Title: 인공지능을 이용한 화학공학

Abstract:

How to design the “optimal” product and process is the central problem in process systems engineering. Although mathematical programming (MP)-based optimization technologies have shown a more systematic design framework than the heuristic approach, there are several critical bottlenecks (e.g., vast design space, uncertainty, non-data-driven, computational cost) to applying the methodology in the real world. For this reason, design methodologies based on machine learning (ML) have been recently proposed, and they show breakthrough performance in some problems that existing methodologies cannot solve. In this talk, we will cover two reinforcement learning (RL), one of the most important ML class, applications performed by our laboratory. In the case of product design, we introduce a fragment combination-based RL agent to discover de novo molecules whose properties are unseen and extrapolated. The results highlight that the proposed RL framework outperforms to generate molecules with unseen properties compared to state-of-the-art molecules inverse design methodologies such as the neural machine translator model (e.g., cRNN) and generative model (e.g., GCT). Second, an autonomous energy management system for optimal planning of hybrid energy storage processes will be discussed. We compare the profit maximization performance between the RL agent and conventional mixed-integer linear programming under uncertainty. Since the proximal policy optimization (PPO) RL algorithm can consider the uncertainty itself, we could confirm that the proposed methodology show more robust performance, under a large uncertainty of the curtailed renewable energy, with a maximizing net profit and stable system.