



Exercise 1

0.1 kg/s of liquid fuel formed by a volumetric mixture of isooctane (80%) and benzene (20%), burns with an excess of air of 10%. Knowing that fuel and air enter at 25°C and 100 kPa and combustion products know at 1727°C and 100 kPa. The molar ratio $CO_2/CO = 5$ and the presence of H_2 (g) is observed in the combustion products.

Carry out a mass and thermodynamic analysis of the combustion process.



Incomplete combustion can occur in rich, lean, or stoichiometric mixtures. In any case, the resolution of the problem can be faced with the previously seen procedures of balance of atomic species and the laws of stoichiometry. Two cases of incomplete combustion that are commonly applied in the operation of thermal plants will be studied: Kissel Combustion, in which the unburned are CO and H₂, and Ostwald Combustion, in which there is only one unburned, the CO. For both cases there are graphic solutions that allow a quick evaluation of the global conditions of combustion, the efficiency of combustion and the production of environmental pollutants. These diagrams can be used to monitor a combustion installation. Large boilers, for example, have instruments to analyze combustion gases.



The hydrocarbon compounds of category C6, C7, C8 and higher, must be at high temperatures and pressures to keep them in a gaseous state.

Normal conditions		
0°C, 1atm (DIN 1343:1990)	•	
0°C, 1atm (DIN 1343:1990) 15°C, 1atm (ISO 2533:1975, ISO 13443:2005) 20°C, 1atm		
25°C, 1atm		
T₀ Dead State P₀ 25.00 ÷ °C 100.00 ÷ kPi	a	

The stable reference environment is defined according to the temperature and pressure conditions of the standard natural environment, that is, 25°C and 1 atm.





Air/fuel ratio (dry air)	Oxygen/Fuel ratio
AIR	OXYGEN -
Theoretical Actual	Theoretical Actual
54.76191 60.23810 mol/mol fuel	(11.50000) (12.65000) [mol/mol fuel
14.76489 16.24138 kg/kg fuel	3.43908 3.78299 🗆 kg/kg fuel
Nitrogen/Fuel ratio	
Theoretical Actual	Reactants (fuel + dry air)
43.26191 47.58810 mol/mol fuel	61.23810 mol/mol fuel
11.32577 12.45835 Kg/kg fuel	(Assume 1 mol fuel is being combusted)

The air-to-fuel ratio is the mount of air needed to completely burn a specific amount of fuel. To determine it, we begin by including the 3.76 kmols of nitrogen that accompany each kmol of oxygen in the combustion equation. This is done by recognizing that the stoichiometric coefficient for nitrogen is always 3.76 times the stoichiometric coefficient of oxygen. Since, in our model, the nitrogen does not take part in the combustion reaction, it usually has the same coefficient on both sides of the reaction equation.

Stoichiometric combustion means that $F_r = 1.0$. Excess fuel produces a rich mixture ($F_r > 1$) and excess air is a lean mixture ($F_r < 1$), the lean mixture is preferred to ensure none of the fuel escapes in an unburnt state.



Carbon monoxide (CO) is produced when combustion reactions are not fully completed, either through lack of oxygen or due to low mixing. Carbon monoxide is a colorless and odorless gas. All combustion sources, including motor vehicles, power stations, waste incinerators, domestic gas boilers, and cookers, emit carbon monoxide. Carbon monoxide is not poisonous but has a temporary effect on the human respiratory system. High concentrations of CO can cause physiological and pathological changes and ultimately death.







FUEL MOLECULAR FORMULA
Normalized form $C_{7.600} H_{15.600} O_{0.000} N_{0.000} S_{0.000}$
GRAVIMETRIC COMPOSITION (1 kg of FUEL)
Normalized form C H O N S
0.853 0.147 0.000 0.000 0.000

FUEL MOLECULAR FORMU	CH _{2.053} O _{0.000} N _{0.000} S _{0.000}
GRAVIMETRIC COMPOSITI	CN (1 kg of FUEL) = O N S O O O O O O O O O O O O O O O O O

Fuel Properties		
Enthalpy of formation	-197.640 kJ/mol fuel	
Absolute entropy (1 atm & 25ºC)	297.6520 J/mol fuel K	
Standard chemical exergy	5069.09 kJ/mol fuel	Kotas (1995)
Standard Gibbs Free Energy of Formation	4664.90 kJ/mol fuel	✓ Thermocombustion database





Enthalpy of formation is the enthalpy change when one mole of substance is formed from its elements in the standard state. By definition, enthalpy of combustion is the enthalpy change (or energy released) when one mole of substance is completely burnt in excess oxygen.

Density of the FUE	L
<i>•API</i> 62.63	<i>Specific gravity</i> 0.7289
Absolu 726.70	<i>te</i> 033) kg/m ³
Compressibility	factor

H/C molar ratio	07C molar ratio	N/C molar ratio
2.0526) mol H/mol C	0.000 mol O/mol C	0.0000 mol N/mol C
Carbon content	Hydrogen content	Oxygen content
0.8531) kg C/kg fuel	0.1469 kg H/kg fuel	0.0000 kg O/kg fuel
C/H mass ratio	C/O mass ratio	C/N mass ratio
5.8054) kg C/kg H	0.000) kg C/kg O	0.000 kg C/kg N

T	ThermoCombustion
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Properties of the AIR

	ity (Normal conditions)	Density (Entry to the chamber)
Dry air	Wet air	Dry air Wet air
1.1843	kg/Nm ³	0.7482 kg/m ³
Mass flo Dry air	w rate kg/s	et air
mol air/mol	products (stq)	kg air/kg products (stq)
(Dry basis)	1.0767	(<i>Dry basis</i>) 1.0217
mol air/mol	products (actual)	kg air/kg products (actual)
(Dry basis)	1.0482	(Dry basis) 1.0161
AIR MOLECU		
C 0.0000	00 23.79405	6.32500 A _r H 0.00000 0.00000
C 0.0000	N 0 23.79405	6.32500 A _r H 0.00000 0.00000
Gas Compressib	N 23.79405	6.32500 A _r H 0.00000 0.00000 Molecular weight
Gas Compressib	N 23.79405	6.32500 Ar 0.00000 0.00000 Molecular weight Wet 28.4109 kg/kmol
Compressib (1.00 Absolute I	N 23.79405	6.32500 Ar 0.00000 0.00000 Molecular weight Wet 28.4109 kg/kmol Dry 29.7623 kg/kmol

The compressibility factor Z is defined as the ratio of the actual volume to the volume predicted by the ideal gas law at a given temperature and pressure. If the compressibility factor is less than 1 then, the gas will show negative deviation and it will be more compressible than expected.

ThermoCombustion	ThermoSuite Technical Software Suite
Density	Flue gas/air ratio
RelativeAbsolute0.98071.1611kg/Nm3	1.0616 kg/kg air 1.0780 mol/mol air
Ideal gas	
Wet 0.9808 1.1613 kg/Nm ³	
Dry 1.0275 1.2166 kg/Nm ³	

Products Temperature)
	(1727.00) °C
Adiabatic Flame	<u>Temperature</u>
For λ = 1.1000 (Actual)	1819.85 °C
For λ = 1.0 (max) (Theoretical)	2132.20 °C (25°C, 1atm)

The adiabatic flame temperature is the maximum temperature of the combustion gas that can be reached by the combustion reaction under the no heat loss to the surroundings in the adiabatic condition. Especially, the theoretical maximum temperature assuming no thermal dissociation and complete combustion is called the adiabatic theoretical flame temperature.

Heat (Released or Abso 242.666 kJ/mol fuel	rbed) i Exothermic ENERGY Exo = release
Reactants	$Q_f = \sum_{\text{Products}} n_{\text{out}} \mathbf{h}_{\text{out}}(\mathbf{T}_{\text{out}}) - \sum_{\text{Reactants}} n_{\text{in}} \mathbf{h}_{\text{in}}(\mathbf{T}_{\text{in}})$
J♥ Products	$(-440.306) kJ/mol fuel (-197.640)$ $Q_f = H_P(T_{outr}P) - H_R(T_{inr}P) = H_P(T_{outr}P) - H_P(T_{adr}P)$
🔽 kJ/mol fuel 🔲 kJ/kg fuel □	kW $H = H_{form} + H(T,P) - H(25^{\circ}C, 1 \text{ atm})$

	hermoC	ombus	tion			Ts	ThermoSuite Technical Software Suite
C ENERGY BA	ALANCE: REACTA	NTS	? X				
0.	kg/mol		Δ.				
N ₂	0.0000	0.0000	÷	۲	ENERGY BA	LANCE: FLUE GAS	? ×
H-O	0.0000	0.0000	1				
1120			R				
TOTAL	0.0000	0.0000				kJ/mol	kJ/mol fuel
C ₈ H ₁₈	-259.3000	-207.4400			CO ₂	-302.0800	-1913.1732
C ₆ H ₆	49.0000	9.8000	F		CO	-53.7910	-68.1353
			U		H ₂ O	-169.1310	-1263.4342
			E		O ₂	59.1990	115.3340
			L		N ₂	56.1410	2671.6433
TOTAL	-210.3000	-197.6400			H ₂	52.9320	17.4595
TOTAL	-210.3000	-197.6400	(AIR+FUEL)		TOTAL	-356.7299	-440.3059

Direct method		
Combustion Efficiency	Reference state: To=25 °C, Po=100 kPa	i
$\eta_{\text{comb}} = \frac{Q_f(T_0)}{LHV}$	90.63 % i (Incomplete Combustion Loss)	
	(100% for complete combustion)	
	Qf(T ₀) 4241.09 kJ/mol fuel	

Combustion efficiency measures the presence of unburnt elements in the combustion process.



The efficiency of the combustion chamber is the ratio between the energy obtained in the combustion process (present in the combustion products) and the heating value of the fuel.

Settings Execute Chemical Equilibrium Plot Format Output summary definition • • • Water gas shift reaction (mass balance) • • • Dissociation ON/OFF • • • Model Substances • • • Reactants at their partial pressure Combustion Products • • Reactants at the same pressure Ignore water condensation • • Reactants at the same pressure Settings Execute Chemical Equilibrium Plot Format Output summary definition • • Products at their partial pressure Dissociation ON/OFF • • Products at their partial pressure Model Substances • • Products at their partial pressure Reactants • • Products at the same pressure Streams of AIR/FUEL • • Separate Streams Sankey or Grassmann • • Sankey or Grassmann	ThermoCombustion
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Entropy Terms (1/mal fuel //)	
Generated Entropy (Sg) Entropy balance Entropy balance S _g = $-\frac{Q_f}{T_f} + \sum_{\text{Products}} n_{\text{out}} S_{\text{out}} - \sum_{\text{Reactants}} n_{\text{in}} S_{\text{in}}$ S _g = $-\frac{Q_f}{T_f} + \sum_{\text{Products}} n_{\text{out}} S_{\text{out}} - \sum_{\text{Reactants}} n_{\text{in}} S_{\text{in}}$ S _g = $-\frac{Q_f}{T_f} + \sum_{\text{Products}} n_{\text{out}} S_{\text{out}} - \sum_{\text{Reactants}} n_{\text{in}} S_{\text{in}}$ S _g = $-\frac{Q_f}{T_f} + \sum_{\text{Products}} n_{\text{out}} S_{\text{out}} - \sum_{\text{Reactants}} n_{\text{in}} S_{\text{in}}$ S _g = $-\frac{Q_f}{T_f} + \sum_{\text{Products}} n_{\text{out}} S_{\text{out}} - \sum_{\text{Reactants}} n_{\text{in}} S_{\text{in}}$	ted Entropy (S _g) f Reactants f Beactants f Reactants f Reac

The entropy generation associated with irreversible phenomena and based on the Second Law of Thermodynamics is of considerable importance in the fields of engineering sciences. Different phenomena give rise to entropy generation, such as heat transfer through finite temperature gradients, heat transfer characteristics, and effects of fluid viscosity.

	ThermoC drocarbon Fuels BALANCE: REACTA	ombust	ion ~ ×		Ts	ThermoSuite Technical Software Suite
O ₂ N ₂	J/mol K 218.0090 193.4619	<i>J/mol fuel K</i> 2757.8142 9206.4844	A I	💽 ENTROPY B	ALANCE: FLUE GA	4s ? ×
TOTAL	411 4709	11964 2988	R			
C _o H ₁₀	301.6962	241.3570			kJ/mol K	J/mol fuel K
CeHe	328.1947	65.6389	-	CO2	328.5627	2080.8972
			F	CO	291.3345	369.0238
			U	H ₂ O	282.5511	2110.6995
			E	O ₂	297.8098	580.2054
			1	N ₂	254.5533	12113.7090
τοται	620,0000	205.0050	-	H ₂	232.2179	76.5966
TOTAL	1041 3618	12271 2047	ATR+FILEL)	TOTAL	1687.0293	17331.1309
Availability Balance (kJ/mol fuel) Boundary temperature T_f 477.0 $\stackrel{\frown}{\longrightarrow}$ °C $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1 - \frac{T_0}{T_f}) Q_f + \sum_{Reactants} n_{out} b_{out}$ $I = \int_f (1$						
(heat transfer process) 146.22000 Exf + Exair ≈ Wrev + Exp Useful exergy (furnace or steam boiler) 0.00000 Exergy of the products, Exp Exergy destroyed (I): >0 Irreversible process Chemical Physical >0 Irreversible process >10 Irreversible process Exergy of the air, Exair >0 Impossible process >0 Impossible process >0.0000						
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C		Thern Hidrocarbon	noCombustio	on		ThermoSuite Technical Software Suite
S	Settings	Execute	Chemical Equilibrium	Plot	Format	E
	Outpu	ıt summary	definition		+	
	Water	gas shift re	action (mass balance)		+	
	Disso	iation ON/	OFF		+	
	Mode	l Substance	s		+	
	Comb	ustion Prod	lucts		+	
	Reactants					Reactants at their partial pressure
Streams of AIR/FUEL				•	 Reactants at the same pressure 	
	Ignore	e water con	densation			
						-
5	Settings	Execute	Chemical Equilibrium	Plot	Format	ł.
	Output summary definition					
	Water gas shift reaction (mass balance)					
	Disso	ciation ON/	OFF		+	
	Mode	l Substance	5		+	
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	Reactants				+	 Products at the same pressure
	Stream	ms of AIR/F	UEL		+	













Combustion products contain CO and molecular hydrogen H_2 (Kissel combustion). The Kissel diagram allows the combustion mass balance to be carried out quickly and effectively, and to obtain its characteristic parameters. The data required by the program are the same as for the Ostwald option, apart from the temperature.







Grebbel diagram shows a family of lines with focus at (0,1) whose intersection with the Grebbel line defines the excess air. In this diagram is shown the Grebbel line and constant excess air lines for complete combustion.

Some sensitivity analyses are performed below:





AXIS X						
Air excess coefficient						
Initial value	1,000 ÷					
Final value	2,500 ÷					
Interval	0,100 🔒					
Background color						
	V					



































