Politechnika Warszawska

Wydział Mechaniczny Energetyki i Lotnictwa

Metody Komputerowe w Spalaniu

Symulation of combusting a fuel and air mixture in variable volume with spontaneous ignition

Author:
Mateusz Skrobek

Supervisor:
Dr. Mateusz Żbikowski

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1 Introduction

Calculation post-shock state and CJ speed in pipe for a specified mixture for a CJ detonation using the algorithm based on minumizing the shock speed. In my studies I focused on three types of inflammable compounds – mixtures of air and methane, ethane and propane. The purpose of my examination was just to examine and calculate post-shock parameters for all these compounds.

2 Model description

2.1 Software

Software used for conducting the study was an open-source chemical kinetics software – Cantera and special Shock and Detonation library - SBToolbox. It is written in C++ and can be used from C++, Python, Matlab and Fortran. I used Python.

2.2 Mathematical model

To calculate the state I use algorithm based on minumizing the shock speed which is defined in library SDToolbox. I could also use algorithm based on the equilibrium sound speed which is faster, however I decided to chose more robust method (it works with large mechanisms).

2.3 Order of activities

At first I created table with temperature values. Next I created three for loops which calculates post-shock parameters for various hydrocarbons and various temperatures. I assume atmospheric pressure in every case.
I also use file operations - I save all results in files.

3 Results

I calculated post-shock parameters for every hydrocarbon and saved results - CJ speed, CJ state and sound speeds. I also have a final composition of exhaust for one case (CH_4, 300K)

3.1 CH_4

CJ state for CH_4					
Parameter	300K	450K	600K	750K	900K
CJ speed	1803 m/s	1791 m/s	1780 m/s	1770 m/s	1760 m/s
CJ Pressure	17,0 atm	11,4 atm	8,58 atm	6,89 atm	5,77 atm
CJ Temperature	2778 K	2806 K	2838 K	2873 K	2909 K
Frozen sound speed	998 m/s	1003 m/s	1009 m/s	1016 m/s	1024 m/s
Equilibrium sound speed	1032 m/s	1040 m/s	1049 m/s	1058 m/s	1068 m/s

3.2 $C2H_6$

CJ state for $C2H_6$					
Parameter	300K	450K	600K	750K	900K
CJ speed	1803 m/s	1791 m/s	1780 m/s	1771 m/s	1763 m/s
CJ Pressure	17,8 atm	11,9 atm	8,97 atm	7,21 atm	6,04 atm
CJ Temperature	2813 K	2839 K	2869 K	2903 K	2938 K
Frozen sound speed	996 m/s	1001 m/s	1007 m/s	1014 m/s	1022 m/s
Equilibrium sound speed	1031 m/s	1039 m/s	1047 m/s	1057 m/s	1067 m/s

3.3 $C3H_8$

CJ state for $C3H_8$					
Parameter	300K	450K	600K	750K	900K
CJ speed	1800 m/s	1788 m/s	1778 m/s	1770 m/s	1762 m/s
CJ Pressure	18,1 atm	12,1 atm	9,11 atm	7,33 atm	6,14 atm
CJ Temperature	2820 K	2846 K	2877 K	2911 K	2946 K
Frozen sound speed	994 m/s	999 m/s	1005 m/s	1012 m/s	1020 m/s
Equilibrium sound speed	1029 m/s	1037 m/s	1046 m/s	1055 m/s	1065 m/s

gri30:

temperature	2778.04	K
pressure	1.72679e+06	Pa
density	2.02409	kg/m^3
mean mol. weight	27.0747	amu

	1 kg	1 kmol	
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enthalpy	8.7096e+05	2.358e+07	J
internal energy	17844	4.831e+05	J
entropy	9462.7	2.562e+05	J/K
Gibbs function	-2.5417e+07	-6.882e+08	J
heat capacity c_p	1547.9	4.191e+04	J/K
heat capacity c_v	1240.8	3.359e+04	J/K

	X	Y	Chem. Pot. / RT
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H2	0.00843033	0.000627692	-22.5172
H	0.00168351	6.26739e-05	-11.2586
O	0.00119339	0.000705217	-15.8874
O2	0.00979597	0.0115776	-31.7749
OH	0.00947959	0.00595474	-27.146
H2O	0.172254	0.114616	-38.4047
HO2	7.36362e-06	8.977e-06	-43.0335
H2O2	8.69925e-07	1.09291e-06	-54.2921
C	7.83613e-14	3.47631e-14	-18.682
CH	1.9807e-14	9.52427e-15	-29.9406
CH2	4.69851e-14	2.43421e-14	-41.1992
CH3	1.05707e-13	5.86999e-14	-52.4579
CH4	3.15105e-14	1.86712e-14	-63.7165
CO	0.0235503	0.0243642	-34.5694
CO2	0.0695851	0.11311	-50.4569
HCO	6.68532e-08	7.16526e-08	-45.8281
CH2O	1.36887e-09	1.51811e-09	-57.0867
CH2OH	5.84395e-14	6.69861e-14	-68.3453
N	6.03521e-07	3.12224e-07	-12.8072
NH	1.6641e-07	9.22856e-08	-24.0658
NH2	6.80856e-08	4.02926e-08	-35.3244
NH3	9.17583e-08	5.7718e-08	-46.5831
NNH	6.80936e-08	7.29897e-08	-36.873
NO	0.0072748	0.00806247	-28.6946
NO2	4.47198e-06	7.59884e-06	-44.5821
N2O	1.59114e-06	2.58658e-06	-41.5019
HNO	9.9345e-07	1.138e-06	-39.9533
CN	4.61687e-11	4.43664e-11	-31.4892
HCN	3.1497e-09	3.14401e-09	-42.7478
H2CN	1.90202e-14	1.96939e-14	-54.0065
HCNO	1.62683e-13	2.58524e-13	-58.6353
HOCN	2.28053e-10	3.62406e-10	-58.6353
HNCO	2.65668e-08	4.2218e-08	-58.6353
NCO	2.54583e-09	3.95086e-09	-47.3767
N2	0.696737	0.720896	-25.6144
[+18 minor]	1.386[illegible]3e-14	1.4229e-14	

4 Analysis and summary

Making use of tables I can conclude that higher initial temperature gives lower CJ speed and lower CJ pressure, but other parameters are growing along with temperature growth. The differences are rather small and for all hydrocarbons CJ speed is about 1750 - 1800 m/s, CJ temperature is about 2800 - 3000 K and sounds speed is around 1000 m/s. Only pressure is significantly changing.
Another conclusion can be that differences in post-shock states for different hydrocarbons are almost invisible, the disparity is just about few percent.
Final conclusion is about post-shock exhaust products. As we can see tens different compounds were created during process of shock-wave.

5 Bibliography

`shepherd.caltech.edu/EDL/public/cantera/html/SD_Toolbox/Cantera_legacy.html`