AC 2012-4013: AN UNDERGRADUATE EDUCATIONAL MODULE ON THERMODYNAMIC ANALYSIS OF PETROLEUM AND BIO-BASED FUELS IN INTERNAL COMBUSTION ENGINES

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An Undergraduate Educational Module on Thermodynamic Analysis of Petroleum and Bio-based Fuels in Internal Combustion Engines

Abstract
This paper describes a newly developed undergraduate educational module on the Thermodynamic Analysis of Petroleum and Bio-based Fuels in Internal Combustion Engines, created as part of an AIChE Grand Energy Challenge Award. The module is designed to introduce undergraduate Chemical Engineering students to the topic of liquid transportation fuels generated from renewable and petroleum based resources from a thermodynamics prospective. Furthermore, the module introduces students to the typical types of internal combustion engines and the thermodynamic principles behind them; provides an overview of the most common petroleum and biobased liquid transportation fuels; and introduces the concept of life cycle assessment as it applies to liquid transportation fuels.

Background

The Grand Energy Challenge is a program launched by the AIChE Center for Energy Initiatives to develop educational materials for equipping chemical engineering graduates with the tools needed to tackle the challenge of providing society with clean, affordable and sustainable energy sources. The Grand Energy Challenge Award is a competitive grant given to faculty to develop innovative educational modules focusing on energy. The first Grand Energy Challenge Award was specifically directed towards developing materials for the chemical engineering thermodynamics course (Keith, *et al.*, 2011).

The module developed by the authors for the Grand Energy Challenge focuses on the thermodynamic properties of both petroleum derived and biomass derived liquid transportation fuels. Liquid fuels are by far the preferred fuel for transportation. Solid phase fuels, like coal, are less convenient; and gas phase fuels present a safety risk due to storage at elevated pressures. Because of these and other factors, liquid fuels – whether biobased or petroleum based - are the most common choice as a transportation fuel and thus were chosen as the basis for the module. In addition to coverage of liquid fuels and their properties, thermodynamic cycles of internal combustion engines, life cycle assessment of biobased and petroleum based fuels, and the solar equivalency of liquid fuels is also presented.

Educational materials that introduce students to concepts of energy generation and usage are important. The National Science Board has recently called the transformation of the U.S. fossil fuel-based energy economy to a sustainable energy economy a critical grand challenge facing the country (NSB, 2009). Furthermore, the US Department of Energy has called for replacing 30% of the nation's fossil-based fuels by 2030 (U.S. DOE 2008). Additionally, the Energy Independence and Security Act of 2007 (EISA 2007) (Public Law, 2007) mandates the production of 36 billion gallons per year of biofuels by 2022, of which 21 billion must come from feedstock other than corn starch and at least 16 billion gallons must come from lignocelluloses (Regalbuto, 2009). Therefore, an understanding of the properties of both biobased and petroleum based fuels as well as understanding their benefits and drawbacks as transportation fuels are important for future engineering graduates.

Module Objectives

The module is intended as a supplement for the traditional Chemical Engineering Thermodynamics course offered as part of the core curriculum at most universities. The objectives of the module are for students, upon completion of the module, to be able to:

- Perform thermodynamic efficiency analyses on conventional and alternative fuel sources in Otto and Diesel cycle engines,
- Critically evaluate the comparative efficiency of biomass derived fuels compared with conventional fuels,
- Compare on a solar energy basis the produced value of biomass fuels compared with fossil fuels and other alternative fuels,
- Perform a life-cycle assessment on biomass derived fuels on an economic basis.

Module Materials

In addition to a complete set of PowerPoint lecture slides with detailed instructor notes, the module includes set of test/homework problems with solutions, solved in class-example problems and a pre-/post-test to assess students understanding of the module material. Also included with the module is a self-guided student inquiry activity that utilizes an interactive spreadsheet application that simulates the performance of Diesel cycle and Otto cycle engines with a variety of petroleum based and biobased liquid fuels under a range of engine operating conditions. The simulator allows students to select an appropriate fuel based on engine selection, change the compression ratio, enter a cylinder volume, select an expansion ratio (for Diesel engines), and even compress the gas mixture entering the cylinder with a turbocharger. Additionally, students can also select a real production vehicle and choose operational parameters to correspond to that vehicle.

Lecture Slides

The lecture slides begin with and overview of liquid fuels and their use as the primary energy source for transportation. As it turns out, however, not all liquid fuels are created equal. Different fuels have different energy content per unit volume due to both differences in density and energy content on a molecular basis. The calculation of higher heating value is incorporated into the module to illustrate this concept.

Next, the concept of thermodynamic cycles is introduced. Most internal combustion engines used for transportation operate on either the Diesel or Otto cycle. These cycles are covered in detail in the module and cycle efficiency and turbo charging is discussed. The effect of engine configuration on fuel economy is also presented.

Figure 1. Solar basis of petroleum based and biobased liquid fuels

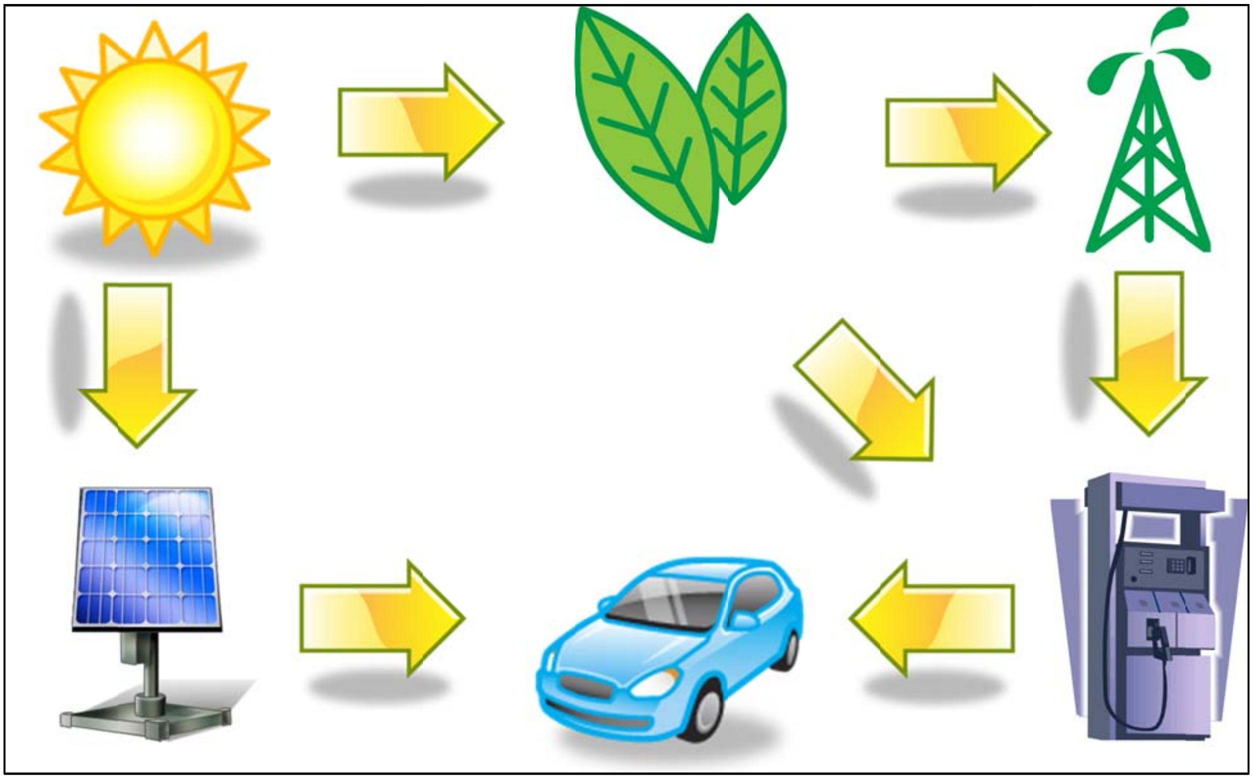

Figure 1. Solar basis of petroleum based and biobased liquid fuels

After the discussion of thermodynamic cycles, an overview of the characteristics of various fuels is presented, along with the pros and cons of their use as transportation fuels. Petroleum based fuels like petroleum diesel, gasoline and methanol and renewable fuels like biodiesel, biobutanol, ethanol and Fischer-Tropsch fuels are covered.

Following the discussion of engines and fuels, an overview of the lifecycles of biobased and petroleum based fuels are presented, as shown in Figure 1, along with the solar basis for liquid fuels. Finally, a set of in-class example problems are provided to illustrate some of the key concepts in the module.

Integrated Inquiry Activity

As a supplement or an alternative to parts of the lecture oriented materials, a pair of interactive inquiry activities designed to allow students to independently explore the effects of different fuels on Otto and Diesel cycle engine performance is included. The activities guide students through the use of a Microsoft Excel-based simulation tool to explore the roles of fuel composition and engine operating parameters in engine performance. A screen shot of the simulator interface that accompanies the inquiry activities is shown in Figure 2. The interface allows students to choose engine parameters with suggestions from a variety of actual commercial engine specifications, including turbocharged and supercharged options, to make the activity more realistic. Multiple fuel options are also available, enabling the student to explore, for example, the effect of using race car fuel in an economy car, or diesel fuel in a gasoline engine. Commentary is provided to caution students about real world performance issues associated with certain parameter choices.

The activities call for the student to first **predict** ideal engine performance under different scenarios. Next, the students will use the simulator to **explore** the effects of changing parameters. Initial changes are specified in detail to acquaint students with the simulator, with subsequent explorations requiring students to make decisions regarding how to determine answers. Students utilizing the activity are frequently encouraged to look at additional options and scenarios according to their interests. Finally, students are asked to **reflect** on both their initial predictions and their explorations from both a thermodynamic and a societal perspective. Possible answers to the questions are provided in an instructor's version of the activities. The modules are modeled after the inquiry activities described by Vigeant (Vigeant, *et al.*, 2011).

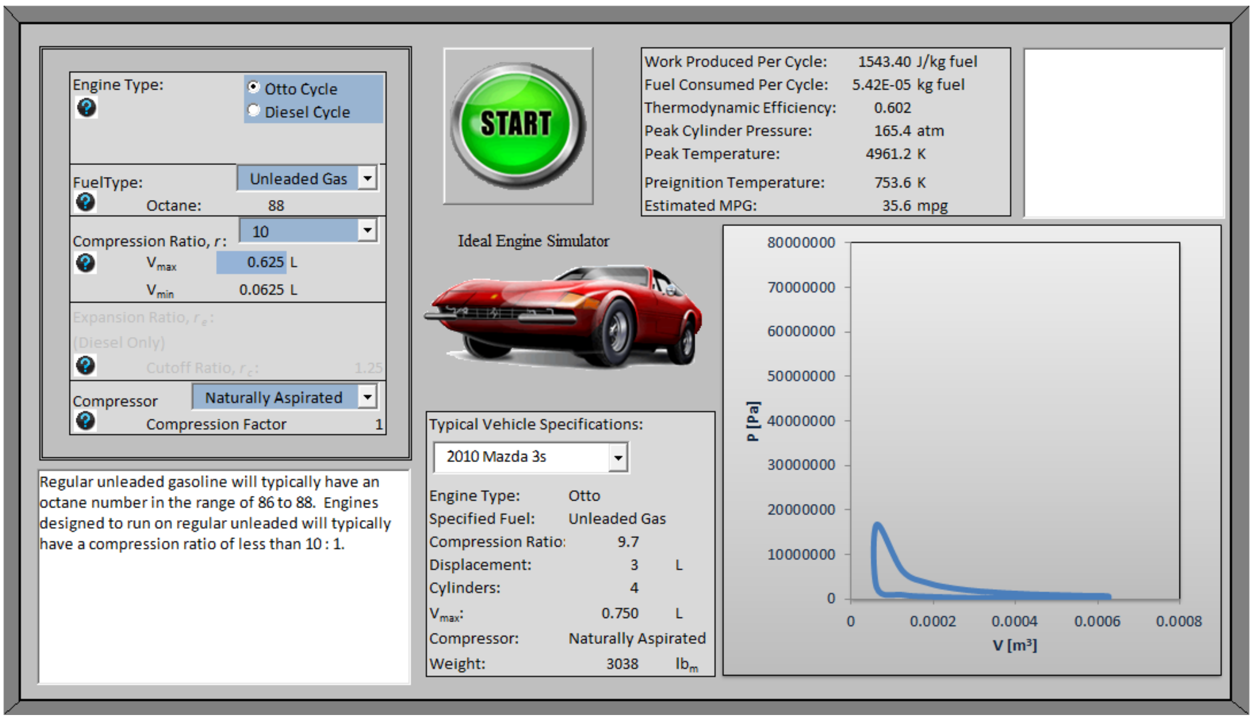

Figure 2. Screen capture of interactive spreadsheet activity.

Homework / Examination Problems

The module includes a set of homework / exam problems that are intended to reinforce the concepts presented in the module. Three problems are available with the module. The problems cover thermal efficiency of biomass, utilizing biomass and fuel, and the efficiency of thermodynamic cycles. Solutions for each of these problems are available to credentialed course instructors.

Outcomes Assessment

Included with the module is a pre- / post- assessment test. This test allows the course instructor to gauge the students' baseline knowledge of the concepts to be presented in the module and the students' retailed knowledge after completing the module. The assessment test consists of 10 multiple choice questions covering each of the major topics presented in the module. The assessment test is shown in Table 1, below. Assessment data from the first class of chemical engineering thermodynamics students to utilize the fully implemented module is currently being compiled and will be made available in a planned future publication.

Table 1. Pre- / Post Assessment Test for Energy Module

1) Modern spark ignition internal combustion engines are based on which one of the following thermodynamic cycles:				
a) Diesel Cycle	b) Rankine Cycle	c) Otto Cycle	d) Carnot Cycle	e) Stirling Cycle
2) Modern compression ignition internal combustion engines are based on which one of the following thermodynamic cycles:				
a) Diesel Cycle	b) Rankine Cycle	c) Otto Cycle	d) Carnot Cycle	e) Stirling Cycle
3) The amount of energy potentially liberated from a fuel by combustion is known as the:				
a) Energy Index Number	b) Octane Number	c) Heating Value	d) Fuel Index	e) Cetane number
4) Which of the following step might be included in a biofuel life cycle assessment?				
a) Production of fertilizer	b) Grain storage	c) Fermentation	d) Production of herbicides	e) All of the above
5) True or False: Both biomass derived and petroleum derived liquid fuels are forms of stored solar energy.				
a) True	b) False			
6) Which of the following liquid fuels has the highest energy content per unit volume?				
a) Ethanol	b) Gasoline	c) Biobutanol	d) No. 2 Fuel Oil	e) Methanol
7) Which of the following liquid fuels has the lowest energy content per unit volume?				
a) Ethanol	b) Gasoline	c) Biobutanol	d) No. 2 Fuel Oil	e) Methanol
8) Which of the following liquid fuels requires the highest compression ratio when burned in an internal combustion engine?				
a) Premium Unleaded Gasoline	b) E85	c) Methanol	d) Regular Unleaded Gasoline	e) Biobutanol
9) The gasification of biomass in the presence of steam produces a product called:				
a) Synthesis gas	b) Biogas	c) Methane	d) Fuel gas	e) Hydrogen
10) Enough solar energy reaches earth every day to more than cover all of our energy needs, however, without concentration and storage this energy is of low value due to the limitations of:				
a) Newton's 1st law of Motion	b) The 2nd Law of Thermodynamics	c) The 1st Law of Thermodynamics	d) Gibbs Free Energy	e) The Joule-Thompson effect

Integration with Leading Textbooks

This module has not been designed with a specific thermodynamics textbook in mind. The coverage of internal combustion engines in popular textbooks used in chemical engineering thermodynamics is limited, and coverage of alternative fuels is essentially absent. Table 2 summarizes coverage in selected textbooks.

Summary

The complete module can be downloaded from http://www.aiche.org/IFS/education.aspx. Instructor materials, including an instructor's version of the inquiry activity and answers to the pre- / post- test, are available to credentialed course instructors by contacting the authors at jseay@engr.uky.edu or silverdl@engr.uky.edu.

Table 2. Coverage of ideal internal combustion engine cycles and alternative fuels in chemical engineering thermodynamics textbooks.

Chemical Engineering Thermodynamics Textbook	**Coverage of internal combustion engine cycles**	**Coverage of alternative fuels**
Elliot, J. Richard, Carl T. Lira, *Introductory Chemical Engineering Thermodynamics*, Prentice Hall, 1999.	Chapter 4	No
Koretsky, Milo D., *Engineering and Chemical Thermodynamics*, Wiley, 2004.	No	No
Kyle, B.G., *Chemical and Process Thermodynamics*, 3rd Ed., Prentice Hall, 1999.	No	No
Sandler, Stanley L., *Chemical, Biochemical, and Engineering Thermodyanmics*, 4th Ed., Wiley, 2006.	No	No
Smith, J.M., H.C.VanNess, M.M. Abbott, *Introduction to Chemical Engineering Thermodynamics*, 7th Ed., McGraw Hill, 2005.	Chapter 8	No

Acknowledgements

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