CHIMIA REPORT/COMPANY NEWS

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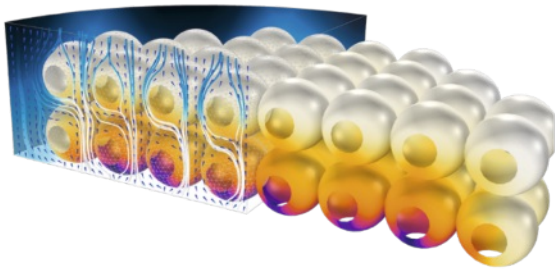
COMSOL: Simulation Drives Understanding

COMSOL Multiphysics® is a general-purpose simulation software used in all fields of engineering, manufacturing, and scientific research. The software offers fully coupled multiphysics and single-physics modeling capabilities, simulation data management, and user-friendly tools for building simulation applications. Spread the value of simulation to your design teams, manufacturing departments, test labs, customers, and other collaborators by distributing your apps using COMSOL Compiler™ and COMSOL Server™. Add-on modules provide specialized functionality for chemical reaction engineering, fluid flow, heat transfer, electromagnetics, structural mechanics, and acoustics. Interfacing products are available for CAD and other third-party software.

Modeling and simulation in chemical engineering is becoming increasingly important and reaches far beyond the abstraction of perfectly mixed, space-independent systems in ideal tank reactors. Researchers and developers in chemistry, chemical engineering, and process engineering can specifically benefit from the ability of the COMSOL® software to couple equations for mass, momentum, energy, and charge in 0D, 1D, 2D, 3D, and beyond in multiscale systems.

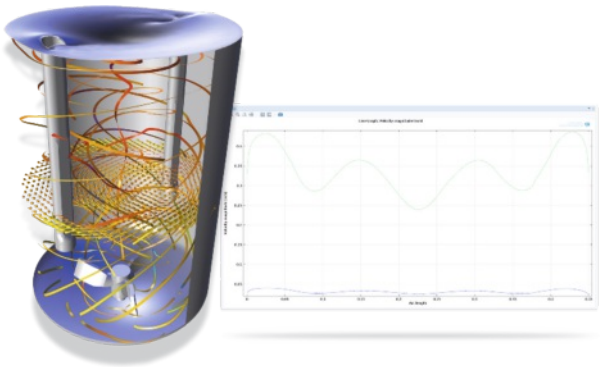


Surface concentration on the porous structure of the ion-exchangemass in an ion-exchange column.

Mathematical models help scientists, developers, and engineers understand processes, phenomena, and designs of reacting systems. The Chemical Reaction Engineering Module, an add-on to the COMSOL Multiphysics® software platform, provides user interfaces for creating, inspecting, and editing chemical equations, kinetic expressions, thermodynamic functions, and transport equations. After developing a validated model, it can be used for studying different operating conditions and designs of reacting systems and transport phenomena. Solving the model equations for a range of different inputs leads to a better understanding of the studied system. Additionally, the software provides tools for optimization and parameter estimation of chemical systems.

Model Realistic Chemical Systems

Too often, chemical reactions are considered to be space-independent and described by 0D models of ideal tank reactors. While such models can be implemented in the COMSOL® software as very coarse first approximations, its specific strength lies in the ability to model realistic reacting systems as they appear in mixing and separation processes, medical technology, food processing, pharmaceutical and environmental processes, and electrochemistry. Such models often involve single- or multiphase flow in laminar and turbulent regimes. The Chemical Reaction Engineering Module also includes ready-made formulations for heterogeneous catalysis, including surface reactions on boundary faces as well as surface reactions distributed over a homogenized porous catalyst. For porous catalysts, multiscale models are predefined to describe bimodal pore structures. The software also contains a thermodynamic properties database, which you can use to calculate properties for gas mixtures, liquid mixtures, gas–liquid systems at equilibrium (flash calculations), liquid–liquid systems, and gas–liquid–liquid systems at equilibrium.



Turbulent mixer with a three-bladed impeller and free surface of the fluid.

Specific Strength in Electrochemistry

COMSOL offers several add-on products to efficiently model electrochemical processes, including migration of species in electrical fields. Such processes are of the highest importance in the understanding of batteries, fuel cells, and electrolyzers. Modeling batteries requires different levels of detail depending on the purpose of the simulations. A large range of modeling scales allows simulations from the detailed structures in the battery's porous electrode to the battery pack scale, including thermal management systems of lithium-ion batteries and electrical impedance spectroscopy. Examples of fuel cell types that can be modeled include PEMFC, AFC, PAFC, SOFC, MCFC, and high-temperature PEMFC, to name a few. Further add-on modules are available for modeling corrosion and electrodeposition. Capabilities such as modeling electrochemical reaction mechanisms, mass transport, and current density distributions enable efficient simulation for applications including electrolysis, electrodialysis, electroanalysis, electrochemical sensors, and bioelectrochemistry.

COMSOL's mission is to provide easy-to-use software solutions to engineering problems and to help our users get the most out of our products. Our branch office in Zurich is available to discuss your specific modeling projects.

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