EVERYDAY EXAMPLES OF ENGINEERING CONCEPTS

T11: Combustion & reacting mixtures

This is an extract from 'Real Life Examples in Thermodynamics: Lesson plans and solutions' edited by Eann A. Patterson, first published in 2010 (ISBN: 978-0-9842142-1-1*) and contains suggested exemplars within lesson plans for Sophomore Thermodynamics Courses. They were prepared as part of the NSF-supported project (#0431756) entitled: "Enhancing Diversity in the Undergraduate Mechanical Engineering Population through Curriculum Change".*

INTRODUCTION

(from *'Real Life Examples in Thermodynamics: Lesson plans and solutions'*)

These notes are designed to enhance the teaching of a sophomore level course in thermodynamics, increase the accessibility of the principles, and raise the appeal of the subject to students from diverse backgrounds. The notes have been prepared as skeletal lesson plans using the principle of the 5Es: Engage, Explore, Explain, Elaborate and Evaluate. The 5E outline is not original and was developed by the Biological Sciences Curriculum Study[1] in the 1980s from work by Atkin & Karplus[2] in 1962. Today this approach is considered to form part of the constructivist learning theory[3].

These notes are intended to be used by instructors and are written in a style that addresses the instructor, however this is not intended to exclude students who should find the notes and examples interesting, stimulating and hopefully illuminating, particularly when their instructor is not utilizing them. In the interest of brevity and clarity of presentation, standard derivations, common tables/charts, and definitions are not included since these are readily available in textbooks which these notes are not intended to replace but rather to supplement and enhance. Similarly, it is anticipated that these lesson plans can be used to generate lectures/lessons that supplement those covering the fundamentals of each topic.

This is the third in a series of such notes. The others are entitled 'Real Life Examples in Mechanics of Solids' (ISBN: 978-0-615-20394-2), 'Real Life Examples in Dynamics'(ISBN: 978-0-9842142-0-4).

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Eann A. Patterson
A.A. Griffith Chair of Structural Materials and Mechanics
School of Engineering, University of Liverpool, Liverpool, UK
& Royal Society Wolfson Research Merit Award Recipient+

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[1] Engleman, Laura (ed.), *The BSCS Story: A History of the Biological Sciences Curriculum Study*. Colorado Springs: BSCS, 2001.

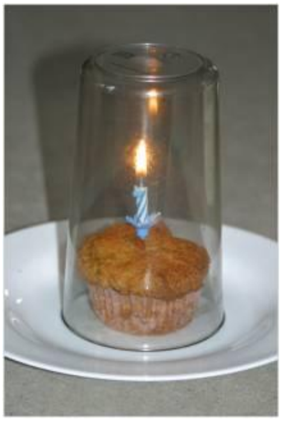
[2] Atkin, J. M. and Karplus, R. (1962). Discovery or invention? *Science Teacher* 29(5): 45.

[3] e.g. Trowbridge, L.W., and Bybee, R.W., *Becoming a secondary school science teacher*. Merrill Pub. Co. Inc., 1990.

THERMODYNAMICS OF CHEMICAL TRANSFORMATIONS

10. Topic: **Combustion & reaction mixtures**

Engage:



Take a cake with a candle, a large glass jar and stop watch into class. Light the candle. Invite the students to make sealed bids on how long it will take the candle to be extinguished when it is covered with the jar. The prize for the nearest correct answer is the cake.

A cup cake would be fine so that you can cover the cake and candle with the jar. Alternatively, if you are feeling generous, use a larger cake that can support the weight of the glass jar when you put it over the candle; and award a slice to the nearest answers.

Explore:

Before placing the jar over the candle, discuss the process that is occurring as the candle burns. The material of the candle is mainly solid paraffin, typically $C_{20}H_{42}$, i.e. with a generic chemical formula of C_nH_{2n+2} which is the same as methane, CH_4 or octane, C_8H_{18} which is the main component of gasoline; so not surprisingly it is very combustible.

Combustion is a chemical reaction between a fuel (paraffin) and an oxidant (oxygen in the air) which results in a set of products (carbon dioxide and water) and heat

$$C_{20}H_{42} + 30.5O_2 \overset{heat}{\rightarrow} 20CO_2 + 21H_2O$$

If sufficient heat is generated, then the products emit light generating the flame observed on the candle.

Invite two students to join you in dowsing the candle; give one the stop-watch and the other the glass jar.

Explain:

When the candle is burning in the room, there is an excess of oxygen available for combustion. This is the state when the jar is initially placed over the candle. When the candle goes out there is no oxygen left to react with the paraffin so combustion is arrested. There is a point somewhere in between when there is exactly the right amount of oxygen; this is known as the ‘theoretical amount of air’.

It is usual practice to idealize air to be 21% oxygen and 79% nitrogen on a molar basis and ignoring the smaller percentages of other gases present, such as argon and carbon dioxide which are less than 1%. So for combustion in air the chemical reaction can be written as

$$C_{20}H_{42} + a(O_2 + [0.79/0.21]\,N_2) \overset{heat}{\rightarrow} bCO_2 + cH_2O + dN_2$$

And the stoichiometric coefficients: a, b, c and d can be found by applying the law of conservation of mass to carbon so $b = 20$; to hydrogen so $c = 21$; to oxygen so $2a = 2b + c$ and $a = 30.5$; and finally to nitrogen so $d = 3.76a = 114.68$. Thus

$$C_{20}H_{42} + 30.5(O_2 + 3.76N_2) \overset{heat}{\rightarrow} 20CO_2 + 21H_2O + 114.68N_2$$

So the number of moles of air required for complete combustion of paraffin is 145.18 (=30.5+30.5×3.76) moles of air per mole of fuel – the theoretical amount of air. It can be turned into an air-fuel mass ratio by multiplying it by the ratio of the molecular masses of air (28.97) and paraffin, (324 [=20×12+42×2]), i.e.,

$$\text{Air-fuel mass ratio} = 145.18 \times \frac{28.97}{324} = 12.98$$

As the candle burns inside the jar, the oxygen is used up until there is insufficient to allow complete combustion of the paraffin and so not all of the carbon is converted into carbon dioxide resulting in the black deposit on the inside of the glass, i.e., soot.

Elaborate:

An energy balance can be used to evaluate the heat generated during the reaction/combustion process. If it is assumed that it is paraffin vapor evaporating from the wick which is reacting with the surrounding air, then this allows a control volume to be considered in which the reactants (paraffin vapor and air) are entering and the products of combustion (carbon dioxide, water and nitrogen) are leaving. Thus for the control volume applying the first law of thermodynamics to equate the change in enthalpy to the net heat transfer and work done

$$\frac{\dot{Q}}{\dot{n}_F} - \frac{\dot{W}}{\dot{n}_F} = \sum_P n_o \left(h_f + \Delta h\right)_o - \sum_R n_i \left(h_f + \Delta h\right)_i$$

where $\dot{n}_F$ is the molar flow rate of the fuel, the subscripts i and o refer to the inlet and outlet gases respectively, and P and R to the products and reactants respectively. h_f is the enthalpy of formation which is the energy released or absorbed when the compound is formed from its elements at the standard reference state (25°C, 1 atm) and Δh is the change in enthalpy relative to the standard reference state.

So work, $\dot{W}$ is zero for the candle and given

$$C_{20}H_{42} + 30.5O_2 + 114.68N_2 \overset{heat}{\rightarrow} 20CO_2 + 21H_2O + 114.68N_2$$

the energy balance becomes

$$\frac{\dot{Q}}{\dot{n}_F} = [\, 20\left(h_f + \Delta h\right)_{CO_2} + 21\left(h_f + \Delta h\right)_{H_2O} + 114.68\left(h_f + \Delta h\right)_{N_2} \,]$$

$$-[\, \left(h_f + \Delta h\right)_{C_{20}H_{42}} + 30.5\left(h_f + \Delta h\right)_{O_2} + 114.68\left(h_f + \Delta h\right)_{N_2} \,]$$

The enthalpy of formation of paraffin ($C_{20}H_{42}$) is -456,000kJ/kmol and treating it as an ideal gas such that $\Delta h = C_p \Delta T$ and $C_p = 2.13$ kJ/kg K. For carbon dioxide, oxygen, nitrogen and water the enthalpy of formation in can be found in thermodynamic tables[4].

i.e. $\left(h_f\right)_{CO_2} = \text{-}393{,}520\,\text{kJ/kgK}$; $\left(h_f\right)_{H_2O} = \text{-}241{,}820\,\text{kJ/kgK}$; $\left(h_f\right)_{O_2} = \left(h_f\right)_{H_2} = \left(h_f\right)_{N_2} = 0\,\text{kJ/kgK}$

Now for the reactants which enter the combustion control volume at 400K:

$$h_R = \left(h_f + C_p\Delta T\right)_{C_{20}H_{42}} + 30.5\left(h_f + \Delta h\right)_{O_2} + 114.68\left(h_f + \Delta h\right)_{N_2}$$

$$h_R = \left(-456000 + 2.13 \times \left[400 - 298\right]\right)_{C_{20}H_{42}} + 30.5 \times \left(0 + 3029\right)_{O_2} + 11468\left(0 + 2971\right)_{N_2}$$

$$h_R = -22{,}684\,\text{kJ/kmol}$$

where Δh values are obtained from the ideal gas data for each gas in the thermodynamic tables[5].

Similarly for the products given a temperature in the candle of 1400K:

$$h_P = 20\left(h_f + \Delta h\right)_{CO_2} + 21\left(h_f + \Delta h\right)_{H_2O} + 114.68\left(h_f + \Delta h\right)_{N_2}$$

$$h_P = 20 \times \left(-393520 + 55907\right)_{CO_2} + 21 \times \left(-241829 + 43447\right)_{H_2O} + 114.68 \times \left(34936\right)_{N_2}$$

$$h_P = -6{,}911{,}821\,\text{kJ/kmol}$$

Hence, from the first law of thermodynamics, remembering $\dot{W} = 0$

$$\frac{\dot{Q}}{\dot{n}_F} = -6911821 - (-22684) = -6889\,\text{MJ/kmol K } (C_{20}H_{42})$$

So if the candle (molecular mass = 324) burns at 1g/min (1.666×10^{-5} kg/s) or 5.14×10^{-8}kmols/s ($=1.666\times10^{-5}/324$), then the heat transfer is 354W ($=5.14\times10^{-8} \times 6889\times10^{6}$).

Evaluate:

Invite students to attempt the following examples:

Example 11.1

What flow rate of natural gas is required to raise two liters of water to boiling point in five minutes in order to cook pasta? You may assume that the gas ring is at a steady temperature of about 450K and the flame temperature is 1600K.

Solution:

The first law of thermodynamics can be used to equate the energy to heat the pan and water to the heat supplied by the gas flame.

Energy input required for water

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[4] e.g. http://v5.sdsu.edu/testhome/Test/solve/basics/tables/tablesComb/formation.html

[5] e.g. http://v5.sdsu.edu/testhome/Test/solve/basics/tables/tablesIG/igN2.html

$$= mC_p\Delta T = 2\times 4.18\times(100-21) = 660.44\,\text{kJ}$$

A stainless steel pan large enough to cook pasta in this quantity of water would have a mass of about 1.8kg,

so energy input required for the pan

$$= mC_p\Delta T = 1.8\times 5.2\times(100-21) = 739.44\,\text{kJ}$$

And the heat transfer rate,

$$\dot{Q} = (660.44+739.44)/(5\times 60) = 4.667\,\text{kW}$$

ignoring the heat losses from the pan.

Now, natural gas is mainly methane so we can approximate the combustion process to

$$CH_4 \;+\; 2O_2 \;+\; 7.58N_2 \;\overset{heat}{\rightarrow}\; CO_2 \;+\; 2H_2O \;+\; 7.58N_2$$

So applying an energy balance based on the first law of thermodynamics

$$\frac{\dot{Q}}{\dot{n}_F} = [\,(h_f+\Delta h)_{CO_2} + 2(h_f+\Delta h)_{H_2O} + 7.58(h_f+\Delta h)_{N_2}\,]$$

$$\text{-}[\,(h_f+\Delta h)_{CH_4} + 2(h_f+\Delta h)_{O_2} + 7.58(h_f+\Delta h)_{N_2}\,]$$

The enthalpy of formation of paraffin ($C_{20}H_{42}$) is -74,850kJ/kmol (from the thermodynamic tables[22]) and treating it as an ideal gas such that $\Delta h = c_p\Delta T$ and $C_p = 2.2\,\text{kJ/kg K}$.

Also $(h_f)_{CO_2} = \text{-}393{,}520\,\text{kJ/kgK}$; $(h_f)_{H_2O} = \text{-}241{,}820\,\text{kJ/kgK}$; $(h_f)_{O_2} = (h_f)_{H_2} = (h_f)_{N_2} = 0\,\text{kJ/kgK}$

Now for the reactants which enter the combustion control volume at 450K

$$h_R = (h_f + C_p\Delta T)_{CH_4} + 2(h_f+\Delta h)_{O_2} + 7.58(h_f+\Delta h)_{N_2}$$

$$h_R = (-74850 + 2.2[450-298])_{CH_4} + 2(4546)_{O_2} + 7.58(4436)_{N_2} = -31799\ \text{kJ/kmol}$$

Similarly for the products given a flame temperature of 1600K

$$h_P = (h_f+\Delta h)_{CO_2} + 2(h_f+\Delta h)_{H_2O} + 7.58(h_f+\Delta h)_{N_2}$$

$$h_P = (-393520+67580)_{CO_2} + 2(-241829+52844)_{H_2O} + 7.58(41902)_{N_2} = -386293$$ Hence, applying the first law of thermodynamics to the flame in a control volume with $\dot{W} = 0$

$$\frac{\dot{Q}_{combustion}}{\dot{n}_F} = -386293 - (-31799) = -354494\,\text{kJ/kmol K}\ (C_{20}H_{42})$$

Now applying the first law of thermodynamics to heating the water and pan

$$\dot{Q}_{required} = \dot{Q}_{combustion} = \left(\frac{\dot{Q}}{\dot{n}_F}\right)\times \dot{n}_F$$

so $$\dot{n}_F = \frac{\dot{Q}_{required}}{\left[\dot{Q}\big/\dot{n}_F\right]} = \frac{4.667}{354494} = 1.316\times10^{-5}\,\text{kmol/s}$$

And for methane, $M = 16$, so $\dot{m} = M\dot{n}_F = 16\times1.316\times10^{-5} = 2.106\times10^{-4}$ kg/s or 0.294 liters/s

Example 11.2

When a car is cruising on the highway at 70mph, its fuel consumption is 35mpg and the engine output is 60hp, estimate the rate of heat transfer from the combustion process if the fuel is assumed to be liquid octane and the temperature in the exhaust is about 900K. Assume the ambient temperature is 25°C.

Solution:

At 70mph the car will use 2 gallons/hour (= 0.007570m^3/hr =2.1×10^{-6}m^3/s)

And, the density of octane is 703kg/m^3 so the mass flow rate,

$$\dot{m} = 703\times2.1\times10^{-6} = 1.48\times10^{-3}\,\text{kg/s}$$

Octane is C_8H_{18} with a molecular mass, $M = 132$,

so by definition $$\dot{n}_F = \frac{\dot{m}}{M} = \frac{1.48\times10^{-3}}{132} = 1.119\times10^{-5}\,\text{kmol/s}$$

Assuming complete combustion

$$C_8H_{18} + 12.5O_2 + 47N_2 \xrightarrow{heat} 8CO_2 + 9H_2O + 47N_2$$

And applying the 1st law of thermodynamics, the energy balance is

$$\frac{\dot{Q}}{\dot{n}_F} - \frac{\dot{W}}{\dot{n}_F} = [\,8(h_f+\Delta h)_{CO_2} + 9(h_f+\Delta h)_{H_2O} + 47(h_f+\Delta h)_{N_2}\,]$$

$$-[\,(h_f+\Delta h)_{C_8H_{18}} + 12.5(h_f+\Delta h)_{O_2} + 47(h_f+\Delta h)_{N_2}\,]$$

The enthalpy of formation of liquid octane is -249,950kJ/kmol and $C_p = 2.23$ kJ/kg K (from the thermodynamic tables[22]).

Also $(h_f)_{CO_2} = \text{-393,520}$ kJ/kgK; $(h_f)_{H_2O} = \text{-241,820}$ kJ/kgK; $(h_f)_{O_2} = (h_f)_{H_2} = (h_f)_{N_2} = 0$ kJ/kgK

Now for the reactants which enter the combustion control volume at 298K

$$h_R = (h_f + C_p\Delta T)_{C_8H_{18}} + 12.5(h_f+\Delta h)_{O_2} + 47(h_f+\Delta h)_{N_2}$$

$$h_R = (-249950)_{C_8H_{18}} + 2(0+0)_{O_2} + 7.58(0+0)_{N_2} = -249950\,\text{kJ/kmol}$$

Similarly for the products given a flame temperature of 900K

$$h_P = 8(h_f+\Delta h)_{CO_2} + 9(h_f+\Delta h)_{H_2O} + 47(h_f+\Delta h)_{N_2}$$

$h_P = 8(-393520 + 28041)_{CO_2} + 9(-241829 + 21924)_{H_2O} + 47(18221)_{N_2} = -4046590$ So, with $\dot{W} = 60\,\text{hp} = 60 \times 745.699\,87 = 44742\,\text{W}$ the energy balance becomes

$$\frac{\dot{Q}}{\dot{n}_F} - \frac{\dot{W}}{\dot{n}_F} = h_P - h_R$$

and $\dot{Q} = \dot{n}_F \left(h_P - h_R\right) + \dot{W} = 1.119 \times 10^{-5}\left(-4046590 - \left(-249950\right)\right) + 44.742 = 2.26\,\text{kW}$