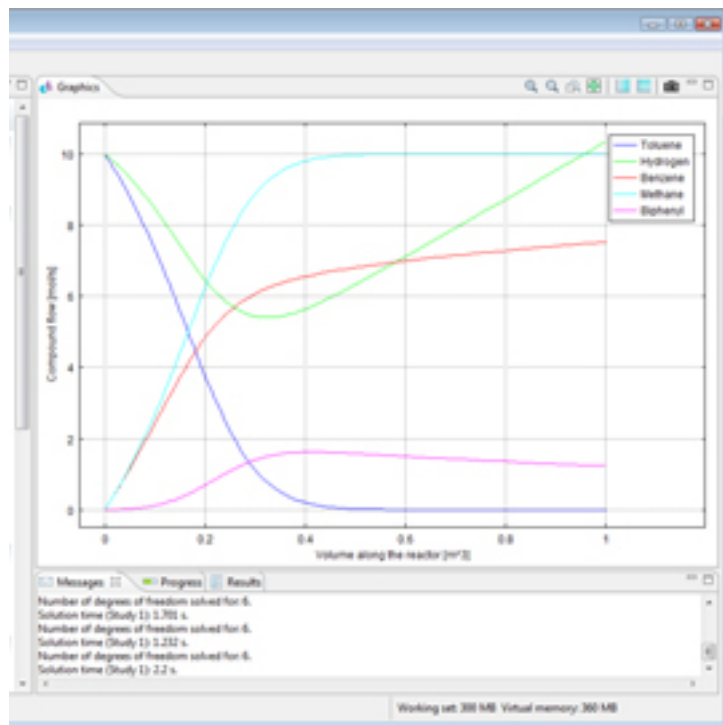


Model & Simulate Reaction Systems & Processes



COMSOL Inc. recently released the chemical reaction engineering module to provide a single environment where engineers and scientists can obtain highly accurate studies of material transport and chemical reactions of a wide assortment of chemistries under different operating conditions. Users can simulate reaction systems ranging from micro-reactors in biotechnology to unit operations in chemical processes, and gain essential knowledge early in the development phase. Other features of the module include:

- Automatic generation of reaction kinetics, mass and energy balances from chemical reaction formulas.
- Allows combinations of perfectly mixed reactor models to detailed time- and space-dependent descriptions in one model.
- Extensive interfaces for simulating mass transport by diffusion, convection and migration in dilute and concentrated solutions as well as in free and porous media.
- Functionality for investigating different chemistries and operating conditions by adding and removing reactions, chemical species and mass transport effects in different studies in a single model.
- Predefined chemical reactor types such as batch and semi-batch reactors, CSTR, and plug flow reactors for continuous volume and variable volume simulations
- User-defined functions and expressions that extend usability for defining arbitrary reaction kinetics and for describing physical properties as a function of composition and temperature

Model & Simulate Reaction Systems & Processes

Published on Chem.Info (<http://www.chem.info>)

- CAPE-OPEN interface for rapid thermodynamics and physical property
- calculations through connecting to third-party chemical engineering
- simulation software
- CHEMKIN file import for combustion, atmospheric chemistry, and
- other gas-phase reacting systems

www.comsol.com [1]

Source URL (retrieved on *01/30/2015 - 5:29pm*):

http://www.chem.info/product-releases/2010/08/model-simulate-reaction-systems-processes?qt-most_popular=0

Links:

[1] <http://www.comsol.com>