

Bayesian Optimization for Reaction Parameter Tuning: An Exploratory Study of Parameter Optimization in Oxidative Desulfurization of Thiophene

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Abstract : The study explores the utility of Bayesian optimization in tuning the physical and chemical parameters of reactions in an offline experimental setup. A comparative analysis of the influence of the acquisition function on the optimization performance is also studied. For proxy first and second-order reactions, the results are indifferent to the acquisition function used, whereas, while studying the parameters for oxidative desulphurization of thiophene in an offline setup, upper confidence bound (UCB) provides faster convergence along with a marginal trade-off in the maximum conversion achieved. The work also demarcates the critical number of independent parameters and input observations required for both sequential and offline reaction setups to yield tangible results.

Keywords : acquisition function, Bayesian optimization, desulfurization, kinetics, thiophene

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