Metody Komputerowe w Spalaniu - Cantera Project: Adiabatic Flame Temperature of a mixture of Methane and Air

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1 Introduction

For a combustion process that takes place adiabatically with no shaft work, the temperature of the products is referred to as the adiabatic flame temperature. This is the maximum temperature that can be achieved for given reactants.

In this Project I am going to show the results on calculating adiabatic flame temperature of a mixture of Methane and Air depending on the concentration of Methane in Air.

Regarding to source [2] the concentration range of flammability for Methane (in Air) is 5,1-15,1 percent. I am going to show changes in adiabatic flame temperatures for these concentrations for different initial conditions.

2 Literature

http://apmonitor.com/che263/index.php
M.Gieras "Spalanie - Wybrane zagadnienia w zadaniach"
3.http://www.cerfacs.fr/cantera/mechanisms/meth.php

3 Description of the Model

I am starting with a stechiometric chemical reaction:

$$CH4 + 2O2 + 7,52N2 \longrightarrow CO2 + 2H2O + 7,52N2$$

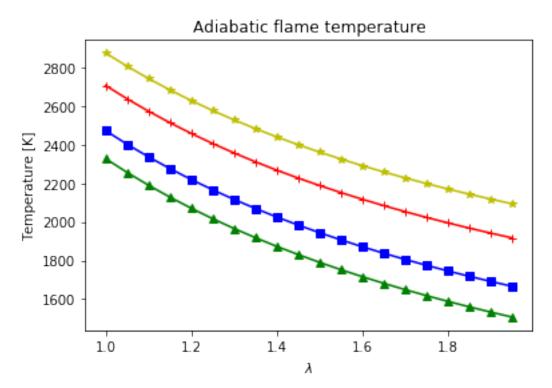
If the reaction is adiabatic it means there is no enthalpy loss, which also means that the products have the same enthalpy as the reactants - so I have hp=hr. To know the products temperature (which is my unknow in this case) I have to solve the problem: f(Tp) = hp-hr = 0.

I am starting with a reactants temperature equal to $300 \mathrm{K}$ (i am also considering other instances of initial temperature further in my project) and calculate the enthalpy of reactants. Then I need to write the function for products enthalpy and then solve $f(\mathrm{Tp})$ so I get the products adiabatic temperature.

Then i have to take into consideration different concentration ranges of flammability from 5,1 percent to 15,1 percent. I am using the excess air coefficient which varies from 0,59 to 1,95 for this case. The variable in my chemical reaction is 'a' which is doubled excess air coefficient and at the same time the amount of moles of air. I am only taking into consideration the stechiometric (excess air coefficient equals to 1) and fuel-lean mixture (excess air coefficient more than 1) which is:

 $CH4+aO2+a3,76N2 \\ \hline \hspace{1cm} CO2+2H2O+a3,76N2+aO2 \\ \hline \hspace{1cm} 2O2 \\ \hline \hspace{1cm} Last step is to do all of the previous steps for different initial reactants temperature – I have chosen: 300K, 500K, 800K and 1000K.$

4 Description of the Results



LEGEND: GREEN - 300 K BLUE - 500 K RED - 800 K YELLOW - 1000 K

In the plot we can see adiabatic flame temperature referred to excess air coefficient. The colors are for different initial temperatures of the reactants.

The highest adiabatic flame temperature we get for stoichiometric mixture.

The higher the initial temperature is the higher adiabiatic flame temperature we get.

5 Summary

According to source [3] all the calculations have been made correctly as both the plots (the one from the source and the one above) looks similar.