Identification of multiple optima for high-throughput screening of combinatorial catalysis using modified particle swarm optimization

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The development of combinatorial technology has enabled synthesis and characterization of a huge amount of chemical compounds in a short time. To discover new catalysts, the automated parallel experimental system for combinatorial catalysis requires efficient optimization algorithms for high-throughput screening and experimental design. Like other algorithms that search for the global optimum of a model predicting catalyst performance, the standard particle swarm optimization (PSO) algorithm based on the concept of the flocking behavior of birds cannot locate more than one solution. However, the model establishing the relationships between the catalyst performance and the affecting factors is hardly robust so that one obtained optimum could be unreliable or inapplicable for synthesizing industrial catalysts. In this study, the niche particle swarm optimization, a modified PSO algorithm, is suggested to locate multiple optima because a specific local or global optimum among multiple optima could be more reliable and applicable to synthesize catalysts. Therefore, this work will contribute to developing new industrial catalysts in combinatorial catalysis.