From Atoms and Molecules
to New Materials and Devices

Chemical Workbench:

software for chemical kinetics model development and conceptual design of processes in reactive media

26 of February 2015

KINTECH LABORATORY

Webinar plan

1. About Kintech Lab Ltd.

2. Conceptual design: principles of modeling
3. Library of reactive media processes models
4. **Demo**: thermodynamic cycle of gas turbine
5. **Demo**: H_2S treatment

6. Instruments for development and verification of chemical mechanisms of processes
7. **Demo**: verification of kinetic mechanism of aviation kerosene combustion – delay time
8. **Demo**: sensitivity analysis of methane combustion mechanism

9. KintechDB Database – storage system of physical ahd chemical properties of substances and processes

About Kintech Lab

KINTECH was founded in 2000 by scientists and engineers from and the Russian Research Center "Kurchatov Institute“ and Moscow State University

Activity fields:

- ✓ Conducting of inventive research and consulting for a wide range of applications
- ✓ Software development for chemistry-intensive modeling and design in complete cycle
- ✓ Customer support in their own research activity using the advanced simulation capabilities of KINTECH's software

About Kintech Lab

Kintech Lab develops methods and special software tools for multilevel modeling in different engineering fields:

- ✓ KintechDB – a network-based database for accumulation of Lab data on substances and processes. ***Applications:*** *information support of kinetic modeling at all levels and stages*
- ✓ Chemical Workbench – an integrated environment for conceptual design of physico-chemical processes, development and reduction of chemical mechanisms. ***Applications:*** *development of detailed chemical mechanisms of pyrolysis, combustion, chemical processes in plasma, processes on surfaces; and conceptual design of processes or devices.*
- ✓ Khimera – a unique tool for calculating microscopic parameters from first-principles calculations ***Applications:*** *development of detailed kinetic mechanisms of combustion, plasmo-chemical processes, interaction of gas and surface.*

Conceptual design: principle of modeling

Optimal conditions for process:
reagents flowrate, temperature, pressure, stages, residence time, geometry…

Engineering design: 3D-design, 3D-modeling

Conceptual design: principle of modeling

Approach to solution:

•Simplified description of process' fluid dynamics
•Emphasys on integral and thermodynamic process conditions
•Emphasys on description of chemical thansformations

Chemical Reactor Networks (CRN)

•**3 basic types of flow**: Batch Reactor (CBR), Plug Flow Reactor (PFR), Well Stirred Reactor (WSR): allow to exclude equations of flow calculation, and operate with integral system characteristics
•A possibility appears to account for **kinetic mechanisms of any complexity**
• **Additional physical phenomena** can be included. For example a non-equilibrium plasma, dispersed media etc.

Chemical Workbench – an integrated environment for conceptual design of physico-chemical processes, development and reduction of chemical mechanisms

Conceptual design: models library

kinetics ...

Well Stirred Reactor (WSR) – chemical kinetic simulator under condition of high intensity turbulent mixing and uniform reagents and temperature distribution in the reactor volume (2 models)

Plug Flow Reactor (PFR) – model permits the user to describe the evolution of reactive mixture composition and parameters along the reactor length in one or quasi one dimensional approximations (3 models)

Calorimetric Bomb Reactor (CBR) – is a zero dimension time dependent model for description of time evolution of chemical composition and gas parameters under effect of chemical reactions and external effects (heating, cooling, plasma interaction, radiation) (4 models)

Flame – is a 1-dimension model for burning that calculates the laminar flame structure and flame speed for a mixture

Conceptual design: models library

. . . thermodynamics

Thermodynamics Equilibrium Reactor (TER) – is designed for calculating the chemical equilibrium, thermodynamics and transport properties of any components of homogeneous or heterogeneous systems (4 models)

Stoichiometric Thermodynamically Equilibrium Reactor (STR) – is designed for calculating the chemical equilibrium of a multicomponent heterogeneous system for a given set of chemical reaction equations (4 models)

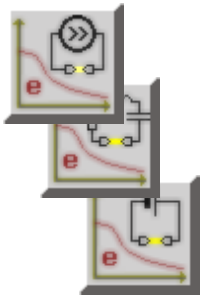
… detonation …

Chapman-Jouguet Detonation Reactor (CJD) – is aimed to compute the static detonation parameters for the given initial thermochemical parameters of a reactive mixture

Zeldovich-Neumann-Doering Reactor (ZND) – is aimed to compute the structure of the steady one dimensional unsupported detonation wave

Conceptual design: models library

… non-equilibrium plasma…



VIBRKIN reactors (VIBR) – is a reactor model for non-equilibrium plasma chemistry reactor including electron stimulated and vibration relaxation reactions

- Glow discharge model (light sources)
- LCR circuit model (laser systems)
- Pulse discharge model (corona discharges, waste treatment)

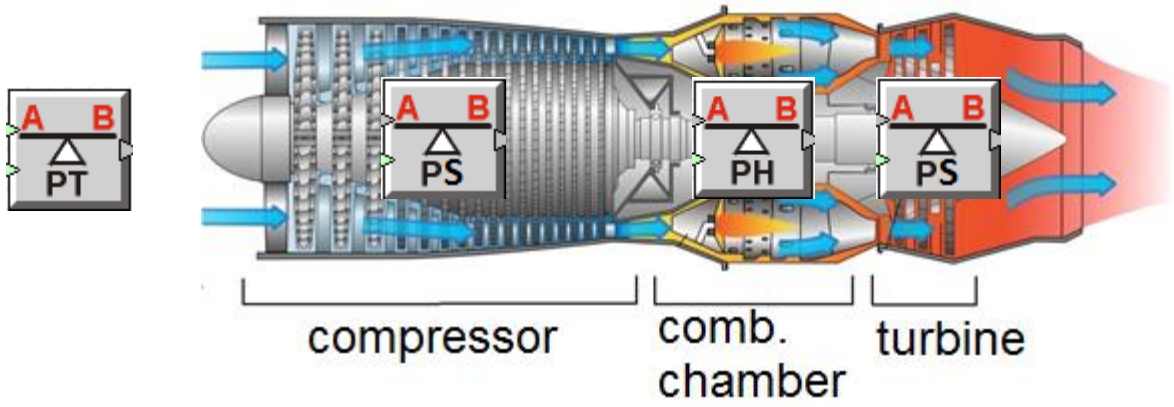
… surface …

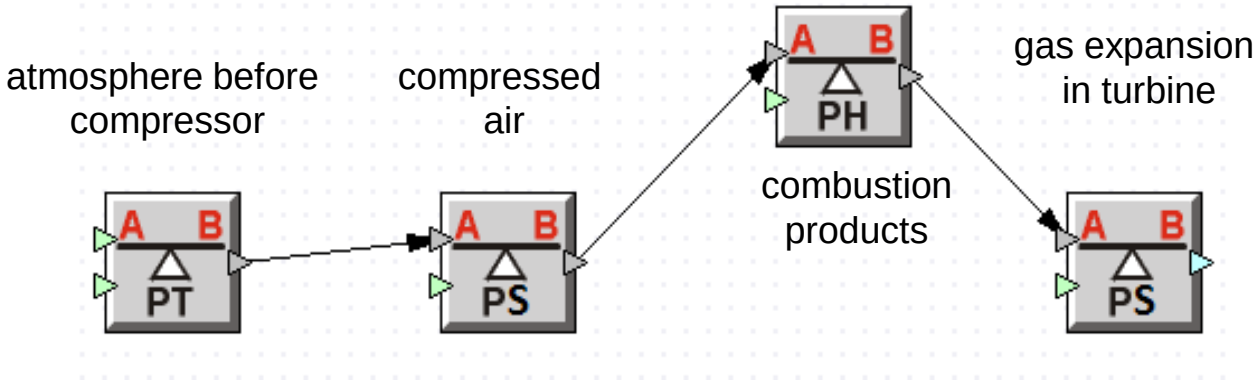
CBR with surface (Extended version of reactor CBR, for simultaneous calculation of reactions in the gas and on the gas-solid interface)

WSR with surface (Extended version of reactor WSR, for simultaneous calculation of reactions in the gas and on the gas-solid interface)

PFR with surface (Extended version of reactor PFR, for simultaneous calculation of reactions in the gas and on the gas-solid interface)

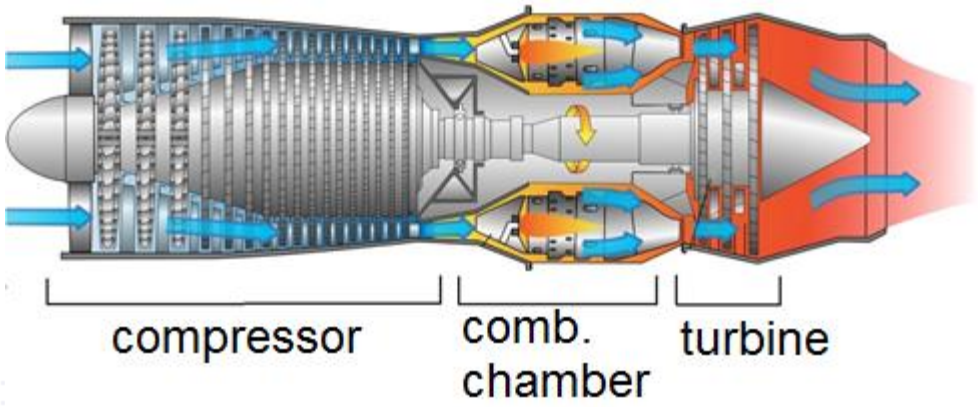
Conceptual design: Gas turbine - 1

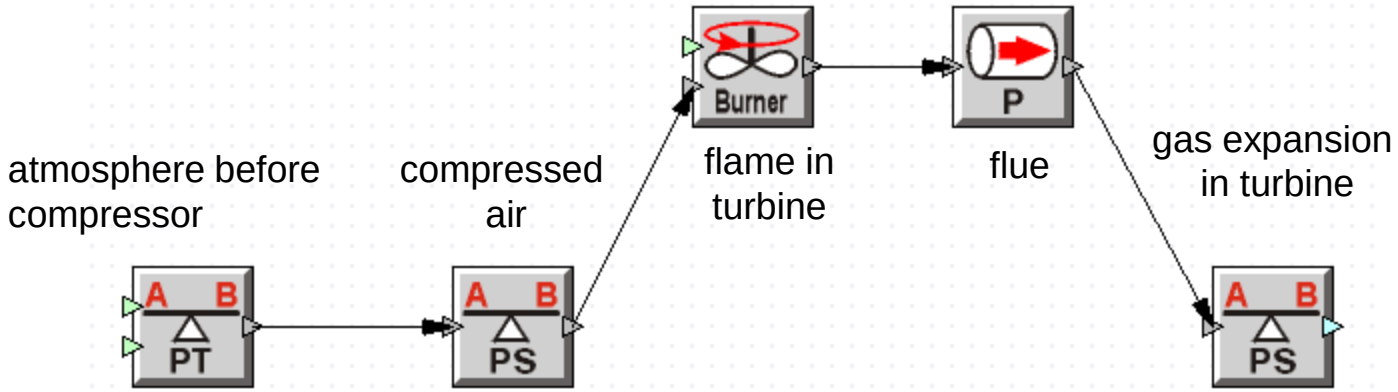




FOCUS: efficiency, temperatures of air behind compressor, combustion products, and exhausts

Conceptual design: Gas turbine - 2





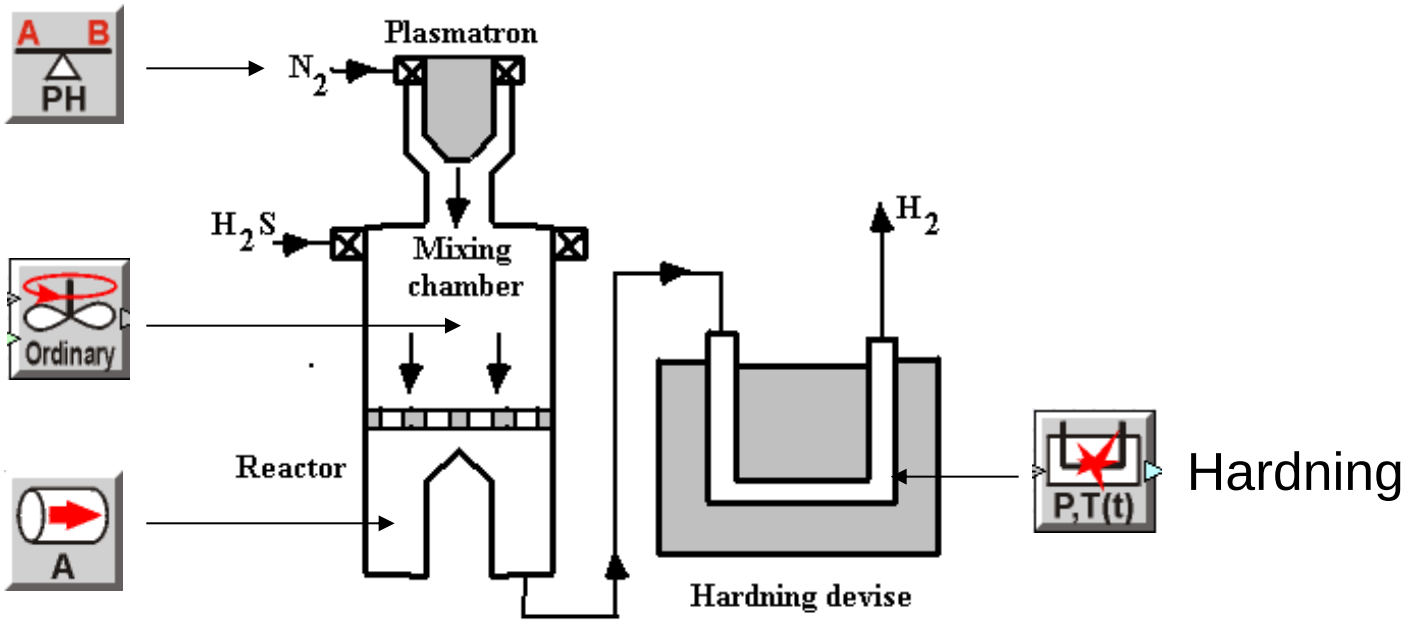
FOCUS: stability of combustion – effects of fuel type, initial temperature, влияния типа топлива, начальной температуры, additives

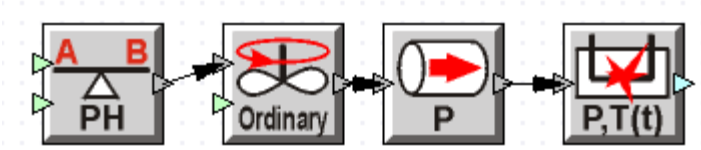
Conceptual design: H_2S treatment

Plasmatron

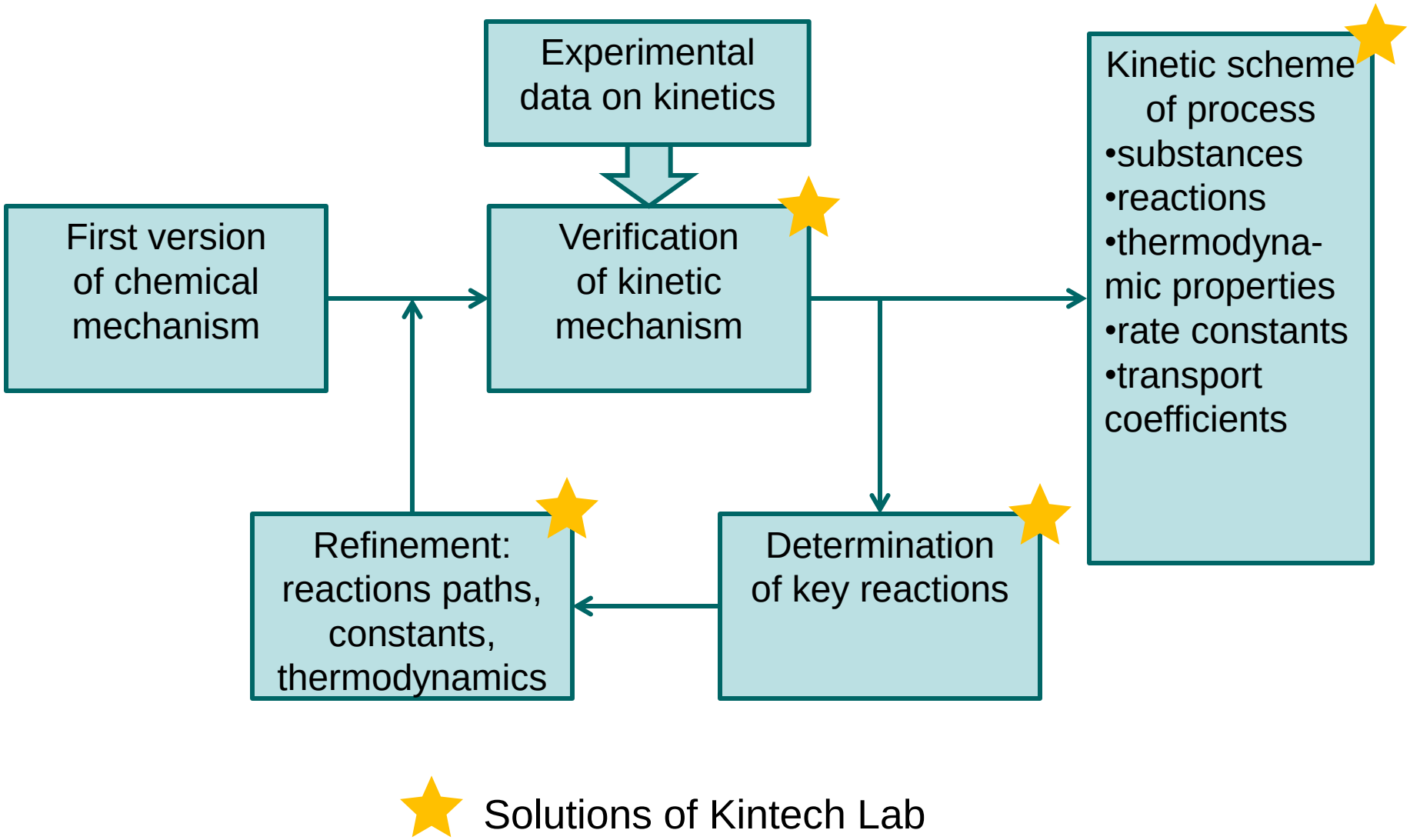
Mixing chamber

Reactor





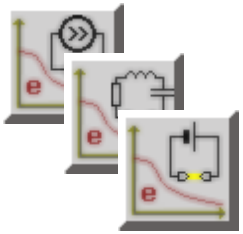
Development & verification of chemical mechanisms



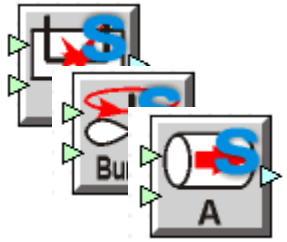
models of kinetic experiments…

- Shock Tube, Rapid Combustion Mashine (CBR),
- Flow Reactor (PFR),
- Jet stirred reactor (WSR)

- Laminar flame in premixed mixture
- Bunsen burner
- Counter-flow Diffusion flame



- Non-equilibrium electrical discharges



- Batch reactor with catalyst (CBR), kinetics is rate-limiting
- Flow reactor with catalyst (PFR), kinetics is rate-limiting
- Jet stirred reactor with catalyst (WSR), kinetics is rate-limiting

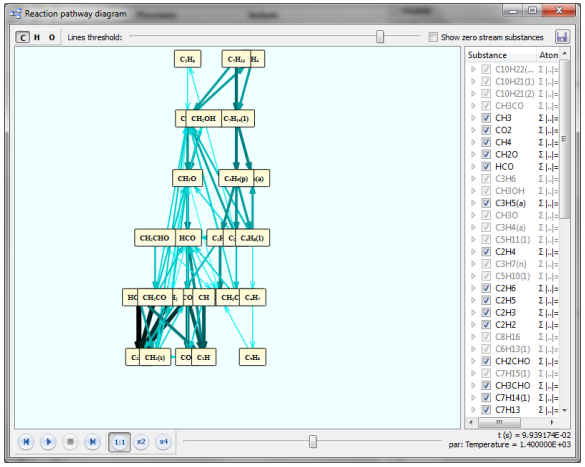
Verification and development of chemical mechanisms

…sensitivity analysis…

Calorimetric Reactor with Deviation (CRD) – Reactor for calculation of global sensitivity based on CBR (4 models)

Calorimetric Reactor with Sensitivity (CRS) – Reactor for calculation of local (differencial) sensitivity based on CBR (4 models)

…reduction



Effective up-to-date reduction methods of kinetic mechanism reduction: DRG, DRGEP, PCA, CSP, etc.

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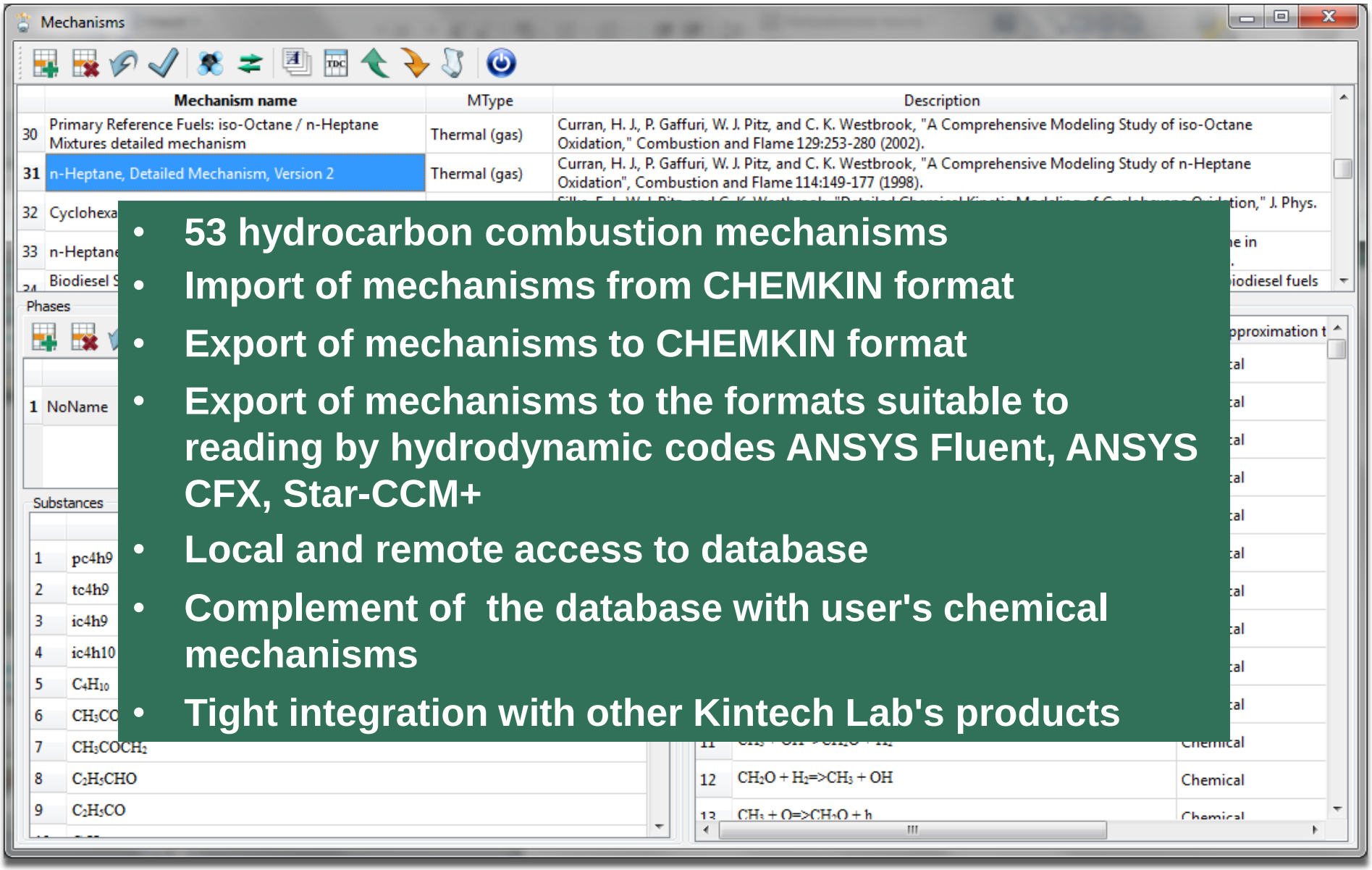
KintechDB



- 53 hydrocarbon combustion mechanisms
- Import of mechanisms from CHEMKIN format
- Export of mechanisms to CHEMKIN format
- Export of mechanisms to the formats suitable to reading by hydrodynamic codes ANSYS Fluent, ANSYS CFX, Star-CCM+
- Local and remote access to database
- Complement of the database with user's chemical mechanisms
- Tight integration with other Kintech Lab's products

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Kintech Lab Contacts

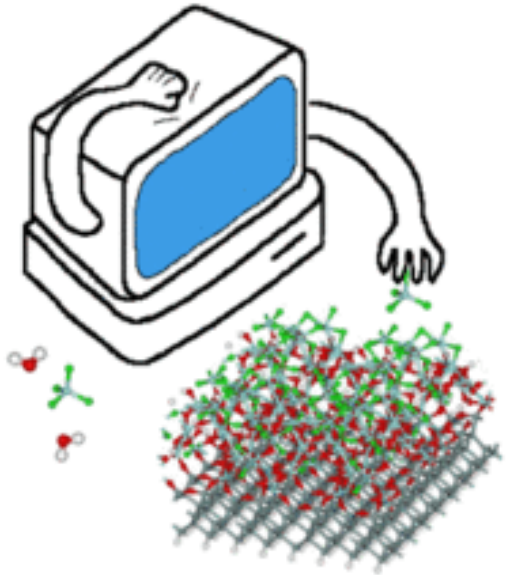
Request evaluation version of the software: evaluation@kintechlab.com

Ask technical questions: support@kintechlab.com

Contact sales: sales@kintechlab.com

Feedback for webinar: webinars@kintechlab.com

Our web-site: www.kintechlab.com



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