From atoms and molecules to new materials and technologies

Reduction of detailed kinetic mechanisms: Introduction to Mechanism Reduction Module for Chemical Workbench and best-practice

July 22, 2014

KINTECH LABORATORY

Overview of the webinar

1. About Kintech Lab
2. What is mechanism reduction and how it works?
3. **Demo**: working with Mechanism Reduction Module
4. Best practice recommendations for mechanism reduction
5. **Demo**: Setting reduction method parameters
6. **Demo**: Reducing mechanisms for a set of conditions
7. **Demo**: Application of several reduction methods

About Kintech Lab

KINTECH was founded in 2001 by scientists and engineers from and the Russian Research Center "Kurchatov Institute“ and Moscow State University

Activity fields:

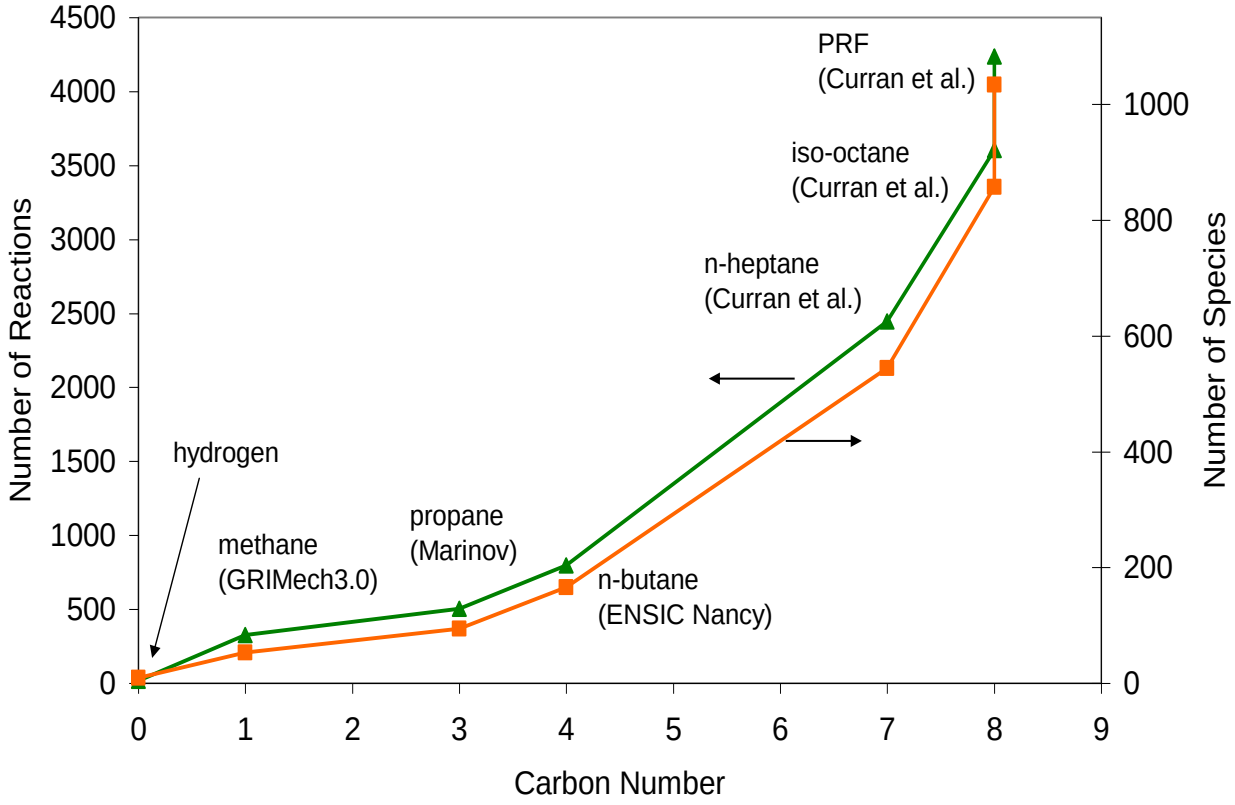
- ✓ Conducting of inventive research and consulting for a wide range of applications
- ✓ Software development for chemistry-intensive modeling and design in complete cycle
- ✓ Customer support in their own research activity using the advanced simulation capabilities of KINTECH's software

About Kintech Lab

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

- ✓ Chemical Workbench – an integrated environment for the development and reduction of chemical mechanisms
- ✓ Khimera – a unique tool for calculating microscopic parameters from first-principles calculations
- ✓ KintechDB – a network-based database for accumulation of Lab data on substances and processes
- ✓ FDTD-II – a tool for modeling the optical properties of metamaterials
- ✓ MD-kMC – an integrated environment for atomistic modeling
- ✓ EtchLab – a tool for modeling and optimization of MEMS fabrication

What is mechanism reduction and how it works?

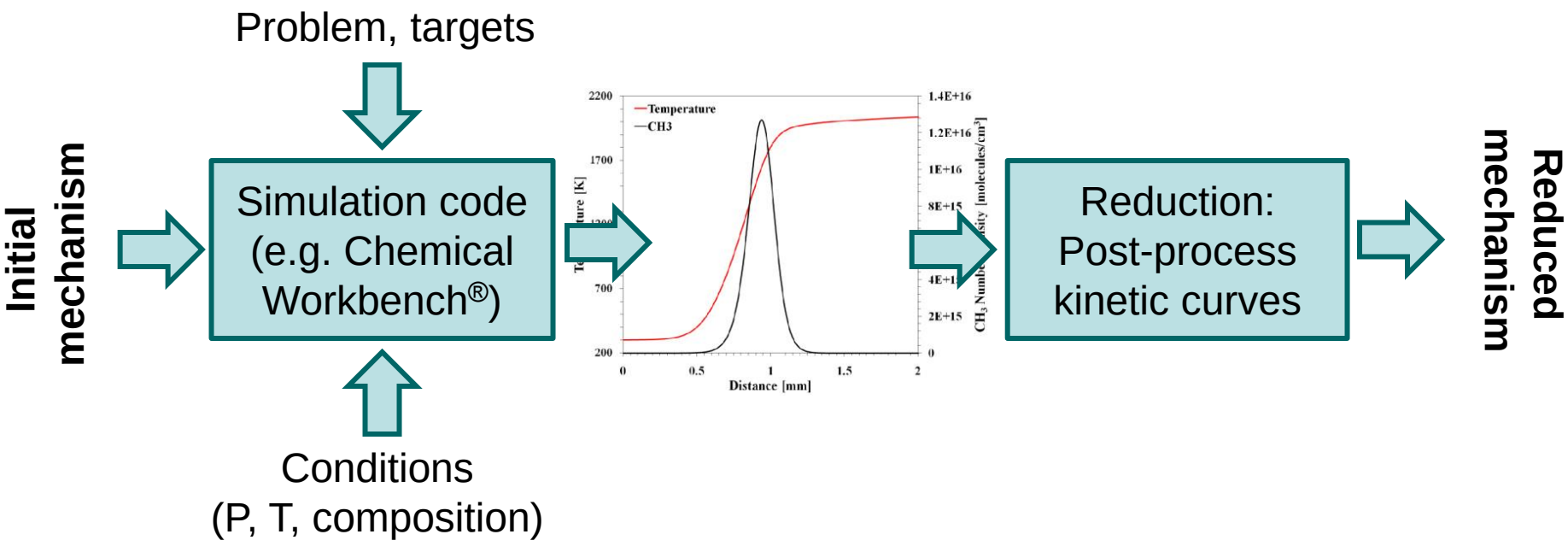


The size of the detailed combustion kinetics mechanisms for surrogates of real fuels makes impossible massive design studies with CFD tools

What is mechanism reduction and how it works?

Type of the mechanism	Applications
Detailed	• Hundreds of spx, thousands of rxns for typical hydrocarbon fuels • Supposed to work in a wide range of conditions • But should be tested
Skeletal	• Tens of spx, tens/hundreds of rxns for typical hydrocarbon fuels • Derived from detailed by removing redundant species and reactions • Derived for narrow range of conditions, sometimes for specific problems Should be tested at desired range of conditions
Reduced	• Tens of spx, tens of rxns for typical hydrocarbon fuels • Derived from detailed/skeletal by application of QSS or QE approximations • Derived for narrow range of conditions, sometimes for specific problems Should be tested at desired range of conditions
Global	• Can not be directly derived from previous one, just a very simple model • Can be applied in a very restricted rage of conditions, only for one type of the problem • MUST be tested every time before applications

What is mechanism reduction and how it works?

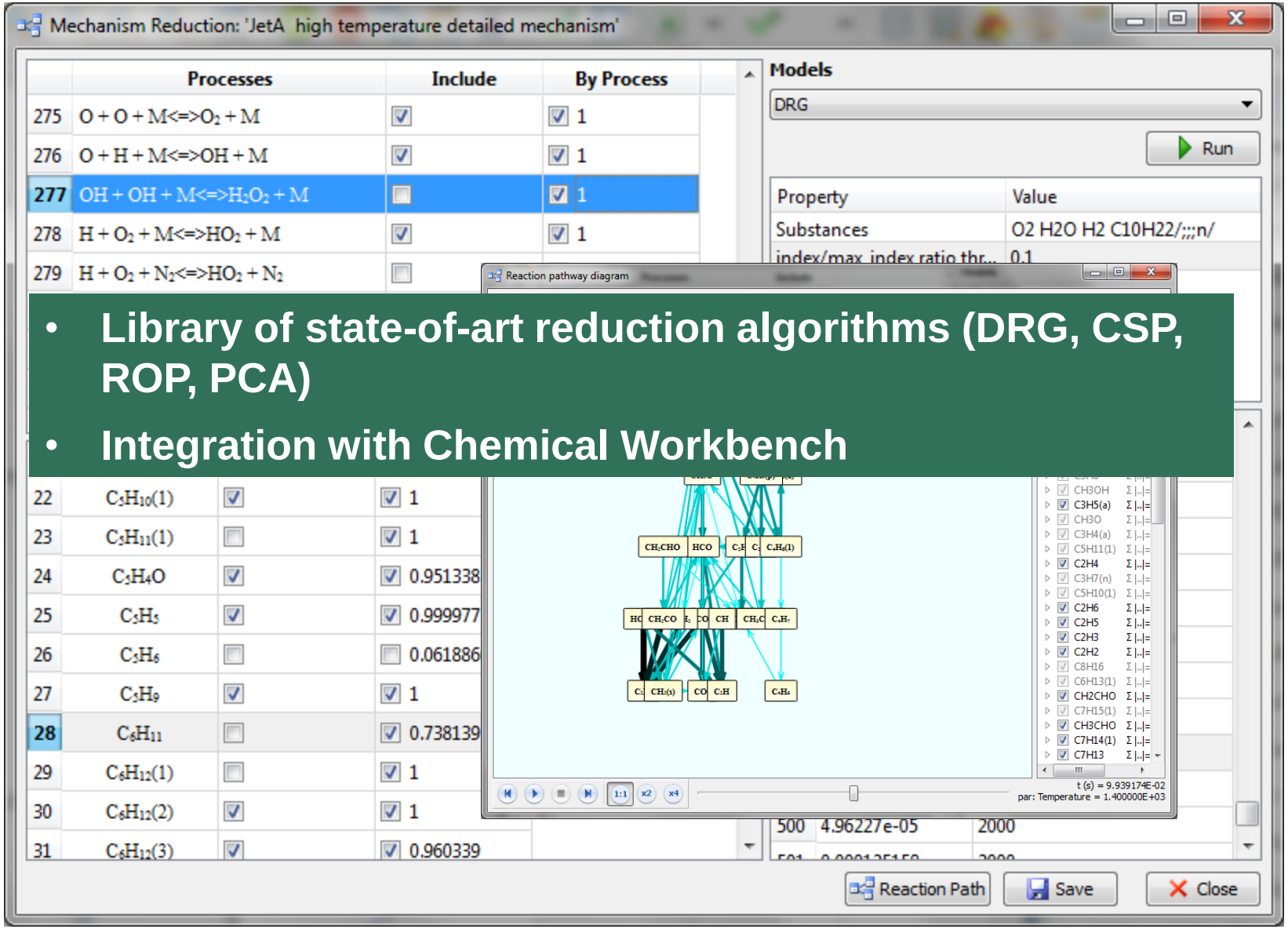


Combustion process	Problem	Targets
Self-ignition	• Shock tube/RCM • Flow reactors	• Ignition delay time • Profiles of species, temperature, pressure
Laminar Flame	• Bunsen burner • Flat flame burner • Diffusion flame	• Laminar flame speed • Extinction strain rate • Profiles of species, temperature, pressure
Turbulent flame	• Jet stirred reactor	• Concentrations of species

What is mechanism reduction and how it works?

Approach	Target for removal	Theoretical framework	Methods of reduction
Element or Species flux analysis	Species, reactions	Reaction paths	ROP, DRG, DRGEP
Time-scale analysis	Species, reactions	CSP	Time scale analysis, importance index analysis
Sensitivity analysis	Species, reactions	PCA	Species or rates sensitivity matrix analysis

Demo: working with Mechanism Reduction Module



- Library of state-of-art reduction algorithms (DRG, CSP, ROP, PCA)
- Integration with Chemical Workbench

Best practice recommendations for mechanism reduction

Test problem:

- Auto-ignition
- stoichiometric n-heptane/air
- 1 bar
- 650 – 2000K

Kinetic mechanism:

- Curran, H. J., P. Gaffuri, W. J. Pitz, and C. K. Westbrook, "A Comprehensive Modeling Study of n-Heptane Oxidation" Combustion and Flame 114:149-177 (1998)

Target:

- Ignition delay time
- 30% - maximum simulation error in comparison with detailed kinetic mechanism

Best practice recommendations for mechanism reduction

Setting numerical parameters for reduction method

Threshold value	Iteration #1(err)	Iteration #2(err)	Iteration #3(err)
0.002	-207(err 0.02%)	-21(err 0.02%)	-2(err 0.02%)
0.004	-241(err 0.02%)	-28(err 0.02%)	-4(err 0.02%)
0.008	-266(err 0.02%)	-27(err 0.02%)	-4(err 0.02%)
0.016	-301(err 0.02%)	-25(err 0.02%)	-2(err 0.02%)
0.024	-327(err 0.03%)	-26(err 0.03%)	-1(err 0.03%)
0.036	-392(err 0.2%)	-36(err 0.3%)	-4(err 0.3%)
0.054	-410(err 1.7%)	-38(err 1.7%)	-1(err 1.7%)
0.081	-413(err 1.5%)	-33(err 0.7%)	-4(err 0.7%)

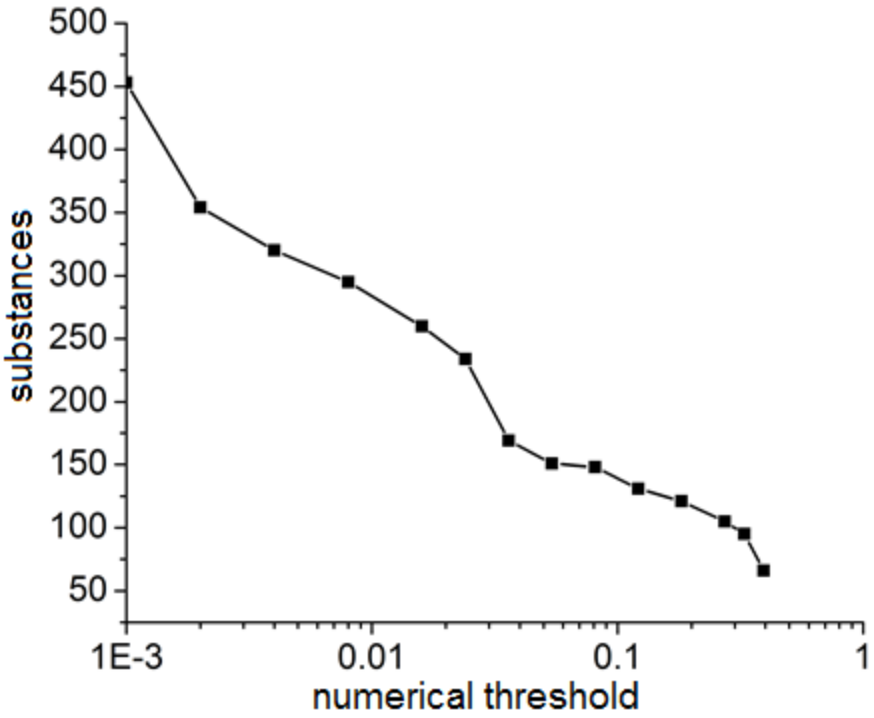
Degree of reduction'

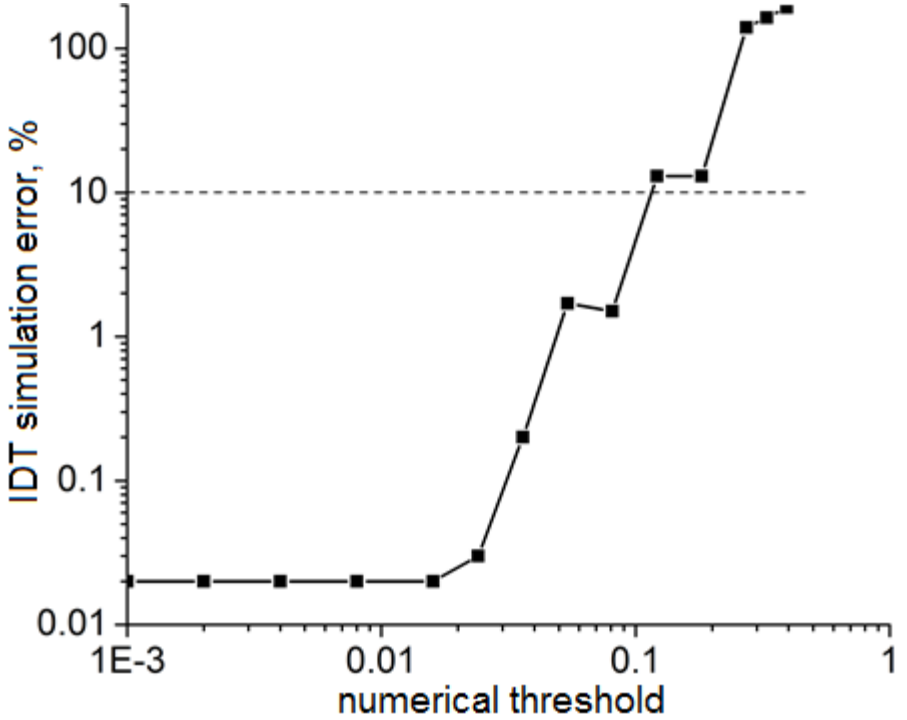
Error of IDT simulation

KAIST LABORATORY

Best practice recommendations for mechanism reduction

Setting numerical parameters for reduction method

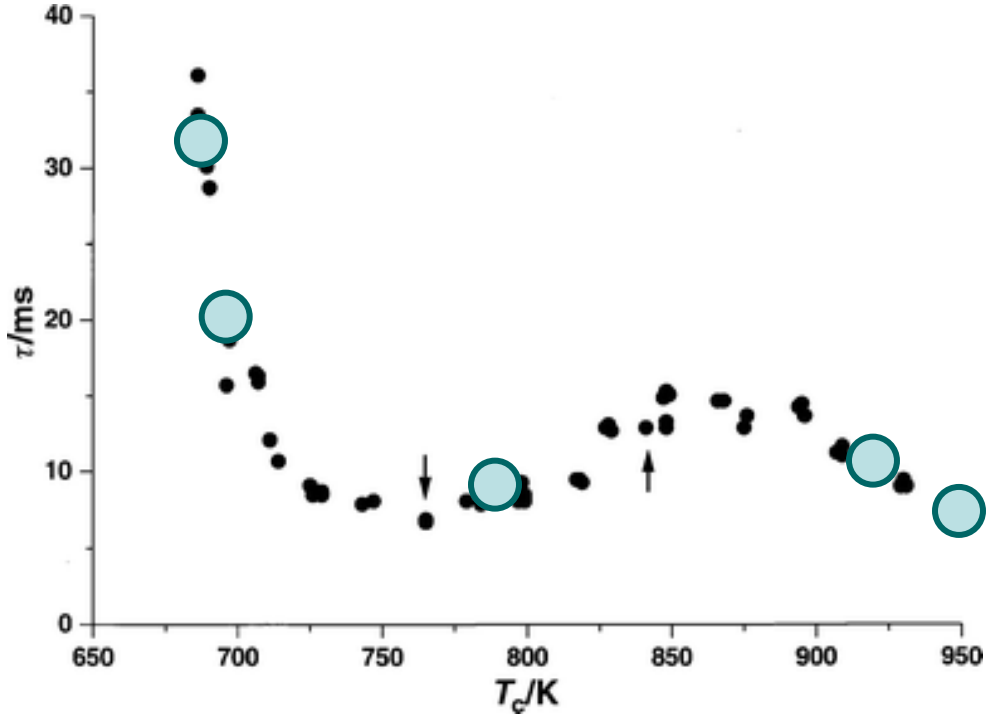




Best practice recommendations for mechanism reduction

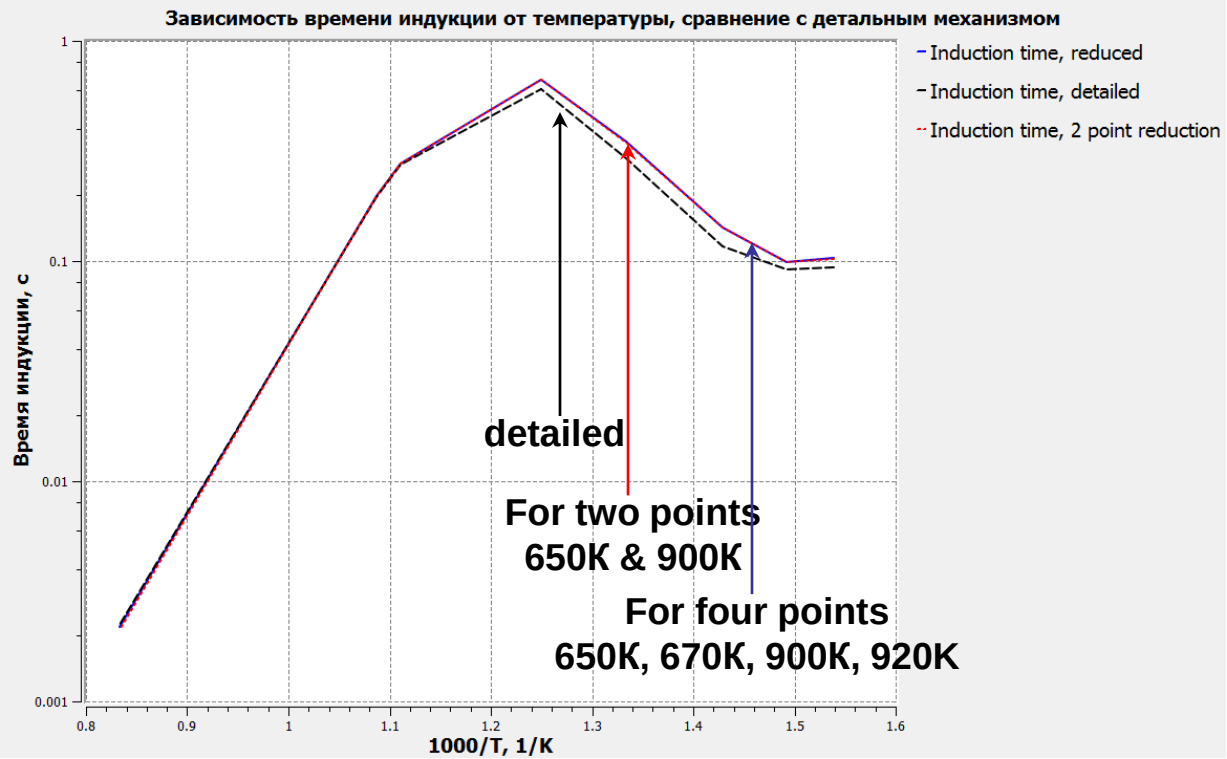
Reducing mechanisms for a range of conditions

Low-to-high temperature ignition and NTC:
How much points should we select for mechanism reduction, keeping the accuracy of reduced mechanism acceptable?



Best practice recommendations for mechanism reduction

Reducing mechanisms for a range of conditions



For efficient generation of the reduced kinetic mechanism in a range of conditions it is enough to take a single point in every characteristic interval of initial conditions.
For example, one point in low-temperature region and one point in high-temperature region

Best practice recommendations for mechanism reduction

Application of several reduction methods

STEP 1

Reduction of redundant species:

- Only species, important at given conditions, will be present in mechanism
- Also a lot of reactions will be removed with species

Connectivity based methods:
DRG, DRGEP

STEP 2

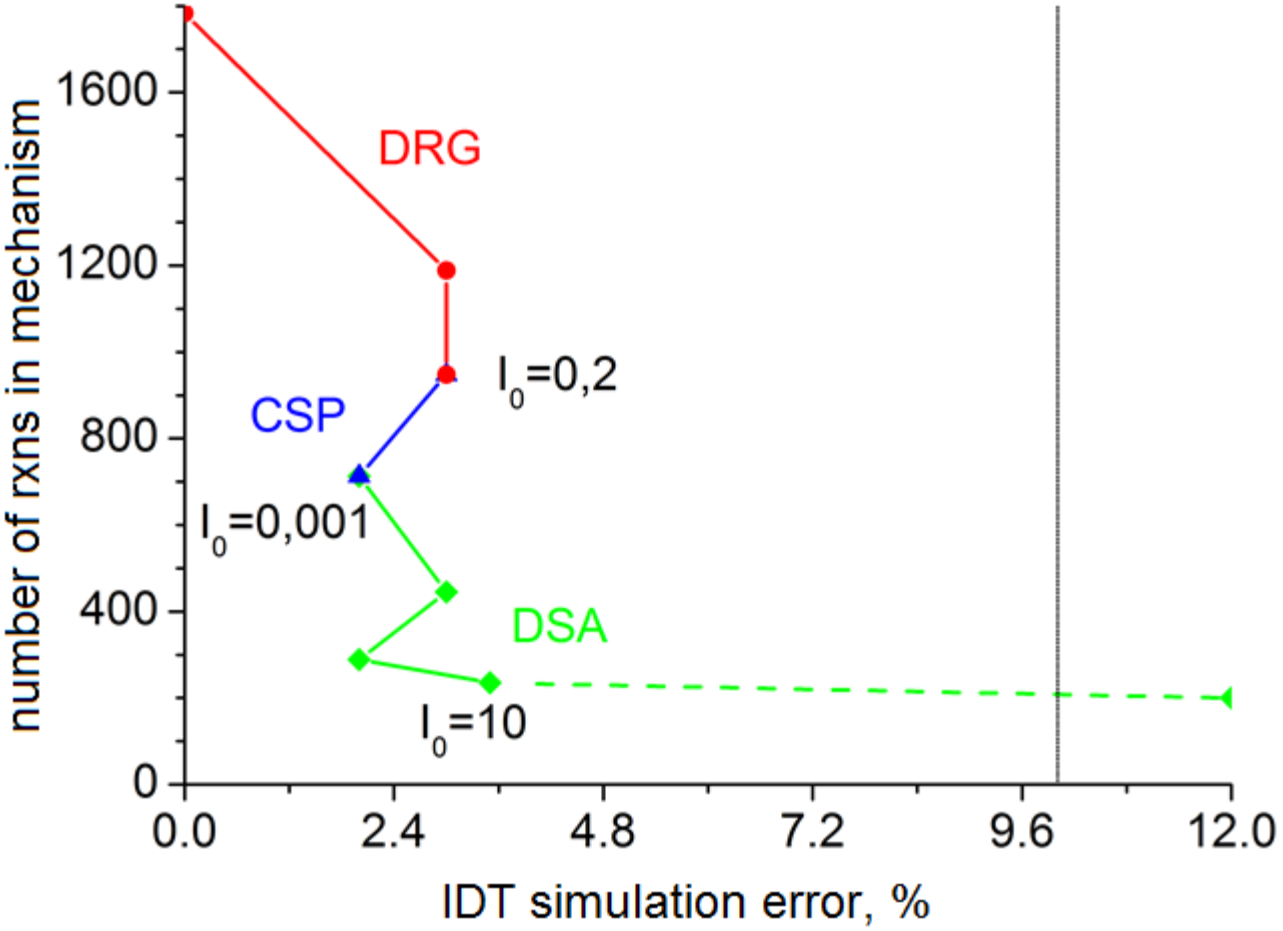
Reduction of redundant reactions

- Still redundant reactions can be removed from mechanism with important species

Time-scale analysis methods:
CSP-based
Sensitivity analysis methods:
PCA-, PCAF-based

Best practice recommendations for mechanism reduction

Application of several reduction methods



Kintech Lab Contacts

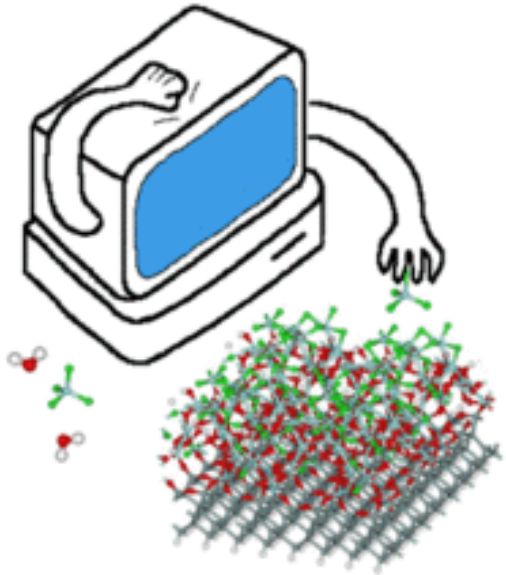
Request evaluation version of the software: evaluation@kintechlab.com

Ask technical questions: support@kintechlab.com

Contact sales: sales@kintechlab.com

Feedback for webinar: webinars@kintechlab.com

Our web-site: www.kintechlab.com



KINTECH LABORATORY