KINTECH LABORATORY

Computing the internal structure of ideal detonation wave

Background

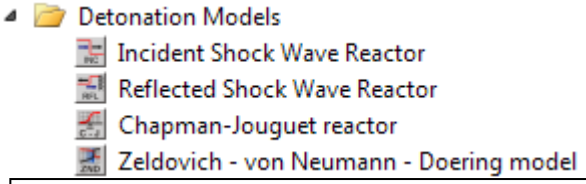
Propagating detonation wave have inherent 3D structure which is expressed as cell structures on the smoked foils at the wall. This structure is characterized by cell size and often used to estimate critical conditions of detonation initiation/re-initiation and propagation (direct initiation, propagation in thing channels, exit from tubes to open space). In a number of theoretical and experimental studies have shown, that there is a correlation of detonation cell size and induction zone length of the internal structure of ideal 1D detonation wave, proposed by Zeldovich, Neumann, Doering.

Problem statement

It is required to calculate the induction zone length of the ideal detonation wave in hydrogen-air mixture at ambient conditions – P = 1 atm, T = 300K (variable stoichiometric ratio □ = 0.5 - 4) and evaluate its correlation with detonation cell size of the same fuel-air mixture.

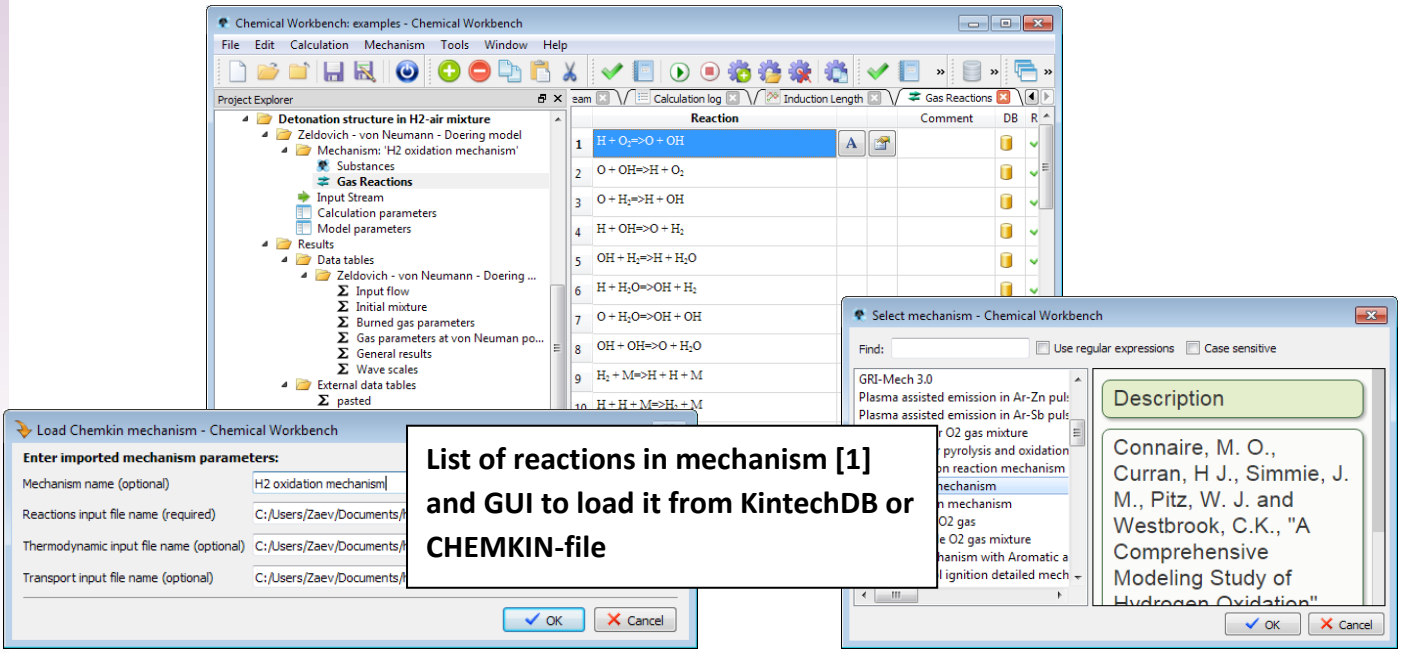
Problem setup in Chemical Workbench

To calculate the induction zone length of the ideal detonation wave, we use the Zeldovich-Neumann-Doering detonation reactor model (**ZND**), available in Chemical Workbench. This model requires information about initial composition of the mixture, chemical kinetic mechanism of fuel-air self-ignition and combustion (specific heat, enthalpy of formation, standard state entropy) and initial conditions.



List of available detonation reactor models in Chemical Workbench

The chemical kinetic mechanism of hydrogen ignition and combustion in air can be loaded from KintechDB database or imported from text file in CHEMKIN format. Loaded mechanism consists of list of species with coefficients to approximate temperature dependence of thermodynamic properties and interaction potentials, and list of reactions with related coefficients to approximate temperature dependence of reaction rate constant. Any of these properties can be visualized.

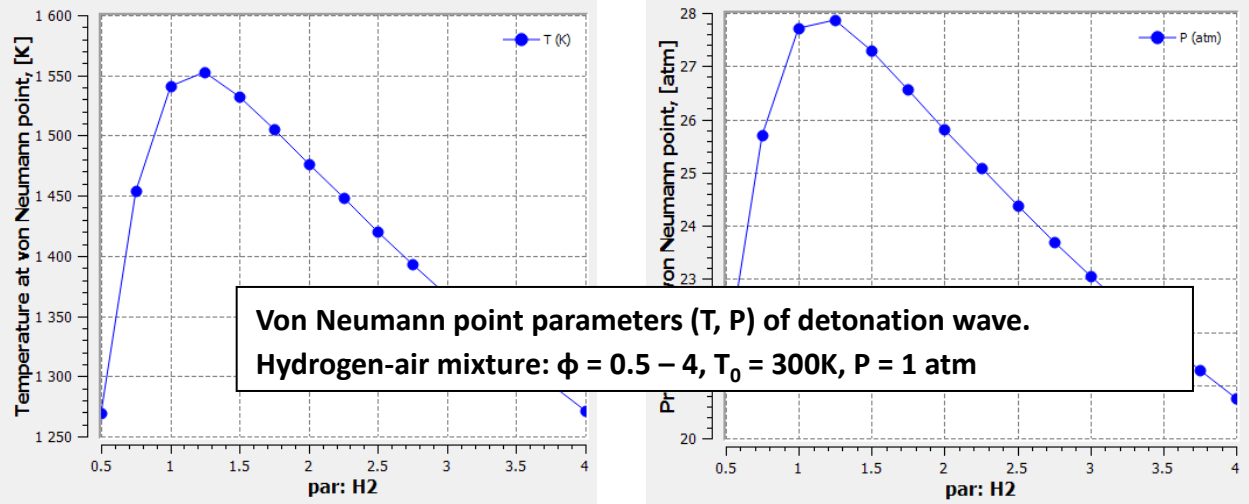


List of reactions in mechanism [1] and GUI to load it from KintechDB or CHEMKIN-file

The **initial mixture** is set in input stream of the reactor with composition xH2 + O2 + 3.76N2 (in moles), where x = 1 – 4 (φ = 0.5 – 4). **Initial temperature** 300K, **reactor pressure** 1 atm

Results

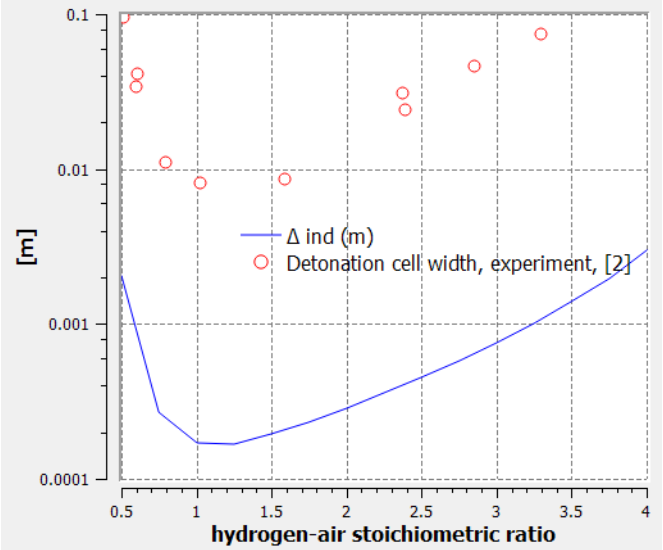
According to ZND model of ideal detonation wave, the reactive mixture is compressed in a viscous layer of leading shock wave, which propagates with the Chapman-Jouget speed DCJ. This compression takes place at the distance of order of mean free path of molecular motion and no chemical reactions happen – mixture composition is frozen. Parameters of the reactive mixture just after compression behind leading chock front – von Neumann point – are computed and can be used in further outside of the Chemical Workbench



Von Neumann point parameters (T, P) of detonation wave.
Hydrogen-air mixture: ϕ = 0.5 – 4, T_0 = 300K, P = 1 atm

After heating in leading shock wave, initial mixture starts to react and after some time/distance, called ignition delay time/induction length, strong heat release with acceleration of combustion products starts. The induction zone length depends strongly on mixture stoichiometric ratio and is minimum at stoichiometric conditions. It is plotted as function of mixture stoichiometric ratio. On the same plot external experimental data [2] are plotted and saved in the project for further use and reference.

As it is seen, the linear correlation of induction zone length and detonation cell size can be derived (their ratio is approximately 13000 and turns to be the save in a wide range of stoichiometric ratios).



Plot of computed and imported experimental data in Chemical Workbench

Next steps

1. Repeat the simulation with a different chemical kinetic mechanism. Compare predictions.
2. Compute induction zone length for different fuel/initial conditions and compare with available experimental data on detonation cell size.

References

1. Connaire, M. O., Curran, H J., Simmie, J. M., Pitz, W. J. and Westbrook, C.K., "A Comprehensive Modeling Study of Hydrogen Oxidation", International Journal of Chemical Kinetics, 36:603-622, 2004
2. G. Ciccarelli, T. Ginsberg, J. Boccio, C. Economos, K. Sato, and M. Kinoshita. Detonation cell size measurements and predictions in hydrogen-air-steam mixtures at elevated temperatures.
3. Combust. Flame, 99(2):212-220, 1994