KINTECH LABORATORY

Reduced mechanism for diesel combustion at engine conditions

Background

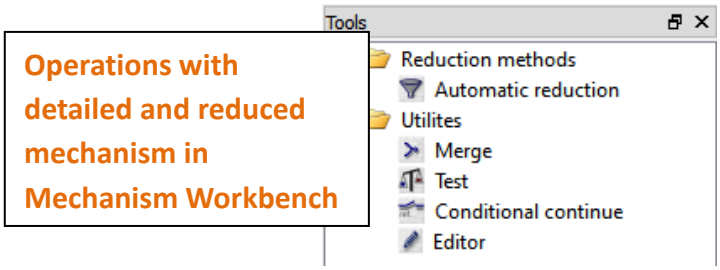
A number of processes take place in diesel engines: self-ignition, turbulent non-premixed flame, NOx and PM formation. Every process is sensitive to the combustion chemistry. In modeling studies these chemistry effects should be captured as accurate as possible. Recently detailed chemical mechanisms of diesel combustion were developed to provide this capability. The only issue is how to use these huge chemical mechanisms (>1000 species, >10000 reactions) in full-scale CFD simulations.

Problem statement

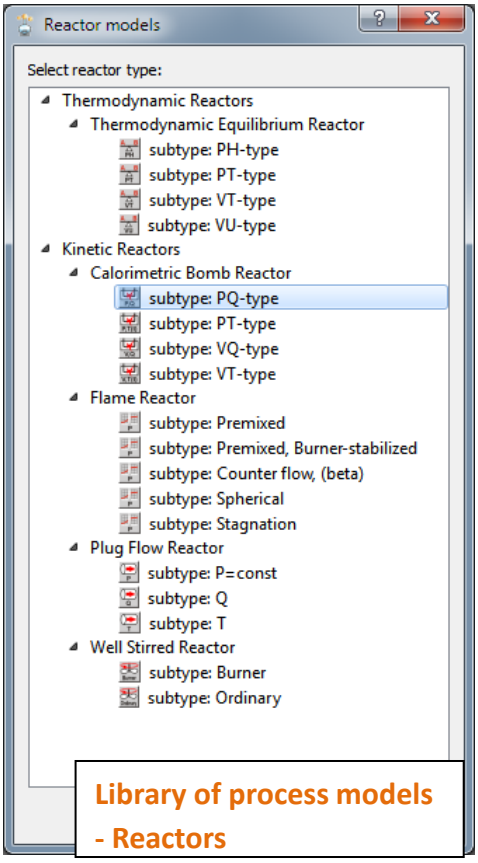
It is required to reduce the size of the diesel surrogate – n-heptane combustion mechanism [1] keeping the deviation of ignition delay time and temperature, predicted with detailed and reduced mechanisms, in the range of 10% and 100K respectively. Target conditions: stoichiometric mixture of n-heptane, range of initial temperatures 600 – 1500K, range of pressures 40 atm.

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



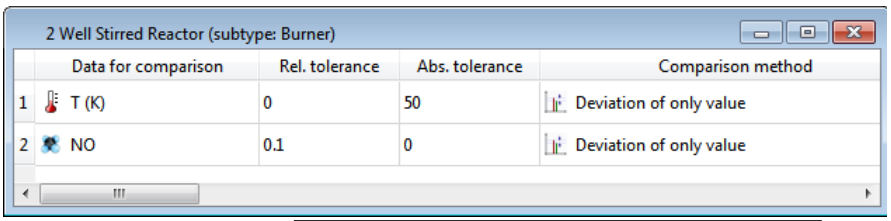
Library of process models - Reactors

The following combustion processes were included as important for reduction

- Ignition (respective process model is Calorimetric Bomb Reactor at constant pressure and adiabatic conditions – CBR_PQ)

The following targets of the reduction were selected:

- For ignition
  - Ignition delay time, maximum introduced error 10%
  - Temperature (maximum introduced error 100K)



Wizard for reduction targets setup

Results

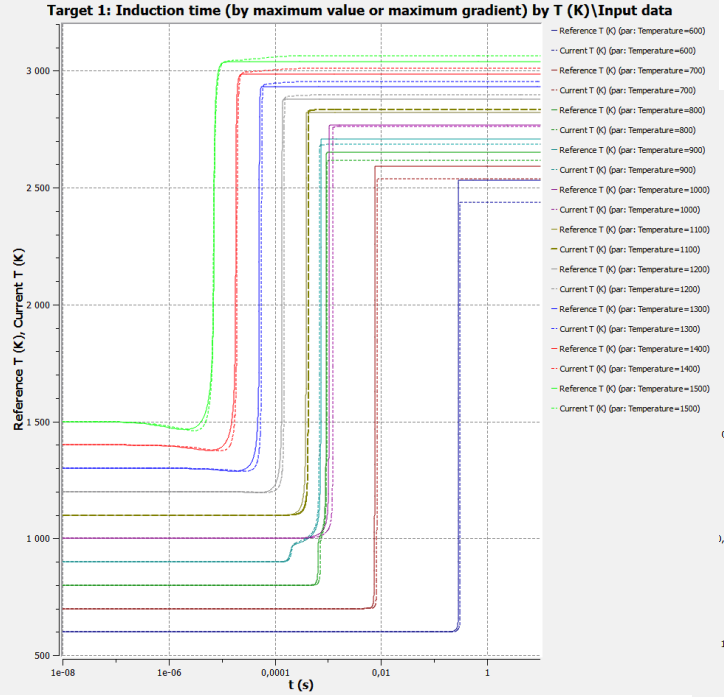
On Intel Core i7 reduction of the mechanism was done in 20 hours. It did not require any run-time monitoring and was done automatically.
The original mechanism included

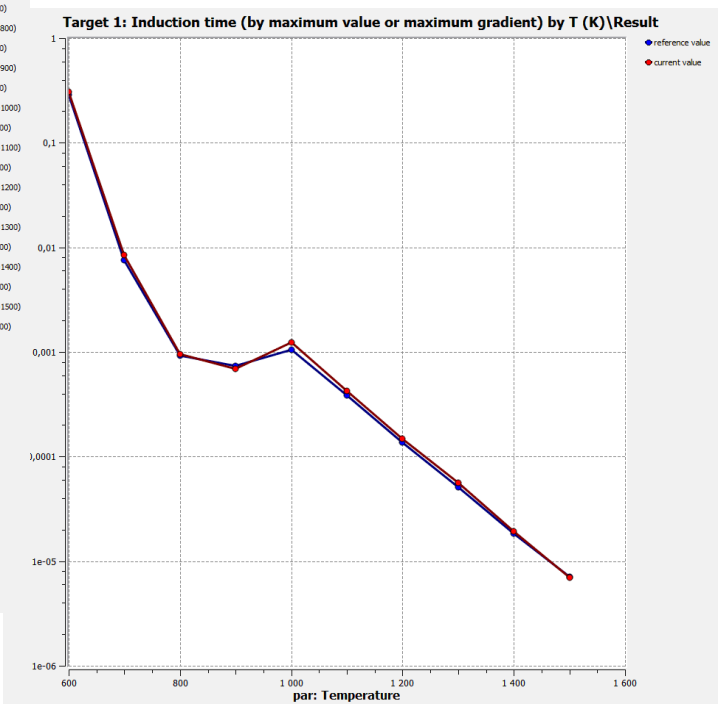
- 651 species
- 5059 reactions

After reduction resulting mechanism incudes

- 111 species
- 249 reactions

The reduced mechanism is able to simulate the requested combustion features (ignition delay time, temperature/heat-release profiles) with requested accuracy at given engine conditions





Reduced mechanism performance

temperature profile/ignition delay time, predicted with detailed and reduced mechanisms

Next steps

This example can be extended further

1. The reduced mechanism can be stored in CHEMKIN format and used directly in any engine CFD software, or used to calculate ignition delay time and laminar flame speed tables for engine combustion models, available in engine CFD codes
2. CO, PAH and unburned hydro-carbons (UHC) can be added as targets of mechanism reduction to extend the capabilities of the reduced mechanism to capture hydro-carbon emissions from diesel engines
3. Prepare new project for reduction of detailed mechanism for gasoline engine simulations

References

[1] 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)