**Module 8 - Energy Content of Fuels: which fuel is “best?”**

**There are many factors to consider when choosing a fuel. In this exercise, your group will work with a set of three different potential fuels and evaluate their performance in terms of price, energy density (per mole, per gram, and per volume) as well as in terms of CO2 emissions. You will then select which of your three fuels is the “best,” realizing that there are several possible considerations to select the “best” fuel. You will have to defend your choice, as well as your definition of “best!”**

**Learning Objectives**: Upon completion of this exercise, you should be able to:

1. Give a basic definition of heat (q) and work (w)
2. Know the relationship between internal energy (U), enthalpy (H), and heat
3. Define a combustion reaction and a formation reaction
4. Mathematically describe a distillation process from a 2-component phase diagram
5. Gain an appreciation for the potential impact/importance of solar energy conversion
6. Use Hess's Law to determine enthalpy changes associated with chemical reactions
7. Use balanced chemical reactions, in combination with other relationships such as density, to derive other useful quantities related to a combustion reaction
8. Account for for the many variables (chemical, societal, and political) associated with picking the "best" chemical fuels as well as for the ways in which your knowledge of thermochemistry and chemical reactions can be applied to understand these variables
9. Draw a reaction coordinate diagram showing the function of a catalyst in a chemical reaction

**Review (material you should know or learn prior to this exercise):** entropy, enthalpy, balancing chemical reactions, one-component phase diagrams

**Terms you should learn while doing this exercise:** heat of formation, combustion reaction, energy density, fuel, greenhouse gas, two-component phase diagram, distillation, catalyst

**Relevant Reading**: Atkins, Jones, & Laverman 7th Ed Topics 4A.1-4A.5, 4B.1, 4C.1, 4D.1, 4D.3-4D.5, 5C.1-5C.3, 3J.2, 3J.4 and Box 4D.1.

**After completing this 3-day module, you should practice your skills on these relevant problems: 4B.1, 4B.3, 4D.1, 4D.5, 4D.9, 4D.13, 4D.15, 5C.9, 5C.11.**

These reading assignments, and the assigned exercises, serve as a *general introduction* to concepts that you will need in order to work on the activities in the coming periods. While we will not collect this work, **you will need to complete the corresponding Sakai assignment to receive credit** for the pre-class reading. Your conceptual understanding and quantitative application of these topics will be assessed during homework, concept quizzes, and exams.

**Reading assignment due by class time Monday Nov 28, 2016**

The pre-class assignment and in-class activities for this day are designed to help you continue to build the skill of reading and digesting technical content. Thus far in the course we have mostly helped you follow the reading by posing targeted questions and providing sample questions. The sample questions set up simple problems that require comprehension of technical concepts in order to do them correctly.

Your pre-class assignment for day one of this module is reversed again. We are assigning the reading and we are asking YOU to create targeted questions that would help guide another student through the material. Thinking about the process in this way will help you engage deeply with the material and will help you practice a skill that will serve you well in your academic career. Some of this material is review of topics from the Haber module.

Skim Topics 4A.1-4A.3 on work and expansion work, and Topics 4A.4-4A.5 on heat. We will not do calculations on heat and work this semester but understand the basic definitions of heat and work so that you can understand internal energy.

Read Topics 4B.1, 4C.1, 4D.1, 4D.3, 4D.4 and 4D.5 on internal energy (U), Enthalpy (H, heat transfer at constant pressure), reaction enthalpy (∆H), standard reaction enthalpies (∆H°) focusing mostly on the combustion reaction (∆Hc°), Hess’s Law, and standard enthalpies of formation (∆Hf°).

Following the model of guided reading questions in the previous modules, create a set of **at least 10 guiding questions** that focus attention on *what you see* as the key concepts in these sections (mostly focusing on the sections we asked you to *READ* not *SKIM*). You should include at least 3 example calculations in your set of questions. Upload those questions to the Sakai assignment and bring a printed copy to class. See Day 1 activity for a description of what you’ll do next.

**In class activity Day 1 Monday Nov 28, 2016**

Using the playing cards, find your new team to partner with for today’s class. You are charged with producing TWO documents today. One is a revised set of guided reading questions that represents your team’s efforts. The second document describes the characteristics of what makes a GOOD guided reading question. Details are outlined below.

**Goal 1:** Split your team of four into two pairs. With your partner, review the 10 or more questions each of you brought to class. What are the similarities? What are the differences? Describe those here.­ *If your group has only three members, you will do this comparison all together, and skip the second round of the activity.*

Settle on a list of questions as a pair *(or group of three)*. At this point, you may even create new or different questions. Create a document (using Google docs, Word, or text editor) with your new set of questions.

After creating your pair’s list, bring your team of four back together. Compare your two lists. What differences do you see? List those here. *If your group has only three members, you will do this comparison all together, and skip the second round of the activity.*

Select one team member as scribe. Now combine your two electronic documents into one set of guided reading questions that encompasses all the important concepts your team selected. Be sure you do *more* than simply copy paste the two documents into one. You need to produce a cohesive set of questions that move the reader through the material in a logical manner.

Include the names of all students in your team at the top of the document.

Name your file using this convention:

*Instructor\_(9am or 10am)\_PlayingCardNumber\_Questions*

For example, if you were all 6’s at 10am in Johnson’s class your file would be

*Johnson\_10am\_6\_Questions.doc (or .pdf etc)*

Upload this final document into the folder Resources / Modules-Reading Guides, Activities, Extras / Module 8 Fuels/Thermo / Student Generated Questions.

**Goal 2:** Now that you have discussed which questions stay and which go, you should have a sense of what makes a good guided reading question. With your team, create a second document that itemizes (lists) the traits of helpful guided reading questions. You may also include traits of particularly bad questions.

Include the names of all students in your team at the top of the document.

Upload the second document to the same folder, but name it as

*Instructor\_(9am or 10am)\_PlayingCardNumber\_traits*

List the traits here as well.

**Wrapping up**

You now have produced both a set of quality guided reading questions for this material AND a higher order analysis of what makes a good guided reading question. To ensure that your group has landed on the key concepts for today’s reading, open the file called

*Module 8 day 1 summary.pdf* located in *Resources/Modules/Module 8 Fuels/Thermo.*

Did you include those concepts in your documents? If not, which did you omit, and why?

**Reading assignment due by class time Wednesday Nov 30, 2016**

Read Topic 5C.1 “The Vapor Pressure of Mixtures.” What is the definition of mole fraction?

What is the equation that relates vapor pressure of a volatile liquid and mole fraction of a liquid?

Do Self-test 5C.1B: calculate the vapor pressure of ethanol in kilopascals at 19 °C for a solution preprared by dissolving 2.00 g of cinnamaldehyde (C9H8O) in 50.0 g of ethanol (CH3CH2OH). The vapor pressure of pure ethanol at 19 °C is 5.3 kPa.

Read Topic 5C.2 “Binary Liquid Mixtures.” Unlike a solution with a non-volatile solute, binary liquid mixtures are a solution where both components are volatile. Each component’s vapor pressure is determined using which law?

The total vapor pressure is determined using which law?

Do self test 5C.2A: what is the total vapor pressure at 25 °C of a mixture of 3.00 mol benzene and 2.00 mol toluene? Pbenzene = 94.6 torr; Ptoluene = 29.1 torr.

The vapor is enriched in the component with the (higher/lower) vapor pressure.

Use the ideal gas law to show that mole fraction of an ideal gas is equal to pressure fraction of an ideal gas.

What is the composition (mole fraction) of the vapor over a solution that is a mxture of 3.00 mol benzene and 2.00 mol toluene? How much is the vapor enriched relative to the starting solution?

Read Topic 5C.3 “Distillation.” What is the function of the horizontal “tie line” drawn in Figure 5C.6? What is the vertical line?

What happens to the boiling temperature of a mixture of compounds as a distillation proceeds?

**In class activity Day 2 Wednesday Nov 30, 2016**

In part one of today’s activity, you will construct a pressure vs. composition curve for a mixture of two volatile liquids. While distillations are normally carried out at constant pressure and changing temperature, it is an easier calculation to determine the vapor pressure of a mixture of liquids at constant temperature.

Given the following data, construct a graph similar to that shown in Figure 5C.2 that shows pressure versus mole fraction. You will then calculate the line that shows the corresponding mole fraction of the vapor.

1-Propanol and 2-propanol form an ideal mixture. The vapor pressures of 1-propanol and 2-propanol at 25 °C are 21.0 and 45.4 torr, respectively. In the template on the next page, draw the curves corresponding to P1P, P2P, and Ptot as a function of mole fraction P1p.

Which component, 1- or 2-propanol, has the higher boiling point?

Which component, 1- or 2-propanol, will be enriched in the vapor during a distillation?

Starting with a mixture of 1-propanol and 2-propanol with mole fractions of 0.75 and 0.25 respectively, calculate the mole fraction of the vapor. Draw a horizontal tie line from the Pvap line to that new mole fraction.

Is the vapor becoming more enriched in the expected compound?

Condense that vapor using a vertical line back to the liquid line. Now, repeat the vaporization and condensation process a 2nd time, drawing two more lines on your diagram.

Repeat a third time. What is the composition of the liquid after three distillation events?

****

Below is a graph of temperature vs. composition for the binary mixture of ethyl acetate and benzene.[[1]](#footnote-1)‡

What is the boiling point of ethyl acetate? Of benzene?

Which species will be enriched during the distillation?

If you start with a mixture that is 10 mol% ethyl acetate and 90 mol% benzene, use the graph to determine the composition and boiling temperature of of the mixture after three distillation events (one series of evaporation and condenstation counts as a single event).

**{T vs mole fraction ethyl acetate graph from reference shown here}**

**Challenge problem**

Here is a temperature vs. composition diagram for the non-ideal mixture of 1,4-dioxane and water;[[2]](#footnote-2)† a similar diagram is obtained for ethanol and water. It is helpful to think of this as two phase diagrams in one, where the solution with composition of about 82% (by mass) dioxane is one end of two phase diagrams, one paired with 100% water and the other with 100% dioxane. Which line corresponds to the composition of the liquid and which line corresponds to the composition of the vapor (and how can you tell?) Hint: at constant composition, does a vapor or a liquid have a higher or lower temperature? Hint 2: at constant temperature, is the vapor or the liquid more enriched in the lower boiling component?

What happens if you distill a mixture of 95% dioxane (by mass)? What happens if you distill a mixture of 35% dioxane (by mass)?

**{dioxane water phase diagram from reference shown here}**

**Reading assignment due by class time Friday Dec 2, 2016**

Read Box 4D.1 “Alternative Fuels.” Based on what you read, is hydrogen a renewable fuel? Are there sources of hydrogen that are renewable? What about methane?

Ethanol is considered to be a renewable fuel. The US government has set a target to reach 1.4·1011 L of ethanol per year. What is the current production of ethanol in the US? How much do we need to increase production?

A quick Google search shows that an acre of US corn field yields 7000 pounds of corn, or 330 gallons of ethanol. How many acres of land are required to reach 1.4·1011 L of ethanol? What percent of the US is this? For more information on this topic, see <https://www.news.cornell.edu/stories/2001/08/ethanol-corn-faulted-energy-waster-scientist-says> and <http://www.forbes.com/sites/jamesconca/2014/04/20/its-final-corn-ethanol-is-of-no-use/#6bab49032ca2>.

Biodiesel is prepared from vegetable oil by transesterification of the triglyceride to make simple esters of fatty acids (we saw this in Module 1a). Why do you think these tend to solidify at low temperatures?

Read Topic 3J.2 “Semiconductors” and examine Figures 3J.4, 3J.5 and 3J.12. Read Topic 3J.4, focusing on the last paragraph on Light-emitting diodes.

Figure 3J.12 shows luminescence (emission of light) by electrons falling from the conduction band to the valence band at a pn junction. This requires electrical energy. What would happen if you shone light onto the device that corresponded to the band gap of the material?

**In class activity Day 2 Friday Dec 2, 2016**

-none-

There will be a lecture and discussion on solar energy conversion

**Reading assignment due by class time Monday Dec 5, 2016**

Do the following practice calculations on the fuel isopropanol (the fuel from Friday’s demo) so you will be able to do them more quickly in class.

1) Write a balanced combustion reaction for isopropanol (CH3)2CHOH (l). Combustion is the process where one mole of fuel reacts with O2 (g) to give CO2 (g) and H2O (l).

2) Use standard enthalpies of formation to determine the enthalpy change (ΔHc°) associated with combustion of isopropanol. ∆Hf° for isopropanol is -318.2 kJ/mol

3) Calculate the energy density of isopropanol. Energy density is defined in four ways, and it is always a positive number so take the absolute value:

1. kJ of heat per mole of fuel
2. kJ of heat per mole of carbon
3. kJ of heat per gram of fuel
4. kJ of heat per milliliter of fuel (isopropanol has a density of 0.786 g/mL)

4) Determine how many mmol of CO2 are produced per |kJ of heat| (absolute value).

5) Determine the price of the fuel, reported in cents (0.01 $) per MJ (1000 kJ) heat produced. Isopropanol costs $1000 per 1000 kg.[[3]](#footnote-3)ξ It is much more expensive ($44/5 gal) when purchased on small scale.

**In class activity Day 2 Monday Dec 5, 2016**

Energy derived from fuels is a complex topic. To properly discuss energy we must consider several interrelated concepts:

 the chemistry of the chemical reaction (combustion)

 the costs of the fuel

 actual costs

 environmental costs (CO2 emission, for example, but also pollution)

 “political squabbles” over a desirable resource

 properties of the fuel

 energy density (energy per g/L/mol C/mol CO2)

 ease of storage and transport

In this exercise, your group will evaluate three potential fuels for use in our society. You will be tasked to choose the “best” fuel, and in order to do that, you will have to define “best” for your group. There is no absolutely correct answer to this question, but each class will vote on the overall “best” fuel based on the arguments you present in class.

**Deliverables:**

- By the end of class, fill out the table on the Google sheet linked from Sakai so the class can evaluate all the fuels

- prepare two to three talking points that allow you to define “best” in the context of fuels

- select your “best” fuel, according to your definition

- during the the last 10 minutes of class, each group will share their definition of “best” and share their chosen “best” fuel

Points to Consider in Formulating Your Recommendation:

1. Energy density in terms of mole, moles of carbon, and mass.
2. Cost of energy in both dollars and societal cost.
3. What is your definition of the “best” fuel?

**Table 1. Standard heats of formation, densities, and prices for common fuels.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Fuel #** | **Fuel** | **ΔfH°(kJ/mol)** | **density (g/mL)** | **Price** |
| 1 | *Hydrogen (H2)* | **0 (gas)** | **8.99·19-5** | **$6/kg** |
| 2 | *Coal (C)* | **0 (solid)** | **1.100** | **$65/metric ton††** |
| 3 | *Natural Gas (methane, CH4)* | **–74.9 (gas)** | **6.67·10-4** | **$2.09/GGE†** |
| 4 | *Methanol (CH3OH)* | **–238.4 (liquid)** | **0.791** | **$6/gallon¶** |
| 5 | *Formaldehyde (CH2O)* | **–177.6 (solid)** | **0.880** | **$16.5/kg** |
| 6 | *Formic acid (HCO2H)* | **–425.0 (liquid)** | **1.220** | **$1250/tonne††** |
| 7 | *Propane (C3H8)* | **–104.7 (liquid)** | **0.582** | **$0.67/pound** |
| 8 | *Octane (C8H18)* | **–208.4 (liquid)** | **0.703** | **$4/gallon¶** |
| 9 | *Biodiesel (C18H31O2CH3)¬* | **-604.88 (liquid)** | **0.889** | **$2.92/gallon¶\*** |
| 10 | *Ethanol (C2H5OH)* | **-277.0 (liquid)** | **0.789** | **$2.13/gallon¶\*** |
| 11 | *Glucose (C6H12O6)* | **-1271 (solid)** | **1.540** | **$1.00/pound\*\*** |
| 12 | *Sucrose (C12H22O11)* | **-2221.2 (solid)** | **1.587** | **$0.50/pound\*\*** |

\*Prices of these fuels include government subsidies; the actual cost is higher by almost $1.50/gallon

\*\*prices of these fuels include government support; the actual cost is lower by about 0.05/pound; a pound is 0.454 kg

† gasoline-gallon equivalent = GGE; one GGE for natural gas = 1 gal CNG \* 0.25

†† one metric ton (tonne) is 1000 kg

¬ Biodiesel is a mixture of straight chain fatty acid esters made by trans esterification (seen in module 1a!); it is modeled here as linoleic acid methyl ester, a liquid.

¶ a gallon is 3.79 liters

**Table 2. Standard heats of formation for other compounds involved in combustion.**

|  |  |
| --- | --- |
| *Oxygen (O2 (g))* | **ΔfH° = 0 kJ/mol** |
| *Carbon Dioxide (CO2 (g))* | **ΔfH° = –393.5 kJ/mol** |
| *Water (H2O (l))*  | **ΔfH° = –285.8 kJ/mol** |

**Exercises**

1) Write a balanced combustion reaction for each of your three assigned fuels. Combustion is the process where one mole of fuel reacts with O2 (g) to give CO2 (g) and H2O (l).

2) Use standard enthalpies of formation to determine the enthalpy change (ΔHc°) associated with combustion of isopropanol.

3) Calculate the energy density of your three fuels. Energy density is defined in four ways, and it is always a positive number so take the absolute value:

1. kJ of heat per mole of fuel
2. kJ of heat per mole of carbon
3. kJ of heat per gram of fuel
4. kJ of heat per milliliter of fuel

For each of your three assigned fuels, determine the energy content in each of the 3 above ways. Fill in your answers on the Google doc linked from Sakai. If your value(s) differ(s) from that of another group, record your value in the cell, separating it with a comma.

4) Due to concerns about global climate change, we are also very interested in CO2 emissions. For each of your three fuels, determine how many mmol of CO2 are produced per |kJ of heat| (absolute value). Enter this value into the spreadsheet.

5) Determine the price of the fuel, reported in cents (0.01 $) per MJ (1000 kJ) heat produced. Enter this value into the spreadsheet.

6) Looking at the class data, can you pick out any trends with respect to the different fuels? What elemental compositions have large ∆­Hr° values?

What fuels or fuel types have large energy densities?

What is the best fuel if we want to minimize CO2 production?

What are potential problems associated with this/these fuels?

7) Considering these points, list approximately three factors that you will use to decide upon your “best” fuel. Select the fuel that you think is “best.”

Your Group’s Fuels:

**Balanced chemical reactions for each fuel:**

1

2

3

**Standard enthalpy of combustion (∆Hc°) for each fuel:**

1

2

3

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Fuel #** | **Fuel** | **Energy Density (kJ/mol)** | **Energy Density (kJ/mol C)** | **Energy Density (kJ/g)** | **mmol CO2 per kJ heat produced** | **Price (0.01$) per MJ heat**  |
| 1 |  |  |  |  |  |  |
| 2 |  |  |  |  |  |  |
| 3 |  |  |  |  |  |  |

**Criteria for “best” fuel:**

**1.**

**2.**

**3.**

**4.**

**Your group’s best fuel:**

1. ‡ Prediction of Solubility of Active Pharmaceutical Ingredients in Single Solvents and Their Mixtures — Solvent Screening, by Ehsan Sheikholeslamzadeh and Sohrab Rohani, in  ["Recent Advances in Thermo and Fluid Dynamics,"](http://www.intechopen.com/books/recent-advances-in-thermo-and-fluid-dynamics) DOI: 10.5772/60982 [↑](#footnote-ref-1)
2. † https://en.m.wikipedia.org/wiki/File:Binary\_phase\_diagram\_dioxane-water.svg [↑](#footnote-ref-2)
3. ξ https://www.alibaba.com/showroom/bulk-isopropanol-price.html [↑](#footnote-ref-3)