447e: Dissolution of Cellulosic Particles: Population Ensemble Modeling Informs Efficient Woody Biomass Processing

Tuesday, October 31, 2017
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A major barrier to the efficient utilization of biomass is the recalcitrance to dissolution of semicrystalline cellulose. The present study addresses the kinetics of swelling and dissolution of cellulose particles in conditions emulating large-scale processing where the particles exhibit a distribution of size and degree of crystallinity. To this end, we have developed a model in which the behavior of a population of particles is obtained from an ensemble of individual cellulose particle dissolution models. The dissolution of individual solid cellulose particles is based on the relevant transport phenomena and kinetics and reveals decrystallization and disentanglement as two important and potentially rate-determinant steps in the process. [Ghasemi, M.; Alexandridis, P.; Tsianou, M., Cellulose dissolution: Insights on the contributions of solvent-induced decrystallization and chain disentanglement. Cellulose 2017, 24 (2), 571-590. DOI: 10.1007/s10570-016-1145-1] The average value or the number distribution of any intra-particle property captured by the individual particle model can be determined by simulation of a sufficient number of individual particles such that ensemble averages are independent of the particle numbers and the computed particle distributions are acceptably smooth. Using this population ensemble model, various cellulose particle size distributions and crystallinity distributions are analyzed for different dissolution parameters. The findings from this study would be useful for the rational design and optimization of pretreatment processes to reduce the particle size and degree of crystallinity, leading to enhanced woody biomass utilization. [Ghasemi, M.; Tsianou, M.; Alexandridis, P., Assessment of solvents for cellulose dissolution. Bioresource Technol. 2017, 228, 330-338. DOI: 10.1016/j.biortech.2016.12.049]

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