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Multi-Agent LLMs for Sustainable Operational Decision Making

A major challenge in the chemicals industry is coordinating decisions across different levels, such as individual equipment, entire plants, and supply chains, to enable more sustainable, autonomous operations. Multi-agent systems, based on large language models (LLMs), have shown potential for managing complex, multi-step problems in software development (Qian et al., 2023). This work investigates translating this success to the chemicals industry: a network of four swing-connected gas-oil-separation plants (GOSPs) serves as a case study, where operational planning requires a trade-off between emissions and economics.

Our multi-agent framework tackles the case study in three stages: i) initial analysis, ii) strategic selection, and iii) operational realization. First, the Optimization Agent gathers inlet feed qualities for a multi-objective optimization in Pyomo. The candidate set points are then debated by Economic and Environmental Agents, using retrieval-augmented generation to support arguments. The Decision Agent then selects the final set-point. Finally, an Operator Agent validates the feasibility using a digital twin in Aspen HYSYS.

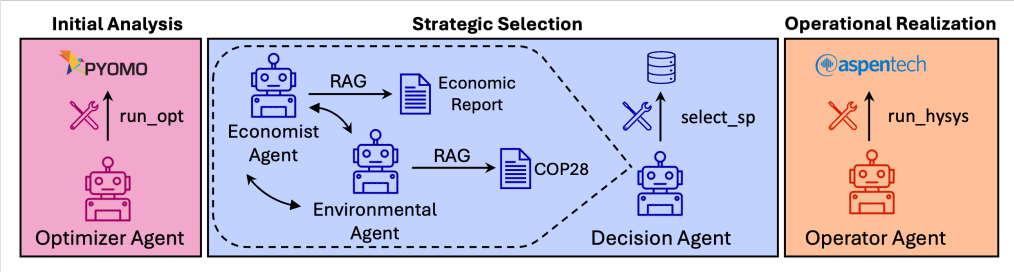

Figure 1: Multi-agent LLM workflow: Initial Analysis) Optimizer Agent utilizes run_opt to calculate the Pareto front for a user-given schedule; Strategic Selection) Decision Agent reviews a debate between RAG-enhanced Economist and Environmental Agent and uses select_sp to choose the operating point; Operational Realization) Operator Agent uses selected operational parameters to run GOSP system using run_hysys.

The results demonstrate how multi-agent LLMs can automate and integrate hierarchical decision-making in the chemicals industry, particularly when balancing sustainability and economic demands. While the baseline runs favour the lowest-emission strategy, imposing an economic directive led to more complex solutions, satisfying cost constraints and minimizing emissions simultaneously. The framework also outputs a rationale for its choice, enhancing transparency and explainability. Future work will consider additional agent roles (e.g., regulatory, safety), the use of reasoning models, and more, paving the way for scalable and ethical adoption of LLM-driven process automation.

Special/ Invited session

Classification

Both methodology and application

Keywords

LLMs, Chemicals Industry, Decision-Making

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Track Classification: Machine Learning