AI-Based Design of Chemical Processes by Deep Reinforcement Learning

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Abstract

Chemical process design is a complex planning problem, characterized by vast search spaces, continuous parameters, and the need for generalization. Machine learning, particularly deep reinforcement learning (RL), has uncovered the potential to design processes without heuristic knowledge or manual modifications. Existing RL algorithms can design flowsheets by sequentially placing and connecting process units until a certain objective, such as maximum plant profitability, is reached [1, 2, 3]. These approaches, however, are limited to single systems of components and do not account for a broad range of chemicals and process units. This work represents a step toward a more generalized RL tool that can learn to synthesize near-optimal flowsheets for a *multitude* of systems, each requiring a substantially different conceptual approach. This is achieved through an algorithmic improvement on AlphaZero, a deep RL algorithm designed to master games such as chess and go, which is trained to synthesize flowsheets for the separation of various binary, azeotropic mixtures [4]. Without prior knowledge, the RL agent learns to add solvents, combine them with distillation columns, decanters, and mixers, and place recycle streams. Achieving capabilities in line with those of graduate students in process engineering, the RL tool learns to propose schemes such as entrainer distillation and azeotropic distillation with decanters and to select solvents for these tasks. On average, the agent can separate more than 99% of the given mixtures into pure components, highlighting the agent's planning flexibility and potential for greater generality. The success of this approach also opens the door to further applications for the RL tool, such as molecular solvent design.

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