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Computer Methods in Combustion

Determination of the maximum impulse and combustion temperature for various types of fuels in liquid rocket engine

Warsaw 02.06.2020

Contents

1 Introduction

The project presents a comparison of two approaches on calculating the specific impulse and the temperature in the combustion chamber for a liquid rocket engine. Two programs were used, MATLAB with the Cantera program and NASA CEA, both are based on the same chemical equations. However, the most important difference between them the degree of simplyfication of reactions and the fact that the data for reactants to MATLAB must be entered and in most cases calculated manually by the user while the CEA uses its own library.

2 Models

2.1 Engine parameters

The calculations were performed for the Merlin 1D engine model from SpaceX. Parameters of this particular engine are presented in *Table 1.*

Properties	Merlin 1
Pressure at exit [atm]	1
Pressure combustion chamber [atm]	95,73
Oxidiser initial pressure [atm]	100
Temperature of reactants [K]	289
Subsonic area ratio [-]	8
Supersonic area ratio [-]	16

Table 1. Engine parameters

2.2 Oxidizer

One oxidizer, nitrous dioxide, was used in all calculations, its properties are summarized in *Table 2.*

Properties	Nitrous dioxide (N_2O)
State of matter	gas
Density $[kg/m^3]$	1,799
Molar mass $[g/mol]$	44,0129
Enthalpy of formation $[J/kg]$	1860000

Tabele 2. Oxidizer properties

2.3 Fuel

The analyzes were carried out for four different fuels, common in aerospace; their properties are summarized in *Table 3.*

Properties	Methane (CH_4)	Hydrogene (H_2)	Hydrazine (N_2H_4)	Kerosene ($RP-1$)
State of matter	liquid	liquid	liquid	liquid
Density $[kg/m^3]$	2.31	70,85	100,30	750,13
Molar mass $[g/mol]$	16,04	2,02	32,04	170,34
Enthalpy of formation $[J/kg]$	-4673750	0	-3046875	-131060
Temperature of reactants $[K]$	111	90	298	298

Table 3. Fuels properties

2.4 Cantera model

Cantera is one of chemical kinetics software which can be used to compute variety of reactions from thermodynamical point of view, including combustion. Any combustion calculation requires entering precalculated formulas for every reactant and product factor. Having given proportions, Cantera can further calculate reaction parameters, for instance, temperature or specific impulses. In this project, Cantera is operated using MATLAB and special toolbox. These things combined allow to write MATLAB code interpreted and ran in Python and to analyse results.

Masses and proportions of products of combustion were calculated using following chemical equations which depend on Oxidiser/Fuel ratio:

O/F	Chemical reaction for $C_{12}H_{26}$
$O/F \leq 3.1$	$a_1 * C_{12}H_{26} + a_2 * N_2O - - > a_3 * CO + a_4 * H_2 + a_5 * N_2 + a_6 * C_{12}H_{26}$
$3.1 < O/F \leq 6.2$	$a_1 * C_{12}H_{26} + a_2 * N_2O - - > a_3 * CO + a_4 * H_2 + a_5 * H_2O + a_6 * N_2$
$6.2 < O/F \leq 9.56$	$a_1 * C_{12}H_{26} + a_2 * N_2O - - > a_3 * CO_2 + a_4 * H_2O + a_5 * N_2 + a_6 * H_2$
$9.56 < O/F$	$a_1 * C_{12}H_{26} + a_2 * N_2O - - > a_3 * CO_2 + a_4 * H_2O + a_5 * N_2 + a_6 * N_2O$

O/F	Chemical reaction for CH_4
$O/F \leq 2.744$	$a_1 * CH_4 + a_2 * N_2O - - > a_3 * CO + a_4 * H_2 + a_5 * N_2 + a_6 * CH_4$
$2.744 < O/F \leq 8.231$	$a1 * CH_4 + a_2 * N_2O - > a_3 * CO + a_4 * H_2 + a_5 * H_2O + a_6 * N_2$
$8.231 < O/F \leq 10.975$	$a_1 * CH_4 + a_2 * N_2O - - > a_3 * CO_2 + a_4 * H_2O + a_5 * N_2 + a_6 * H_2$
$10.975 < O/F$	$a_1 * CH_4 + a_2 * N_2O - - > a_3 * CO_2 + a_4 * H_2O + a_5 * N_2 + a_6 * N_2O$

O/F	Chemical reaction for H_2
$O/F \leq 5.458$	$a_1 * H_2 + a_2 * N_2O - - > a3 * H_2O + a_4 * NH_3$
$5.458 < O/F \leq 21.835$	$a_1 * H_2 + a_2 * N_2O - - > a3 * H_2O + a_4 * NH_3 + a_5 * N_2$
$21.835 < O/F$	$a_1 * H_2 + a_2 * N_2O - - > a_3 * H_2O + a_5 * N_2 + a_6 * H_2 + a_4 * N_2O$

O/F	Chemical reaction for N_2H_4
$O/F \leq 2.75$	$a_1 * N_2H_4 + a_2 * N_2O - - > a_3 * H_2O + a_4 * NH_3 + a_5 * N_2$
$2.75 < O/F$	$a_1 * N_2H_4 + a_2 * N_2O - - > a_3 * H_2O + a_4 * N_2O + a_5 * N_2$

Table 4. Chemical reactions of fuel and oxidant in the combustion chamber

Based on above reactions and standard enthalpies of formation for adequate substances, the heat revealed during combustion process has been computed. Due to the fact that all products are defined in Cantera,the temperature in combustion chamber has been evaluated considering the fact that specific heat strongly depends on temperature. Also the phenomenon of fuel vaporization has been omitted what results in approximation that heat of vaporization for kerosene is close to zero.
As a result of above reactions and temperature the specific impulse could be computed based on following equation:

$$Isp = \sqrt{\frac{kR_{gas}T_c}{k-1}\left[1 - \left(\frac{p_e}{p_c}\right)^{\frac{k-1}{k}}\right]}$$

where:
k = ratio of specific heats, cp/cv
p_e = nozzle exit pressure
p_c = combustion chamber pressure
T_c = combustion chamber temperature
R_{gas} = exhaust flow specific gas constant

2.5 NASA CEA model

The NASA Computer program CEA (Chemical Equilibrium with Applications) calculates chemical equilibrium compositions and properties of complex mixtures. Applications include assigned thermodynamic states, theoretical rocket performance, Chapman-Jouguet detonation parameters, shock tube parameters, and combustion properties. Chemical equations used in the NASA CEA program are partly analogous to the equations used in the program created in Cantera. However, there is no need to enter them because the program is based on its own library with material properties.

3 Results

3.1 Cantera results

O/F	Methane		Hydrogene		Hydrazine		Kerosyne	
	T	Isp	T	Isp	T	Isp	T	Isp
[-]	[K]	[s]	[K]	[s]	[K]	[s]	[K]	[s]
1	1307,85	115,76	715,98	100,59	1311,55	145,38	1614,42	101,97
2	1380,36	136,80	1053,36	153,86	2515,22	180,77	1989,10	131,36
3	1466,36	147,10	1408,40	189,53	2866,85	187,31	2176,81	146,02
4	1944,20	163,19	1716,25	209,72	2403,94	181,87	2699,10	156,53
5	2418,52	175,24	1982,37	220,94	2072,08	176,12	3056,65	160,86
6	2777,05	182,06	2206,80	224,25	1833,25	170,99	3248,15	161,70
7	3040,62	185,80	2397,75	223,89	1653,70	166,46	3323,28	160,62
8	3213,47	187,25	2565,31	223,20	1513,77	162,45	3336,59	158,80
9	3303,53	186,94	2712,01	222,28	1401,91	158,90	3323,03	156,85
10	3327,42	185,36	2840,33	221,21	1311,07	155,78	3297,63	154,98
11	3317,65	183,31	2952,24	220,04	1236,10	153,02	3266,79	153,22
12	3290,53	181,12	3049,40	218,79	1174,04	150,62	3233,62	151,61
13	3255,57	178,97	3133,02	217,47	1121,55	148,48	3199,61	150,11
14	3216,81	176,90	3204,22	216,10	1077,32	146,60	3165,54	148,72
15	3176,58	174,94	3263,59	214,67	1040,30	144,99	3131,89	147,43

Table 5. Cantera Results

3.2 NASA CEA results

O/F	Methane		Hydrogene		Hydrazine		Kerosyne	
	T	Isp	T	Isp	T	Isp	T	Isp
[-]	[K]	[s]	[K]	[s]	[K]	[s]	[K]	[s]
1	764,30	166,56	469,79	249,39	1706,25	228,42	930,65	171,85
2	899,54	183,94	705,63	2530,10	2377,82	249,04	1059,09	184,69
3	974,91	191,04	996,29	264,66	2486,73	247,17	1219,56	191,51
4	1260,77	197,96	1248,79	271,31	2269,04	226,26	1730,37	206,26
5	1684,64	212,58	1466,87	276,32	2060,08	210,23	2150,57	223,10
6	2013,65	225,37	1657,04	279,51	1883,06	197,55	2441,19	233,44
7	2267,35	233,84	1823,95	281,29	1735,42	187,24	2606,40	240,03
8	2451,05	239,71	1970,52	282,29	1611,85	178,63	2657,41	243,90
9	2556,60	243,84	2098,71	282,80	1507,47	171,34	2647,81	245,04
10	2587,88	246,30	2210,11	282,98	1418,35	165,06	2611,22	240,76
11	2574,26	246,23	2306,36	282,91	1314,48	159,58	2560,29	234,50
12	2537,85	240,42	2389,11	282,66	1274,51	154,76	2500,12	228,31
13	2488,85	234,44	2459,84	282,26	1215,68	150,47	2433,39	222,42
14	2432,19	228,73	2519,74	281,81	1163,59	146,63	2362,19	216,88
15	2370,79	223,34	2569,64	281,26	1117,14	143,16	2288,61	211,71

Table 6. NASA CEA Results

4 Comparision

Comparison for each one of four cases looks similar. Specific impulse calculated in Cantera program is always lower than the one calculated in NASA CEA. The bigger difference occurs for RP-1, around 30 percents. The opposite is true for temperature calculations in the combustion chamber, where temperatures are higher in Cantera. The differences are around 25-30 percents for all substances burned except for methane for which the difference between the two calculation methods is about 15 percents. The percentage differences resulting from different calculation methods have been collected and presented in *Table 7*.

Methane		Hydrogene		Hydrazine		Kerosyne	
T [%]	Isp [%]	T [%]	Isp [%]	T [%]	Isp [%]	T [%]	Isp [%]
28,58	23,98	27,01	20,75	15,29	24,79	25,56	34,01

Table 7. Results comparasion

Charts 1-4 show the results of calculations performed in each software. It is noticeable that results seem to be similar in a qualitative way. For both calculation methods, the maximum temperature and maximum specific impulse appear for the same ratio of oxidant to fuel.

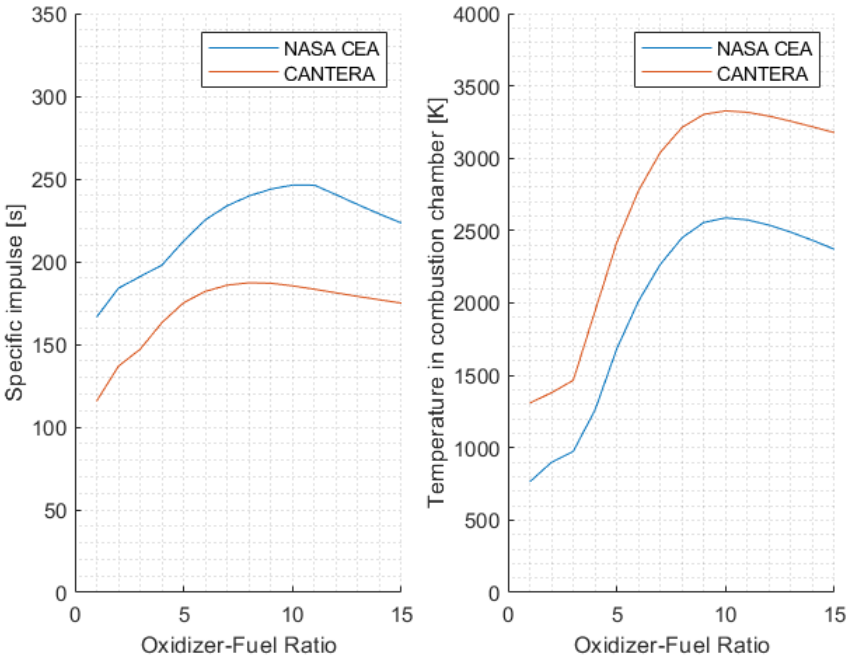

Chart.1 Comparasion of results from NASA CEA and Cantera CH_4

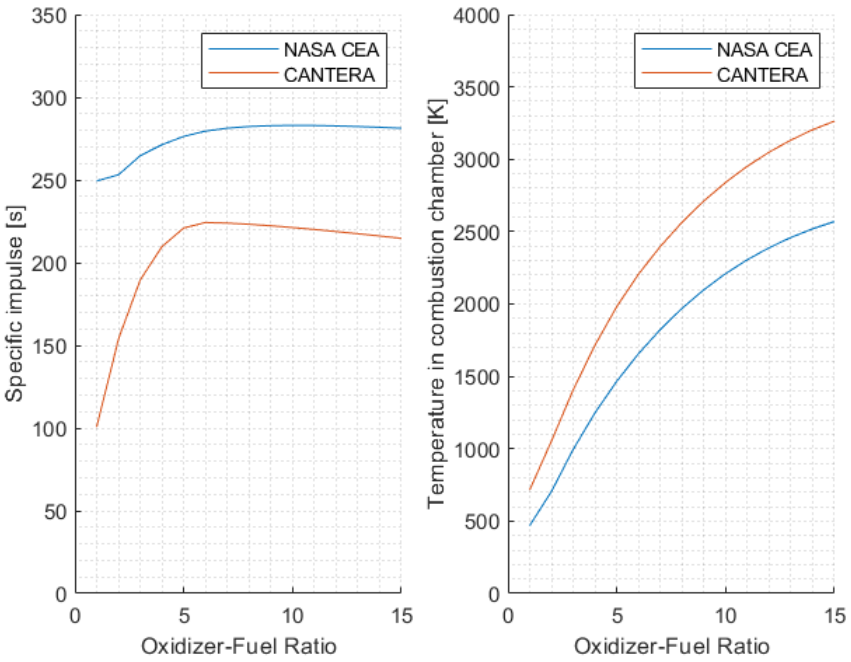

Chart.2 Comparasion of results from NASA CEA and Cantera H_2

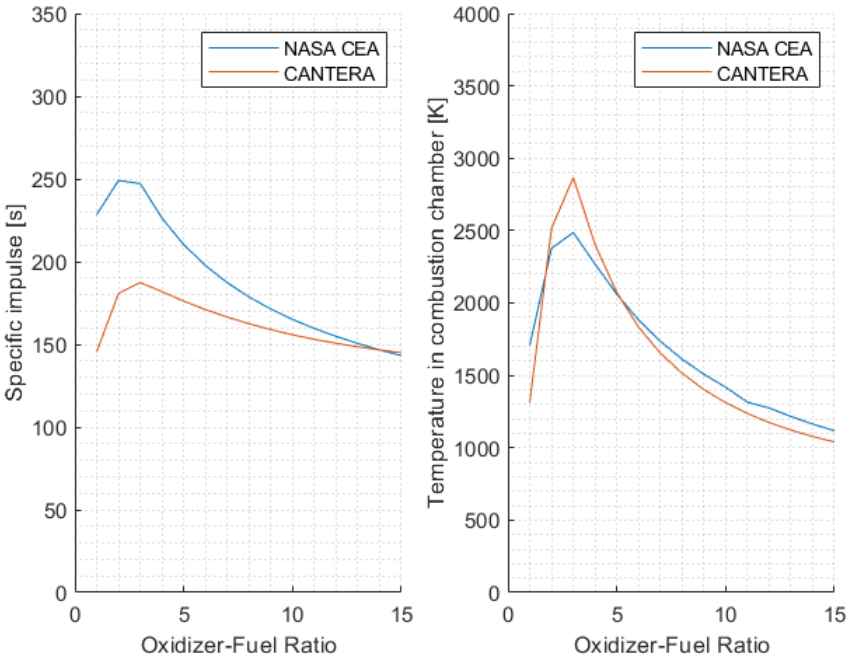

Chart.3 Comparasion of results from NASA CEA and Cantera N_2H_4

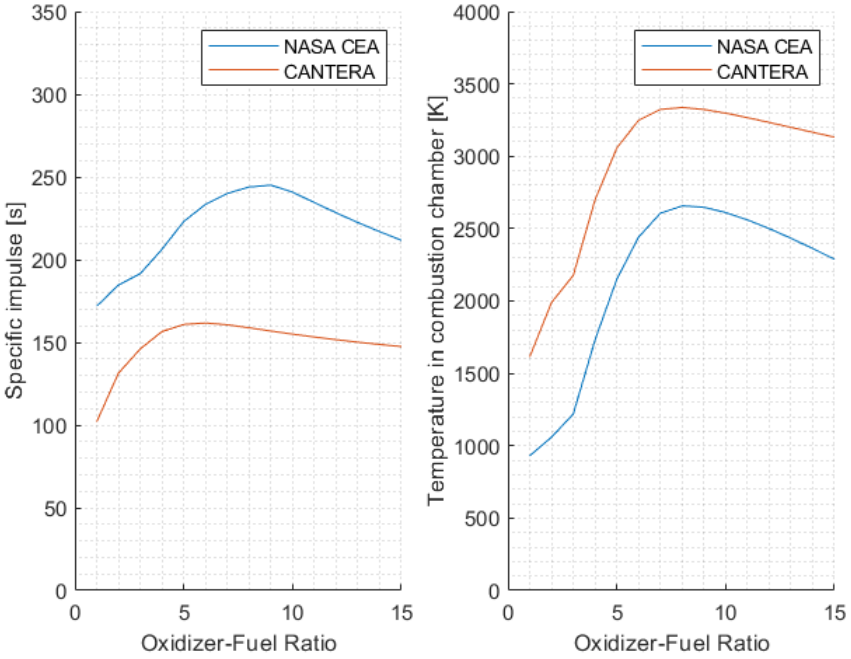

Chart.4 Comparasion of results from NASA CEA and Cantera $RP-1$

5 Conclusions and summary

Not all parameters of chamber are used in Cantera, that might cause differences in way software sees the place of combustion, which might have slight impact on results. Both Cantera and NASA CEA are different softwares so they might have different attitude to same issues.

Another thing that may cause differences are collections of data. NASA CEA is quite old software, the last update was 15 years ago, where time from the latest update of Cantera is counted of months. The methods of calculations may not be changed drastically in perspective of years, but parameters of gases and substances used in combustion may vary as there are new researches still made.

In case of temperatures, MATLAB program written to use Cantera has the 100K range of accuracy (later changed to 50 kelvins). This draws attention on the fact, that programs are not exactly accurate, both have different outcomes than reality, the sum of these might be significant.

Another reason of differences might be the degree of simplification of equations and processes during combustion. Cantera takes into account problem of inadequate ammount of oxidiser, but does not consider temporary conditions and grading of the reaction (i.e. temporary existing of OH- in combustion of carbohydrates).

All these factors may not cause much difference separately, but combined might be the reason of such gaps in values during calculations in project.

6 Code

Matlab code for all calculated cases is available on GitHub in the project repository.
Link: https://github.com/OlaMochol/MKWS_Siemionek_Mochol_2020

7 Sources

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