Integrated Computational Strategies for the Analysis, Design and Synthesis of Chemical and Biological Systems

by

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ABSTRACT

Continuous efforts of application and development of computational strategies in various research fields, e.g. fuel cell, pressure swing distillation (PSD), hydrogen production from energy resources other than fossil fuel, and cell metabolism have been the focus of much attention in the chemical engineering and science community for decades. At the heart of this problem, one of the continuous demands in order to improve and realize these computational efforts is the application of optimization methods to handle problems appeared in different mathematic forms, such as linear, nonlinear, and differential. These optimization methods can be used to evaluate reaction parameters in complex reactor form such as adiabatic plug flow reactor, generate brand new thermal cycle to be further evaluated, improve the economy of PSD, and reveal the metabolism of cell culture. I will present work which shows that four optimization applications applied in the developments of computational strategies. The first is parameter estimation for reaction kinetics of PROX reaction in fuel cell. The second is evaluation of hydrogen production by thermal cycle with sensitivity analysis and searching of potential new and feasible thermal cycle with optimization technology. The third is to improve the PSD economy with the optimal heat and power integration for PSD. The fourth is revealing the dynamic behavior of cell metabolism with the application of dynamic optimization. These results highlight the importance of optimization applications in development of computational strategies. However, some further works are required to meet more realistic demand from the view points of industry. Therefore, I will also outline future work with a goal of improving the application of optimization to match more realistic situation, as well as other potential optimization technology which is potentially suitable to the application of new computational strategies for other important topics in chemical and biological engineering fields.