



Slovak Society of Chemical Engineering
Institute of Chemical and Environmental Engineering
Slovak University of Technology in Bratislava

PROCEEDINGS

51st International Conference of the Slovak Society of Chemical Engineering SSCHE 2025

Hotel DRUŽBA
Jasná, Demänovská Dolina, Slovakia
May 27 - 30, 2025

Editors: Assoc. Prof. Mário Mihaľ

ISBN: 978-80-8208-158-2, EAN: 9788082081582

Published by the Faculty of Chemical and Food Technology Slovak Technical University in Bratislava in Slovak Chemistry Library for the Institute of Chemical and Environmental Engineering; Radlinského 9, 812 37 Bratislava, 2024

Szatmári, K., Németh, S., Kummer, A.: Reinforcement learning for chemical process control, Editors: Mihaľ, M., In *51st International Conference of the Slovak Society of Chemical Engineering SSCHE 2025*, Jasná, Demänovská Dolina, Slovakia, 2025.

Reinforcement learning for chemical process control

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Key words: reinforcement learning, chemical process control, multi-agent reinforcement learning, resilience engineering, explainable reinforcement learning

Reinforcement learning (RL) algorithms are well-suited for sequential decision-making tasks, making them an excellent choice for chemical process control, where making decisions is required continuously. In this paper, we explore the application of RL at different levels of hierarchical process control to assess its potential to improve efficiency and robustness. We present two case studies of chemical process control applications, one with resilience engineering and explainable reinforcement learning, and one with multi-agent reinforcement learning. In the first case study, an intervention action is designed with RL to prevent reactor runaway in a batch reactor, and resilience is applied as a reward function. Two explainable reinforcement learning methods are investigated, a decision tree, as a policy-explainer, and the Shapley value as a state-explainer. The decision boundary of the decision tree is compared with the runaway boundaries defined by runaway criteria, and the Shapley value explains how different state variables influence the agent's decisions over time. The results show that this method is applicable to the development of a resilience-based mitigation system, and can be explained and presented transparently. In the second case study, two RL controllers are applied, one RL controller varies the feed rate in the feed phase of a semi-batch reactor, while the other RL controller in the mixing phase works as a master controller in a cascade control structure. The multi-agent structure enables the handling of more complex chemical processes beyond the capabilities of a single agent. The developed RL controllers perform effectively and can keep the temperature at the desired setpoint.

Acknowledgement

This work has been prepared with the professional support of the Co-operative Doctoral Program of the University Research Scholarship Program of the Ministry of Culture and Innovation financed from the National Research, Development and Innovation Fund. The work was supported by the 2024-2.1.1-EKÖP University Research Scholarship Programme of the Ministry for Culture and Innovation from the Source of the National Research, Development and Innovation Fund.