

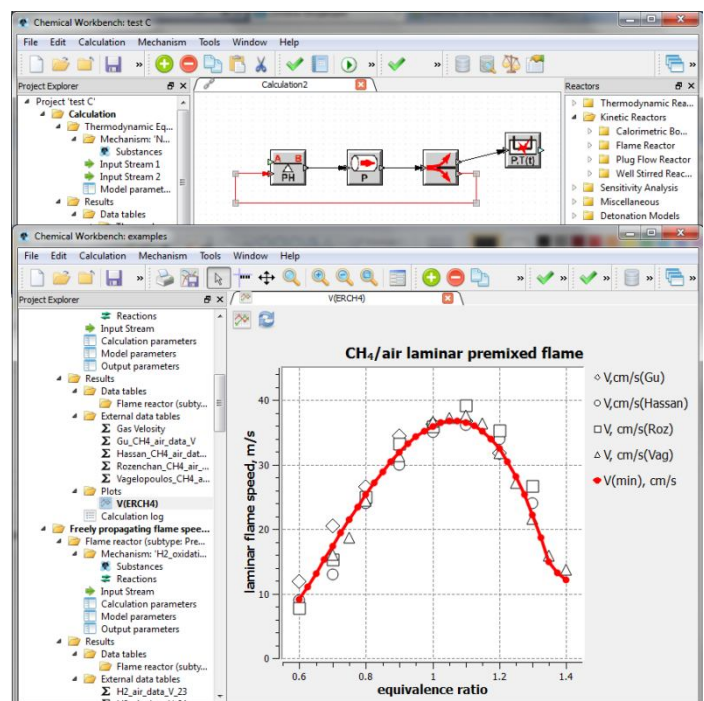
## Chemical Workbench®

### Integrated Environment for Conceptual Design of Complex Physical-Chemical Processes and Kinetic Mechanisms Development

**Chemical Workbench®** is an integrated easy-to-use simulation software tool aimed at the modeling of homogeneous gas phase and heterogeneous processes with chemical transformations and kinetic mechanisms development. It can be effectively used for modeling, optimization and design of a wide range of industrially and environmentally important chemistry-loaded processes such as combustion, waste treatment, metallurgy, microelectronics, plasma light sources etc. Chemical Workbench® is a modeling environment, based on advanced scientific approaches, complementary databases and accurate solution methods.

#### Chemical Workbench® Highlights

- Comprehensive library of basic physical-chemical models – **reactors** – for simulation of multi-phase thermodynamic equilibriums, homogeneous gas phase, heterogeneous and non-equilibrium chemical active plasma kinetics
- Interactive Model explorer for building multi-stage process flow as a chain of reactors with recycles, automatic data transfer between reactors
- Extensive set of tools for manipulation and analysis of kinetic mechanisms: comparison, analysis and basic reduction techniques
- Multiple options for reaction-rate approximations in kinetic simulations including user-defined expressions
- Customizable and flexible post-processing tools: user-defined manipulation of simulation results, templates for data post-processing and plots
- Automated parametric simulations with multi-core CPU support
- Integration with databases on thermodynamic properties of substances, kinetic data, individual chemical mechanisms
- Export/import of the chemical kinetic mechanisms to/from CHEMKIN® file format



#### Chemical Workbench® Library of Physico-Chemical models for Process simulation

##### Rich collection of models for process conceptual design and mechanism analysis

- Thermodynamic chemical equilibrium models
- Kinetic models for batch, flow and stirred reactors
- Sensitivity analysis models for batch reactor and flame models
- Laminar flame reactor for calculation of the structure of laminar premixed and non-premixed flame
- Detonation models for estimation of the detonation static and dynamic parameters
- Gas-solid surface kinetic models for calculation of the steady-state and time dependent chemical processes in gas phase and at the phases boundary
- Plasma reactors models for simulation chemical processes in the non-equilibrium homogeneous or one-dimensional plasmas
- Membrane model for calculation of the separation characteristics of the membrane elements
- Flow divider and mixer models

##### Ideal tool for researchers and engineers, working in industries

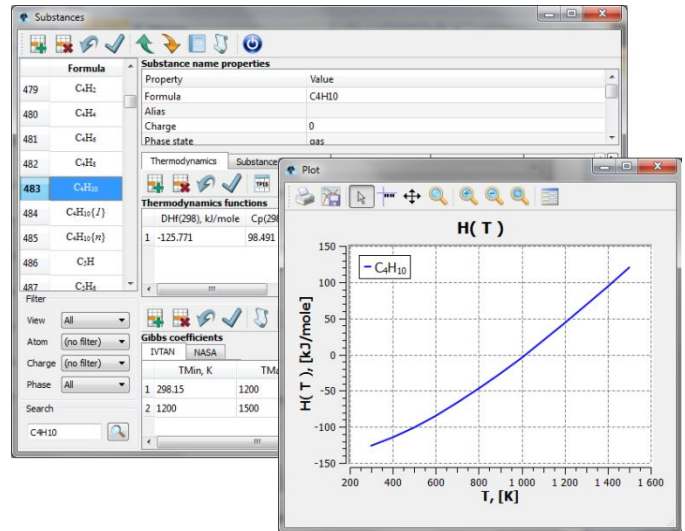
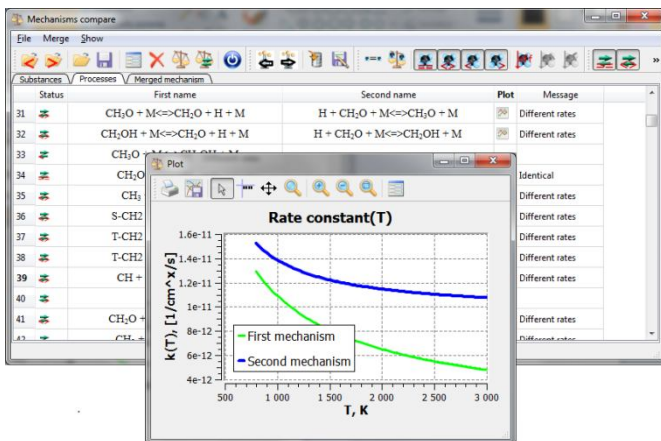
- General chemical kinetics and thermodynamics
- Catalysis and chemical engineering
- Combustion, detonation and pollution control
- Waste treatment and recovering
- Thin films growth for microelectronics
- Plasma light sources and plasma chemistry
- High temperature chemistry
- Nanotechnology
- Education

# Chemical Workbench® Tools for Kinetic Mechanisms Analysis and Reduction

Chemical Workbench® contains extensive set of tools for kinetic mechanism development from detailed mechanism construction to mechanism reduction

## Integrated Database for easy mechanism construction

- Thermodynamic property data for 4500 pure substances
- Physical properties for 1700 species
- Molecular data for 800 species
- Rate coefficients for 6500 gas phase and liquid phase reactions
- Automatic data transfer from Database to Chemical Workbench® calculations
- Saving data from Chemical Workbench® to the Database for future use



## Mechanism comparison and merging

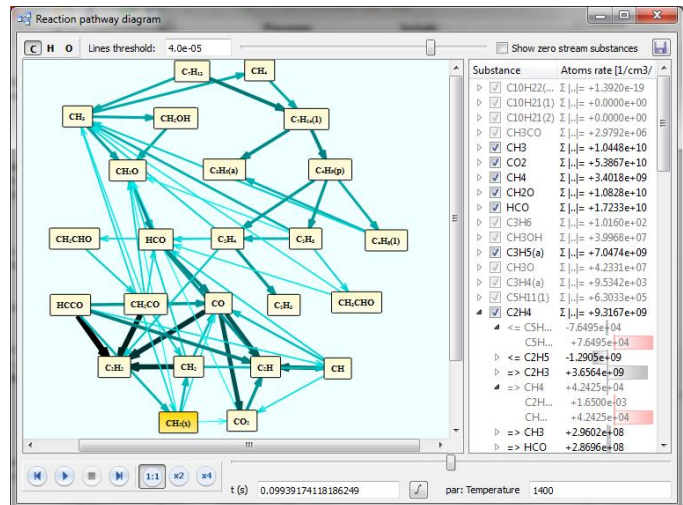
- Identification of identical species and reactions (name and physical properties)
- Identification of similar species with different thermo-chemical properties, reactions with different rate constants
- Merging of the mechanism based after comparison

## Models for sensitivity analysis of the chemical kinetic models

- Global sensitivity analysis for batch reactor and laminar flame model
- Differential sensitivity analysis and calculation of the sensitivity matrices for batch reactor model

## Advanced post-processing tools for kinetic mechanism analysis and automatic reduction

- Elements flux analysis (Reaction Pathway Diagrams, Steady-Species Index)
- Basic Mechanism reduction algorithms for kinetic mechanism simplification (Rate-of-Production analysis, Direct Reduction Method, Principle Component Analysis, Computational Singular Perturbation, Directed Relation Graph)



## Chemical Workbench® Configurations and Purchase options

- A multiple packages, which include different subsets of available reactor models, are available to fit project needs and resources:
  - Basic set (includes thermodynamic equilibrium and chemical kinetic models, mechanism reduction and standard database)
  - Combustion, Plasma, Chemical Engineering Packages (+ models of Basic Set)
  - Full package.
- Chemical Workbench® can be run on Windows PC, Unix-family PC and Mac OS X

## Contacts

Kintech Lab, Ltd.,  
1, Kurchatov Sq., Moscow,  
123182, Russian Federation

+7 (499) 704-25-81  
+7 (499) 704-25-81  
info@kintechlab.com  
www.kintechlab.com