

Sensitivity analysis of propane ignition in air at low temperatures

Background

Combustion is a complex phenomenon, characterized by interaction and competition of various physical and chemical processes. The correct description of chemical changes requires the application of reaction mechanisms consisting of several hundred or thousand reactions. For example the combustion of natural gas (mixture of methane, ethane and propane) is described by detailed mechanism amounted approximately 130 species and 1300 reactions. This means that the chemistry of combustion processes is described by a huge number of parameters and hence the application of sensitivity analysis techniques is very useful for its understanding.

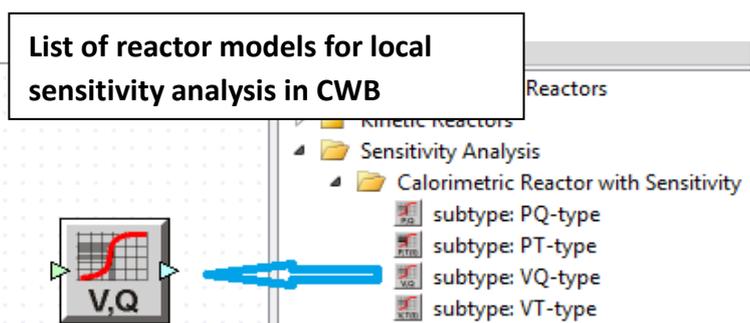
Problem statement

It is required to carry out the sensitivity analysis of propane/air stoichiometric mixture ignition at initial pressure 10 atm and initial temperature 700 K to understand the governing reactions peculiar for low temperature ignition.

Problem setup in Chemical Workbench

To carry out the sensitivity analysis of ignition delay times of propane/air mixture we use the **Calorimetric Reactor with Sensitivity** (subtype:VQ-type), available in Chemical Workbench.

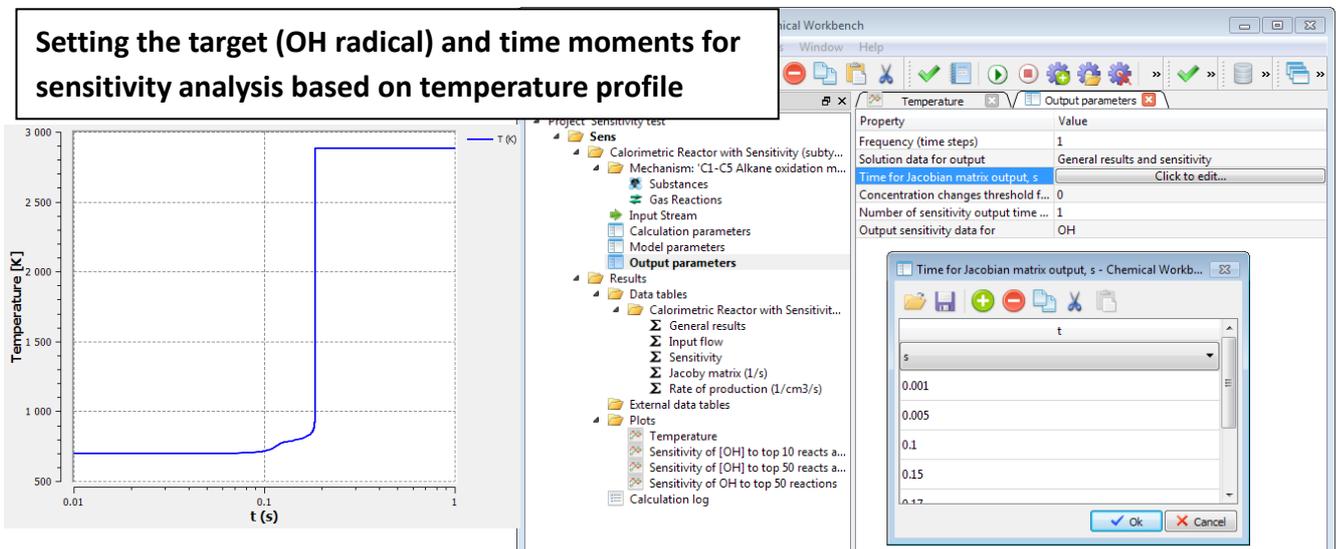
The chemical kinetic **Mechanism** is loaded from KintechDB database. Original mechanism was imported from CHEMKIN file, available at [http://c3.nuigalway.ie/mechanisms.html/Natural gas to/including nC5 \(2010\)](http://c3.nuigalway.ie/mechanisms.html/Natural%20gas%20to/including%20nC5%20(2010).).



For **Input stream** the stoichiometric mixture of propane and air at initial temperature 700 K was set. Initial pressure of the process was set to 10 bar.

For the sensitivity analysis the OH radical was set as target to produce the sensitivity coefficients. The **Time for Jacobian matrix output** was selected to print sensitivity coefficients based on time moment, where the temperature behavior experience significant changes.

Setting the target (OH radical) and time moments for sensitivity analysis based on temperature profile

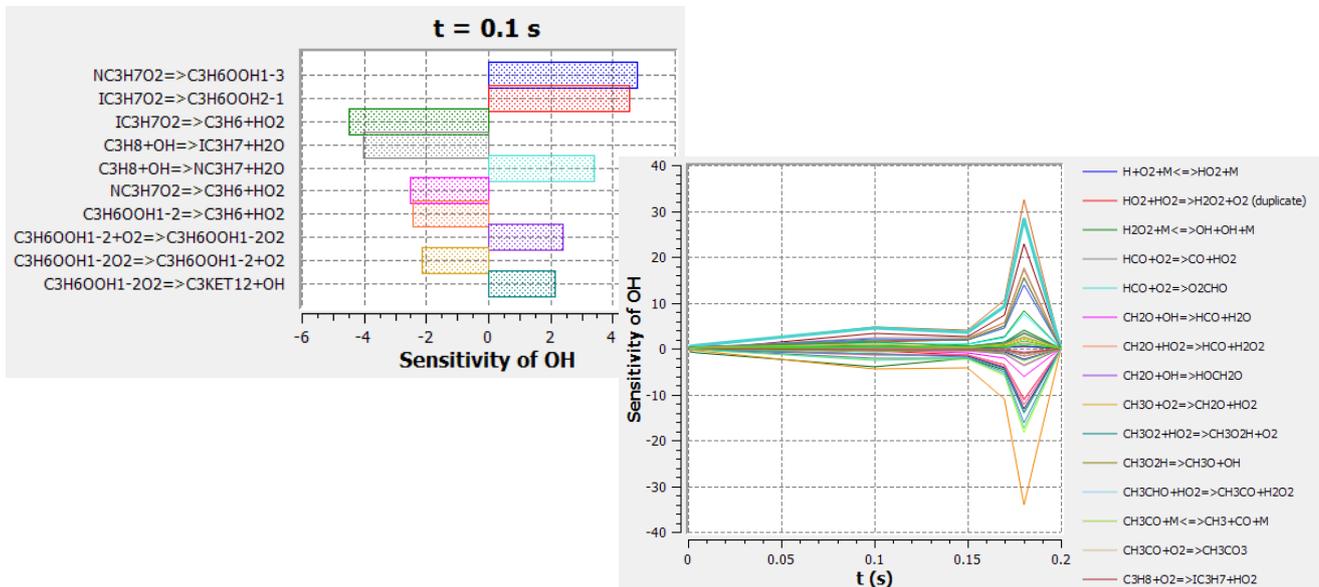
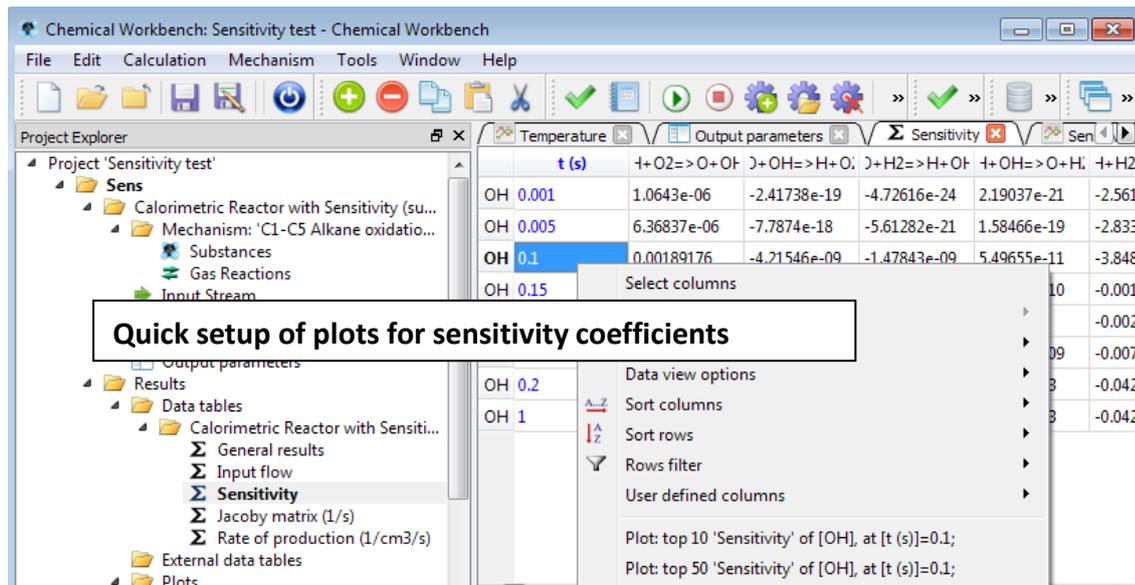


The figure displays the Chemical Workbench interface. On the left, a plot shows Temperature [K] versus time t (s) on a semi-log scale. The temperature starts at 700 K, remains constant until approximately 0.1 s, then rises sharply to about 2800 K. A vertical dashed line is drawn at t = 0.1 s. On the right, the 'Output parameters' dialog box is open, showing the 'Time for Jacobian matrix output, s' property. The 'Value' field is set to 0.15. Below the dialog, a list of time moments is shown: 0.001, 0.005, 0.1, 0.15, and 0.17. The '0.15' value is highlighted.

Results

After the calculation is finished three tables are produced (more tables can be produced if Jacoby matrix output is required): **Input flow**, **General results** (which contain kinetic curves of the system) and **Sensitivity coefficients** at requested time moments. Using Sensitivity table it is possible to obtain plots with 10 and 50 main reaction, which mostly affect the OH radical concentration at selected time moment. Also time variation of sensitivity coefficients can be tracked through the stages of ignition by plotting them at different time moments.

As sensitivity analysis show, at time moment of 0.1 s, when first temperature rise occurs, low temperature reactions path dominate (internal isomerization, chain propagation and branching characteristic to low-temperature chemistry).



Next steps

1. Analyze sensitivity coefficients at time moment t = 0.18 s, when most of the heat is released
2. Setup sensitivity analysis for peroxide radicals (HO₂, RO₂·)
3. Change fuel and mechanism to more complex (for example, n-heptane) and build the same project and analysis.