

From atoms and molecules – to new materials and technologies

Chemical Workbench®4.2: what's new?

Reactor models

All models

- 1. NASA9 format support
- 2. Input of process rate, different from law of mass action (only for direct reactions)

Laminar flame models

- 1. New premixed laminar flame model:
 - adaptive mesh has no limitations on the mesh size and calculating area
 - precise model of multicomponent transport properties
 - fast calculation of sensitivity coefficients
 - automatic and manual assignment of initial approximation

Detonation and Shock wave models

- Added incident and reflected shock waves models
- 2. Added ZND model
- 3. Updated Chapman-Jouget model

Thermo-chemical equilibrium models

- 1. New procedure of equilibrium state calculation in thermodynamic equilibrium reactors:
 - PT, VT (iso-thermal)
 - PH, VU (adiabathic)
 - PS, VS (isentropic)

GUI

New results tables and plots

- 1. Plotting graphs by context menu in results table
- 2. Flexible settings of graph view (font sizes, curve settings, legend)
- 3. Improved interface of sensitivity graphs
- 4. Automatic plotting of graphs will draw the most important components
- 5. Graph export settings

Calculation wizard

1. New calculation wizard

ChemKin converter

- 1. NASA9 format support
- 2. Selection of units at export to ChemKin format
- 3. General bugs fixed:
 - Diagnostics of wrong ChemKin files
 - Import of reactions with units for specific reaction

New license manager

- Floating licenses support (license server, start of the license-allowed number of simulation from any computer in the network)
- 2. Support of licensing of CWB components: database, reactor models
- 3. Licensing of multithread calculations (for floating licenses)

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