KINTECH LABORATORY

Computing static parameters of the detonation wave in gases

Background

Detonation waves are harmful phenomena, related with fast propagation of reaction waves in gases, accompanied by strong pressure and temperature rise. Estimation of the detonation wave parameters, which include propagation speed and pressure/temperature rise is important at evaluation of detonation consequences.

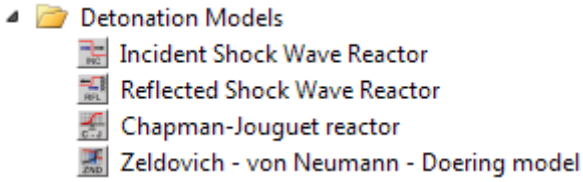
Problem statement

Calculate the parameters of detonation wave, propagating through fuel-lean, stoichiometric (φ= 1) and fuel-rich hydrogen-air mixture.

Problem setup in Chemical Workbench

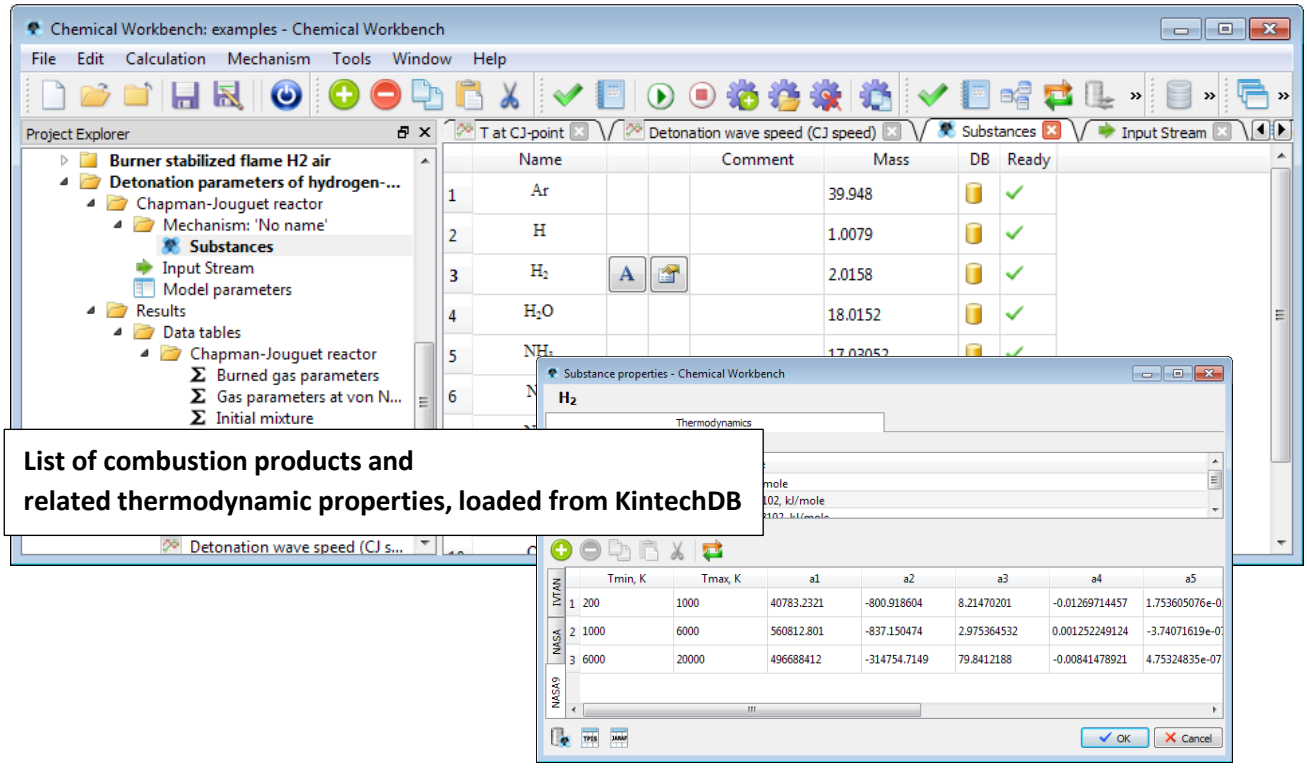
The parameters of the self-supporting detonation wave (propagation speed, pressure and temperature rise), propagating through the reactive gaseous mixture are determined by initial thermodynamic conditions (pressure, temperature) and by reactive mixture composition.

The given problem is solved in Chemical Workbench software with Chapmann-Jouget reactor model (CJR). This model calculates the following parameters of the steady detonation wave: equilibrium combustion products composition, speed of self-supporting detonation – so called Chapman-Jouget speed, temperature and pressure just behind the detonation wave – Chapman-Jouget pressure and temperature.



List of detonation-related reactor models

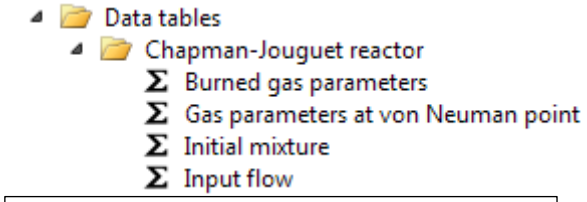
The combustion state and composition of reactiove Mixture is defined in Input Stream by molar mixture composition: [O2]:[N2] :[H2] = 1:3.76:X, where X = 0.5 - 4. The initial temperature of reactive mixture is set to 300K, initial pressure is 1 atm.
Thermodynamic properties of air components and combustion products are extracted from Kintech DB database.



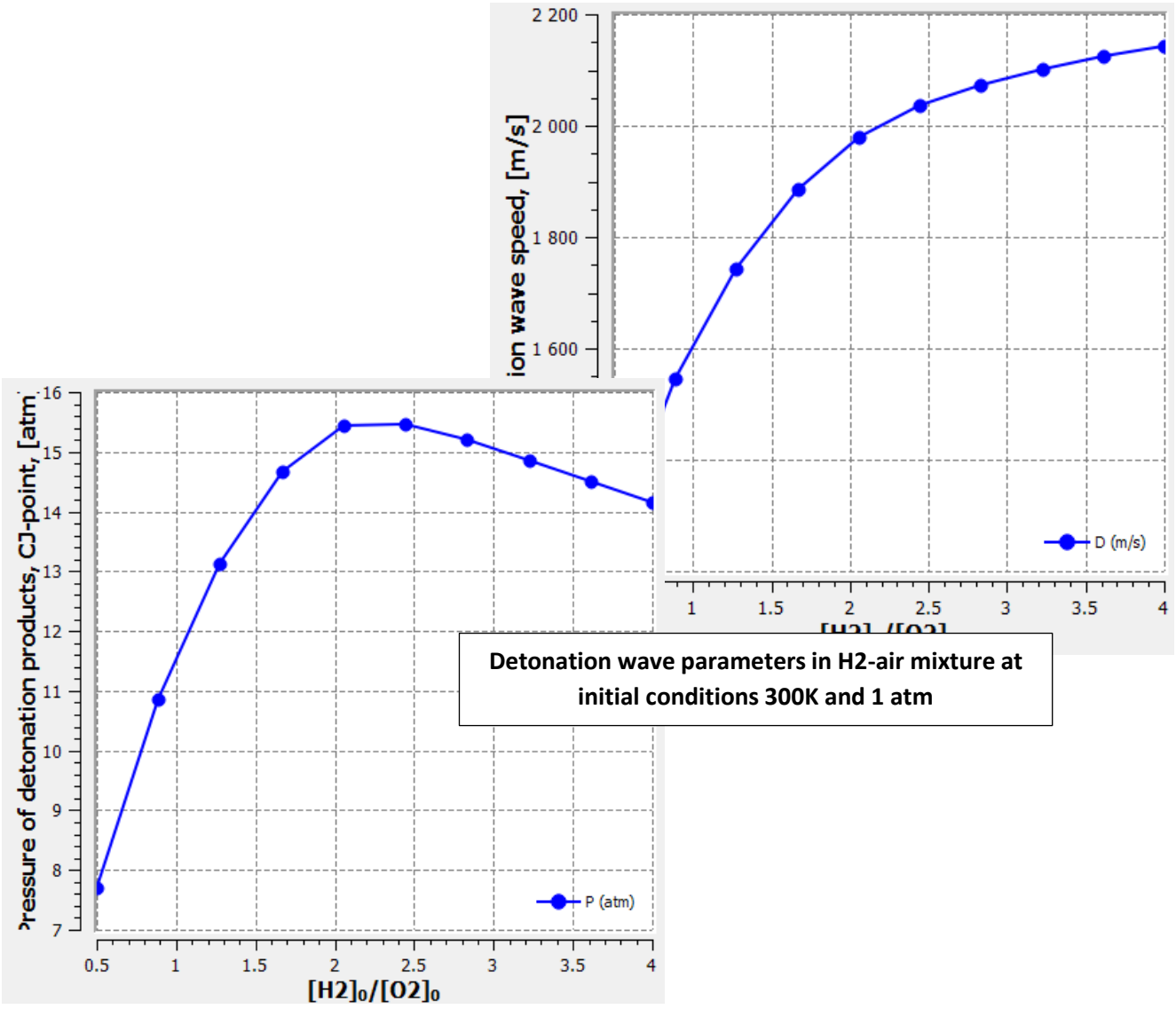
List of combustion products and related thermodynamic properties, loaded from KintechDB

Results

State of the reactive mixture after combustion behind detonation wave (Chapman-Jouget point) are given in **Burned Gas Parameters table**. Properties of the initial mixture, including Chapman-Jouget speed of detonation wave, are given in table **Initial mixture**. In addition to the Chapman-Jouget point, the gas properties are computed at conditions of von Neumann point (state of initial mixture behind shock wave, propagating with the CJ speed) and given in table **Gas parameters at von Neumann point**



Available tables of results in CJR



Detonation wave parameters in H2-air mixture at initial conditions 300K and 1 atm

Next steps

1. Simulate detonation parameters of the methane, ethane and propane mixtures with air. Estimate, how the detonation velocity depends upon hydrocarbon molecule
2. Plot dependence of von-Neumann point parameters vs stoichiometry of the mixture
3. Evaluate detonation parameters of any real fuel: non-integer x and y in brutto-formula CxHy