# Basic Chemistry & Overview

Lecture 8 – Fuel Chemistry

When you have a chance please visit the shown link and read about the Capstone CMT-380 Hybrid Supercar. This car is powered by a turbine instead of an internal combustion engine. It is a hybrid vehicle and the turbine is used to drive an electric motor. This makes it fuel flexible and gives it outstanding mileage and power. In some ways, it is one of the most compelling developments in hybrid car technology in quite some time.

http://www.gizmag.com/capstone-cmt-380-an-electric-hybrid-featuring-wind-turbines/13517/

## Week 3 – Basic Chemistry & Overview
## -Learning Objectives-

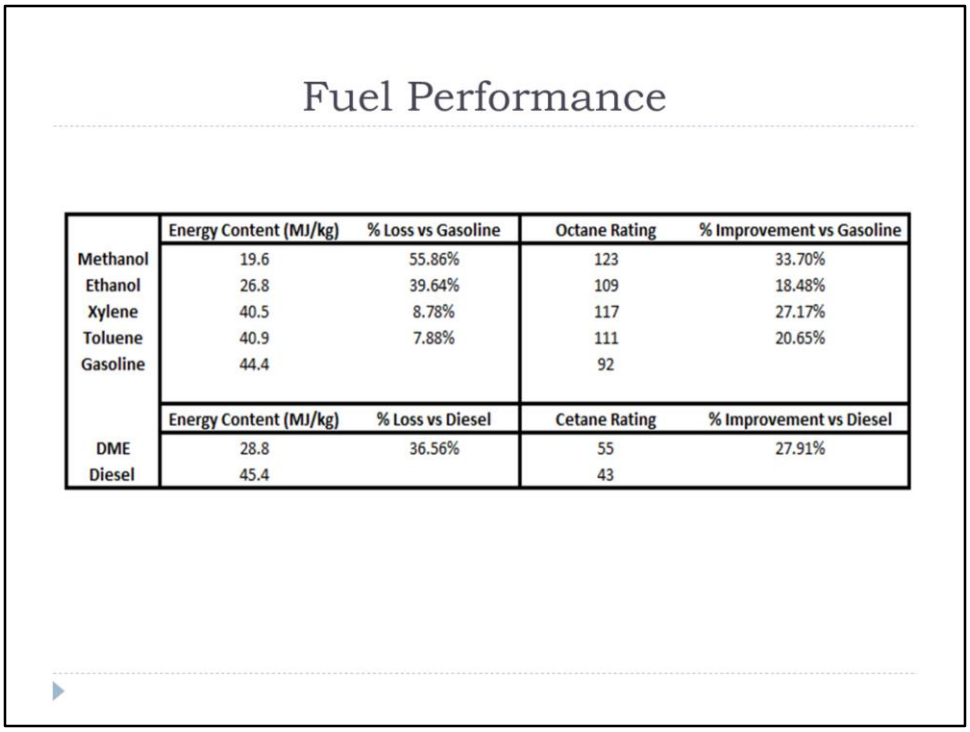
- Recall the 4 common denominators of the bioenergy industry and list their subsets.
- Recognize the basic chemical characteristics of biomass and fuels.
- Describe what makes a good fuel

## Lots of confusing fuel names

- Bio-oil is not the same thing as biological oils
- Biogas is not the same thing as bio-gasoline
- Biodiesel is not the same thing as renewable diesel
- Blendstock is not the same thing as drop-in



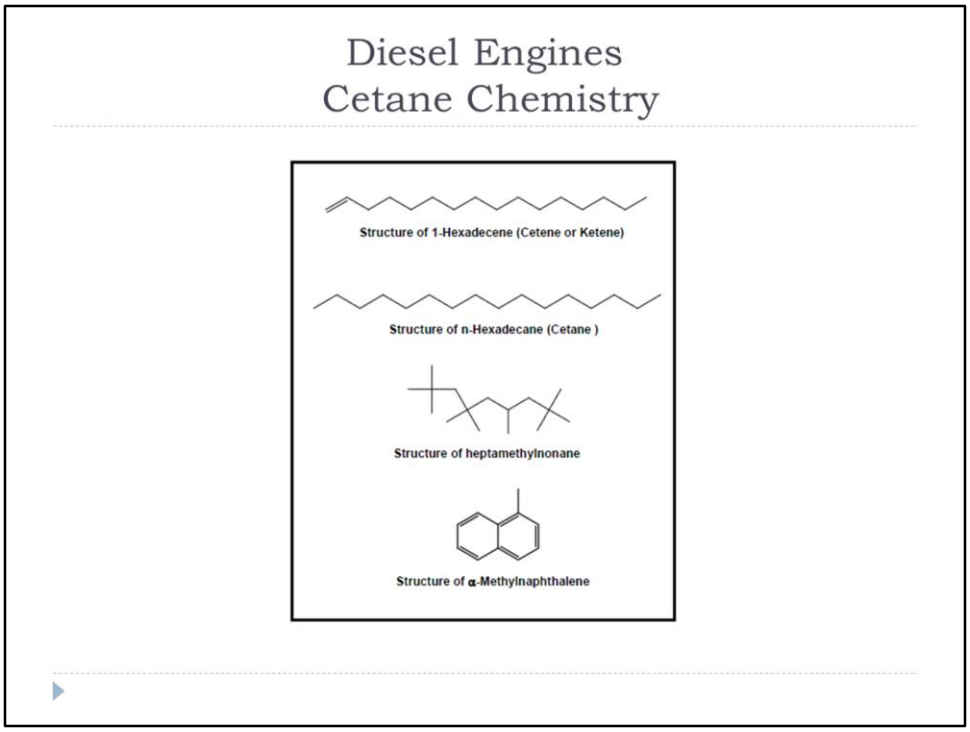
As you learn about bioenergy you will almost certainly find yourself confused by the various naming conventions. Like most names they have been largely based on marketing and not on facts. For example, bio oils generally mean pyrolysis oils which have no chemical similarity to petroleum or vegetable oils. Biogas actually means biologically produced methane, or natural gas, and has nothing to do with gasoline. Biodiesel is an interesting one because it almost exclusively composed of something called fatty acid methyl esters which makes it a very pure fuel, compared to renewable diesel which is a mixture of hydrocarbon components more like regular diesel. Finally the word blendstock is thrown around a lot because most biofuels are in fact blendstocks. This means it has to be mixed with regular gasoline or diesel at some level to be a fuel that works well in the engines commonly available today. If there are any questions about these terms as we learn more about different conversions, please ask. It is much easier to understand everything when the terms are clear.




DME is dimethyl ether and it is commonly regarded as a renewable diesel alternative.

It is very important to remember that diesel and gasoline engines have been designed for different kinds of fuel. This means that each engine has a preferred type of fuel for its design and this type of fuel has its own engine specific fuel performance characteristics (octane value or cetane value). Octane and Cetane value describe how well a fuel will perform in an engine, not the energy content of the fuel.

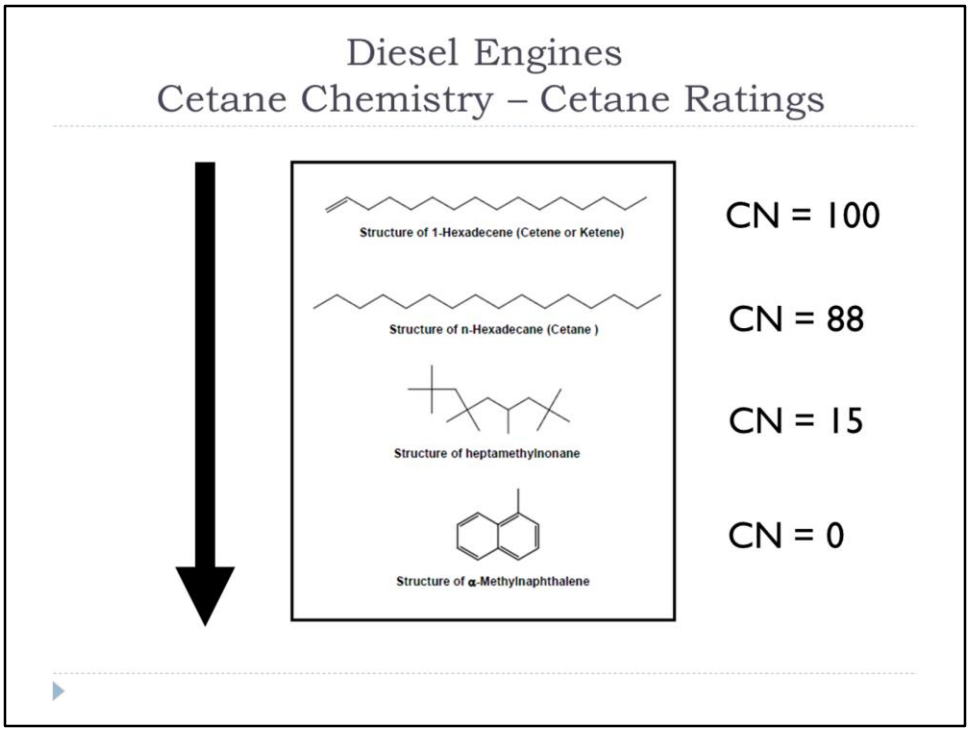
Energy content and engine performance (octane/cetane) cannot be separated and in fact must always be considered together when considering new fuels, or how an engine type will perform on a new fuel.




http://en.wikipedia.org/wiki/Cetane_number

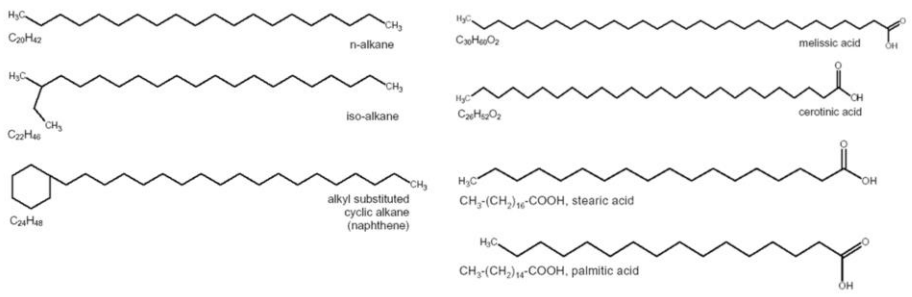
From Wikipedia:

Cetane is a chemical compound, alkane (named hexadecane after IUPAC rules; chemical formula n-C16H34), molecules of which are un-branched and with open chain. Cetane ignites very easily under compression, so it was assigned a cetane number of 100, while alpha-methyl naphthalene was assigned a cetane number of 0. All other hydrocarbons in diesel fuel are indexed to cetane as to how well they ignite under compression. The cetane number therefore measures how quickly the fuel starts to burn (auto-ignites) under diesel engine conditions. Since there are hundreds of components in diesel fuel, with each having a different cetane quality, the overall cetane number of the diesel is the average cetane quality of all the components (strictly speaking high-cetane components will have disproportionate influence, hence the use of high-cetane additives).



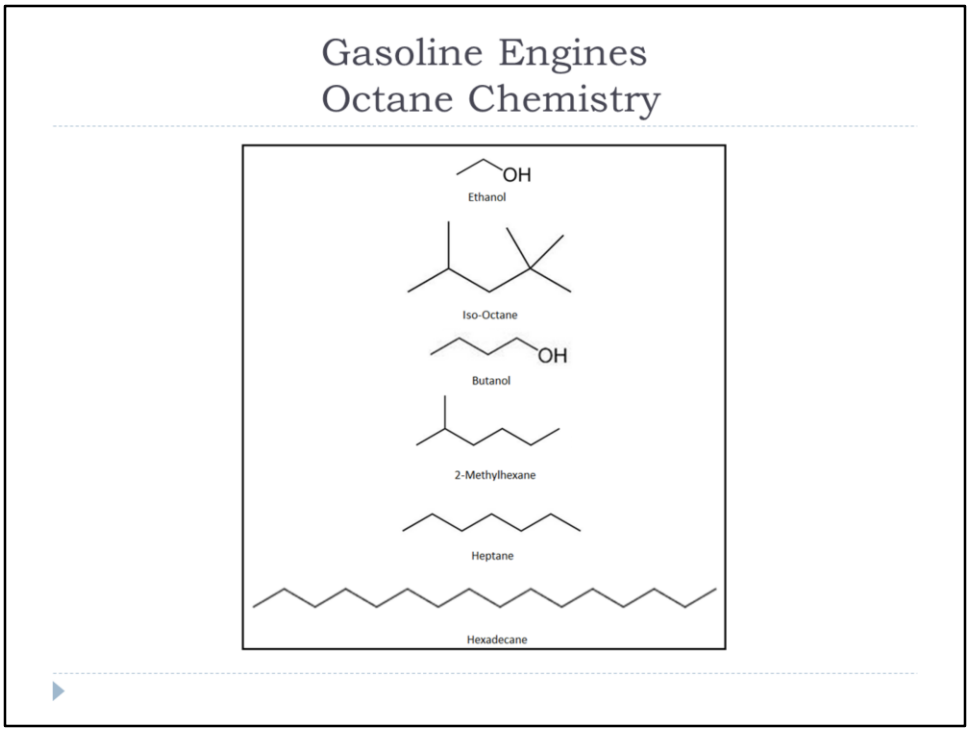

These are the decreasing CN numbers for these fuel chemicals. Notice how as the chemical structure changes the CN changes.

# You can see why oil and biological oils can be good resources for diesel fuels




Petroleum Oils

Biological Oils



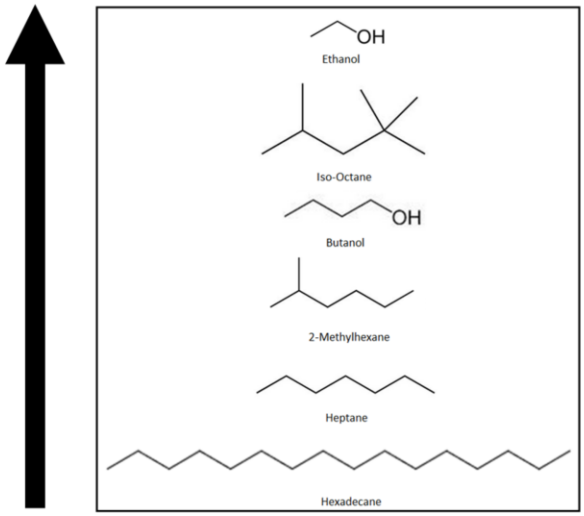

http://en.wikipedia.org/wiki/Octane_rating

From Wikipedia:

The octane rating of gasoline is measured in a test engine and is defined by comparison with the mixture of 2,2,4-trimethylpentane (iso-octane) and heptane that would have the same anti-knocking capacity as the fuel under test: the percentage, by volume, of 2,2,4-trimethylpentane in that mixture is the octane number of the fuel. For example, petrol with the same knocking characteristics as a mixture of 90% iso-octane and 10% heptane would have an octane rating of 90.[2] A rating of 90 does not mean that the petrol contains just iso-octane and heptane in these proportions, but that it has the same detonation resistance properties (generally, petrol sold for common use never consists solely of iso-octane and heptane; it is a mixture of several different hydrocarbons, and often other additives). Because some fuels are more knock-resistant than pure iso-octane, the definition has been extended to allow for octane numbers greater than 100.

Octane ratings are not indicators of the energy content of fuels. (See Effects below and Heat of combustion). They are only a measure of the fuel's tendency to burn in a controlled manner, rather than exploding in an uncontrolled manner. Where the octane number is raised by blending in ethanol, energy content per volume is reduced. Ethanol BTUs can be compared with gasoline BTUs in heat of combustion tables.

# Gasoline Engines
## Octane Chemistry – Octane Ratings




RON = 108.6

RON = 100

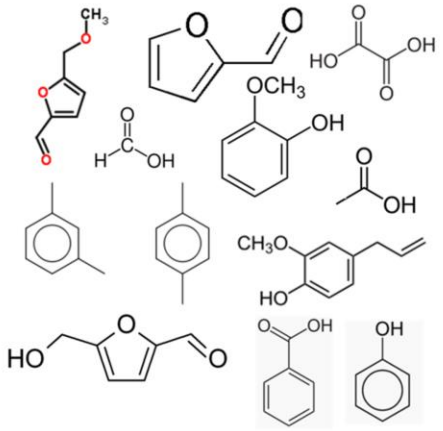
RON = 92

RON = 44

RON = 0

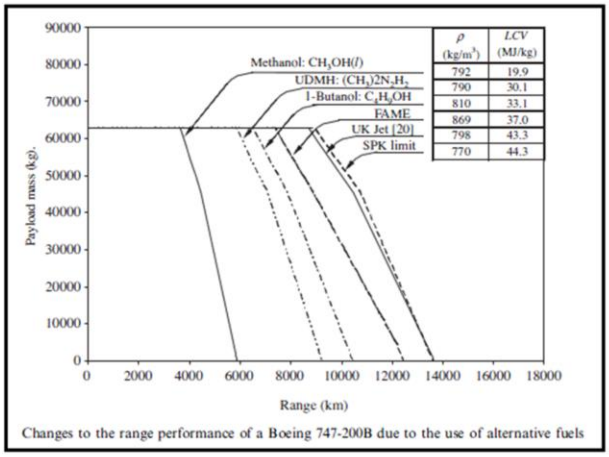
RON = -30

# Bio-oils are closest to gasoline, but they have too much oxygen and are extremely acidic




- If you react bio-oil with high levels of hydrogen you can make it look more like gasoline (remove $O_2$ as $H_2O$ and $CO_2$)

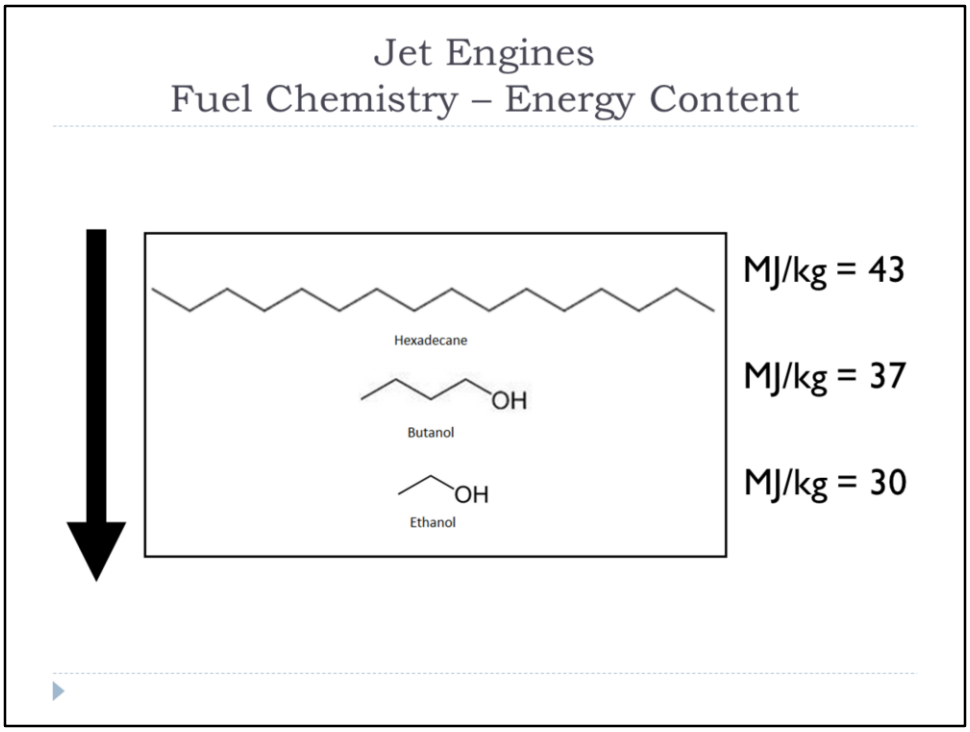
## Jet Engines
## Fuel Chemistry



Changes to the range performance of a Boeing 747-200B due to the use of alternative fuels

Blakey, Simon, Lucas Rye, and Christopher William Wilson. "Aviation gas turbine alternative fuels: A review." Proceedings of the combustion institute 33.2 (2011): 2863-2885.

Jet fuel has almost nothing to do with internal combustion engine fuels – the most important thing for a jet fuel is energy content.

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# Fuel is almost always a mixture!

**Aromatic Species Analysis by ASTM D6379 for Alternative Fuels**

| aromatics (vol %) | JP-8 | Shell FT | Sasol FT | Rentech FT | R-8 HRJ | tallow HRJ | camelina HRJ |
|---|---|---|---|---|---|---|---|
| monoaromatics | 15.1 | <0.2 | 0.4 | 1.5 | 0.3 | <0.2 | <0.2 |
| diaromatics | 1.6 | <0.1 | <0.1 | <0.1 | <0.1 | <0.1 | <0.1 |
| total aromatics | 16.7 | <0.2 | 0.4 | 1.5 | 0.3 | <0.2 | <0.2 |
| total saturates | 83.3 | >99.8 | 99.6 | 98.5 | 99.7 | >99.8 | >99.8 |

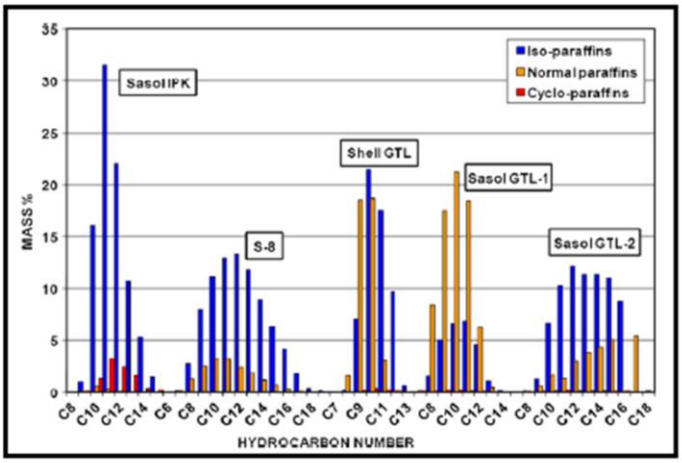
**Hydrocarbon Type Analysis by ASTM D2425 for Alternative Fuels**

| hydrocarbon type (vol %) | JP-8 | Shell FT | Sasol FT | Rentech FT | R-8 HRJ | tallow HRJ | camelina HRJ |
|---|---|---|---|---|---|---|---|
| paraffins (normal + iso) | 50 | >99 | 88 | 92 | 92 | 98 | 90 |
| *cyclo*-paraffins | 34 | <1 | 12[a] | 7[a] | 8[a] | 2 | 10 |
| alkylbenzenes | 12 | <0.3 | 0.4 | 1.3 | <0.3 | <0.3 | <0.3 |
| indans and Tetralins | 3 | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 |
| indenes and $C_nH_{2n-10}$ | 0.4 | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 |
| naphthalene | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 |
| naphthalenes | 1.4 | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 |
| acenaphthenes | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 |
| acenaphthylenes | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 |
| tricyclic aromatics | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 | <0.3 |
| total | 100 | 100 | 100 | 100 | 100 | 100 | 100 |



Corporan, Edwin, et al. "Chemical, thermal stability, seal swell, and emissions studies of alternative jet fuels." Energy & Fuels 25.3 (2011): 955-966.

## Fuel is almost always a mixture!



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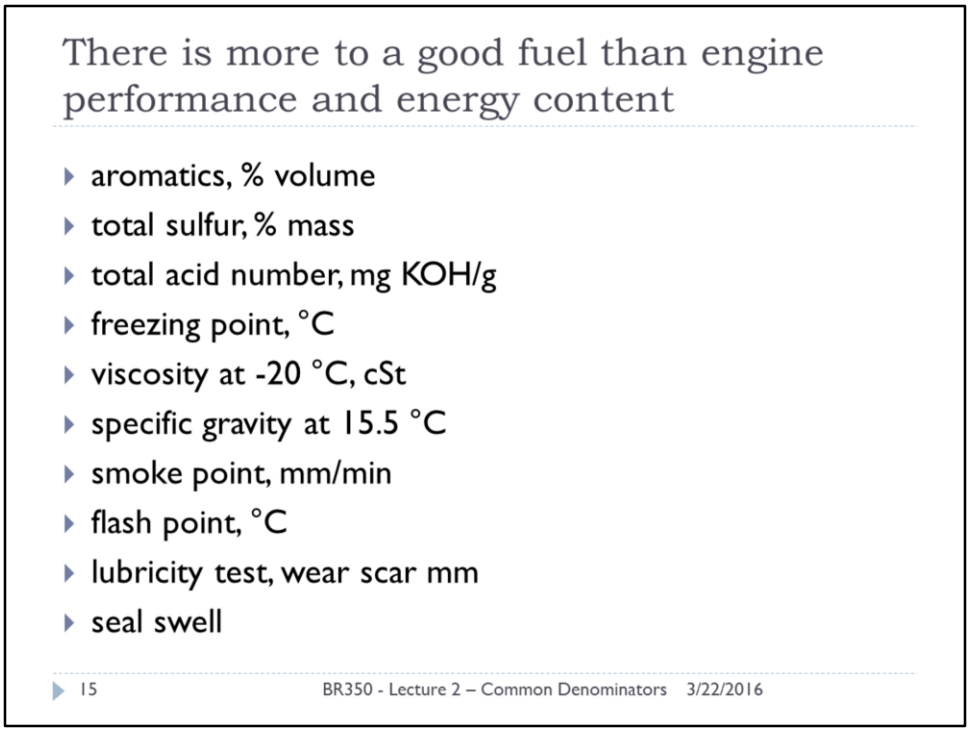


A good fuel can be an exotic cocktail of organic chemistries meant to provide good overall vehicle performance and meet regulations. A good fuel serves the needs of the entire vehicle and not just the engine.

## Next Lecture – Bioenergy Industry Overview




http://www.hybridcars.com/electrified-hybrid-turbine-powered-trucks-in-walmart-future/

Turbine powered semi – maybe the future?