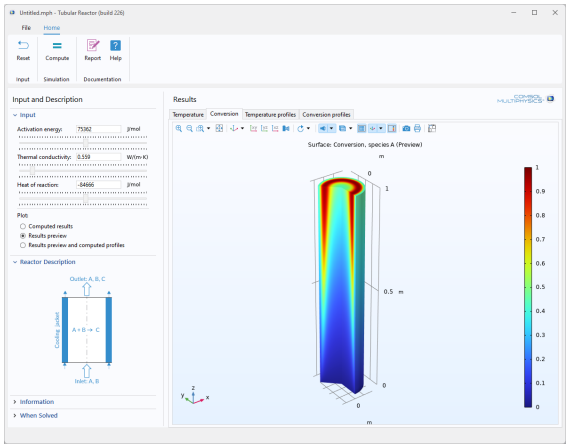
A Digital Laboratory for Flow Chemistry – How Multiphysics Simulation Drives Research and Process Innovation

Shahab Eghbali

Applications Specialist (COMSOL Multiphysics GmbH, Technoparkstrasse 1, 8005 Zürich, Switzerland)
shahab.eghbali@comsol.com

Chemical process education, research and development have long relied on the foundational pillars of theory and experimental laboratory work, both of which have been instrumental in shaping our understanding and advancing chemical technologies. While these traditional methods remain invaluable, leveraging state-of-the-art tools is crucial for fostering innovations and process optimization.



Analytical methods can sometimes be challenging in capturing the intricate multiphysics nature of flow chemistry, which involves convoluted interactions between reaction kinetics, species transport, flow, and heat transfer within a system. While laboratory experiments can help with providing tangible insights into the outcome and spark inspirations, iterating on ideas often remains limited within discrete scenarios and entails high costs; in material, time and logistics. Multiphysics simulation, grounded in fundamental chemical and physical principles, offers a powerful complementary approach. It serves as a digital laboratory, enabling the exploration of complex systems without any need for physical equipment or materials, and is free from safety hazards. This approach not only aids in understanding system behavior but also facilitates the prediction and optimization of outcomes for industrial scale-up.

In our talk, we will demonstrate the general workflow of the modeling process using COMSOL Multiphysics® software, highlighting its capabilities in parametric, optimization and reliability studies. We will provide examples of simulated flow chemistry across various processes, e.g., mixing, chromatography, etc. Furthermore, we will highlight advanced methods, e.g. incorporation of machine learning and the possibility of turning sophisticated chemical models into user-friendly simulation apps that allow a broader audience to benefit directly from modeling results and insights to monitor, design and improve the chemical systems[1].

In conclusion, the talk will underscore the growing significance of modeling and simulation as the third pillar of process engineering, complementing experiment and theory. By focusing on methodology rather than specific software, we aim to illustrate current advances in the technology and inspire dialogue among leading chemical industries and researchers, paving the way for future innovations.

[1] E. Fontes, *Chimia*, **2025**, *79*, 698.