

# Calculation of Jet A surrogate ignition at high temperatures

## Background

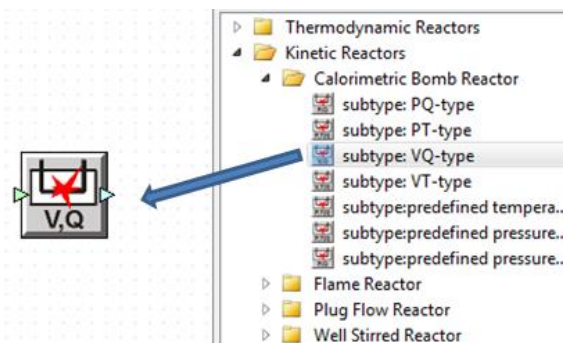
Aviation kerosene Jet A is multi-component fuel consisting of several hundreds of hydrocarbons. Modeling of such fuel ignition in propulsion systems such as ramjets, scramjets, pulse detonation and gas turbine engines demands its exchange on more simple fuel model with well-defined and reproducible composition (surrogate), which exhibits an ignition behavior similar to kerosene and can be used instead of the actual Jet A fuel.

## Problem statement

It is required to calculate the induction times, temperature and main concentrations behavior during the combustion of Jet A surrogate ( n-decane C<sub>10</sub>H<sub>22</sub> /n-hexane C<sub>6</sub>H<sub>14</sub> / benzene C<sub>6</sub>H<sub>6</sub> for a range of mixture equivalence ratio. Initial temperature of kerosene-air is 1000K – 1800 K, initial pressure 1, 10 atm. Mixture equivalence ratio - 0.5, 1, 2.

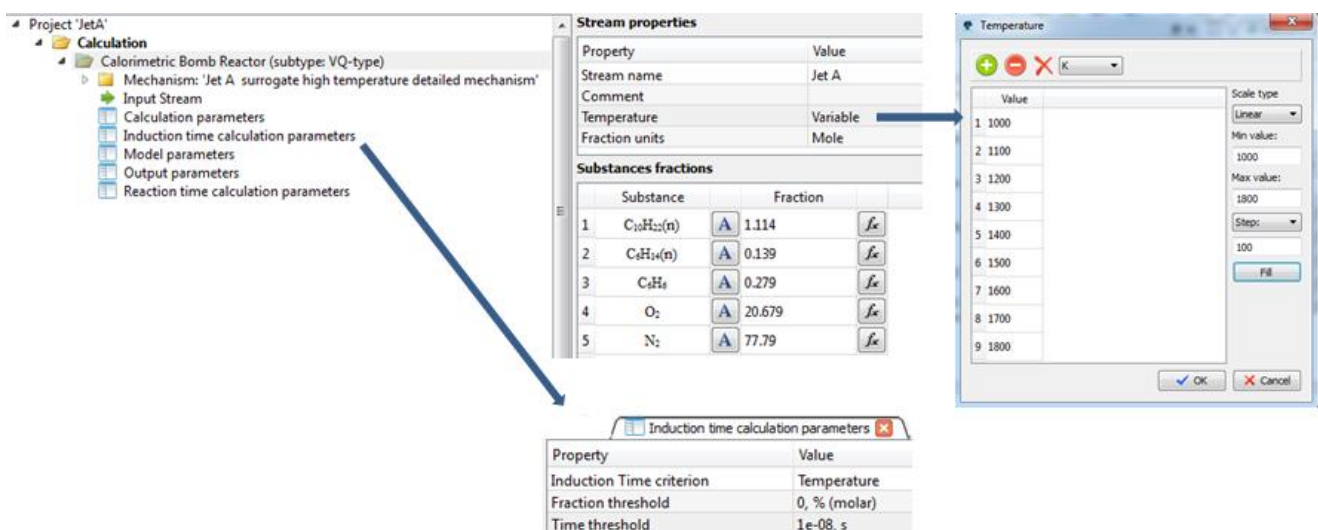
## Problem setup in Chemical Workbench

To calculate the induction times, temperature and main concentrations behavior during the combustion of Jet A surrogate, we use the **Calorimetric Bomb Reactor VQ-type** (combustion at adiabatic conditions and constant volume), available in Chemical Workbench.



This model requires information about **Input stream**, kinetic mechanism, induction time criterion.

**The Mechanism** is loaded from KintechDB database, which is tightly integrated with Chemical Workbench and provide kinetic mechanisms elaborated by Kintech or taken from available data . **The initial mixture** is set in the same input stream of the reactor with composition  $\phi = 1$ . **Initial temperatures** 1000 - 1800K, **initial reactor pressure** 10 atm. Ignition delay time (Induction time) is determined by max grad (Temperature).



**Stream properties**

Property	Value
Stream name	Jet A
Comment	
Temperature	Variable
Fraction units	Mole

**Substances fractions**

Substance	Fraction
1 C <sub>10</sub> H <sub>22</sub> (n)	1.114
2 C <sub>6</sub> H <sub>14</sub> (n)	0.139
3 C <sub>6</sub> H <sub>6</sub>	0.279
4 O <sub>2</sub>	20.679
5 N <sub>2</sub>	77.79

**Induction time calculation parameters**

Property	Value
Induction Time criterion	Temperature
Fraction threshold	0, % (molar)
Time threshold	1e-08, s

**Temperature**

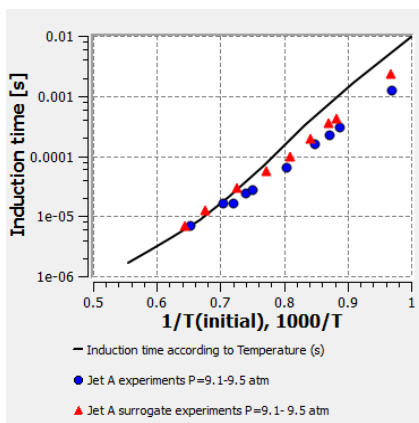
Value	Scale type
1 1000	Linear
2 1100	
3 1200	
4 1300	
5 1400	
6 1500	
7 1600	
8 1700	
9 1800	

Experimental data can be included in **Results/External data tables** for validation of calculated results.

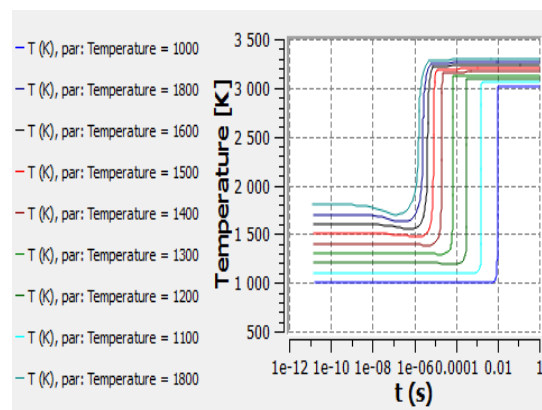
	1000/T	tau, s
1	0.653	7e-06
2	0.705	1.6e-05
3	0.72	1.65e-05
4	0.74	2.4e-05
5	0.751	2.75e-05
6	0.805	6.35e-05
7	0.848	0.000159
8	0.871	0.000217
9	0.888	0.000296
10	0.969	0.00125

## Results

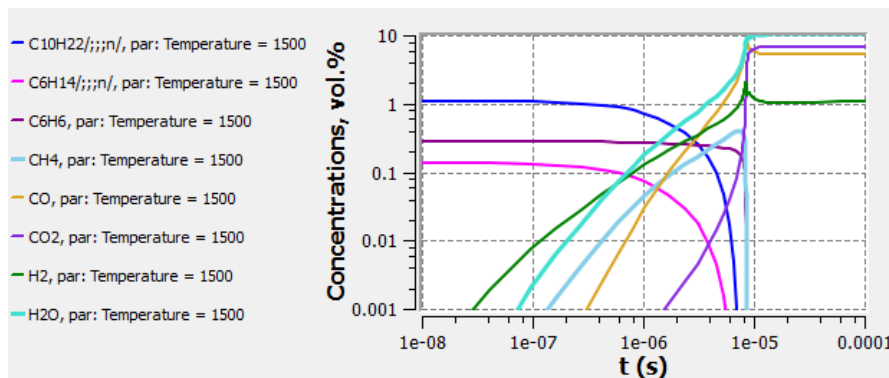
Simulated results are shown at below pictures at  $Po=10$  atm. Experimental results of ignition delay times are taken from O.G. Penyazkov, K.L. Sevrouk, V. Tangirala, N. Joshi, Autoignitions of Diesel Fuel/Air Mixtures Behind Reflected Shock Waves, in Proceedings of the Fourth European Combustion Meeting, Vienna, Austria, 2009.



(a) Induction time vs. initial temperature



(b) Temperature behavior during combustion at different initial temperatures



(c) Main concentrations behavior during the combustion at  $T_0=1500$  K

## Next steps

1. Change criteria for ignition delay time (e.g. time, when H radical concentration is maximum) and repeat simulation to see, how ignition delay time is dependent on it
2. Repeat simulation in constant pressure adiabatic reactor to see the sensitivity of the ignition delay time to constant pressure/constant volum conditions

## References

[1] O.G. Penyazkov, K.L. Sevrouk, V. Tangirala, N. Joshi, Autoignitions of Diesel Fuel/Air Mixtures Behind Reflected Shock Waves, in Proceedings of the Fourth European Combustion Meeting, Vienna, Austria, 2009.