

Chapman-Jouguet conditions in ethane-air mixture

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1 Introduction

Estimating activation energy of explosive mixtures is one of the most difficult cases modern computer fluid dynamics and thermodynamics applied methods. The insufficient computational power limits complexity of differential equations, both in quality and quantity, therefore there is a demand in simplifying the math while staying accurate with an output.

This report presents study of the CJ conditions in various starting temperatures and pressures.

2 Model

Numerical model uses `adiabaticTemp`, `cvCJInd`, `explosionInd` and finally, `activationEnergy` functions to calculate minimal energy needed to activate detonation. Overlooking the reaching to the final formula, the equation for the activation energy is calculated from:

$$E_a \approx RT_0 \left(-\frac{T_0}{\tau_i} \frac{(\tau_i' - \tau_i)}{T'} \right) + (n + 1)$$

Where:

R -> universal gas constant [J/mol/K]

T0 -> 0,9 of starting adiabatic temperature [K]

i -> Chapman - Jouguet induction time in constant volume for T0 [s]

T' -> slightly larger temperature (T0 + 30) [K]

i' -> Chapman - Jouguet induction time in constant volume for T' [s]

n -> effective reaction order, for ethane it equals 3

After calculating approximate activation energy for a few points in explosibility range

Although the output is approximately correct for only narrow range of explosibility around stoichiometric values, it can help in developing explosion preventing systems.

3 Results

- a) Activation energy at 300 K and 1 atmosphere pressure
- b) Activation energy at 300 K and 2 atmosphere pressure
- c) Activation energy at 400 K and 1 atmosphere pressure
- d) Activation energy at 400 K and 2 atmosphere pressure

4 Summary

The results for higher temperatures and/or pressures should be significantly lesser than corresponded at lower pressure/temperature. However, the outcome seems to be at the safe side of the margin of aberration (values lower than experimental ones), which makes an output of a program a good initial approximation for the further research at explosion safety.

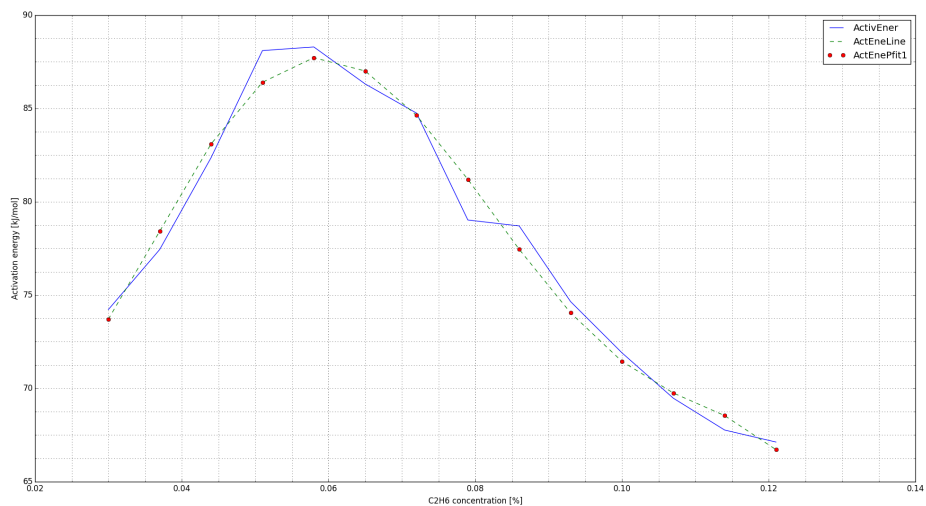


Figure 1: Activation energy at 300 K and 1 atmosphere pressure

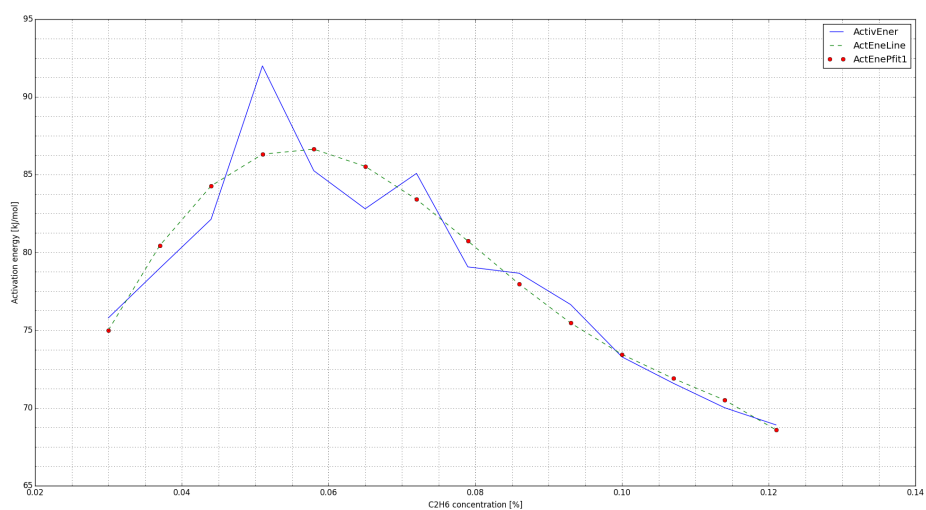


Figure 2: Activation energy at 300 K and 2 atmosphere pressure

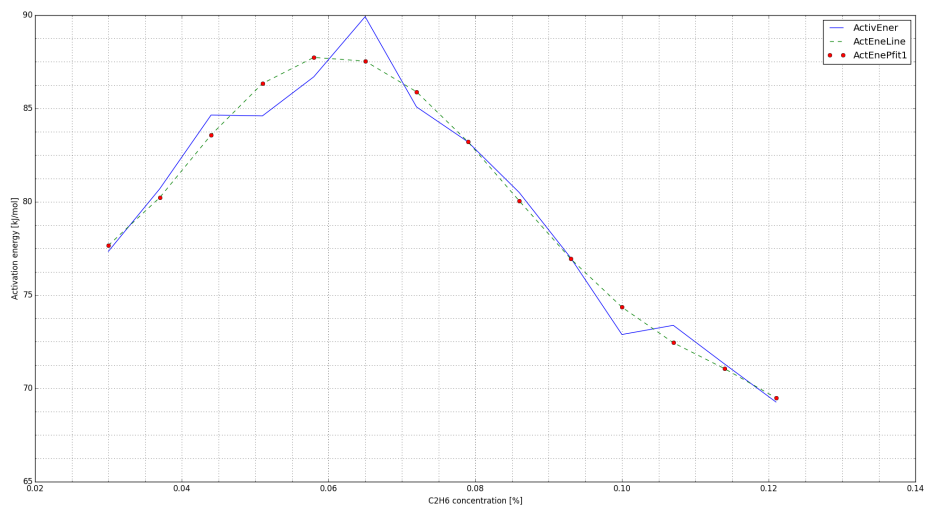


Figure 3: Activation energy at 400 K and 1 atmosphere pressure

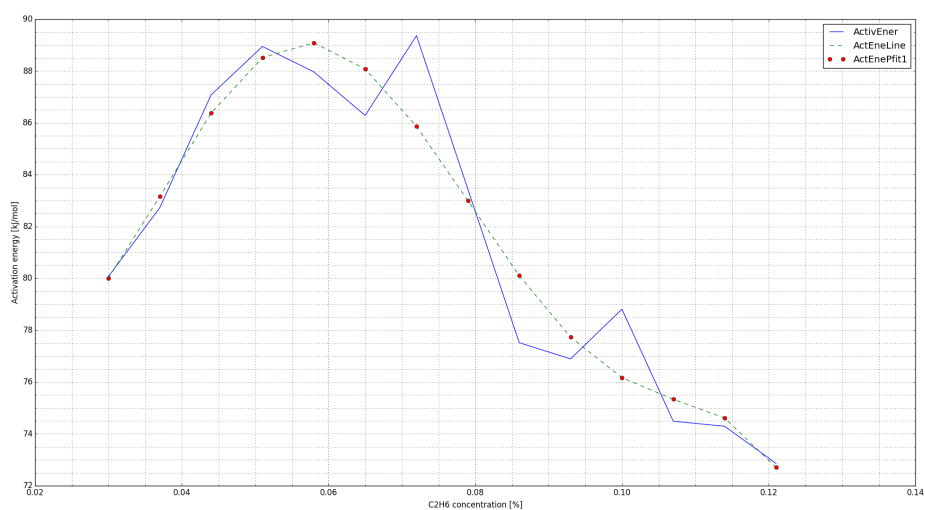


Figure 4: Activation energy at 400 K and 2 atmosphere pressure