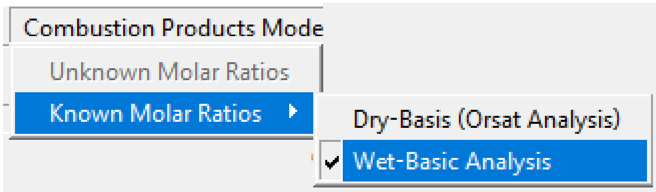
Exercise 4 (Effect on NOx)

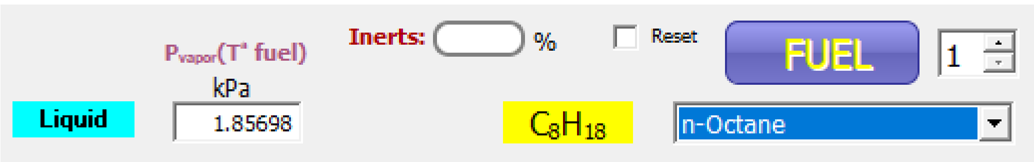
Some products of a combustion process of the octane in chemical equilibrium in volumetric composition are the following:

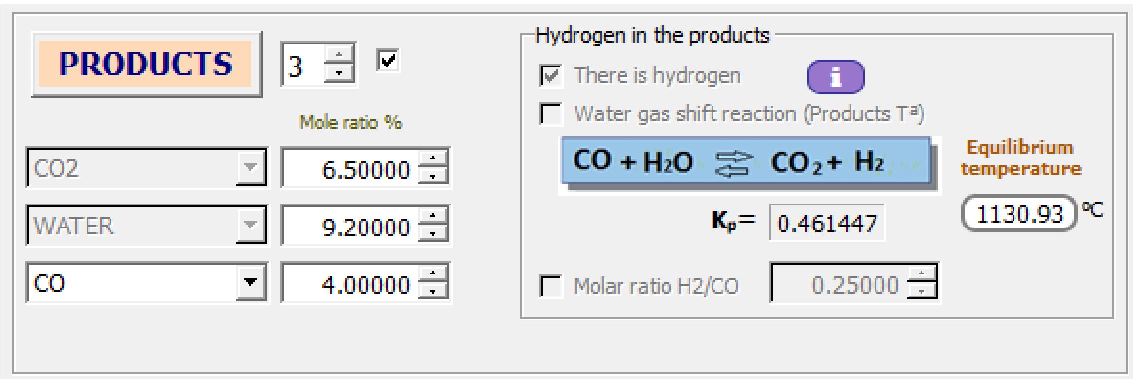
CO_2	6.5 %
H_2O	9.2 %
CO	4.0 %

a) Obtain the composition of H_2
b) Study the effect of the temperature of combustion products on NOx
c) Obtain the effect of the excess air coefficient on NOx

(excerpted from Introduction to Internal Combustion Engines by Richard Stone)







ThermoCombustion
Hidrocarbon Fuels

ThermoSuite
Technical Software Suite

FLUE GAS (Combustion Products)

☑ On wet basis ☐ On dry basis

	☑ mol/mol fuel	☐ kg/kg fuel	Mole %	Mass %
CO_2	4.952381	1.908046	6.5000	10.3302
CO	3.047619	0.747310	4.0000	4.0460
H_2O	7.009524	1.105492	9.2000	5.9852
N_2	54.645429	13.401294	71.7221	72.5551
O_2	4.545048	1.273251	5.9654	6.8934
SO_2				
H_2	1.990476	0.035128	2.6125	0.1902
Ar				
Unburned				
TOTAL	76.1905	18.4705	100.00 %	100.00 %

Dew Point (and P_{sat})

58.27 ºC

18.40 kPa

H_2O (liquid) ☐ 100% ___ % ___ mol/mol fuel ___ kg/kg fuel

Excess Air Coefficient

1.16208

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FLUE GAS (Combustion Products) ☐ On wet basis ☑ On dry basis

	☑ mol/mol fuel	☐ kg/kg fuel	Mole %	Mass %
CO_2	4.952381	1.908046	7.1586	10.9879
CO	3.047619	0.747310	4.4053	4.3035
H_2O				
N_2	54.645429	13.401294	78.9891	77.1742
O_2	4.545048	1.273251	6.5698	7.3323
SO_2				
H_2	1.990476	0.035128	2.8772	0.2023
Ar				
Unburned				
TOTAL	69.1810	17.3650	100.00 %	100.00 %

Dew Point (and P_{sat})

58.27 ºC

18.40 kPa

H_2O (liquid) ☐ 100% %

mol/mol fuel

kg/kg fuel

Air/Fuel ratio (dry air)

AIR

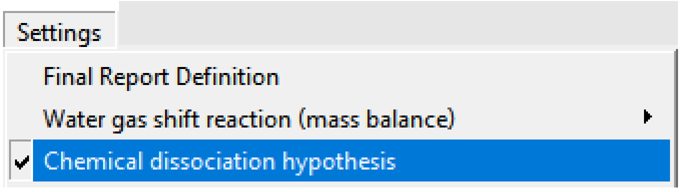
Theoretical	*Actual*	
59.52381	69.17143	☐ mol/mol fuel
15.03393	17.47063	☐ kg/kg fuel

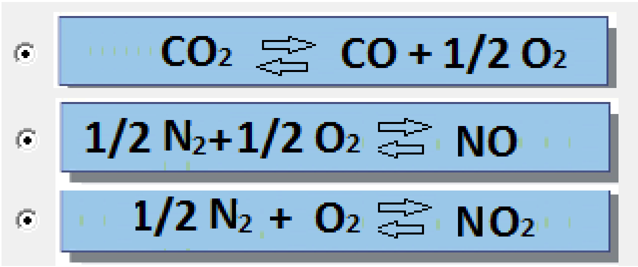
Oxygen/Fuel ratio (dry air)

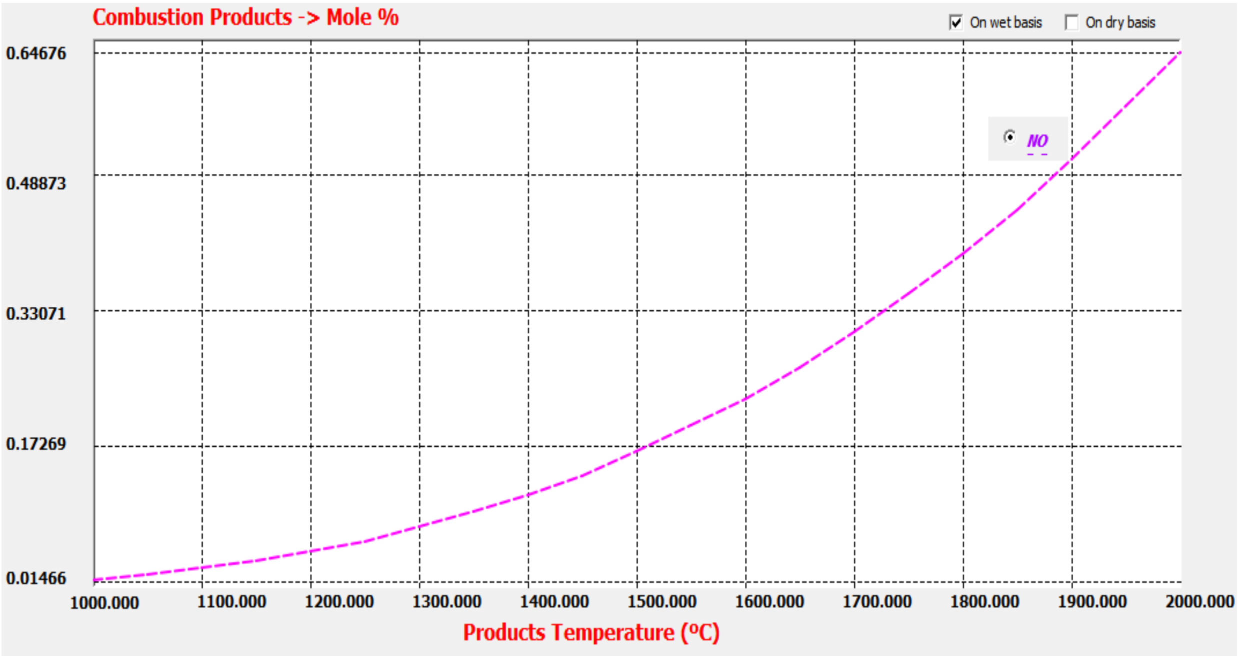
OXYGEN

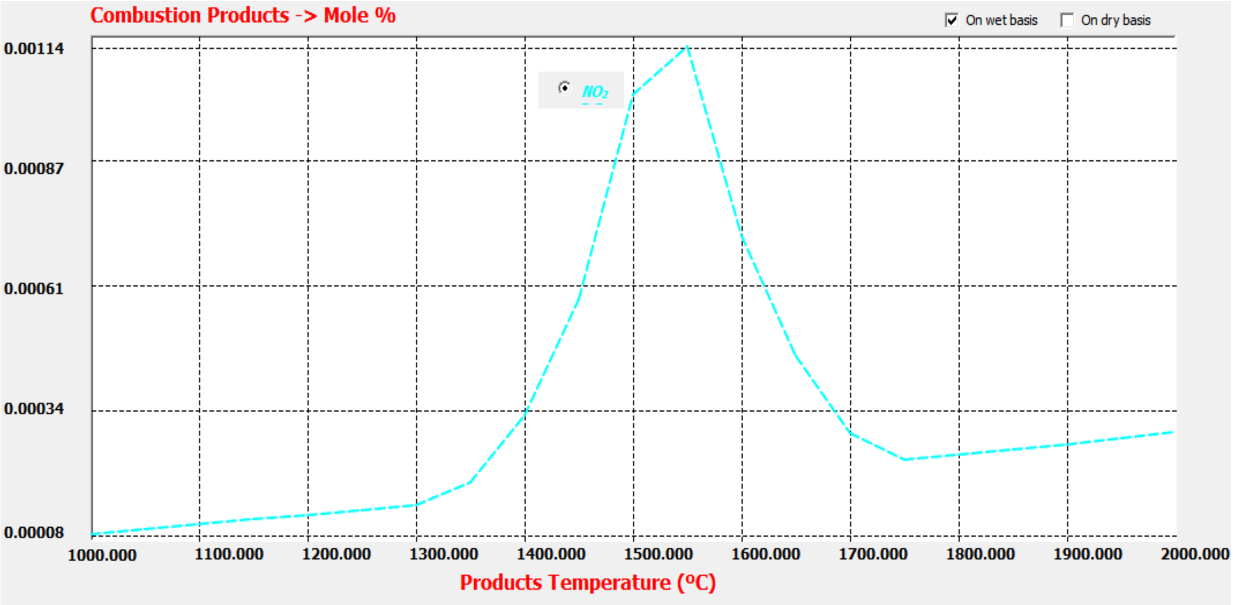
Theoretical	*Actual*	
12.50000	14.52600	☐ mol/mol fuel
3.50175	4.06931	☐ kg/kg fuel

b) Effect of product temperature


Settings
Final Report Definition
Water gas shift reaction (mass balance)
Chemical dissociation hypothesis

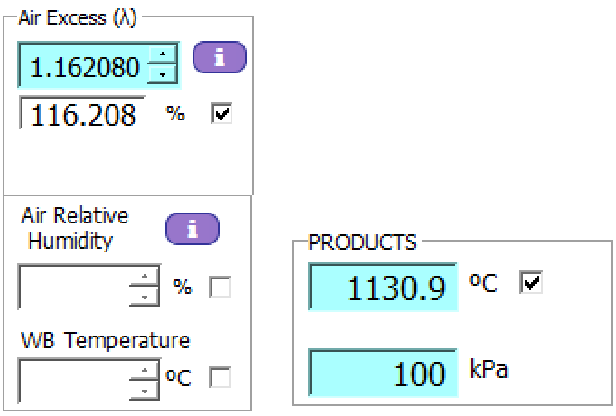

$CO_2 \rightleftarrows CO + 1/2\ O_2$
$1/2\ N_2 + 1/2\ O_2 \rightleftarrows NO$
$1/2\ N_2 + O_2 \rightleftarrows NO_2$


Combustion Products -> Mole %
On wet basis
On dry basis
0.64676
0.48873
0.33071
0.17269
0.01466
NO
1000.000
1100.000
1200.000
1300.000
1400.000
1500.000
1600.000
1700.000
1800.000
1900.000
2000.000
Products Temperature (ºC)

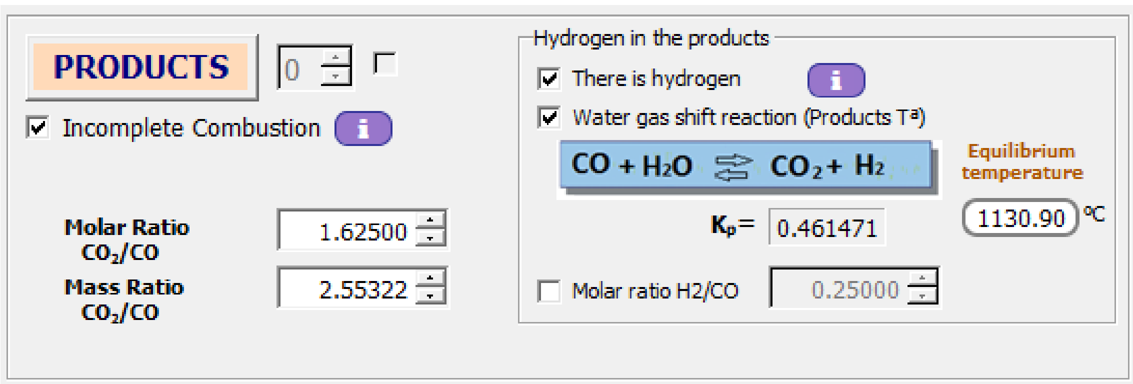


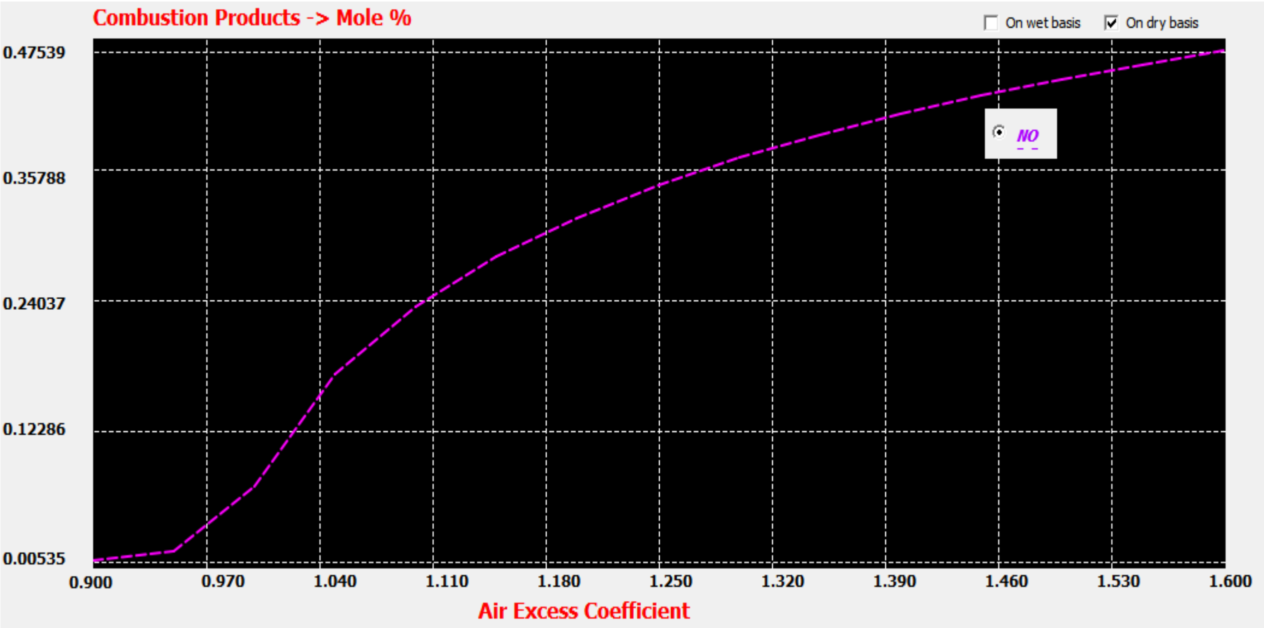
c) Incidence of the excess air coefficient on NOx

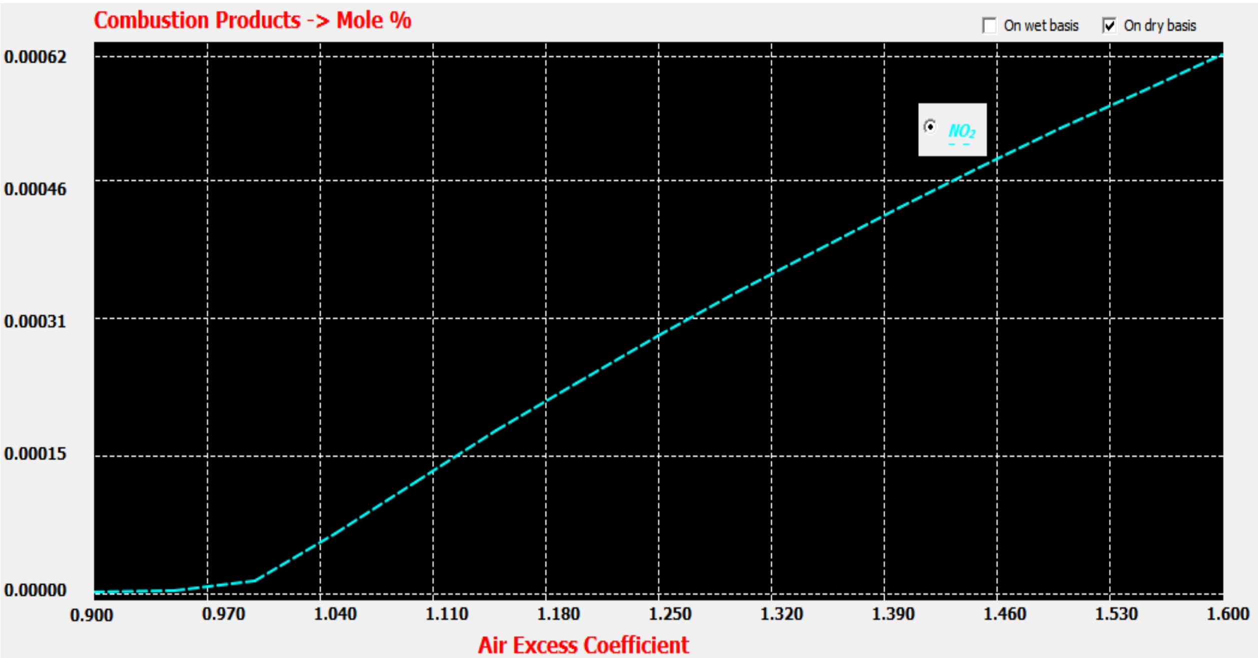
To have the excess air coefficient tab active, this must be an input variable, so you have to start the problem again, in this case without knowing the mole fractions of the products. Notice that the problem has the same results as in the previous case.



Calculating: CO_2/CO (mole) = 4.952381/ 3.047619 = 1.625







NOx emissions require both oxygen and high temperatures to form. Higher temperatures will occur with rich mixes, then drop as the mix becomes lean. However, only with lean mixtures will there be significant amounts of free oxygen. Therefore, as the mixture becomes lean from stoichiometric, there is a trade-off between increasing oxygen level and decreasing temperature.