Revealing molecular-level interplays during copyrolysis of macromolecular mixtures

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The development of enabling technologies for efficient production of renewable fuels and chemicals is projected to grow over the next decades. Pyrolysis is a simple thermochemical method to upcycle under-utilized macromolecular resources, such as lignocellulosic biomass, plastics, and food waste, into high-value products. The molecular picture of copyrolysis of waste mixtures, however, is still lacking due to the complex nature of the systems, making the technology nonselective. In this talk, mixtures of cellulose and various synthetic plastics are selected as model systems to reveal the fundamental interplays between two immiscible macromolecular components during their copyrolysis. It was found that the mixing of the two phases has a significant impact on their synergy during copyrolysis. Three molecular-level interactions were discovered based on our experiments and density functional theory calculations. First, the molten plastic layers, which have a much longer decomposition timescale, serve as a trapping agent surrounding the fast-pyrolyzing cellulose, inhibiting the escape of the primary cellulose pyrolysis products and promoting secondary cellulose pyrolysis reactions. Second, the functional groups of the molten plastic phase alter cellulose pyrolysis pathways by changing the local environments of the reaction centers. Third, the biochar remains from the fast-pyrolyzing cellulose catalyze the pyrolysis of molten plastics at a later stage. Our findings suggest that the interplays between chemical kinetics and mass transfer during copyrolysis of macromolecular mixtures can be manipulated to promote yields of desired products or to reveal decomposition pathways of other less-studied, fast pyrolyzing carbohydrate polymers.

Bio: Hsi-Wu Wong is an Associate Professor in the Department of Chemical Engineering at UMass Lowell. His research group focuses on using chemical reaction engineering principles to manipulate reaction and mass transfer pathways for converting under-utilized feedstocks into high-value products. Dr. Wong received his PhD from Northwestern University and worked as a postdoctoral researcher at MIT. He has authored or co-authored more than 50 peer-reviewed papers and is the recipient of the National Science Foundation CAREER award, North American Symposium on Chemical Reaction Engineering Early Career Faculty Travel Award, and B. J. Martin Dissertation Year Fellowship at Northwestern University.