

Ensuring GenAI Works for Chemical Process Systems: Perspectives on Use Cases and Alignment

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ABSTRACT

Recent years have seen the rapid proliferation of generative AI tools, from chatbots to autonomous “agents.” These tools have transformative potential in all parts of society, including the chemical process industry. However, deploying these tools to their full effect will require careful consideration of the areas where generative AI can enhance, rather than replace existing chemical engineering knowledge, and how it can be deployed in a safe manner given the current limitations in generative AI technology. The first half of this talk reviews some promising use cases of generative AI in process systems engineering emphasizing areas where first principles knowledge is insufficient for the task. In particular, efforts utilizing AI for generating new decompositions of large-scale optimization problems, explaining optimization outcomes, and incorporating hard-to-quantify sustainability objectives into decision making frameworks are discussed. In the second half of the talk, I transition to considering the alignment of generative AI models, an

essential quality of AI systems to ensure they support real industry objectives and are deployed in a safe manner. I note that the process systems community is particularly well suited for addressing these issues given its expertise in constrained optimization, model predictive control, multi-objective optimization, and dynamic systems. The need to move from soft-constrained to hard-constrained AI models to ensure alignment is emphasized, and efforts in the chemical process systems community towards constrained AI are highlighted, including new methods for constrained network structure detection and neural network training.

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