# Calculation of hydrogen-air mixtures detonation parameters using EDL Shock & Detonation Toolbox

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**Abstract**

The aim of this report was to calculate detonation cell size using ZND in SD Toolbox for Cantera 2.1 and detonation parameters as a function of variable initial temperature.

## 1 Detonation theory

The one-dimensional detonation model developed independently by Zeldovich, von Neumann and Doring (called ZND for short) during World War II assumes that a detonation wave consist of a planar shock wave, which raises the density above the ignition value, followed by a reaction zone in which reaction proceeds. Experiments data confirms the model only qualitatively, because one-dimensional detonation waves are unstable.[1]. The model is simple to implement computationally.

It was proposed by Schelkin and Torshin in 1963 that detonation cell size can be related to reaction zone length $\Delta$ calculated using the ZND model [2] via simple equation: $\lambda = A * \Delta$ (where $\Delta = (V_{CJ} - u) * t_{ind}$, $V_{CJ}$ is C-J speed and $u$ is the particle velocity behind the shock wave). However experiments prove that constant $A$ ratio cannot be accurate. Instead, it was proposed that $A$ should be a function of initial conditions. Shepherd in 1986 proposed, that $A = f(\Phi)$, because large variations of this parameter with equivalence ratio are observed [3].

## 2 Part 1 - ZND calculations

### 2.1 Model

The computation was made in Matlab for hydrogen − air mixture (file: $ZNDCJ.m$) with equivalence ratio ranging from 0.4875 to 3.57 in points taken from experiments performed by Guirao et al.[4]. (Not all points were tested). The initial conditions were: pressure = 101300 Pa , temperature= 293 K.Then knowing that cell size is proportional to reaction zone lenght , and that the constant of proportionality $A$ was determined to be equal to 51 by Ciccarelili et al.[2]. Cell size can be calculated based on induction zone length, which is a output data for ZND program in SD Toolbox.

### 2.2 Results

Figure 1 shows the output data, and Figure 2 compares the acquired cell size with experimental data taken from work of Guirao et al.[4] [5]. The error was ranging from 7.35% to 68.88% with mean error for all points of 46%.

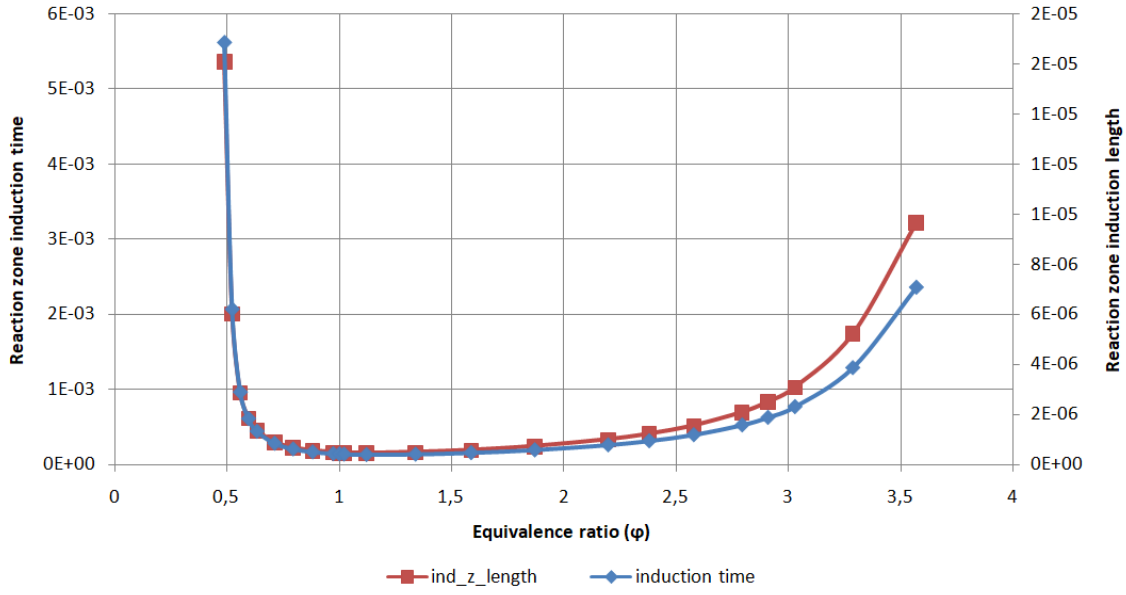


Figure 1: Induction time and ind. length as a function of equivalence ratio

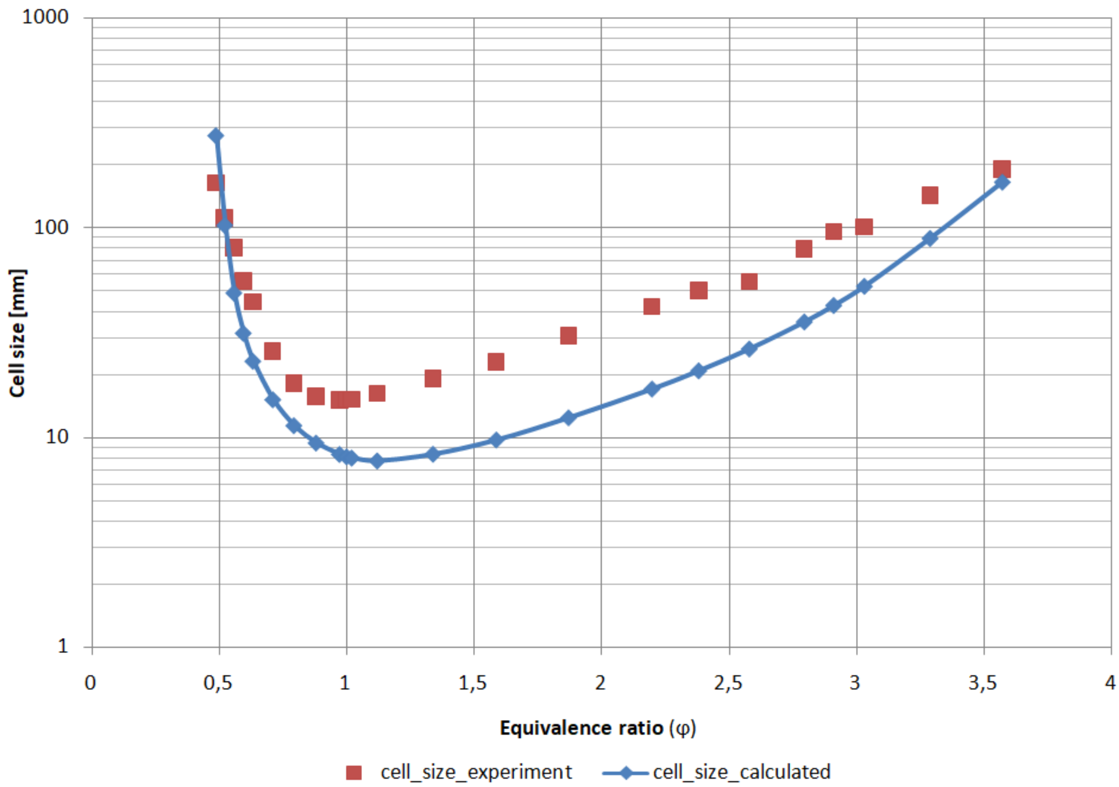


Figure 2: Calculated detonation cell size as a function of equivalence ratio

Plotting the A factor, which was calculated basing on actual cell size from experiment ([4]) and computed induction lengths as a function of equivalence ratio yields Figure 3. As can be observed the A factor varies to the greatest extent below $\Phi = 1.12$ and above $\Phi = 2.38$. Between those points the average A factor is equal to 119.1, which is two times higher than the value obtained in experiment by Ciccarelili et al.[2].

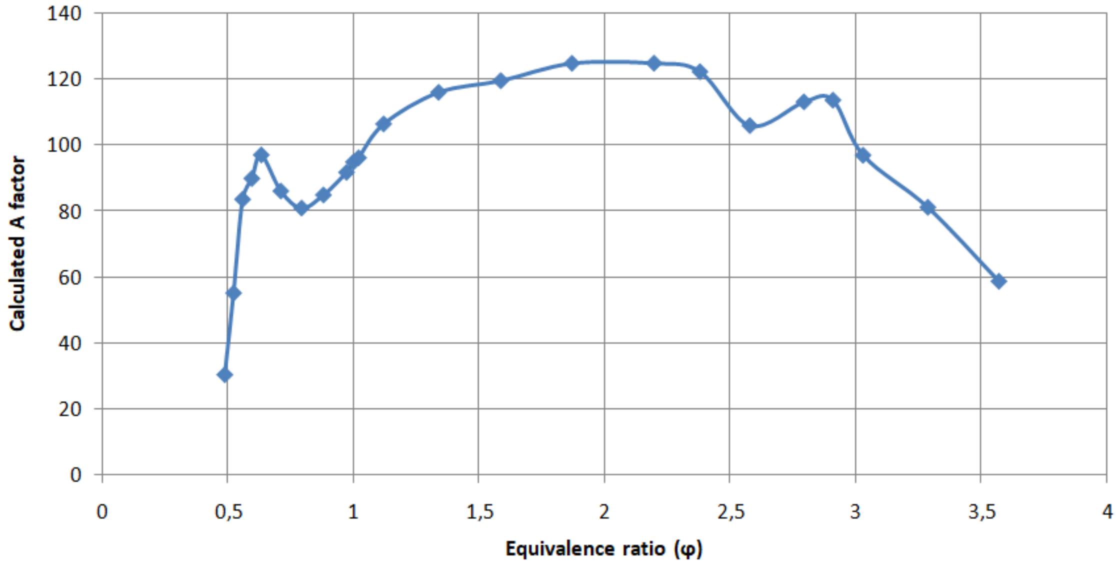


Figure 3: Calculated factor of proportionality $A$ as a function of equivalence ratio

# 3 Part 2 - Detonation parameters as a function of initial temperature

## 3.1 Model

The second task was to determine detonation parameters with variable initial temperature. This was done using SD Toolbox in Matlab, using modified example code (file: $Temperature\_Series.m$) The temperature was ranging from $300K$ to $1000K$ with a step of $50K$. Pressure was set to $100000Pa$. The equivalence ratio was constant and equal to 1.

## 3.2 Results

Results are shown on Figures 4 to 8.

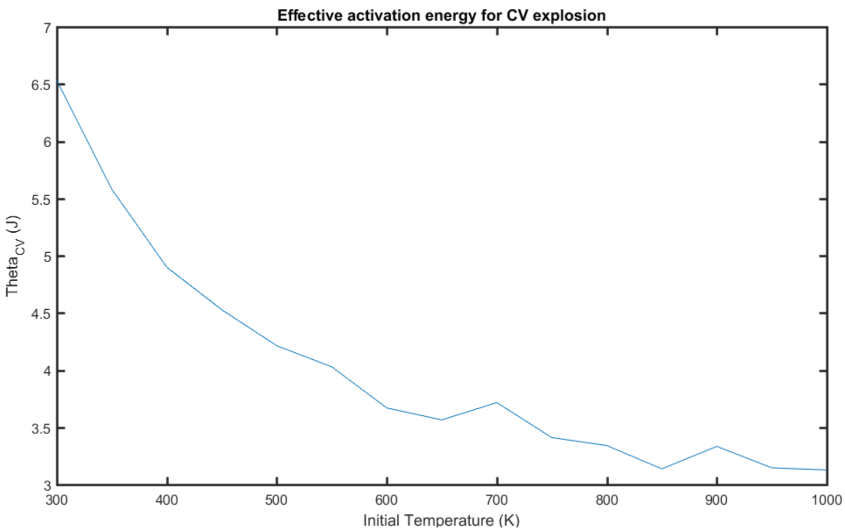


Figure 4: Calculated effective activation energy for CV explosion as a function of temperature

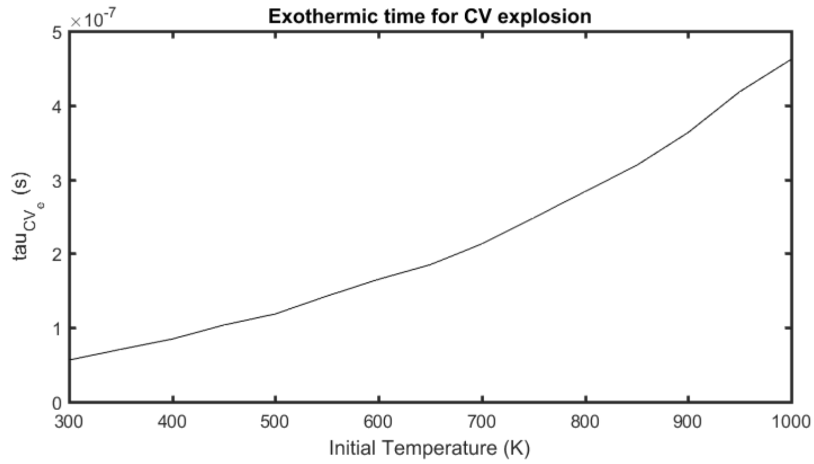


Figure 5: Calculated exothermic time as a function of temperature

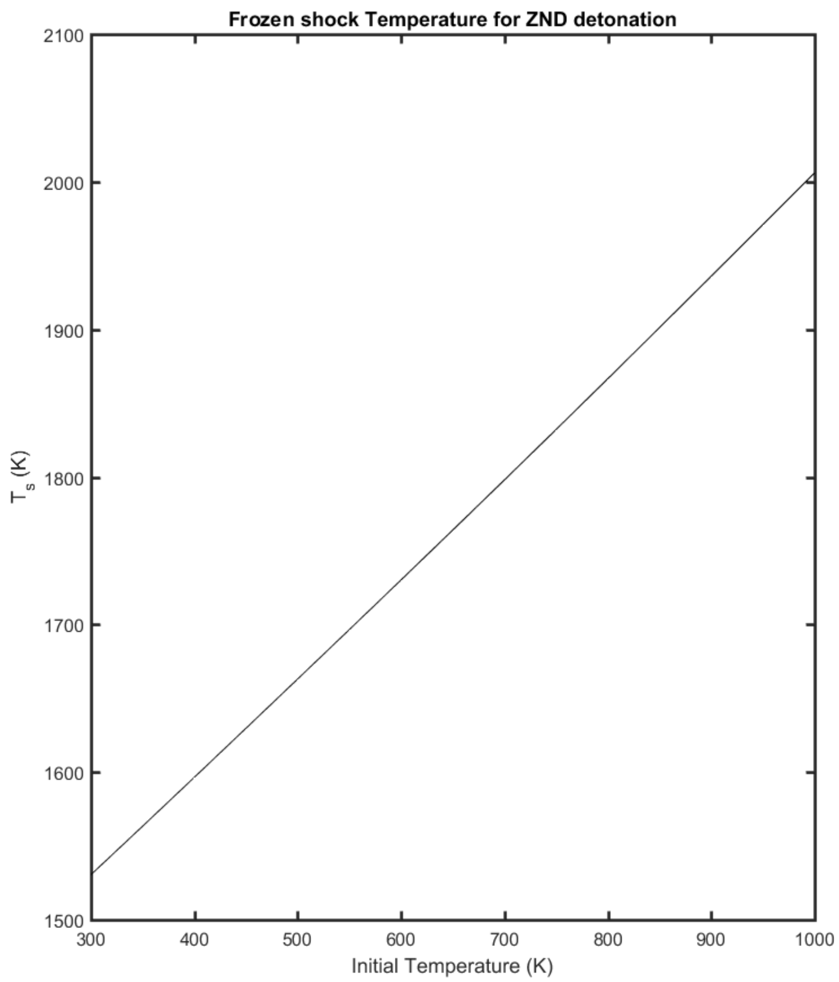


Figure 6: Calculated frozen shock temperature as a function of temperature

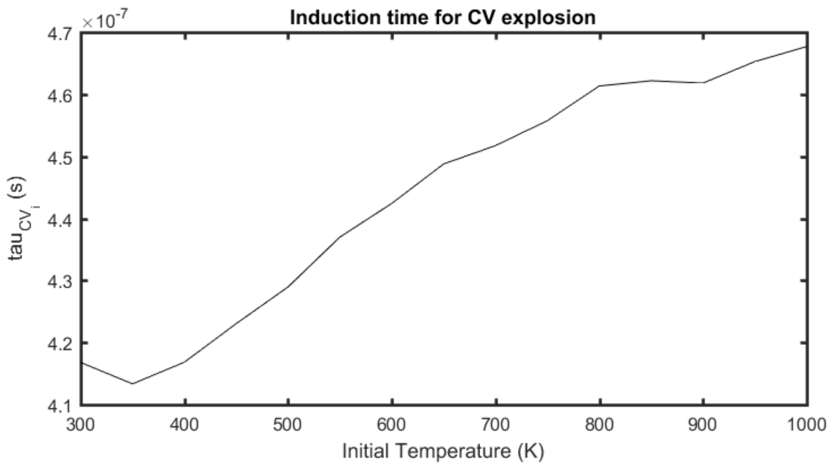


Figure 7: Calculated as a function of temperature

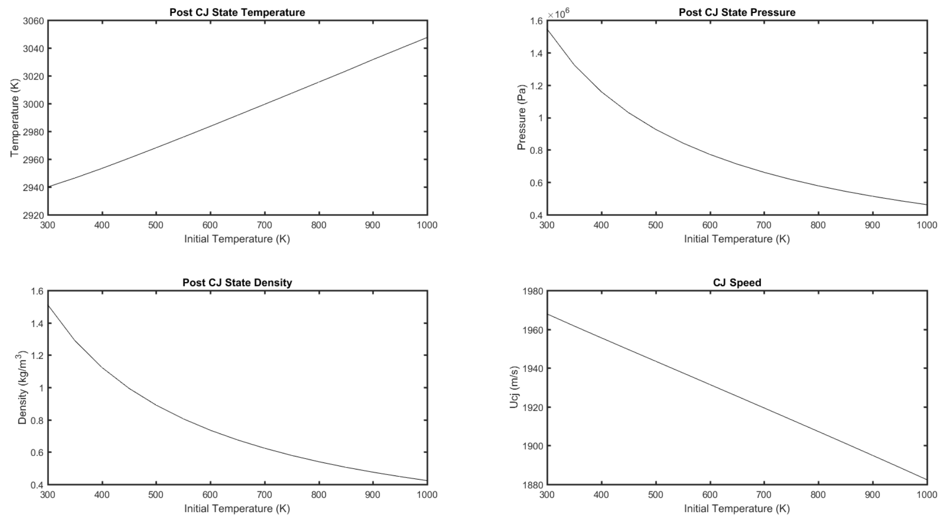


Figure 8: Calculated induction time as a function of temperature

# 4 Conclusions

Calculations from the first part of the report prove that using constant $A$ factor, independent from $\Phi$ will not accurately predict real cell sizes.

In the second part of the report we can see that effective activation energy is dropping non-linearly with rising temperature and exothermic time is rising non-linearly. Frozen shock Temperature is linearly related to initial temperature by equation $T_S = 0.679 * T_1 + 1324$. Induction time for CV explosion and post CJ state temperature rise with the rise of initial temperature. Rise of post CJ state temperature is linear and governed by equation: $T_2 = 0.155 * T_1 + 2891$. Post CJ pressure and density declines with the rise of initial temperature. The drop of CJ speed with rising temperature is linear and can be described as $V_{CJ} = -0.121 * T_1 + 2004$.

# References

[1] C.M. Guirao, R. Knystautas, and J. Lee. A summary of hydrogen-air detonation experiments. page 1, 1987.

[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. *Combust. Flame*, 99(2):212–220, 1994.

[3] Rémy Mével, Fabien Lafosse, Laurent Catoire, Nabiha Chaumeix, Gabrielle Dupré, and Claude-Etienne Paillard. Induction delay times and detonation cell size prediction of hydrogen-nitrous oxide-diluent mixtures. *Combustion Science and Technology*, 180:10-11:1858–1875, 2008.

[4] C.M. Guirao, R. Knystautas, J. Lee, W. Benedick, and M. Berman. Hydrogen-air detonations. *19th Symp. Int. Combust. Proc.*, pages 583–590, 1982.

[5] Caltech. Detonation database – Cell width - H2 fuel, 2002.