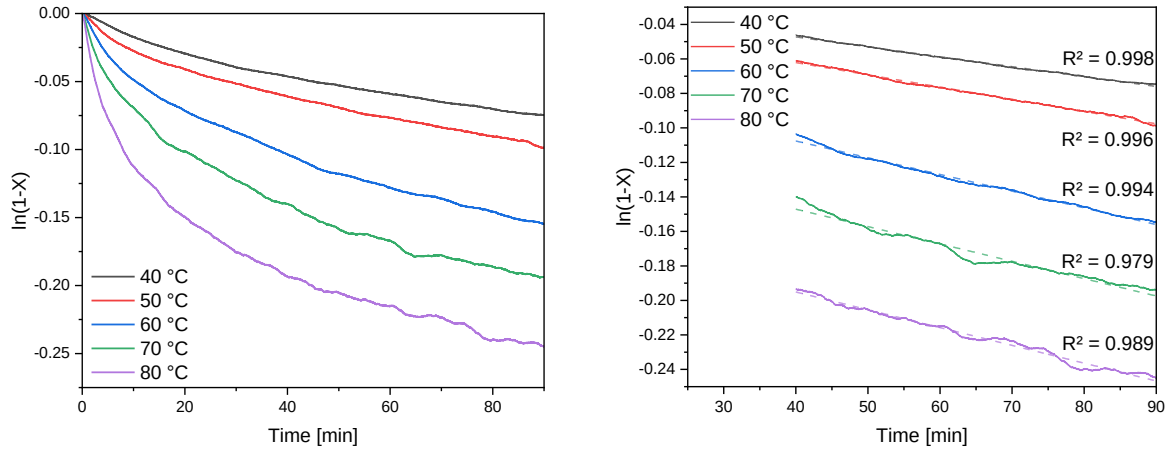

Figure S5. Linearized plot of the evolved O_2 volume as a function of time for TBHP decomposition experiments at different temperatures (left) and the selected linear time ranges for the determination of the reaction constant k (right). Reaction conditions: 50 mg commercial $CoFe_2O_4$, 20 mL acetonitrile, 500 µL TBHP, 40/50/60/70/80 °C, 700 rpm.

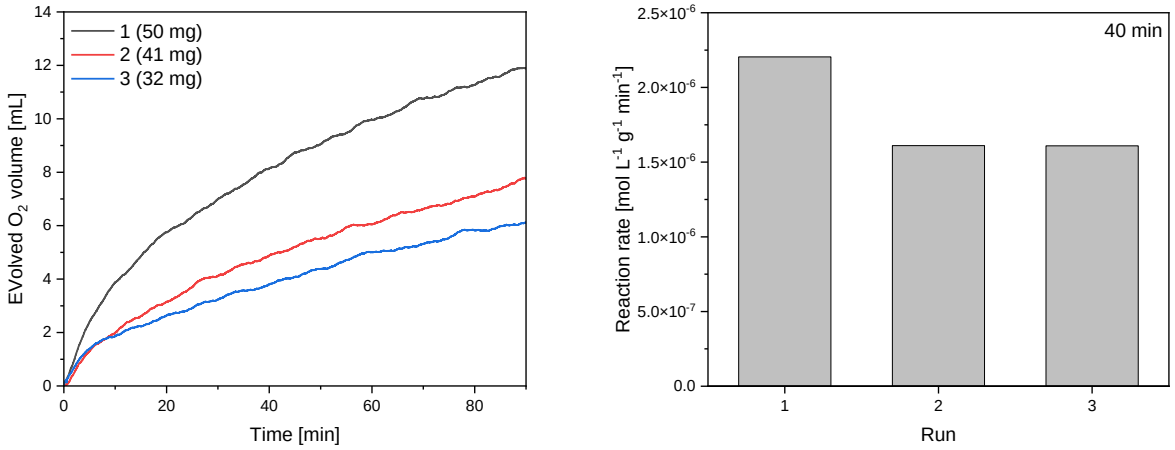

Figure S6. Evolved O_2 volume as a function of time for TBHP decomposition experiments using the same catalyst for three reaction runs under identical reaction conditions to test its stability and reusability (left) and the corresponding reaction rates normalized to the catalyst amount after 40 min (right). Reaction conditions: 50 mg commercial $CoFe_2O_4$, 20 mL acetonitrile, 500 µL TBHP, 60 °C, 700 rpm, 3 × 90 min.

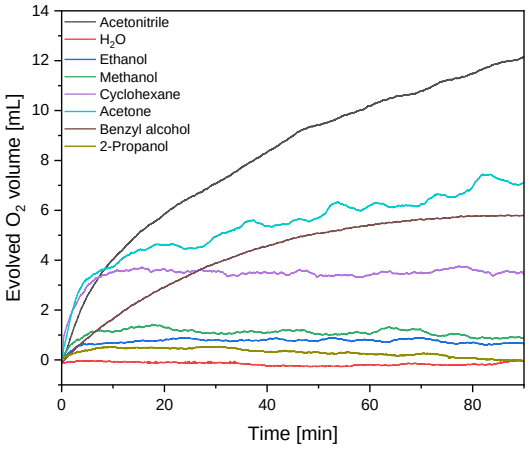

Figure S7. Evolved O_2 volume as a function of time for TBHP decomposition experiments using different solvents. Reaction conditions: 50 mg commercial $CoFe_2O_4$, 20 mL solvent, 500 µL TBHP, 60 °C, 700 rpm.

