Warsaw University of Technology
Faculty of Power and Aeronautical Engineering
Division of Aircraft Engines

Computer Methods in Combustion

Simulation of detonation of kerosene-air mixture using SD Toolbox package for Cantera

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1 Introduction

The purpose of this work is to evaluate model of kerosene surrogate-air mixture detonation in conditions described in previous project about combustion in turbine engine chamber. It is done by comparison of shock wave speed and level of compression with experimental data for stoichiometric air to fuel ratio to verify the model for different combustion mechanisms, and then parameters behind shock wave are computed for $\lambda = 1{,}5$, like in previous projects. Initial temperature and pressure are $T_0 = 800$ K and $p_0 = 1{,}4$ MPa.

2 Literature survey

Numerical code used for computation is variation of example demo_CJstate.py, which is available on page of SD Toolbox package ([1]). Like in previous project, combustion mechanisms are taken from [2]. Experimental study of kerosene-oxidizer mixtures detonation, including combustion of kerosene in air, can be found in publication [3] and those results are used for validation of numerical calculations.

3 Model description

Firstly, it was assumed that initial pressure and temperature doesn't affect significantly shock wave speed and level of compression. For Dagaut's mechanisms, the kerosene surrogate has a mole composition of 74% $NC_{10}H_{22}$ (n-decane), 15% PhC_3H_7 and 11% CYC_9H_{18}. In JetSurf mechanism this surrogate is made up entirely of n-decane. Stoichiometric number of moles of O_2 and N_2 are respectively 13,6675 and 51,3898 for the first surrogate, 15,5 and 58,28 for the second one. Program calculates results using 2 functions: CJspeed and PostShock_eq, based on the Chapman-Jouguet model of detonation.

4 Results

Comparison of calculated results with experimental data for stoichiometric conditions is placed in Table 1; chem_pecs is the name of Dagaut's mechanism derived to be valid under high pressure.

Case	Experiment	Dagaut_Ori	chem_pecs	JetSurf
Shock wave speed $\left(\frac{\mathrm{m}}{\mathrm{s}}\right)$	1843	1842,17	1854,73	1834,47
Level of compression	≈ 7	7,61	7,69	7,5

Table 1: Comparison of data for stoichiometric condition

As it is clearly visible, the detonation speed predicted from applied model agrees very well with experiment. Level of compression is a bit overrated, but there is agreement in terms of order of magnitude. It is also difficult to calculate experimental value precisely from plot with high amplitude of oscillations.
After validation of the model, it is possible to compute shock wave speed and parameters behind it for $\lambda = 1{,}5$. Results are presented in Table 2.

Case	Dagaut_Ori	chem_pecs	JetSurf
Shock wave speed, $\lambda = 1{,}5$ $\left(\frac{\mathrm{m}}{\mathrm{s}}\right)$	1702,55	1718,43	1685,84
Level of compression, $\lambda = 1{,}5$	6,39	6,48	6,2
Temperature, $\lambda = 1{,}5$ (K)	2861,11	2902,8	2808,48
Temperature, stoichiometric (K)	3177,32	3215,49	3171,67

Table 2: Calculated results for $\lambda = 1{,}5$

5 Conclusions

The first noticeable result is that temperature in detonation process in comparison with deflagration is about 800 K higher for case $\lambda = 1{,}5$. The decrease in exhaust fumes temperature caused by increased air-fuel equivalence ratio is also significantly lower for detonation. But due to problems with causing detonation process and the fact that it is connected with sudden pressure jump, deflagration is the dominating mechanism in industrial combustion.
Interesting conclusion is as well that JetSurf and Dagaut's high pressure mechanism changed places in comparison with the previous projects and chem_pecs predicts highest temperature behind shock wave. It is likely the result of higher number of O_2 and N_2 molecules in model based on JetSurf mechanism.

References

[1] `http://shepherd.caltech.edu/EDL/public/cantera/html/SD_Toolbox/`

[2] `http://www.cerfacs.fr/cantera/mechanisms/kero.php`

[3] Kindracki, J.: Study of detonation initiation in kerosene–oxidizer mixtures in short tubes. Shock Waves 24, 603-618, Springer International Publishing (2014)