# KINTECH LABORATORY

# Reduced mechanism of methane combustion for gas turbine combustor simulations

## Background

Design of the low-emission burners for gas turbine (both industrial and for transportation) is hardly possible without computational analysis. This analysis allows to capture both heat release and pollutants formation and helps to understand system behavior from inside. In modeling studies these chemistry effects should be captured as accurate as possible. Recently detailed chemical mechanisms of natural gas combustion were developed to provide this capability. The only issue is how to use these huge chemical mechanisms in full-scale CFD simulations.

## Problem statement

It is required to reduce the size of the methane combustion mechanism [1] keeping the deviation of temperature in turbulent combustion, predicted with detailed and reduced mechanisms, in the range of 100K. Target conditions: from lean to rich mixture of methane and air, initial temperature 650 K, pressure 17 atm, range of residence time in turbulent eddies $10^{-8} - 1$ s.

## Problem setup in Chemical Workbench

For mechanism reduction in frame of Mechanism Workbench software the **Automatic Reduction** tool with Kintech Lab highly efficient algorithm was used. Both redundant species and reaction were subject to removal.

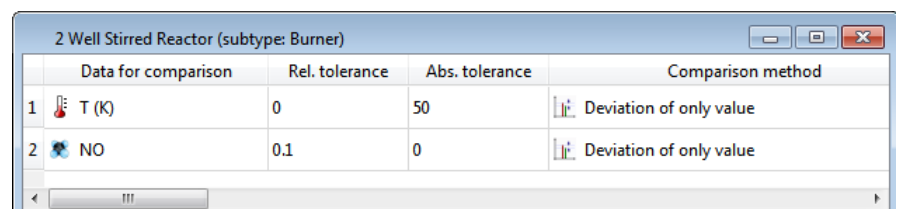**Operations with detailed and reduced mechanism in Mechanism Workbench**
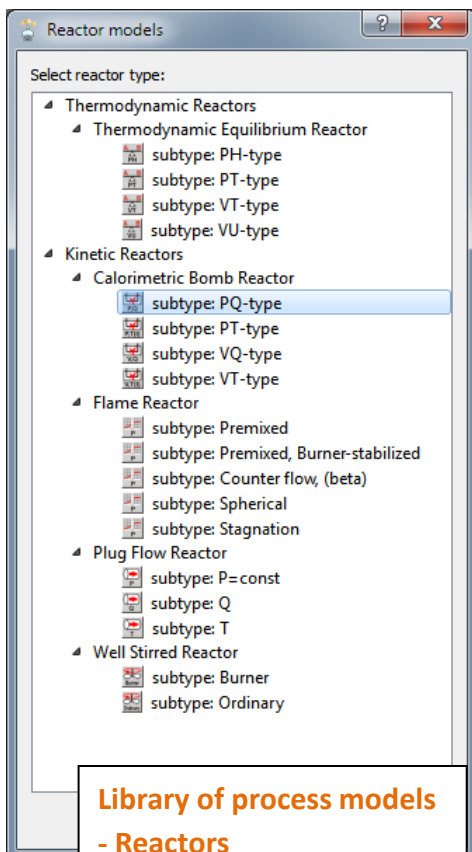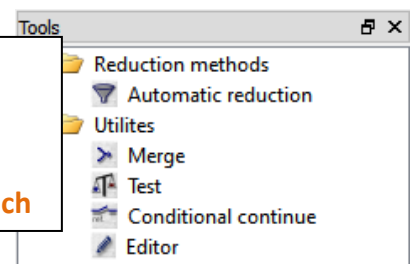


**The following combustion processes** were included as important for reduction

- Turbulent combustion: respective process model is well-Stirred Reactor – **WSR_Burner**, range of residence time covers all possible residence time values in turbulent eddies

**The following targets of the reduction** were selected:

- For turbulent combustion
  - Temperature (maximum introduced error 100K)
  - Correct capture of the critical residence time, when reaction quenches

**Library of process models - Reactors**

| | Data for comparison | Rel. tolerance | Abs. tolerance | Comparison method |
|---|---|---|---|---|
| 1 | T (K) | 0 | 50 | Deviation of only value |
| 2 | NO | 0.1 | 0 | Deviation of only value |

2 Well Stirred Reactor (subtype: Burner)

**Wizard for reduction targets setup**

## Results

On Intel Core i7 reduction of the mechanism was done in 5 minutes. It did not require any run-time monitoring and was done automatically.
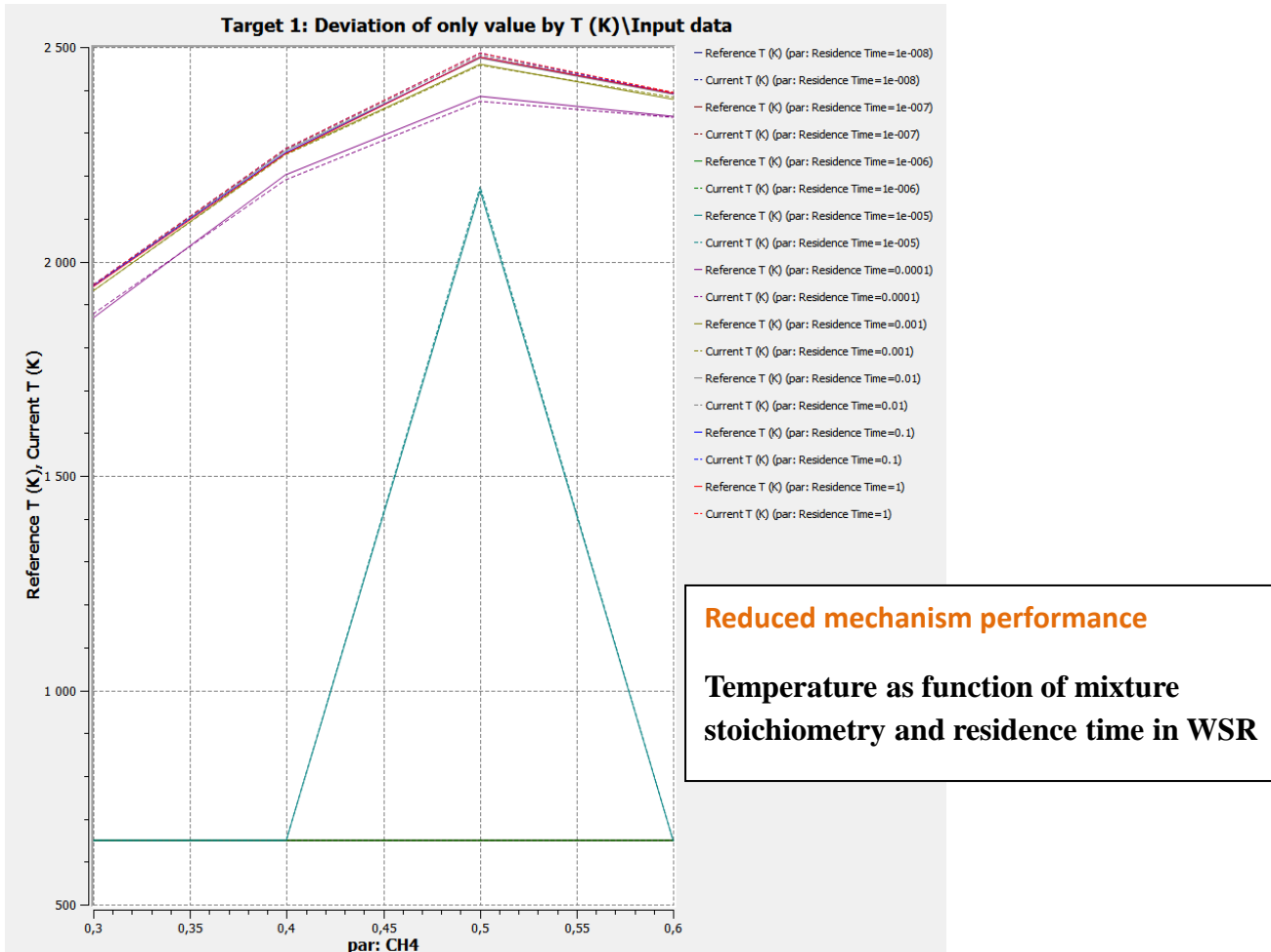
The original mechanism included

- 53 species
- 325 reactions

After reduction resulting mechanism incudes

- 19 species
- 27 reactions

The reduced mechanism is able to simulate the requested combustion features (temperature value and reaction quench) with requested accuracy at given engine conditions



**Reduced mechanism performance**

**Temperature as function of mixture stoichiometry and residence time in WSR**

## Next steps

This example can be extended further

1. Add NO and CO concentrations as targets to extend the mechanism for pollutants formation predictions

## References

[1] Gregory P. Smith, David M. Golden, Michael Frenklach, Nigel W. Moriarty, Boris Eiteneer, Mikhail Goldenberg, C. Thomas Bowman, Ronald K. Hanson, Soonho Song, William C. Gardiner, Jr., Vitali V. Lissianski, and Zhiwei Qin http://www.me.berkeley.edu/gri_mech/