1st assignment: Flame Temperature Analysis and NOx Emissions for different Fuels and combustion conditions

Concepts: Adiabatic flame temperature, theoretical air, EGR percent, Diesel and gasoline engine kinds of combustion

Problem Motivation

For a combustion process that takes place with no heat loss to the surrounding, the temperature of the products is referred to as the adiabatic flame temperature. It is found that with an increase in the adiabatic flame temperature, there is increase in NOx emissions from internal combustion engines. As we know, vehicles are a major source of air pollutants such as nitric oxides, hydrocarbons, carbon dioxide, etc., there is a growing shift in the fuels from the petroleum-based fuels such as gasoline and diesel fuel to the alternative fuels such as natural gas, ethanol, methanol, liquefied petroleum gas and hydrogen. So, in order to study NOx emissions, the change in adiabatic flame temperature values for conventional fuels in comparison to the alternative fuels with various equivalence ratios and various EGR rates is studied in this module. Depending on how the process is completed, adiabatic flame temperature can be of constant volume or constant pressure type.
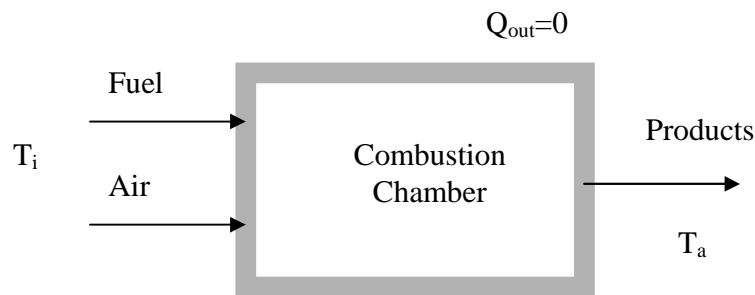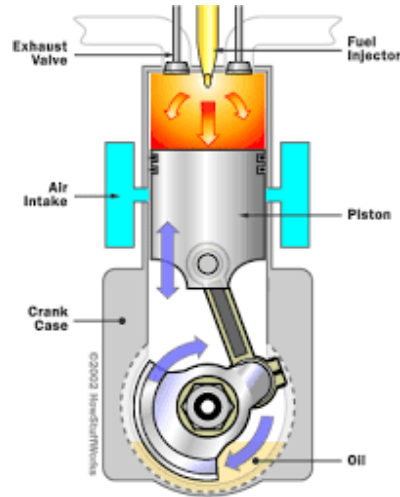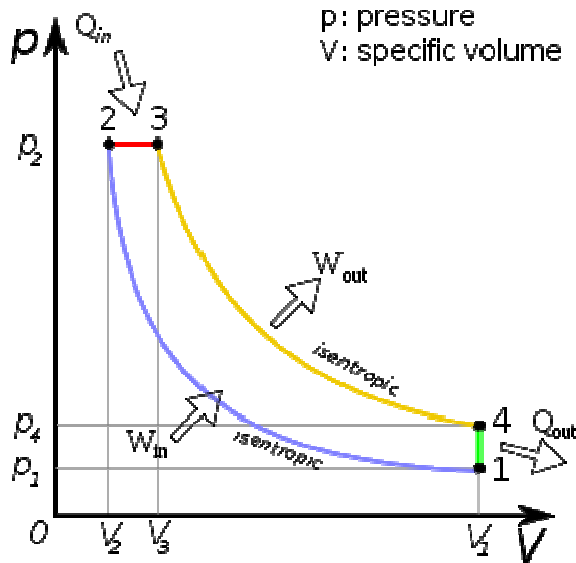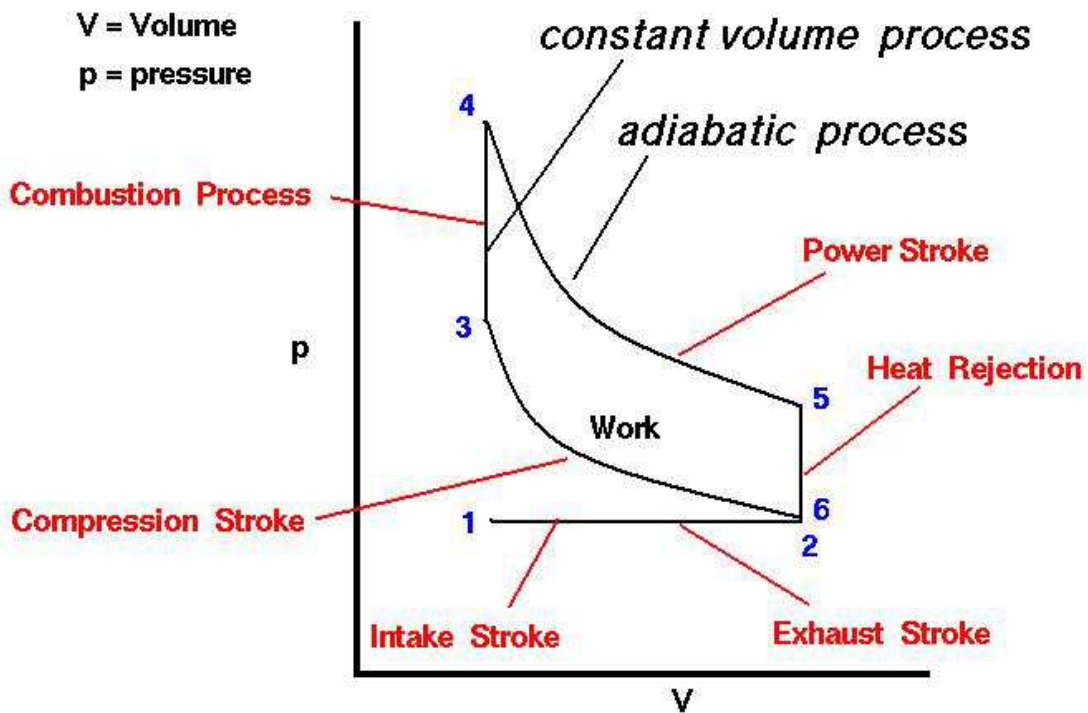

Figure 1 adiabatic combustion chamber, for adiabatic flame calculation [1]

Constant pressure combustion occurs for example in Diesel engines (see the P-v diagram), and constant volume combustion in gasoline engines (see P-v diagram).

Diesel theoretical P-v diagram
Q_{in} from combustion 2-3

Gasoline theoretical P-v diagram
Q_{in} from combustion 3-4

Exhaust Gas Recirculation (EGR)[2]:

Exhaust gas re-circulation i.e. EGR is EGR decreases the adiabatic flame temperature and so the NOx emissions. It is the most effective technique used to reduce NOx emissions in internal combustion engines. As shown in figure 2, a fraction (x_1) of the exhaust gases is re-circulated with the intake air into the engine. This is a technique commonly used in Diesel engines.
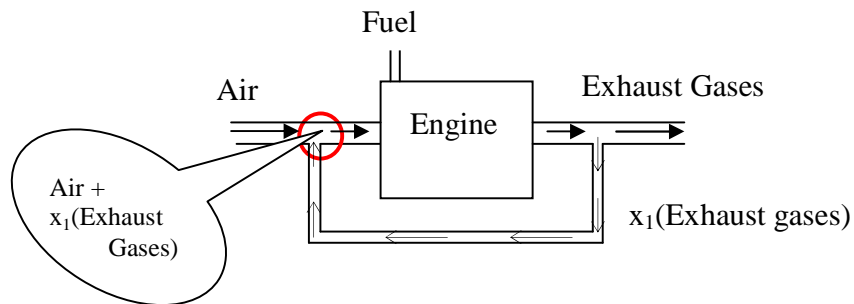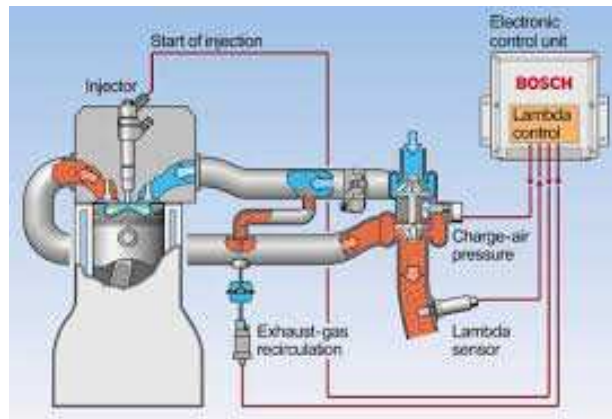

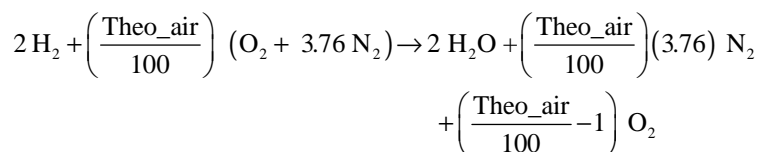Figure 2: Exhaust Gas Re- circulation

Question # 1 (influence of different fuels, excess air, constant volume or constant pressure, dissociation and initial conditions):

(a) Compute the adiabatic flame temperature of H_2- air at constant pressure and at constant volume for 40, 60, 80, 100, 120, 140, 160, 180, 200 and 250 percent theoretical air. Consider that both the fuel and the air enter the combustion chamber at $T_{in} = 25$ °C. Discuss the difference between the adiabatic flame temperature values at **constant pressure** and **constant volume** case.

(b) Compute the adiabatic flame temperature of gasoline- air, CH_4-air and ethyl alcohol-air mixtures at **constant pressure** for 100, 120, 140, 160, 180, 200 percent theoretical air. Obtain and compare a combined plot of adiabatic flame temperature vs % theoretical air (100 – 200 %) for H_2- air, CH4-air, gasoline- air and ethyl alcohol- air mixture.

(c) Using **Cantera** [3]*, free-open source combustion software, compute the adiabatic flame temperature and **equilibrium composition** of H_2-air, CH_4-air for 40, 60, 80, 100, 120, 140, 160, 180, 200 and 250 percent theoretical air. And different inlet premixed conditions: **T_{in} ranging from 250 K to 350 K**. Mark the values you found on a) and b) for Lambda influence and compare against Cantera. Discuss the dissociation influence on adiabatic flame temperature.

Hints:

▪ The combustion of hydrogen for two cases (i.e. for Lambda>=1 or for Theo_air/100 >= 100% and for Lambda< 1 or for Theo_air/100< 100%) can be explained with the following combustion equations.

1) Lambda>=1 or for Theo_air/100 >= 100%

$$2\,H_2 + \left(\frac{Theo\_air}{100}\right)(O_2 + 3.76\,N_2) \rightarrow 2\,H_2O + \left(\frac{Theo\_air}{100}\right)(3.76)\,N_2$$
$$+ \left(\frac{Theo\_air}{100} - 1\right)O_2$$

2) Lambda< 1 or for Theo_air/100 < 100%

$$2\,H_2 + \left(\frac{Theo\_air}{100}\right)(O_2 + 3.76\,N_2) \rightarrow 2\left(\frac{Theo\_air}{100}\right)H_2O + \left(\frac{Theo\_air}{100}\right)(3.76)\,N_2$$
$$+ \left(2 - 2\left(\frac{Theo\_air}{100}\right)\right)H_2$$
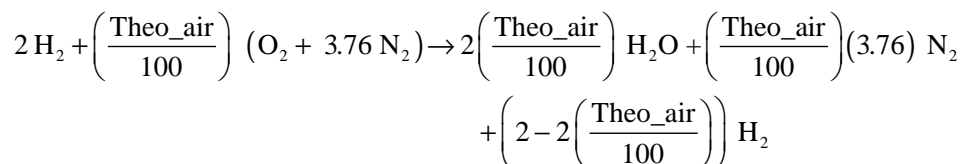
▪ The combustion of gasoline and ethyl alcohol for Lambda>=1 or for Theo_air/100 >= 100% can be explained with the following combustion equations.

Gasoline

$$C_8H_{18} + 12.5\left(\frac{\text{Theo\_air}}{100}\right)(O_2 + 3.76\, N_2) \rightarrow 8\, CO_2 + 9\, H_2O + 12.5\left(\frac{\text{Theo\_air}}{100}\right)(3.76)\, N_2$$

$$+ 12.5\left(\frac{\text{Theo\_air}}{100} - 1\right) O_2$$

Ethyl Alcohol

$$C_2H_5OH + 3\left(\frac{\text{Theo\_air}}{100}\right)(O_2 + 3.76\, N_2) \rightarrow 2\, CO_2 + 3\, H_2O + 3\left(\frac{\text{Theo\_air}}{100}\right)(3.76)\, N_2$$
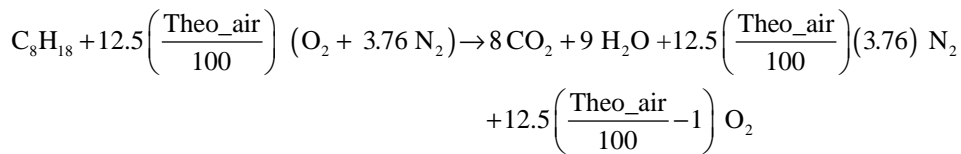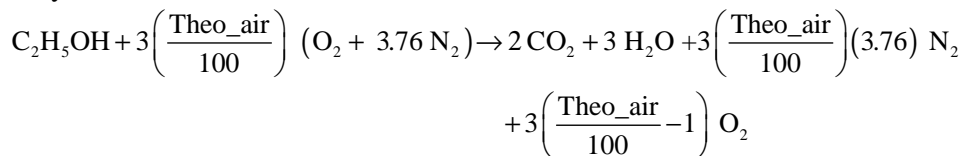
$$+ 3\left(\frac{\text{Theo\_air}}{100} - 1\right) O_2$$

- **Cantera   freeware/open   source**
  http://www.cantera.org/docs/sphinx/html/index.html

"Anaconda and Miniconda are Python distributions for which Cantera is available through the `conda` package manager. "

1st install: https://www.anaconda.com/download/

2nd install pycharmhttps://www.jetbrains.com/pycharm/download/#section=windows

3rd in pycharm set Conda **environment "combustion"**

4th Anaconda prompt:
    activate combustion
    conda install –c cantera cantera
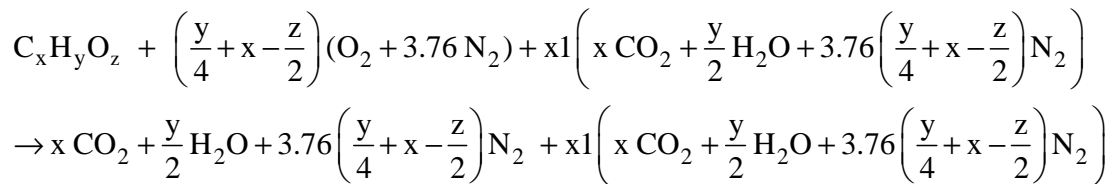   conda install ipython matplotlib

5th copy example
http://www.cantera.org/docs/sphinx/html/cython/examples/multiphase_adiabatic.html

Question # 2 (influence of different fuels, excess air, constant volume or constant pressure, dissociation and initial conditions):

(a) Compute the adiabatic flame temperature of the poor mixture (140% percent theoretical air) of diesel- air, and biodiesel- air at **constant volume** using 0, 5, 10, 15, 20, 25, 30% EGR percent. Assume that each fuel is burned with the stoichiometric amount of air in the combustion chamber. Obtain and compare a combined plot of adiabatic flame temperature vs EGR percent for diesel- air and biodiesel- air mixture. Assume that the recirculation does not change the air feed temperature to the exhaust.

(b) Is it possible to do the same calculations assuming that the recirculation change the air feed temperature to 350 K?. If so do-it.

(c) What engine would you guess to have higher NOx emissions? Gasoline engine working at stoichiometry (100% theoretical air) with no EGR or diesel engine working with excess air (140% theoretical air) and 20-30% EGR? Justify.

(d) Biodiesel blend with diesel would increase NOx emissions or not? Discuss.

Hints:

▪ Generalized equation for combustion of fuel $C_xH_yO_z$ including EGR is given by

$$C_xH_yO_z + \left(\frac{y}{4} + x - \frac{z}{2}\right)(O_2 + 3.76\,N_2) + x1\left(x\,CO_2 + \frac{y}{2}H_2O + 3.76\left(\frac{y}{4} + x - \frac{z}{2}\right)N_2\right)$$

$$\rightarrow x\,CO_2 + \frac{y}{2}H_2O + 3.76\left(\frac{y}{4} + x - \frac{z}{2}\right)N_2 + x1\left(x\,CO_2 + \frac{y}{2}H_2O + 3.76\left(\frac{y}{4} + x - \frac{z}{2}\right)N_2\right)$$

▪ EGR (fraction) and the number of moles of the exhaust gas mixture to be re-circulated per mole of fuel $C_xH_yO_z$ (x1) are related to each other by an equation,

$$x1 = \frac{EGR}{1\text{-}\,EGR}$$

Diesel chemical formula: $C_{10.8}H_{18.7}$; Biodiesel from sunflower: $C_nH_{2n}O_2$ (assume it is mainly composed by Linoleic acid, C18:2).

Ideal gas phase thermodynamic properties of species involved in surrogate fuels
Linoleic acid, C18:2 (In [4])

Species	$\Delta_f H^\circ_{298K}$	S°_{298K}	C_p (T)						
			300 K	400 K	500 K	600 K	800 K	1000 K	1500 K
N₂	0.00	45.77	6.95	7.01	7.08	7.19	7.50	7.83	8.32
CH₄	−17.92	44.52	8.49	9.81	11.15	12.50	15.13	17.43	21.07
C₂H₆	−20.29	54.85	12.59	15.76	18.67	21.31	25.80	29.37	36.24
C₃H₈	−24.88	64.51	17.64	22.60	26.99	30.85	37.10	41.83	49.95
C₄H₁₀	−30.23	74.12	23.36	29.69	35.31	40.25	48.24	54.24	64.51
n-C₇H₁₆	−44.96	102.01	39.81	50.57	60.02	68.25	81.49	91.28	105.73
n-C₁₀H₂₂	−59.81	129.96	56.05	71.35	84.71	96.29	114.75	128.16	149.00
n-C₁₄H₃₀	−79.62	167.35	77.94	99.18	117.69	133.68	159.11	177.51	205.99
n-C₁₆H₃₄	−89.49	186.10	88.88	113.06	134.14	152.35	181.27	202.13	234.41
MCYH	−36.05	81.00	32.43	44.53	55.09	64.21	78.62	88.83	103.11
PCYH	−45.40	99.73	43.36	58.44	71.56	82.89	100.78	113.48	131.56
BCYH	−50.35	109.07	48.86	65.38	79.80	92.25	111.89	125.81	145.82
Toluene	11.95	78.45	24.89	33.31	40.62	46.79	55.96	62.36	71.38
PBZ	1.91	95.61	36.28	47.53	57.18	65.38	78.03	86.74	99.77
BBZ	−3.38	104.76	42.07	54.85	65.81	75.13	89.50	99.43	114.54
OBZ	−22.83	142.37	63.65	82.30	98.39	112.12	133.48	148.40	170.97
NP	35.91	82.35	31.99	42.94	52.06	59.58	70.73	78.26	93.19
MNP	28.24	92.58	37.14	49.34	59.65	68.27	81.32	90.25	105.91
BNP	13.13	119.41	54.44	70.57	84.59	96.59	114.95	126.67	133.62
C₁₄:0	−157.81	192.42	87.49	109.90	129.63	146.74	173.56	191.28	201.94
C₁₆:0	−167.70	211.13	98.44	123.81	146.10	165.43	195.74	215.94	230.42
C₁₈:0	−177.60	229.85	109.37	137.73	162.59	184.12	217.90	240.60	258.92
C₁₈:1	−149.48	226.47	104.94	132.69	157.02	178.07	210.95	232.85	249.88
C₁₈:2	−120.84	224.25	101.97	128.98	152.66	173.14	205.10	226.31	241.97
C₁₈:3	−92.20	222.02	99.00	125.28	148.30	168.20	199.25	219.78	234.02
C₂₀:0	−187.49	248.56	120.34	151.59	179.04	202.82	240.10	265.22	287.41
C₂₀:1	−159.38	245.18	115.87	146.60	173.50	196.75	233.12	257.52	278.38
C₂₂:0	−197.38	267.27	131.27	165.52	195.53	221.50	262.26	289.90	315.91
C₂₂:1	−169.27	263.90	126.82	160.51	189.98	215.44	255.29	282.17	306.87

$\Delta_f H^\circ_{298K}$ is expressed in kcal mol^{-1} and S°_{298K} and C_p (T) are given in cal mol^{-1} K^{-1}.

Table H.2 Curve-Fit Coefficients for Fuel Specific Heat and Enthalpy[a] for Reference State of Zero Enthalpy of the Elements at 298.15 K and 1 atm:

$$\bar{c}_p \text{ (kJ/kmol · K)} = 4.184(a_1 + a_2\theta + a_3\theta^2 + a_4\theta^3 + a_5\theta^{-2}),$$
$$\bar{h}^\circ \text{(kJ/kmol)} = 4184(a_1\theta + a_2\theta^2/2 + a_3\theta^3/3 + a_4\theta^4/4 - a_5\theta^{-1} + a_6),$$
$$\text{where } \theta \equiv T \text{ (K)}/1000$$

Formula	Fuel	Molecular Weight	a_1	a_2	a_3	a_4	a_5	a_6	a_8^*
CH₄	Methane	16.043	−0.29149	26.327	−10.610	1.5656	0.16573	−18.331	4.300
C₃H₈	Propane	44.096	−1.4867	74.339	−39.065	8.0543	0.01219	−27.313	8.852
C₆H₁₄	Hexane	86.177	−20.777	210.48	−164.125	52.832	0.56635	−39.836	15.611
C₈H₁₈	Isooctane	114.230	−0.55313	181.62	−97.787	20.402	−0.03095	−60.751	20.232
CH₃OH	Methanol	32.040	−2.7059	44.168	−27.501	7.2193	0.20299	−48.288	5.3375
C₂H₅OH	Ethanol	46.07	6.990	39.741	−11.926	0	0	−60.214	7.6135
C₈.₂₆H₁₅.₅	Gasoline	114.8	−24.078	256.63	−201.68	64.750	0.5808	−27.562	17.792
C₇.₇₆H₁₃.₁		106.4	−22.501	227.99	−177.26	56.048	0.4845	−17.578	15.232
C₁₀.₈H₁₈.₇	Diesel	148.6	−9.1063	246.97	−143.74	32.329	0.0518	−50.128	23.514

[a]To obtain 0 K reference state for enthalpy, add a_8 to a_6.
[b]Source: From Heywood, J. B., *Internal Combustion Engine Fundamentals*, McGraw-Hill, New York, 1988, by permission of McGraw-Hill, Inc.

[2]

1st assignment (6 val)   Carla Silva   Tecnologias de combustão

References

[1]   Turns SR. An introduction to combustion: concepts and applications. System 2000;499:411. doi:10.1016/j.ijhydene.2008.07.121.

[2]   Heywood JB. Internal Combustion Engine Fundamentals. vol. 21. 1988.

[3]   Goodwin DG, Moffat HK, Speth RL. Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes. Http://www.cantera.org 2017. doi:10.5281/zenodo.170284.

[4]   Glaude PA, Fournet R, Bounaceur R, Moli??re M. Adiabatic flame temperature from biofuels and fossil fuels and derived effect on NOx emissions. Fuel Process Technol 2010;91:229–35. doi:10.1016/j.fuproc.2009.10.002.