Continuous hydrodeoxygenation of neat poplar lignin oil to jet-range aromatic hydrocarbons with molybdenum carbide

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The aviation industry requires sustainable aviation fuels (SAF) capable of reducing greenhouse gas emissions while satisfying strict safety and quality standards. Lignin is a promising renewable feedstock for the production of aromatic hydrocarbons, the missing fraction needed to achieve 100% SAF. The use of lignin in SAF hinges on reducing oxygen content while limiting ring hydrogenation and maximizing yields of C8-C20 hydrocarbons. Herein, we utilize molybdenum carbide (Mo_2C) catalysts to hydrodeoxygenate lignin oil produced via reductive catalytic fractionation (RCF) of untreated poplar. We designed a 3-phase trickle-bed reactor that generates steady-state partial-conversion kinetic data to analyze catalyst activity while deoxygenating complex lignin feeds, concluding that surface oxidation is the key catalyst limitation while processing neat lignin oil. At 350°C, complete deoxygenation is achieved in a single-pass at steady-state, with 94.2% selectivity of monomeric products to propylbenzene and methylpropylbenzene and 70.8 C-mol% recovery of whole oil. While achieving high monomer recovery, single-pass reactions at 350°C have low recovery of dimers and larger oligomers. We hypothesize this is due to high reactivity of oxygenated oligomers toward unwanted side reactions at 350°C. To recover larger oligomers, a multi-pass reaction was performed in which 50% of oxygen was removed at 300°C, an additional 25% oxygen was removed at 325°C and the remaining oxygen was removed in a third pass at 350°C. This multi-pass experiment resulted in an oil containing 49.5 wt.% 1-ring aromatics, 25.6 wt.% 2-ring aromatics, and 14.1 wt.%

cycloalkanes. Deoxygenation of neat RCF oil corresponded to an increase in carbon content from 65.4 to 88.7 mass %, a decrease in oxygen content from 26.8 to 0.7 mass %, an increase of lower heating value from 21.73 to 39.99 MJ/kg, and a decrease in viscosity at 40°C from 231 to 1.04 cP.

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