Autoignition time

Artur Kuriata

May 16, 2017

1 Introduction

This section will be dedicated to simulation of autoignition time of ethane. Using Cantera program to analize influence of pressure and concentration of water in the mixture on autoignition time.

2 Mathematical model

The mixture of ethane and water is located in ideal reactor with total mol mass of : Nitrogen - 3.76 mol , Oxygen - 1 mol , ethane -1 mol and water with 0 - 1.44 mol. In first part reactor temperature is changed from 1176 K to 1538 K and the changes of temperature in function of distance where measured.In second part pressure is changed from 0,8 bar to 1 bar and the changes of pressure in function where measured. In the third part we add water to methane with 0 - 20 percent and the the changes of water percentage in mixture in function is measured.

3 Program description

3.1 Basic part of program

Importing libraries

import sys
import numpy as np
from cantera import *
import cantera as ct
from pylab import *
import csv

Creating gas object used to evaluate all thermodynamic, kinetic, and transport properties.

gas = Solution('gri30.cti')

Specifying the number of time steps,the time step size and borders of each parameter

nt = 100000
dt = 1.e-6
Tmin = 0.65
Tmax = 0.85
npoints = 11
pmin= 0.8
pmax = 1
wmin=0
wmax=1.44
$Autoignition_cas = np.zeros(npoints,' d')$
$FinalTemp_cas = np.zeros(npoints,' d')$
$mfrac_cas = np.zeros([npoints, gas.n_spepcies],' d')$

Looping over the three variables

for l in range(npoints):
    $w[l] = wmin + (wmax + wmin) * l/(npoints - 1)$
    $procent = (w[l]/(5.76 + w[l])) * 100$

for k in range(npoints):
$pi[k] = pmin + (pmax - pmin) * k/(npoints - 1)$
$one_atm = one_atm * pi[k]$
for j in range(npoints):
$Ti2[j] = Tmin + (Tmax - Tmin) * j/(npoints - 1)$
$Ti[j] = 1000/Ti2[j]$
Set gas state, always at stoichiometry
$gas.TPX = Ti[j], one_atm, ('C2H6 : 1, O2 : 1, N2 : 3.76, H2O :' + str(w[l]))$
Create the ideal batch reactor
$r = ct.IdealGasReactor(gas)$
create a reactor network consisting of the single batch reactor
$sim = ct.ReactorNet([r])$
Initial simulation time
$time = 0.0$
Loop for nt time steps of dt seconds.
for n in range(nt):
$time+ = dt$
$sim.advance(time)$
$tim[n] = time$
$temp_cas[n] = r.T$
$mfrac_cas[j][:] = r.thermo.Y$

Getting time of autoignition

$Dtmax = [0, 0.0]$
for n in range(nt - 1):
$dtemp_cas[n] = (temp_cas[n + 1] - temp_cas[n])/dt$
$if(dtemp_cas[n] > Dtmax[1])$:
$Dtmax[0] = n$
$Dtmax[1] = dtemp_cas[n]$ **Printing the result of calculation**
Autoignition = ((tim[Dtmax[0]] + tim[Dtmax[0] + 1]) / 2.)
print ('For ' + str(Ti[j]) +',p='+str(pi[k])+',st='+str(w[l])+ ', Autoignition time = (s) ' + str(Autoignition))
$Autoignition_cas[j] = Autoignition * 1000$
$FinalTemp_cas[j] = temp_cas[nt - 1]$

Making plot of the results of calculations

$plot(Ti2, Autoignition_cas,' , color =' orange')$
$xlabel(r'Temp[1000/K]', fontsize = 20)$
$ylabel("Autoignition[ms]")$
$title(r'Autoignitionof C_2H_6 + Airmixtureat Phi = 1, P =' + str(pi[k]) +' barand H_2O -'$
$+str(procent) +' ofmixture', fontsize = 22, horizontalalignment =' center')$
$axis([0.60, 0.90, 0.0, 100.0])$
$grid()$
$show()$

4 Results

Program returns plot returns time of autoignition of mixture of ethane and water of mixture temperature in the reactor.

5 Conclusion

Results from calculations for different pressures and concentration of water estabilished division indicates that increasing these parameters extend time of mixture autoignition.

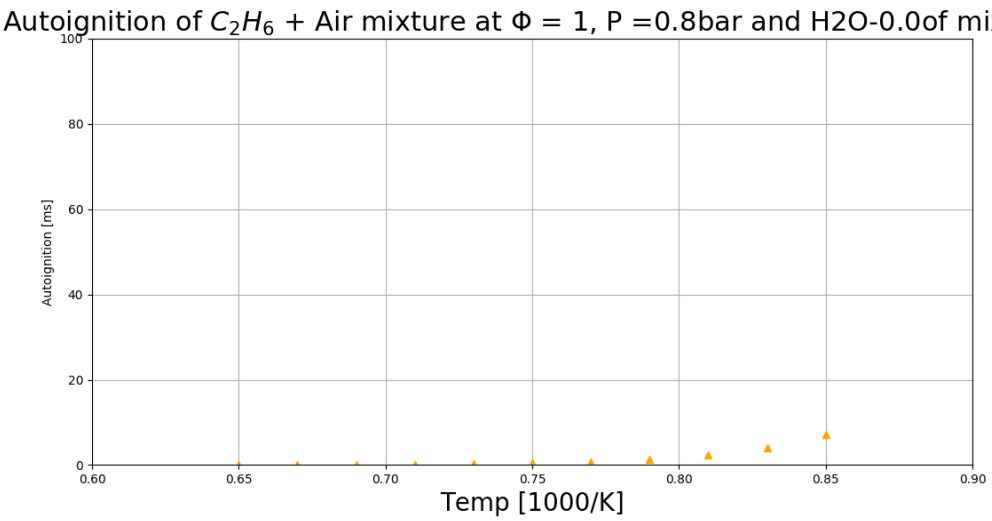

Figure 1: Autoignition time of an ethane mixture with water in function of reactor temperature.