Form atoms and molecules
to new materials and devices

Development of the kinetic mechanisms for combustion, catalysis and environment: software tools from Kintech Lab

May 5, 2015

KINTECH LABORATORY

Overview

1. Stages of kinetic mechanism development for processes in reactive media

2. Collection and analysis of reference data
3. **Demo**: database KintechDB, comparison of kinetic mechanisms – species-by-specie, reaction-by-reaction

4. Computational models for verification of the mechanisms based on experimental data
5. **Demo**: methane combustion mechanism

6. Analysis of the kinetic mechanisms: sensitivity analysis, reaction paths identification based on reduction techniques
7. **Demo**: reduction of kinetic mechanisms

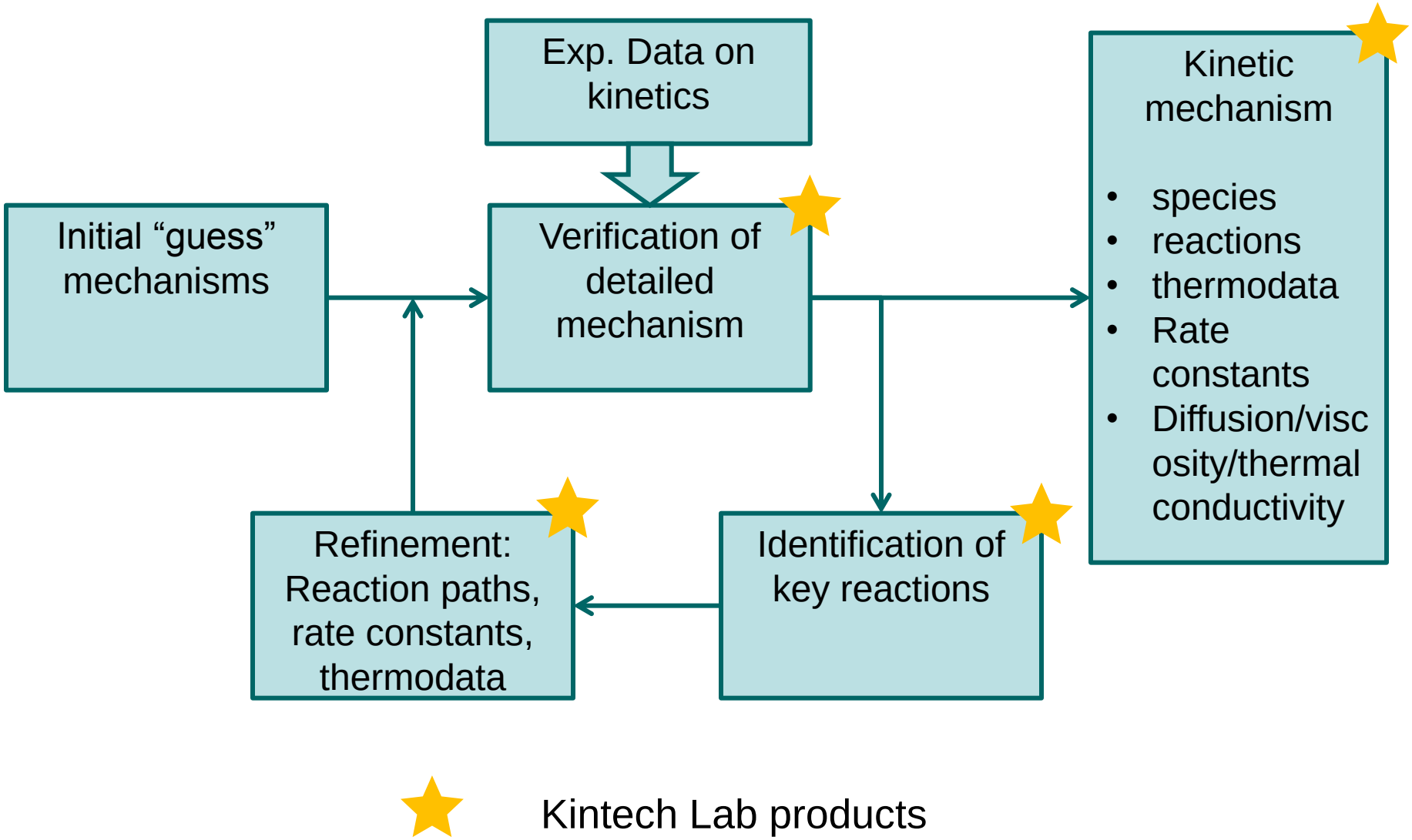
8. Refinement of the thermodynamic properties of substances and reaction rate constants based on first-principles simulations
9. **Demo**: calculation of reaction rate constant in Khimera

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.*

Stages of mechanisms development



Collection of reference data

Research Papers

- Combustion and Flame, Physica Chemistry Chemical Pjysics, Int. J. Chemical Kinetics, …
- Reviews, collection of evaluated data: Baulch review, …

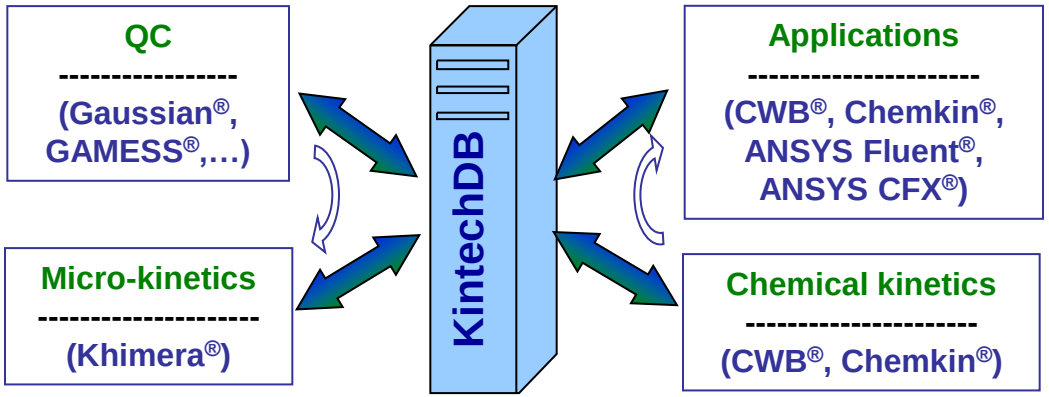
Open databases in internet, commercial databases

- NIST, Burkat Millenium database, NASA CEA, ИВТАНТЕРМО

Web-sites of research groups

- Combustion Chemistry at LLNL web site: combustion chemistry from C1 to C16, bio-fuel, pure and surrogate mixtures https://www-pls.llnl.gov/?url=science_and_technology-chemistry-combustion-mechanisms
- Combustion Chemistry Centre at NUI Galway: combustion chemistry from C1 to C5 http://c3.nuigalway.ie/mechanisms.html
- Chemical Reaction Engineering and Chemical Kinetics group at Politecnico di Milano: small and large hydrocarbons, bio-fuels, NOx and PAH http://creckmodeling.chem.polimi.it/index.php/kinetic-schemes
- Chemical reaction mechanisms for catalytic systems, developed at Karlsruhe Institute of Technology http://www.detchem.com/mechanisms.html
- Master Chemical Mechanism of tropospheric chemistry http://mcm.leeds.ac.uk/MCM/

Collection of reference data



- > 4500 – thermodata of substances,
- > 800 – molecular properties of substances,
- > 6000 – elementary processes, rates, cross-sections,
- > 80 detailed kinetic mechanisms of combustion, chemically active and radiating plasma
- Tools for analysis, comparison and visualization
- Global search
- Extesion of the database by customer, e.g. CHEMKI files
- Export into CHEMKIN format
- Local and remote acces to database
- Tight integration with other software by Kintech Lab

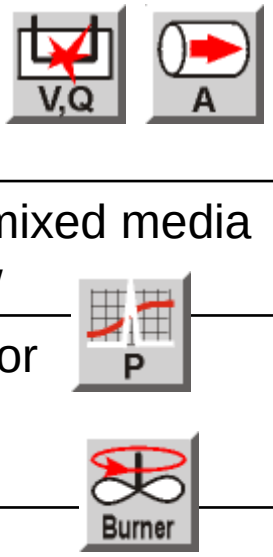
Verification of kinetic mechanisms

Application

Source of data For mechanism testing

Models of experiments

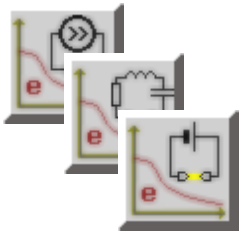
Process	Experimental setup	Theoretical model
Self-ignition/uniform flow	• Shock tube • Rapid compression machine	• Calorimetric (batch) reactor • Plug flow reactor
Flame	• Bunsen flame • Flat flame burner	• Laminar flame in premixed media • Diffusion counter-flow
Turbulent flame/stirred reactor	• Jet stirred reactor	• Perfectly stirred reactor



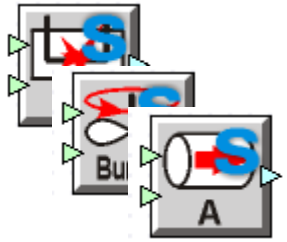
Models of kinetic experiments…

- Shock tube, Rapid compression machine (CBR),
- Flow reactor (PFR),
- Jet stirred reactor (WSR)

- Laminar flame in premixed media,
- Bunsen flame
- Counter flow flame

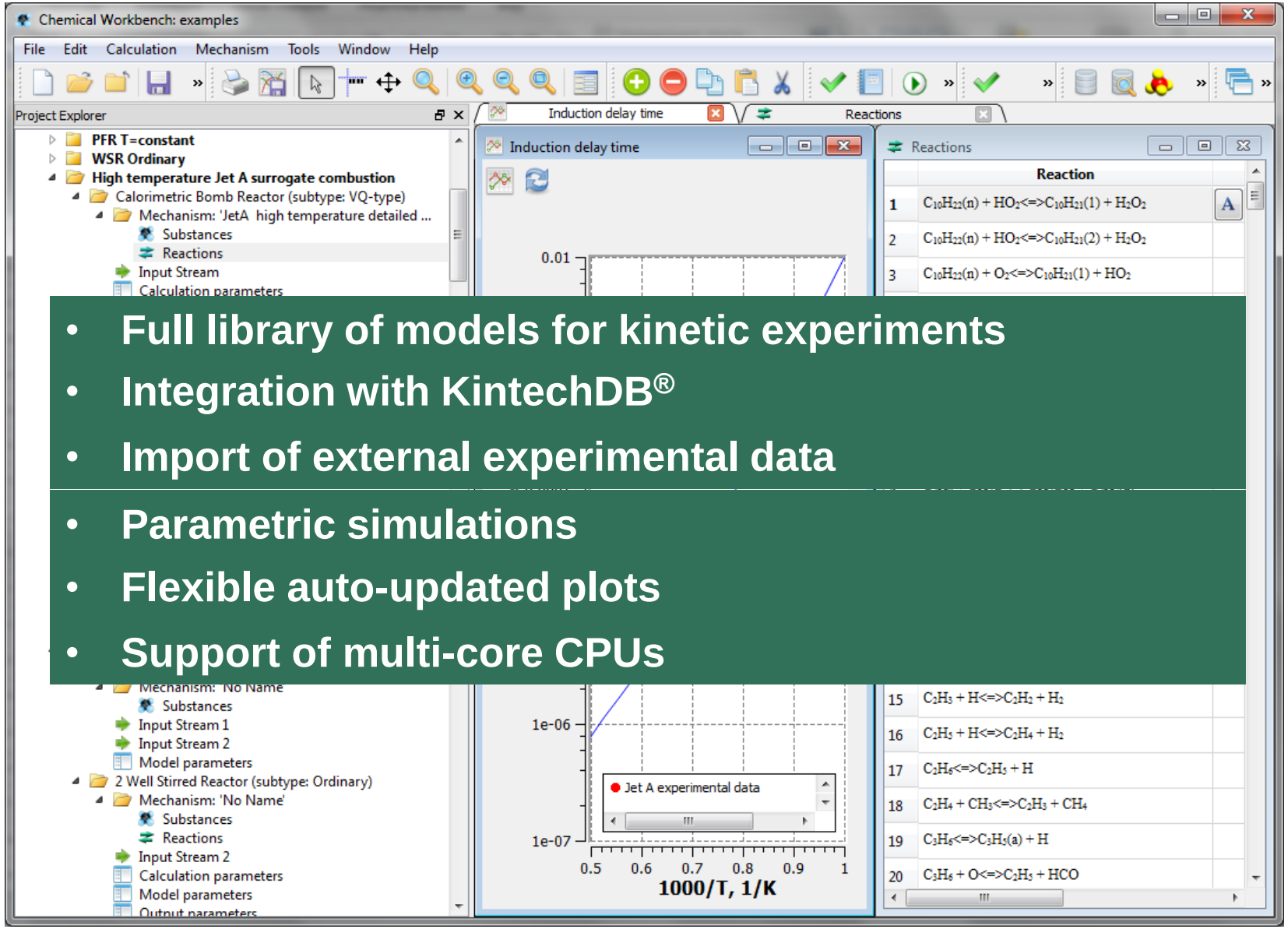


- Non-equilibrium electric discharges



- Batch reactor with catalyst (kinetic limiting)
- Flow reactor with catalyst (kinetic limiting)
- Jet-stirred reactor with catalyst (kinetic limiting)

Verification of kinetic mechanisms



- Full library of models for kinetic experiments
- Integration with KintechDB®
- Import of external experimental data

- Parametric simulations
- Flexible auto-updated plots
- Support of multi-core CPUs

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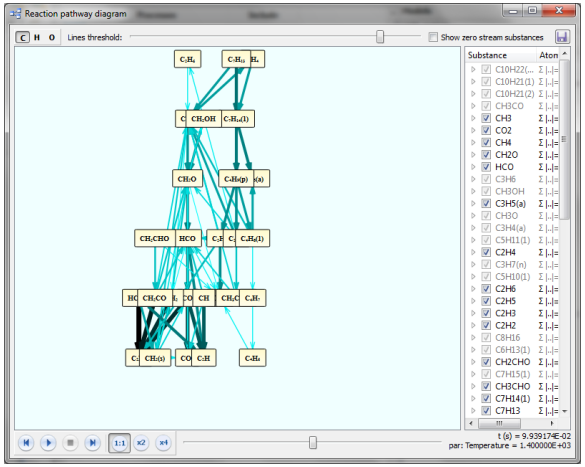
Analysis of kinetic models

…sensitivity…

Calorimetric Reactor with Deviation (CRD) – global sensitivity calculation CBR (4 models)

Calorimetric Reactor with Sensitivity (CRS) – local (differential) sensitivity calculation CBR (4 models)

…reduction



- Reaction paths diagrams
- Modern mechanism reduction techniques: DRG, DRGEP, PCA, CSP, и т.д.

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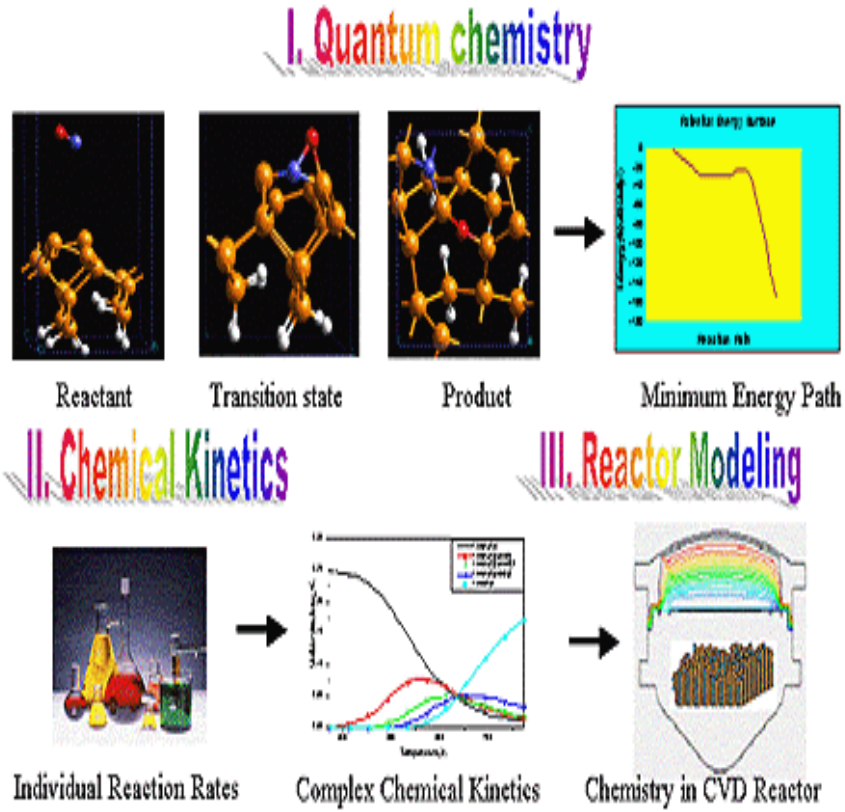
Recovery of properties from data of first-principles simulations



Heavy particles
- Direct bimolecular reactions
- Bimolecular reactions through the long-living complexes
- Multi-channel reactions
- Dissociation of di-atomic molecules
- Ion-molecular reactions
- Surface diffusion and reactions

Electron-molecular reactions
- Excitations
- Ionization
- Attachment

V-V' energy transfer

Photo-chemical reactions
- Photo-dissociation
- quenching
- isomerisation

RRCM

Surface diffusion

Thermodynamic and transport properties of multi-component gases and plasma

Contacts

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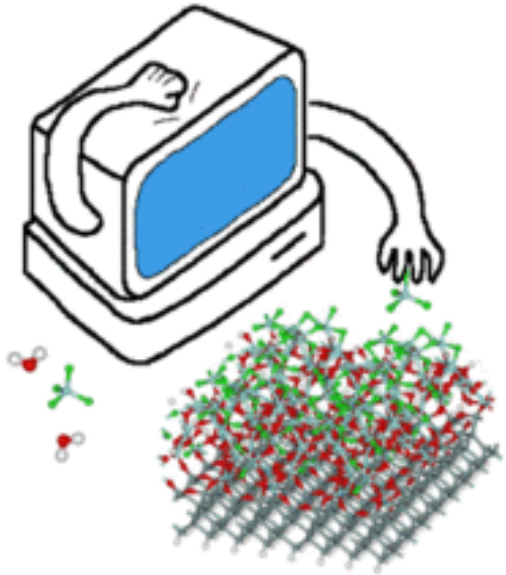
Our web-site: www.kintechlab.com



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