Chapman Jouguet Speed and State

Mateusz Sienicki
Lotnictwo i Kosmonautyka
Metody Komputerowe w Spalaniu

1 Introduction

Shock and detonation play an important role in nowadays studies. We cannot imagine combustion processes without them. It is no wonder that more and more projects focus on them, because detonation or deflagration can be used for example in modern millitary matters and prospective communication. In this project I'm going to analise detonation of a mixture of methane and air. Methane is the major constituent of natural gas as well as the smallest hydrocarbon fuel. Methane has been in use on specific combustion devices like internal combustion engines and industrial gas turbines operated at high pressure and temperature. Methane has a boiling point of 164 C at a pressure of one atmosphere. As a gas it is flammable over a range of concentrations (5.4 to 17%) in air at standard pressure.

Combustion of stoichiometric methane mixture in air:

$CH_4 + 2(o_2 + 3.76N_2) \longleftrightarrow CO_2 + 2H_2) + 7.52N_2$

The aim of this simulation is measurement the Chapman Jouguet speed for a mixture of air and methane. We will consider how it changes depending on initial external conditions and also check the state of a gas after detonation.

2 Description of phenomenon

The Chapman Jouguet condition holds approximately in detonation waves in high explosives. It states that the detonation propagates at a velocity at which the reacting gases just reach sonic velocity (in the frame of the leading shock wave) as the reaction ceases.

David Chapman and Emile Jouguet originally stated the condition for an infinitesimally thin detonation. A physical interpretation of the condition is usually based on the later modelling by Yakov Borisovich Zel'dovich, John von Neumann, and Werner Dring (the so-called ZND detonation model).

In more detail (in the ZND model) in the frame of the leading shock of the detonation wave, gases enter at supersonic velocity and are compressed through the shock to a high-density, subsonic flow. This sudden change in pressure initiates the chemical (or sometimes, as in steam explosions, physical) energy release. The energy release re-accelerates the flow back to the local speed of sound. It can be shown fairly simply, from the one-dimensional gas equations for steady flow, that the reaction must cease at the sonic ("CJ") plane, or there would be discontinuously large pressure gradients at that point. The sonic plane forms a so-called choke point that enables the lead shock, and reaction zone, to travel at a constant velocity, undisturbed by the expansion of gases in the rarefaction region beyond the CJ plane.

Let's focus now on CJ speed. There are two different definitions of that:

1. **Definition I**: The Chapman-Jouguet detonation velocity is the minimum wave speed for which there exists a solution to the jump conditions from reactants to equilibrium products traveling at supersonic velocity.

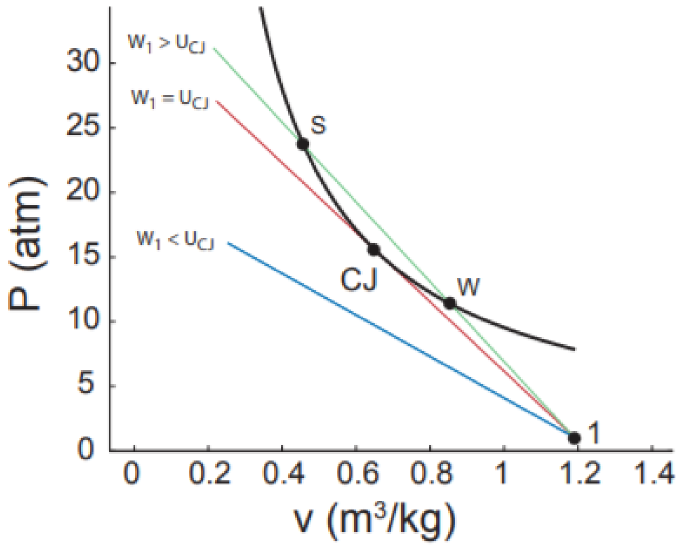

Figure 1: Hugoniot and three representative Rayleigh lines illustrating w1 = UCJ as the minimum wave speed and tangency of Rayleigh line and Hugoniot at the CJ point.

   From the geometry (Fig. 1), it is clear that the minimum wave speed condition occurs when the Rayleigh line is tangent to the Hugoniot.

2. **Definition II**: The Chapman-Jouguet detonation velocity occurs when the flow in the products is sonic relative to the wave. This is equivalent to the tangency of the Rayleigh line, Hugoniot, and equilibrium isentrope at the CJ point.

   The equilibrium isentrope and equilibrium sound speed appear in this formulation because the problem has been approached in a purely thermodynamic fashion with no consideration of time-dependence or detonation structure.

3 Simulation

The simulation was conducted using Cantera, which is a software tool for Python language. In addition I annexed SDToolbox that is a shock and detonation package for Cantera.

The chemical kinetic model utilized in the study includes GRI Mech 3.0. There are 325 elementary chemical reactions and associated rate coefficient expressions and thermochemical parameters for the 53 species in GRI Mech 3.0. It includes the detailed combustion reaction mechanism for hydrogen. What is more simulation uses this model with high temperatures correction.

3.1 Detailed CJ state analysis for common condition

Temperature was set to $300K$
Pressure : $1000kPa$
Mole composition: CH_4: 1, O_2: 1, N_2: 3,76

After calculations we achieved many information about the state of mixture after detonation, CJ speed and also equilibrium and frozen velocities of sound. All is shown below:

```
CJ State

  gri30:

       temperature          2159.78  K
          pressure      1.48382e+06  Pa
           density          1.87426  kg/m^3
  mean mol. weight          22.6825  amu

                          1 kg             1 kmol
                       -----------      ------------
          enthalpy      5.2362e+05        1.188e+07     J
   internal energy     -2.6806e+05        -6.08e+06     J
           entropy           10398        2.359e+05     J/K
    Gibbs function     -2.1934e+07       -4.975e+08     J
 heat capacity c_p          1702.6        3.862e+04     J/K
 heat capacity c_v          1336.1        3.031e+04     J/K
```

Figure 2: Major properties of gas after detonation

	X	Y	Chem. Pot. / RT
H2	0.166914	0.0148343	-18.8344
H	0.000476965	2.11948e-05	-9.41718
O	9.684e-08	6.83073e-08	-21.8132
O2	3.16002e-08	4.45792e-08	-43.6264
OH	4.81931e-05	3.61351e-05	-31.2304
H2O	0.128588	0.102129	-40.6475
HO2	8.76018e-11	1.27475e-10	-53.0436
H2O2	2.73082e-10	4.09513e-10	-62.4607
CH	3.88567e-14	2.23023e-14	-21.0934
CH2	5.36973e-12	3.32064e-12	-30.5105
CH2(S)	2.53739e-13	1.56912e-13	-30.5105
CH3	1.02973e-09	6.82544e-10	-39.9277
CH4	1.86757e-08	1.32088e-08	-49.3449
CO	0.128636	0.158851	-33.4894
CO2	0.019254	0.0373576	-55.3026
HCO	2.30278e-07	2.946e-07	-42.9066
CH2O	1.27511e-07	1.68794e-07	-52.3237
CH2OH	6.44426e-12	8.81704e-12	-61.7409
CH3O	3.23831e-13	4.43065e-13	-61.7409
CH3OH	2.67464e-11	3.77829e-11	-71.1581
C2H2	8.68285e-12	9.96728e-12	-42.1867
C2H4	6.2576e-14	7.7394e-14	-61.0211
HCCO	2.14639e-13	3.88251e-13	-54.5827
CH2CO	1.06434e-11	1.97254e-11	-63.9999
N	1.49589e-09	9.23731e-10	-12.5482
NH	7.89898e-09	5.22872e-09	-21.9653
NH2	1.083e-07	7.65019e-08	-31.3825
NH3	1.19756e-05	8.99159e-06	-40.7997
NNH	1.02495e-08	1.31139e-08	-34.5135
NO	3.76584e-06	4.98173e-06	-34.3614
NO2	7.57317e-12	1.53602e-11	-56.1746
N2O	6.78847e-10	1.31723e-09	-46.9095
HNO	1.70248e-09	2.32781e-09	-43.7785
CN	1.32607e-10	1.52105e-10	-24.2244
HCN	1.62447e-06	1.93552e-06	-33.6415
H2CN	9.95877e-12	1.23082e-11	-43.0587
HCNO	7.98517e-14	1.51466e-13	-55.4547
HOCN	1.21246e-09	2.29984e-09	-55.4547
HNCO	4.89201e-07	9.27936e-07	-55.4547
NCO	4.95397e-10	9.17675e-10	-46.0375
N2	0.556065	0.686754	-25.0963

Figure 3: List of almost all components of mixture methane air after detonation

```
For CH4:1 O2:1 N2:3.76 with P1 = 1.00 atm & T1 = 300.00 K using gri30_highT.cti
CJ Speed is 1738.49 m/s
The CJ State is 14.64 atm & 2159.78 K
The sound speeds are: af = 1004.44 m/s & ae = 1001.89 m/s
```

Figure 4: Conclusion. Index f means frozen and e means equilibrium. We can see here a huge rise of temperature and pressure. 2 different sound velocities are quite similar.

3.2 CJ speed and state depending on initial pressure

Next step is a comparizon between different initial pressures. I made 15 measurements increasing pressure of 1000 kPa. First pressure was set to 1000 kPa, which is close to one atmosphere. Temperature and mole composition were constant.

Let's look at the results:

Pressure [atm]	CJ speed [m/s]
1.0	1738.5
2.0	1738.9
3.0	1739.1
3.9	1739.3
4.9	1739.3
5.9	1739.4
6.9	1739.4
7.9	1739.5
8.9	1739.5
9.9	1739.5
10.9	1739.5
11.8	1739.5
12.8	1739.5
13.8	1739.6
14.8	1739.6

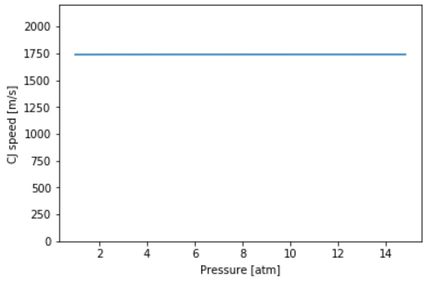

Figure 5: CJ speed remains constant for every pressure. Little change is caused probably by numerical mistake.

During calculations program saved also state of gas for every initial pressure. The most important parameters are pressure and temperature after detonation and so they are gathered together in a combined table:

Pressure [atm]	CJ state pressure [atm]	CJ state temperature [K]
1.0	14.5	2159.8
2.0	28.9	2160.9
3.0	43.4	2161.4
3.9	57.8	2161.7
4.9	72.3	2161.9
5.9	86.8	2162.1
6.9	101.2	2162.2
7.9	115.7	2162.4
8.9	130.1	2162.5
9.9	144.6	2162.5
10.9	159.1	2162.6
11.8	173.5	2162.7
12.8	188.0	2162.7
13.8	202.5	2162.8
14.8	216.9	2162.9

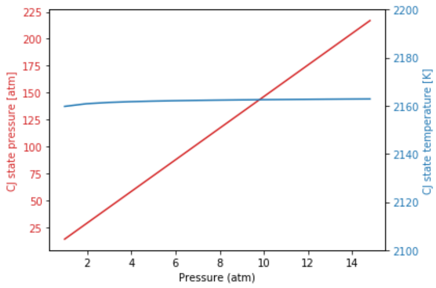

Figure 6: Temperature of gas is high and constant for every initial pressure. On the other side pressure rises enormously quick. For about 7 atm we have gas pressure about 100 atm. This kind of value is measured in a piston after work stroke in an engine.

3.3 CJ speed and state depending on initial temperature

Last calculations affect the influence of initial temperature on CJ speed and state. First value is set to 300 K and 15 times it is rised of 100 K. Pressure remains the same for every measurement and equals 1000 kPa. Mole composition is also just like earlier. Results may be interesting:

Temperature [K]	CJ speed [m/s]
300.0	1738.5
400.0	1748.4
500.0	1758.9
600.0	1770.2
700.0	1782.0
800.0	1794.0
900.0	1805.7
1000.0	1816.8
1100.0	1826.9
1200.0	1835.7
1300.0	1843.2
1400.0	1849.3
1500.0	1854.1
1600.0	1857.7
1700.0	1860.2

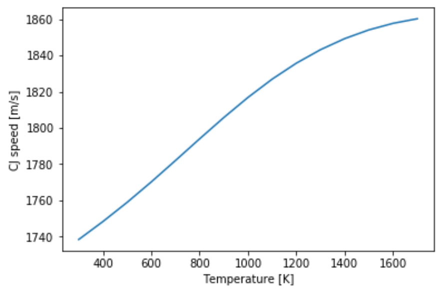

Figure 7: For every rise in temperature there's a significant rise in CJ speed. Generally in the range of 300 K to 1700 K CJ speed may be higher up to 130 m/s.

Like in 3.2 program also saved CJ state for every temperature:

Temperature [K]	CJ state pressure [atm]	CJ state temperature [K]
300.0	14.5	2159.8
400.0	11.1	2226.9
500.0	9.1	2296.0
600.0	7.8	2367.2
700.0	6.8	2439.8
800.0	6.1	2512.9
900.0	5.6	2585.2
1000.0	5.1	2655.9
1100.0	4.8	2723.1
1200.0	4.5	2786.3
1300.0	4.2	2845.2
1400.0	4.0	2899.6
1500.0	3.8	2949.6
1600.0	3.6	2995.9
1700.0	3.4	3038.7

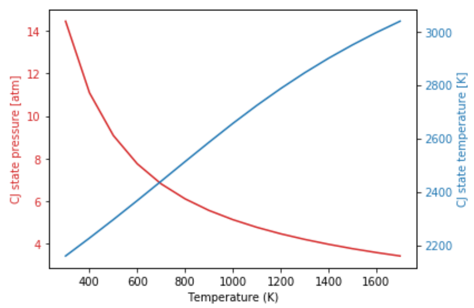

Figure 8: Now results are a bit different. CJ state pressure decreases, but CJ state temperature rises. For a temperature that occurs in nowadays turbine engines after combustor we're getting a value of about 3000 K of CJ state. It is such high that only very few materials can bear.

4 Observation and Conclusion

- CJ speed strictly depends on initial temperature but pressure doent's affect on it
- CJ state strictly depends on both pressure and temperature
- After detonation a lot of new compounds appear.
- Not all of methane discharged after combustion.
- CJ speed and state are important parameters in combustion issues.

5 Analised literature

1. Numerical Solution Methods for Shock and Detonation Jump Conditions by S. Browne, J. Ziegler, and J. E. Shepherd
2. pl.wikipedia.org