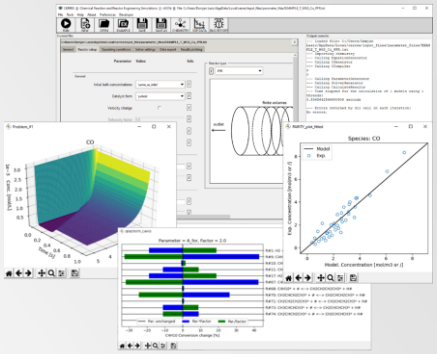
NATIONAL INSTITUTE OF CHEMISTRY

RESEARCH DOMAINS: Mathematical modelling/simulations

INDUSTRIES: Chemicals production industries

CERRES
Chemical Reaction and Reactor Engineering



The invention is a software application designed for the simulation of various types of chemical reactors under different operating conditions with user-supplied chemistry, allowing for complex bulk and surface reaction (micro)kinetics. Furthermore, it provides additional modes of operation such as the comparison of the model results to experimentally measured values and reaction rate parameter optimization (fitting). The software is used through a user-friendly interface, which requires no coding skills whatsoever. CERRES can be used in various different scenarios, from academic applications to study chemical kinetics to the design of industrial scale reactors. The main goals of the software are computing efficiency, ease of use and wide functionality. Please visit www.cerres.org for more information.

Technology

The software is written in a combination of Python, C++ and C. Efficient computation is one of the main focuses of the software, which allows fast simulations even for large systems with highly stiff numerical characteristics. This is achieved through a powerful backend written in C, which includes robust BDF solvers, multi-threading, automatic generation of Jacobian matrices for the differential equations and on-the-fly dynamic generation and compilation of critical code segments. In addition, CERRES defines its own human-readable standard for input chemistry and experimental data files, which can be edited by any '.csv' editing tools, and can be interchanged and mixed with different reactor models at different operating conditions in a modular way. The software also provides its own chemistry and experimental data editors. CERRES is closed-source, and it's installer can be downloaded from www.cerres.org. The software is free to use for academic, teaching and research purposes, while a paid license can be acquired for use of CERRES for commercial purposes (e. g. in industry).

Main advantages

- Simulation of 14 different types of chemical reactors
- Complex user-defined chemical reactions and kinetics
- User friendly interface focused on ease-of-use

Key words

Chemical reactor, Reaction kinetics, Modeling, Simulations, Software

TYPE OF COOPERATION
R&D cooperation and technology licensing opportunity

DEVELOPED BY
Department of Catalysis and Chemical Reaction Engineering

CONTACT
Knowledge Transfer Office
P: 00386 1 4760 529
E: knowledge.transfer@ki.si

MORE INFORMATION ABOUT THE INVENTION

EUROPEAN UNION
EUROPEAN REGIONAL DEVELOPMENT FUND
INVESTING IN YOUR FUTURE

REPUBLIC OF SLOVENIA
MINISTRY OF EDUCATION, SCIENCE AND SPORT