

<u>Catalyst and Reactor Design Considerations for Selective Production</u> <u>of Acids by Oxidative Cleavage of Alkenes with H₂O</u>₂

Background/Objective

- The oxidative cleavage of bio-based unsaturated fatty acids (UFAs) with the oxidant hydrogen peroxide (H_2O_2) offers a more efficient and lower environmental impact process to create bioproduct precursors than current methods with more caustic chemicals.
- Here we proposed a semi-batch reactor for high acid yields from UFAs based on reactor engineering principles and prior insights elucidating the reaction mechanism.

Approach

Derived kinetic model equations for each reaction step, fit them to experimental batch data to obtain kinetic parameters, optimized the oxidant feed rate (F_{H2O2}) of semi-batch operation using model prediction, and validated the model with experimental data.

Results

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Semi-batch operation with a low F_{H2O2} into the reactor increases product selectivity.

Significance/Impacts

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Science

Determined reaction conditions where low concentrations of H_2O_2 , along with solid oxide catalysts like tungstates, will be effective for stable and selective oxidative cleavage reactions to produce bioproduct precursors.

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Selectivities toward oxidative cleavage products and H_2O_2 during oxidative cleavage of 4-octene as functions of H_2O_2 feed rate over aluminasupported tungstate catalyst (WO_x -Al₂O₃). Dashed lines signify model predictions, and black and green arrows indicate selectivities measured in the batch-stirred tank reactor (BSTR).