

CHIMIA REPORT/COMPANY NEWS

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Companies present themselves and their products

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Swiss Chemical Society, info@scg.ch, +41 31 306 92 92

COMSOL: New Release Brings Chemical Modeling Updates

COMSOL is a global provider of modeling and simulation software for product design, engineering, and research at technical enterprises, labs, and universities. The COMSOL Multiphysics® platform product is an integrated environment for creating physics-based models and simulation apps. Add-on products connect seamlessly via the platform to bring specialized functionality for chemical engineering, electrochemistry, fluid flow, heat transfer, electromagnetics, structural mechanics, and acoustics. Simulation apps can be distributed to colleagues and customers worldwide via COMSOL Server™ and COMSOL Compiler™.

Mathematical models help scientists, developers, and engineers understand processes, phenomena, and designs of reacting systems. The Chemical Reaction Engineering Module add-on to the COMSOL Multiphysics® software platform makes it straightforward to create, inspect, and edit 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.

Precipitation and Crystallization

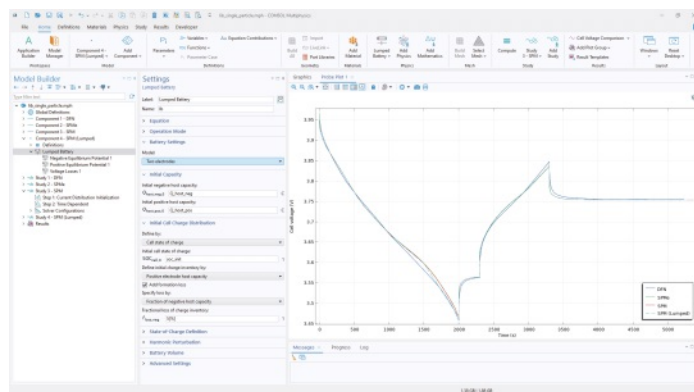
The latest version of COMSOL Multiphysics, version 6.3, introduces new functionality in the Chemical Reaction Engineering Module for modeling precipitation and crystallization processes, where liquid or solid particles form in liquid or gaseous solutions due to changes in temperature or pressure, or through additives or seed particles. The software solves for the number density of all particle sizes by accounting for particle nucleation, particle growth, and fluid transport. This capability allows for the analysis of separation processes in industries such as fine chemicals, bulk chemicals, and pharmaceuticals. For ideal reactors, it can be used to track the generation and growth of particles.

Electrochemistry and Battery Design News

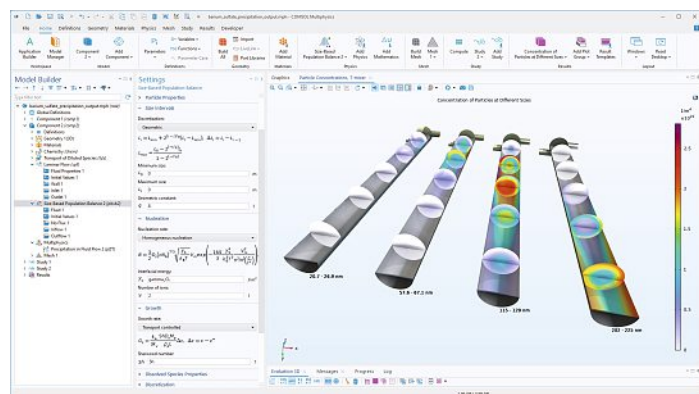
COMSOL Multiphysics version 6.3 also brings new and enhanced functionality to the add-on products for modeling electrochemistry. All of the

add-on products for electrochemistry offer new functionality for modeling transport in any concentrated electrolyte solution with an arbitrary number of charged and uncharged species. Common electrolytes that can be modeled with this functionality include ionic liquids, salt melts, and highly concentrated solutions. In addition, these products now include parameter estimation functionality, used for reverse engineering, that is determining model parameters by fitting simulations to experimental data.

The Battery Design Module, an add-on product for modeling batteries at the microscale, battery cell scale, battery module scale, and battery pack scale, introduces a two-electrode lumped model for single-particle electrode modeling. This model is especially helpful when defining the electrode potential, initial host capacity, and degree of conversion individually for the two electrodes in a battery. It also allows for users to define individual electrode properties to account for ohmic activation and concentration overpotentials. In addition, there is a new thin porous electrode feature for defining electrodes at domain boundaries instead of defining a domain as well as a simulation app that demonstrates how to use a surrogate model function for predicting the cell voltage, open-circuit cell voltage, and internal resistance of a lithium–nickel–manganese–cobalt (NMC111)–graphite battery cell undergoing a battery test cycle. A surrogate model is a simpler, usually computationally less expensive model that is used to approximate the behavior of a more complex, and often more computationally expensive, model.



Voltage-vs.-time plots for a number of different model types, modeled using the new single-particle modeling features in COMSOL Multiphysics version 6.3.



The COMSOL Multiphysics® software user interface (UI) in version 6.3, featuring a model of transport-controlled growth in a process for barium sulfate precipitation in 3D.

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. You can also learn more about the latest version of COMSOL Multiphysics here: <https://www.comsol.com/release/6.3>

Contact

COMSOL Multiphysics GmbH
Technoparkstr. 1
8005 Zürich
Switzerland
Phone: +41-44 515 78 00
Email: info-ch@comsol.com
Website: www.comsol.com

