Autonomous Exploration of Catalyst Shape with Blender-CFD based Multi-Objective Bayesian Optimization

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In the field of chemical processes, fixed-bed reactor is generally used. Recently, advances of devices and methods in computational fluid dynamics (CFD) simulations, enabled consideration of particle shape rather than using porosity of reactor. This study aims to determine optimal catalyst shape for specific reactions by using closed-loop system consisted of automated packed bed reactor (PBR) generator part and optimization applied CFD simulation part. PBR generator part is handled with Bullet Physics Library and rigid-body model (both in the open-source software Blender) and CFD simulation part used multi-objective Bayesian optimization for the catalyst shape optimization. It is shown that random PBR packing using the Blender achieved quite exact simulation for porosity and particle orientation compared to experimental one with much faster calculation. Further, we developed model to maximize conversion and selectivity for reactions, such as VOCs oxidation, by adopting different shapes of catalyst such as cylinder, sphere, Raschig ring, and several more others. Finally, this model significantly reduced simulation time respect to discrete element method with comparable precision.