KINTECH LABORATORY

From atoms and molecules -
to new materials and technologies

Chemical Workbench® 4.1: New features

Reactor models

New fast and accurate one dimensional flame models solver

CWB 4.1 Flame model redesigned to fully comply with modern demand in terms of solution time and size of chemical mechanism which the model is capable to calculate.

Sensitivity coefficients calculation in flame models

Calculation of the species sensitivity coefficients in flame models is implemented. Sensitivity data obtained from flame models can be used for chemical mechanism optimization and reduction.

Recombination boundary conditions for premixed flame models

Recombination boundary conditions on the left boundary are implemented which allows more accurate description of the radicals profiles close to burner surface.

Calculation results post processing and visualization

User defined columns in results table

Possibility to add columns to results tables with values calculated based on user defined formula is implemented. Any calculation results from current CWB project can be used in user defined formula. Columns values are updated automatically when any of calculation results is changed. User defined column values as well as reactor models calculation results can be plotted using CWB plot tool. User defined columns formulas are saved in CWB project and can be transferred between CWB session or installations.

Calculation results filter and sorting

Filter tool to tune calculation results representation is implemented. It allows to specify a set of user defined filter criteria to select calculation data to display and set columns sort order.

Reaction path diagram

Reaction path diagram tool were redesigned. A tree dialog with rate of production data is implemented which allows visualize relative importance of different reaction paths on diagram.

Sensitivity data output

New criteria for sensitivity data output are implemented. It allows more accurate specification of the solution point for the sensitivity data output and significantly reduce the amount of data for analysis.

Tools for mechanism development

Mechanism comparison and merge tool

Tool for detailed mechanism comparison and merge is implemented. It allows comparing two chemical mechanisms in terms of species and reactions lists and it's parameters. Merge tool allows combining the data from two mechanisms based on user choice.

Import/Export

Chemical mechanism parameters units

Possibility to specify units used for chemical mechanism parameters exported to Chemkin format is implemented.

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