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

PROCEEDINGS

52nd International Conference of the Slovak Society of Chemical Engineering SSCHE 2026

Hotel SOREA TRIGAN
Štrbské Pleso, Slovakia
May 26 - 29, 2026

Editors: Assoc. prof. Mário Mihaľ

ISBN: 978-80-8208-177-3, EAN: 9788082081773

Published by the Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava in Slovak Chemistry Library for the Institute of Chemical and Environmental Engineering; Radlinského 9, 812 37 Bratislava, 2026

Herda, A., Labovský, J., Labovská, Z.: Enhancing the safety of chemical processes using a dynamic digital system, Editors: Mihaľ, M., In *52nd International Conference of the Slovak Society of Chemical Engineering SSCHE 2026*, Štrbské Pleso, Slovakia, 2026.

Enhancing the safety of chemical processes using a dynamic digital system

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Key words: chemical process safety; Aspen HYSYS; dynamic simulation; nonlinearity; multiple steady states; Morris method

The work is focused on verifying the possibilities of using Aspen HYSYS for the analysis of steady-state and dynamic system behavior, on assessing its practical applicability for modeling a chemical process from the viewpoint of hazardous states, and at the same time on evaluating whether the use of a commercial simulation program can accelerate calculations and reduce the time required for a more extensive safety analysis. Part of the solution was the development of a mathematical model in MATLAB, which served as a reference and comparative basis for the results obtained in the commercial simulation environment Aspen HYSYS. In Aspen HYSYS, models of a CSTR, a CSTR with an external heat exchanger, and subsequently a CSTR approximated by a PFR model with heat exchange were developed step by step. In the case of the simple CSTR model, it was shown that Aspen HYSYS does not allow a sufficiently realistic description of heat transfer between the reaction mixture and the cooling medium, since heat removal could only be defined by a fixed heat duty. Therefore, a CSTR model with an external heat exchanger was created, although it enabled cooling by means of cooling water, it did not fully correspond to the behavior of an ideally mixed reactor. For these reasons, a PFR model was finally selected and configured to approximate CSTR behavior as closely as possible, while also providing a more suitable description of heat transfer and showing very good agreement with the reference MATLAB model. Using this model, continuation diagrams of selected input parameters were analyzed under steady-state conditions, namely reactant flow rates, inlet temperatures, cooling-medium flow rate, and cooling-medium inlet temperature. The results showed that all analyzed parameters exhibit nonlinear behavior accompanied by the occurrence

of multiple steady states. Since the steady-state calculations indicated the sensitivity of the system to changes in input parameters, the next part of the analysis focused on system behavior in the dynamic regime. In the dynamic regime, attention was paid to the system response to deviations from the operating point, as well as to the effect of their duration on the system's ability to return to the original steady state. The simulations confirmed that the dynamic model in Aspen HYSYS is able to reliably describe system behavior on individual solution branches, although transitions between the individual branches of steady states could not be captured reliably. The final step of the nonlinearity analysis consisted in the use of the Morris method as a tool of global sensitivity analysis. Based on this method, the input parameters with the most significant influence on the model outputs were identified, with the flow rates of both reactants showing the strongest nonlinearity. The obtained results indicate that a model-based approach in Aspen HYSYS makes it possible to analyze the safety aspects of a chemical process reliably and at the same time more time-efficiently, which is particularly important when modeling larger-scale chemical plants.