Non-Traditional Fuels for High-Efficiency, Clean-Combustion Engines

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Research Supported by
US DOE Office of FreedomCAR and Vehicle Technologies (Kevin Stork) and Caterpillar Inc. (David Milam, Michael Radovanovic)

Western States Section of the Combustion Institute, Fall Technical Meeting
Sandia National Laboratories, Livermore, CA
October 16, 2007

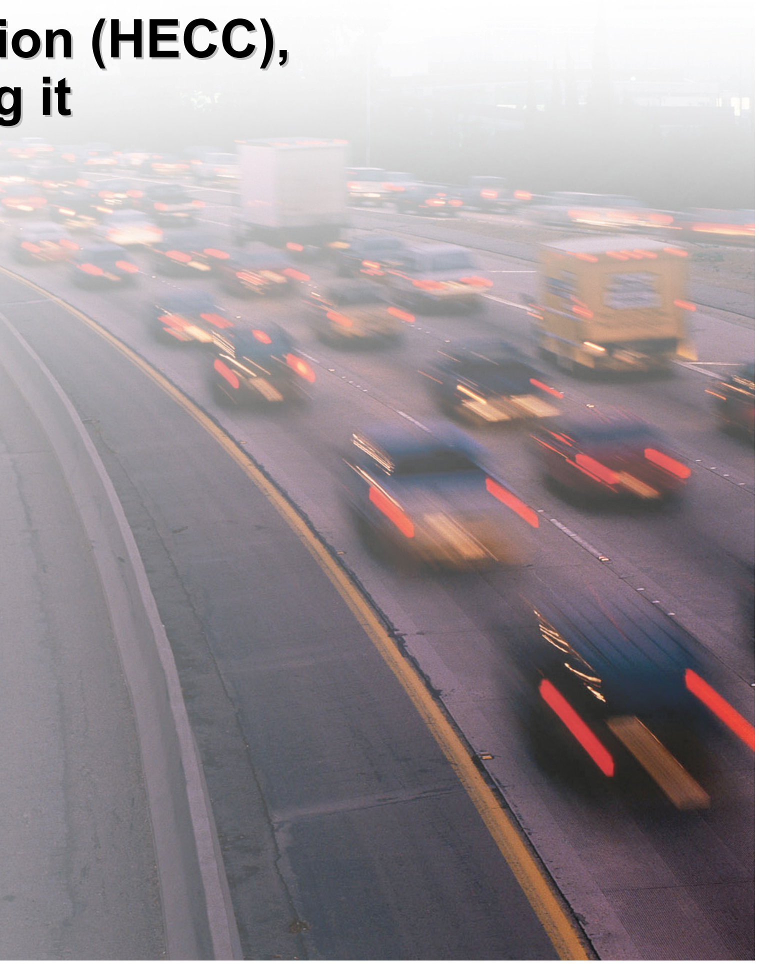
Opening Thought

More than any other time in history, mankind faces a crossroads. One path leads to despair and utter hopelessness. The other, to total extinction. Let us pray we have the wisdom to choose correctly.

— *Woody Allen*, "My Speech to the Graduates"

Presentation Outline

- Discuss factors that are driving changes in fuels and engines
- Outline transportation fuel options for the next 3-6 decades
- Explain high-efficiency, clean combustion (HECC), and show some strategies for achieving it
- Touch on some recent results from the Sandia Advanced Fuels Laboratory
- Propose some challenging and important research topics for world-class combustion scientists
- Summarize

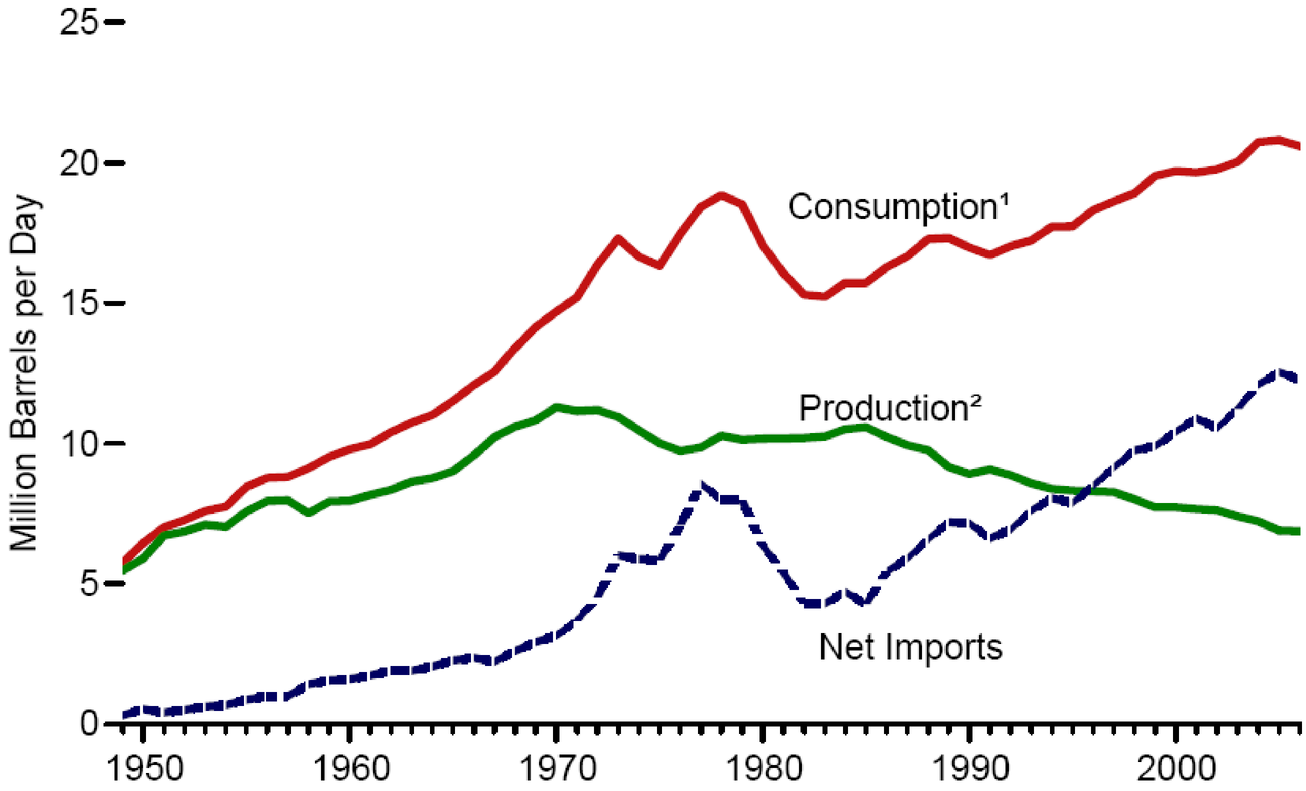


Factors Driving Changes to Transportation Fuels and Engines

1. Energy security
2. Sustainability
3. Air quality

Energy Security:
"Houston, We Have a Problem"

US Petroleum Consumption, Production, and Imports

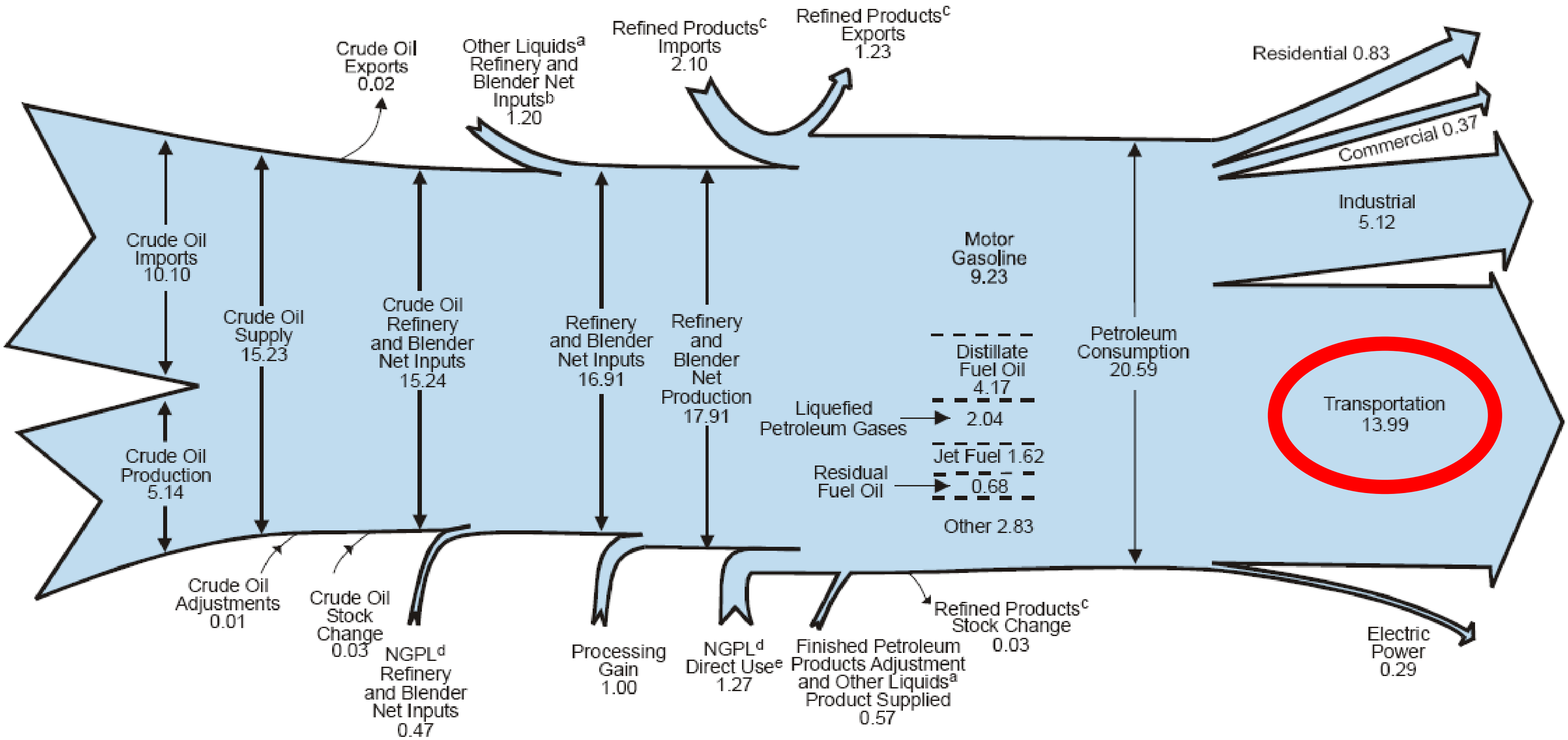


Source: EIA Annual Energy Review, 2006, Fig. 5.1

20 million barrels of oil would cover an American football field (100 x 53.3 yds) to a depth of 2341 feet – nearly half a mile deep!

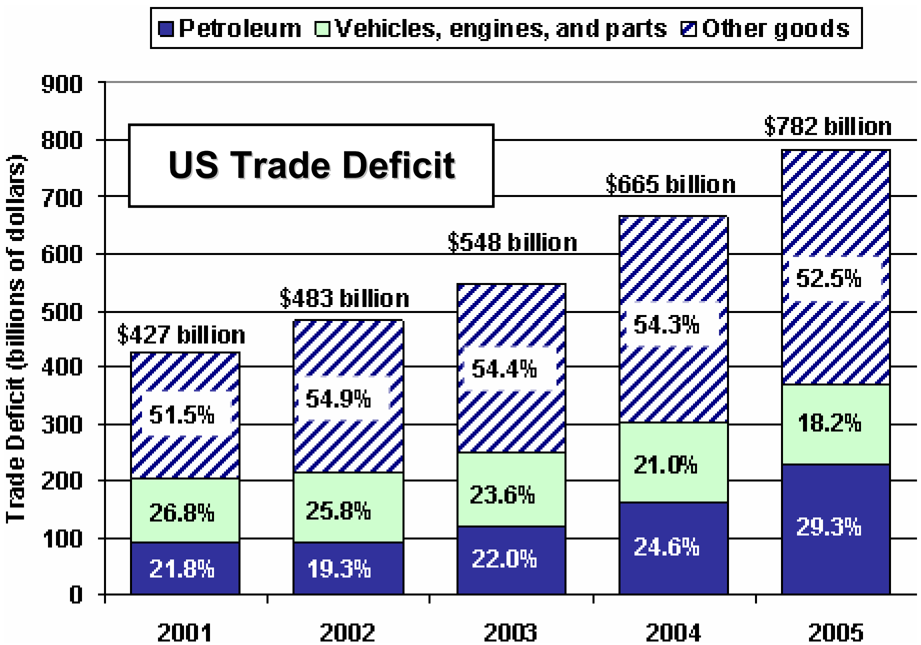
Energy Security: Where Is All of That Petroleum Going?

US Petroleum Flow (Million Barrels per Day)

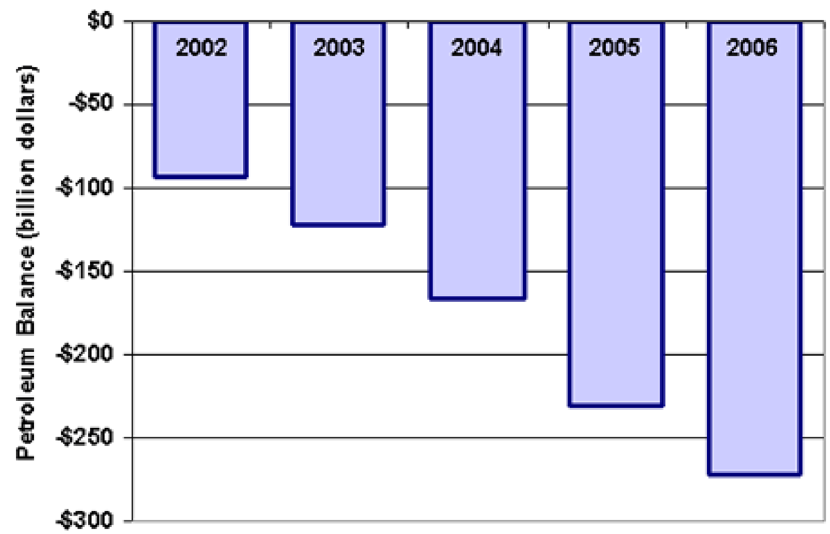


Source: EIA Annual Energy Review, 2006, Diagram 2

Energy Security:
Why Should We Care about Petroleum Use?



Source: U.S. Department of Commerce, Bureau of Economic Analysis, "U.S. International Trade in Goods and Services," Exhibits 6 and 9, November 2004, March 2005, March 2006 editions.

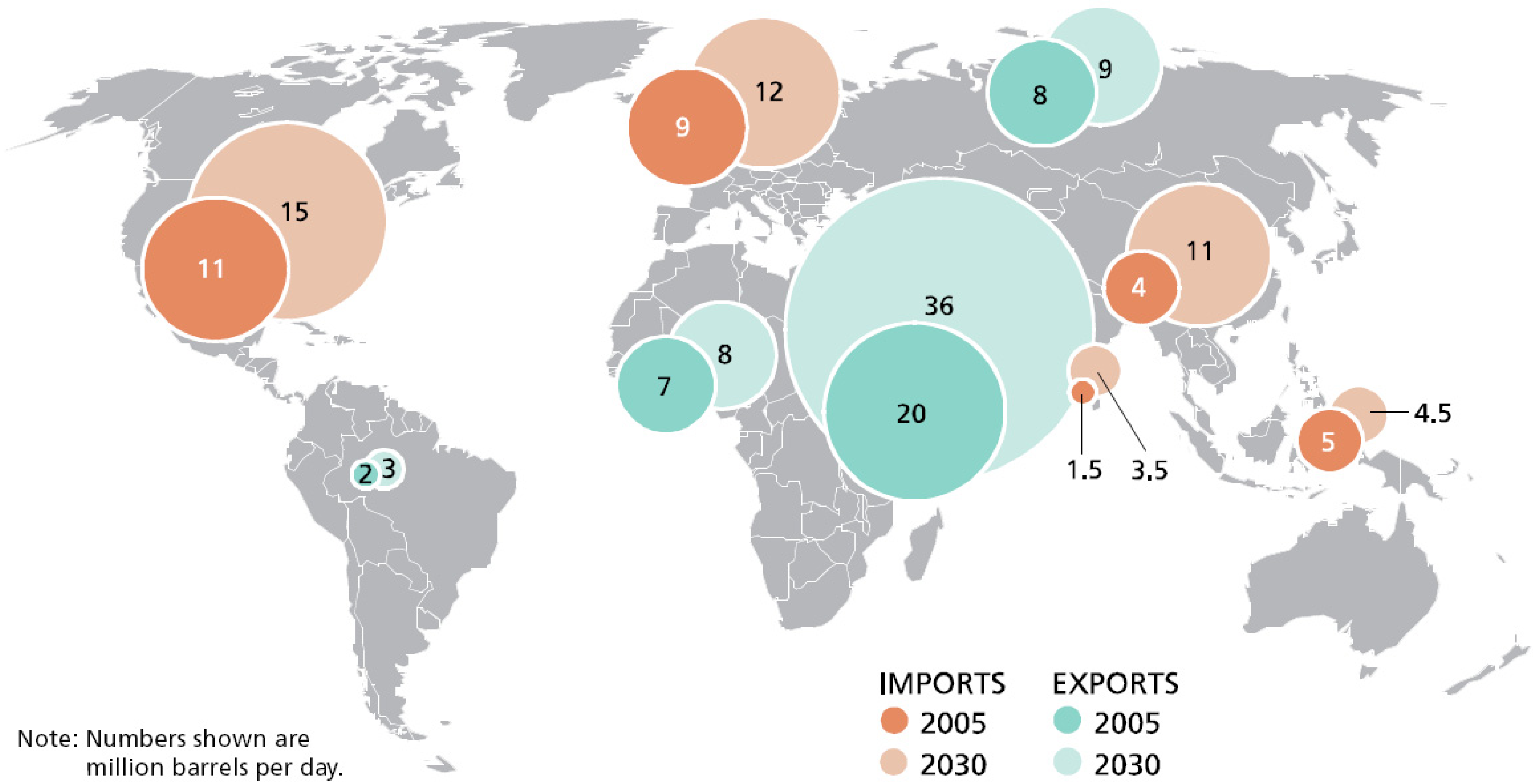


Source: EIA, Monthly Energy Review, March 2007, Table 1.5

Estimated cost of Iraq war (3/20/2003 – 9/26/2007): $454 Billion

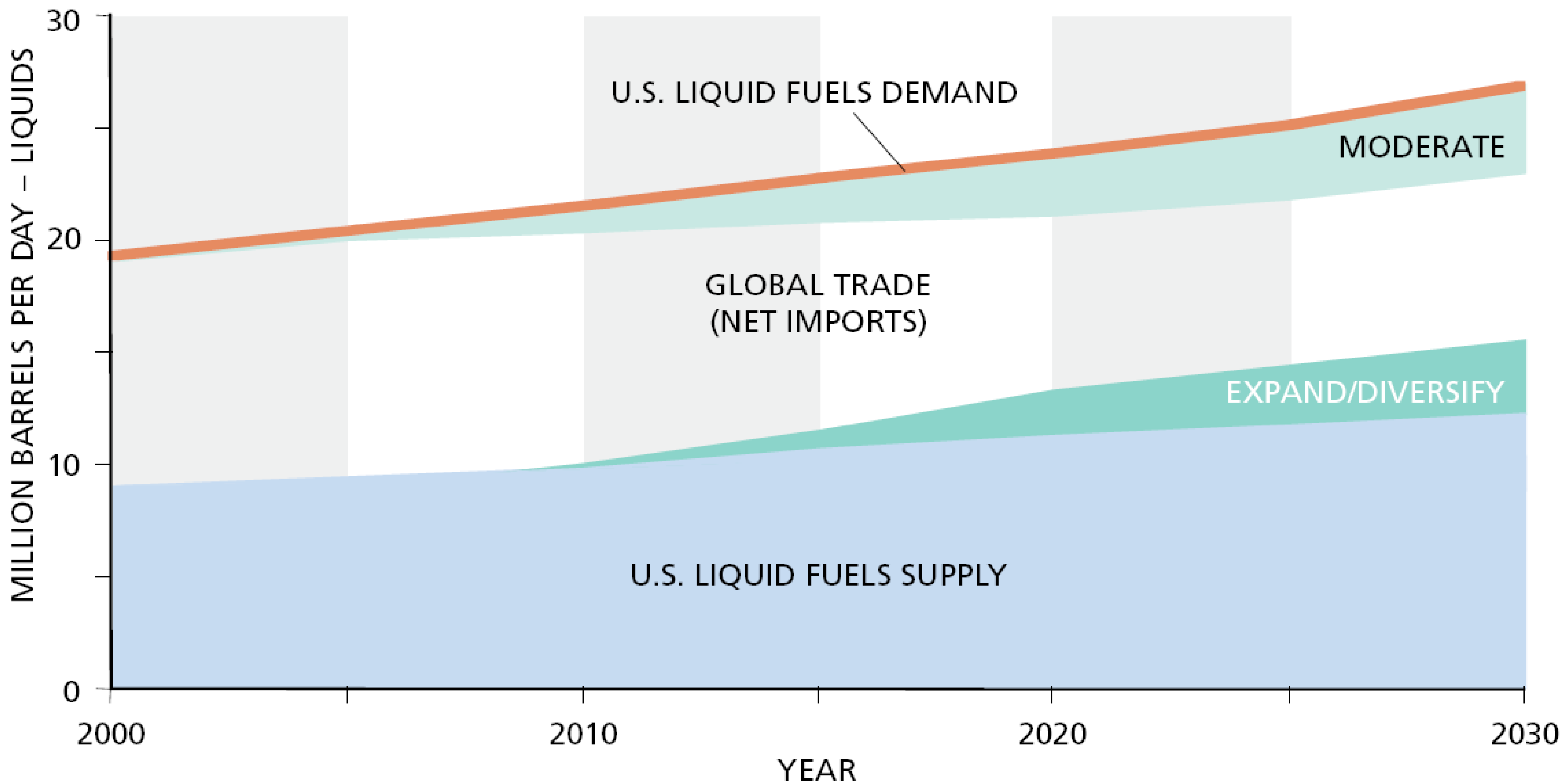
Source: Wikipedia, "Financial Cost of the 2003 Iraq Conflict"

Energy Security: The Middle East Will Remain a Hot Spot



Source: National Petroleum Council, "Facing the Hard Truths about Energy," Executive Summary, Fig. ES-6

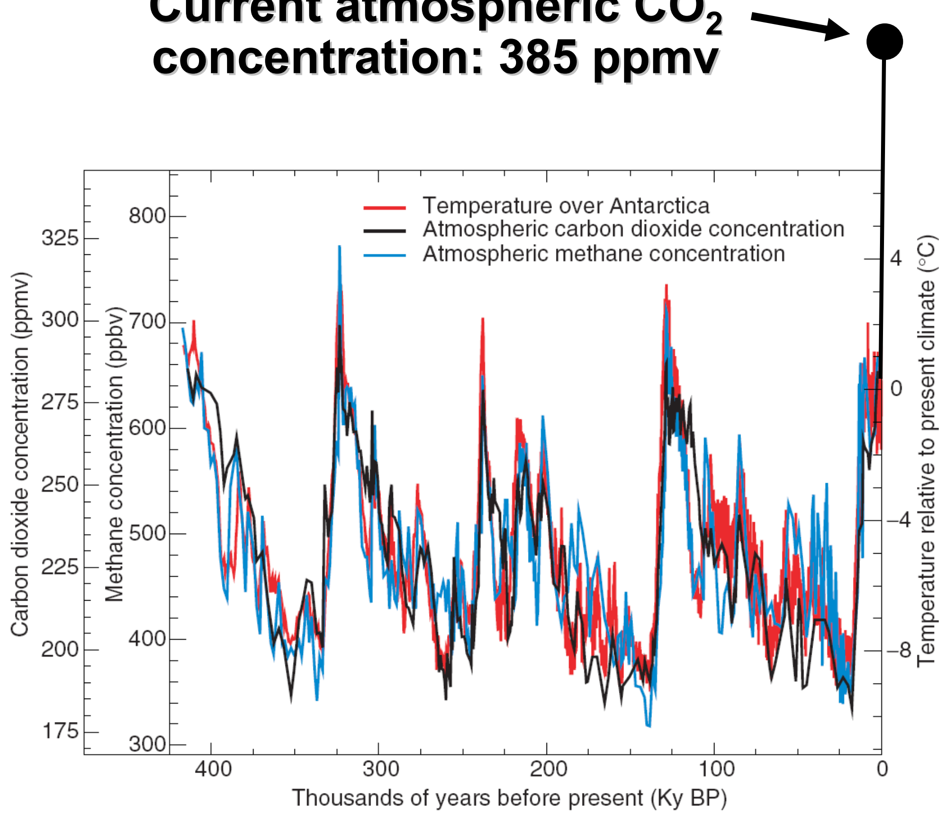
Energy Security: US "Energy Independence" Not Probable on 25-Year Timescale



Source: National Petroleum Council, "Facing the Hard Truths about Energy," Executive Summary, Fig. ES-15

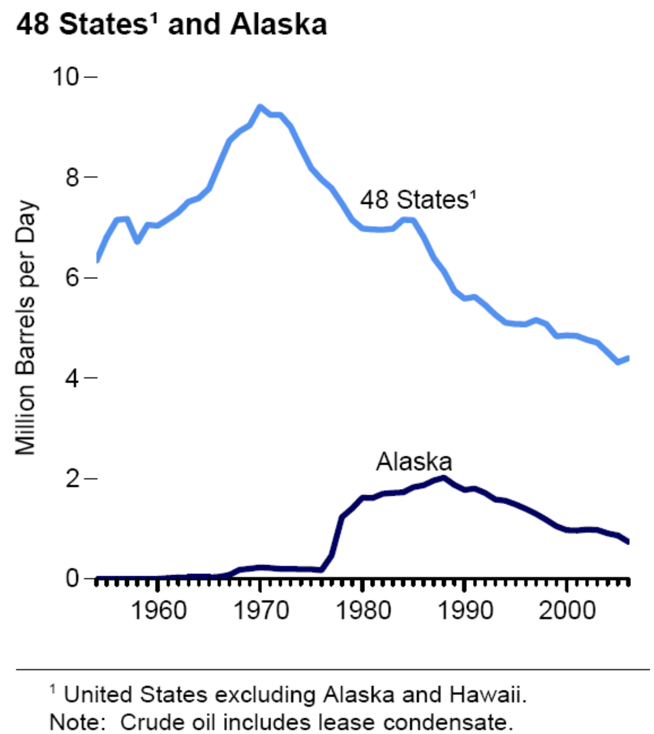
Sustainability

Current atmospheric CO_2 concentration: 385 ppmv



Source: "Climate Change 2001: The Scientific Basis," Fig. 2.22

Peak Oil? US Crude Oil Production, 1954 – 2006



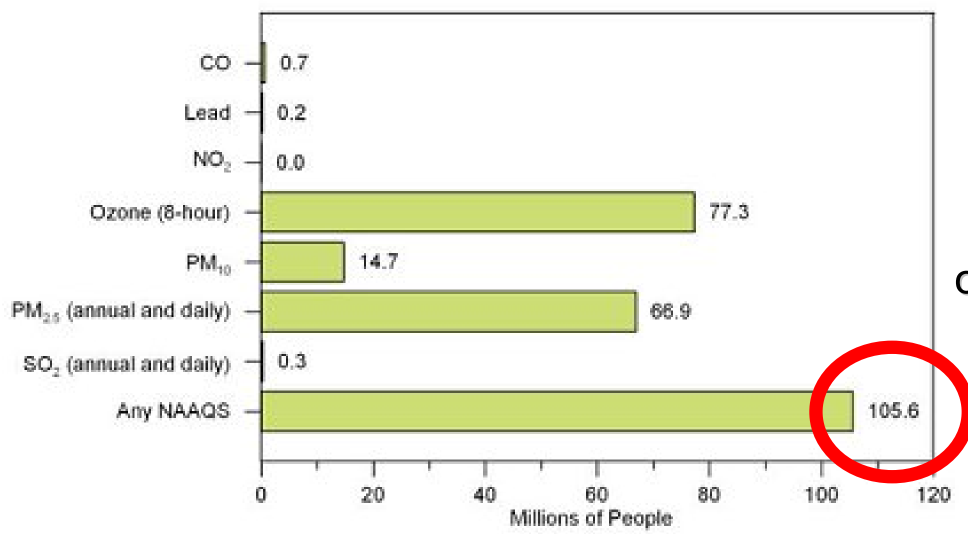
Source: EIA Annual Energy Review, 2006, Fig. 5.2

Air Quality

"…on a typical warm day in LA, the exhaust gases of a vehicle such as a Honda Insight Hybrid will be cleaner on average than the surrounding air the engine draws in."

— Ricardo Quarterly Review, Q3 2007

Number of People Living in Counties with Pollutant Concentrations above the Primary NAAQS in 2006



More than 1/3 of US residents live in non-attainment areas

Source: US EPA, http://www.epa.gov/air/airtrends/sixpoll.html

Take-Home Message #1

We must increase transportation system efficiency while continuing to improve air quality.

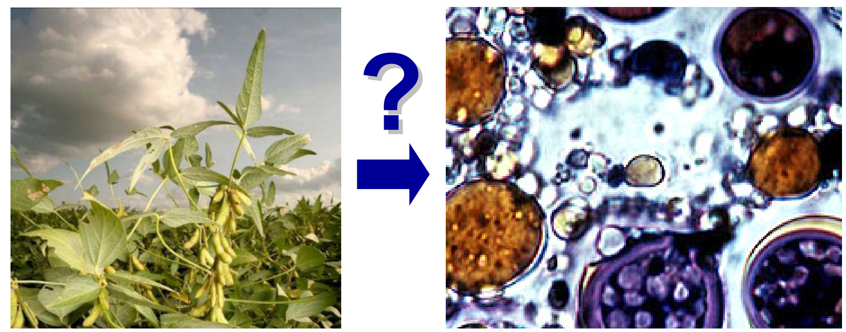
Liquid Transportation Fuels for the Next 30 to 60 Years

Transportation Fuels Are Changing

- **World demand for petroleum is ↑, supplies are finite and ↓**
  - **As prices increase, so will diversity of fuel options**
- **Many fuel streams from which to choose**

Near-term → Long-term

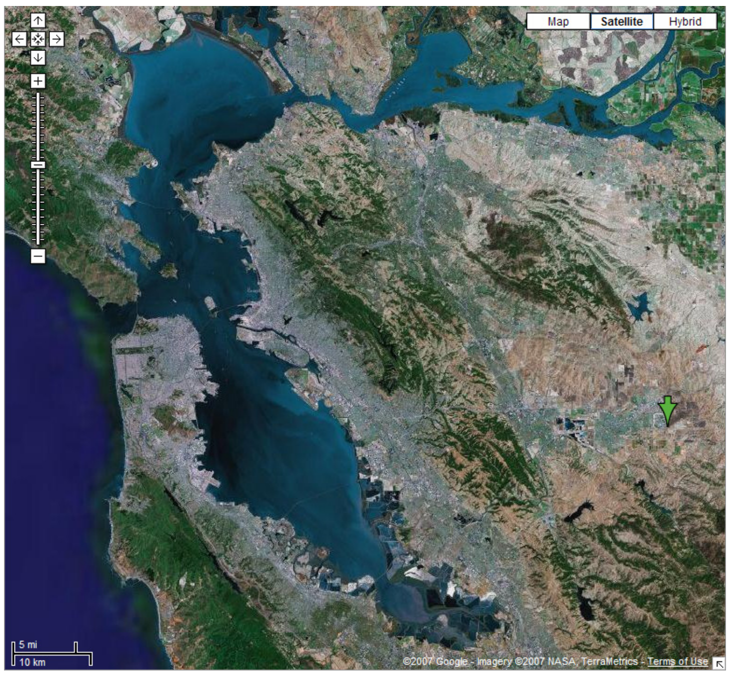
  - **Heavy, sour crude**
  - **Fischer-Tropsch: natural gas (methane hydrates?)**
  - **Ethers: not MTBE!**
  - **Alcohols: methanol, ethanol, butanol**
  - **Biodiesel, renewable diesel**
  - **Oil sands from Canada**
  - **Coal-to-liquids**
  - **Biomass-to-liquids (pyrolysis, gasification)**
  - **Oil shale from Western US**
  - **Hydrogen (50 years away?)**



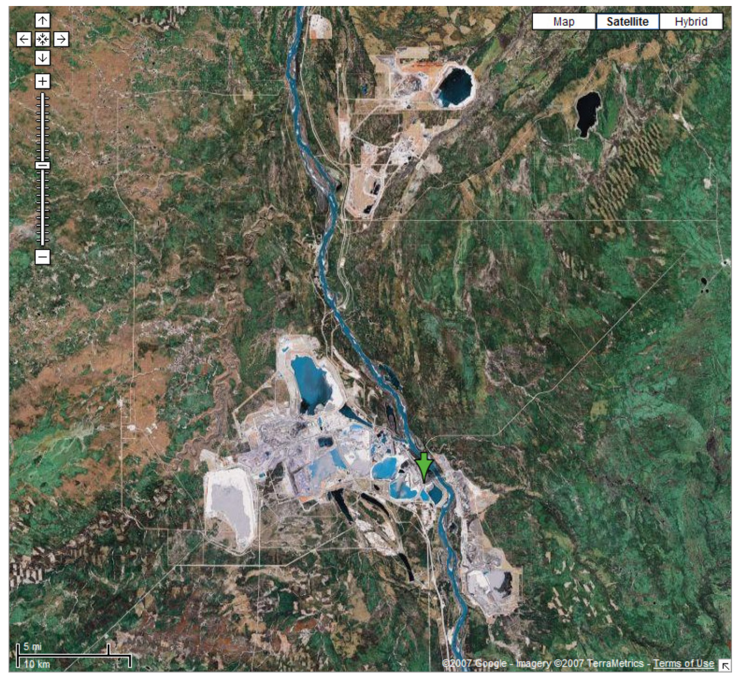
Chronicle / Brant Ward

Canadian Oil Sands

- **Arguably the most important unconventional fuel stream in large-scale use today**
  - **179 Gbbl recoverable reserves (2nd only to Saudi Arabia @ 262 Gbbl)**
  - **US imported 1.1 Mbpd of oil-sands-derived crude in 2006**



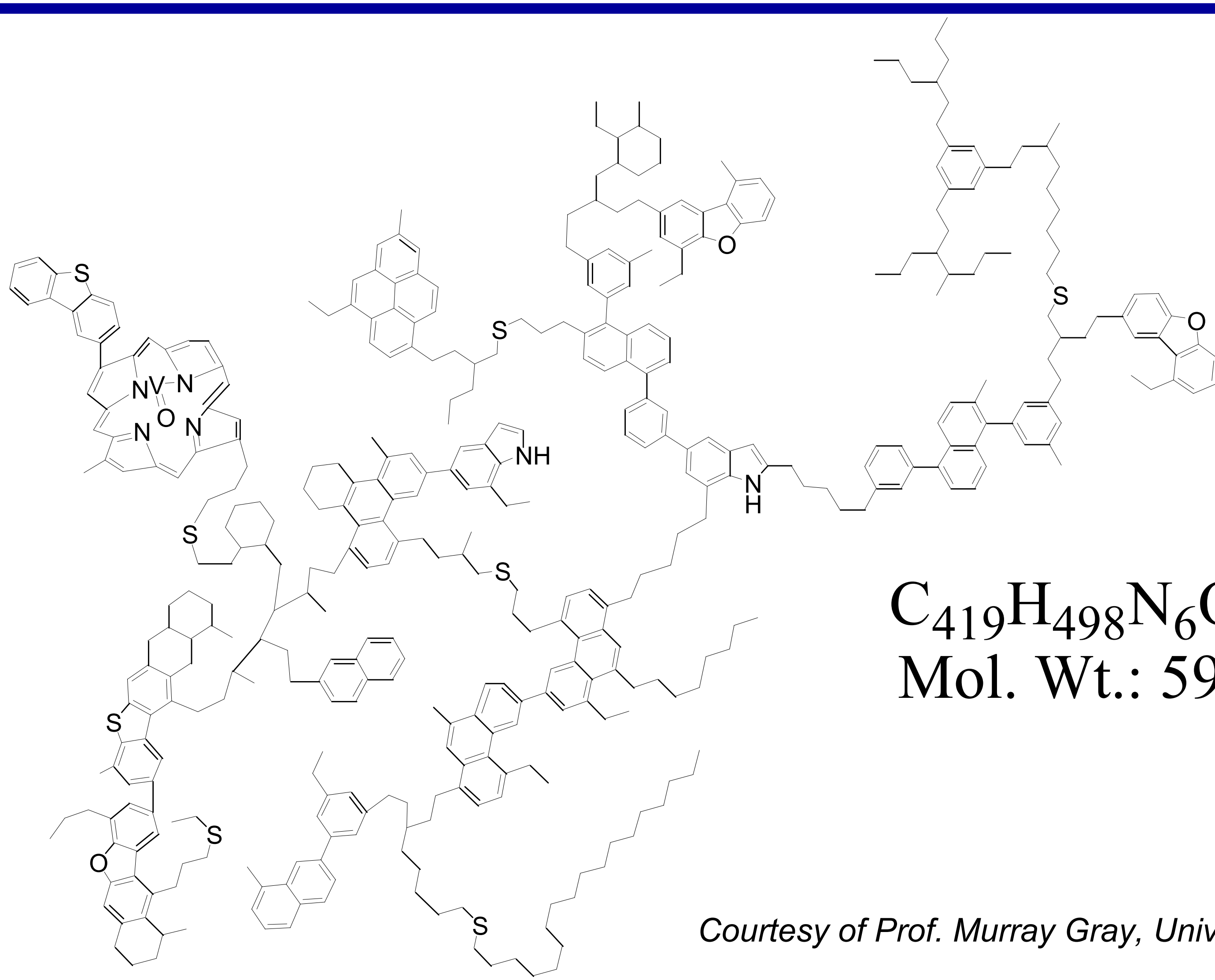
San Francisco Bay Area



Fort Mackay, Alberta, Canada

Source: Google Maps (http://maps.google.com)

Representation of an Asphaltene Molecule from Oil-Sands Bitumen



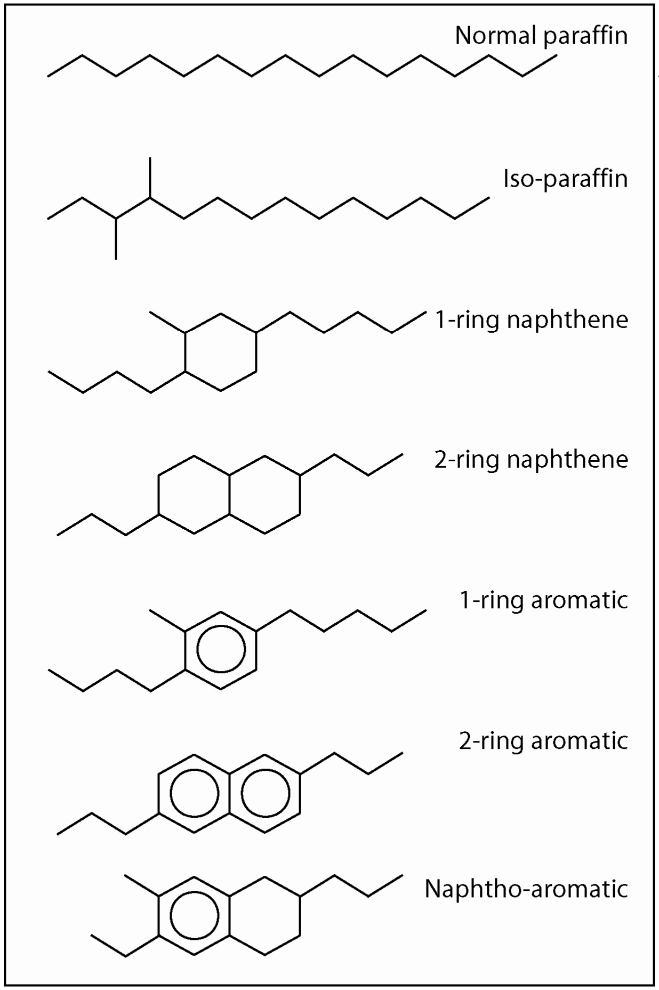
$C_{419}H_{498}N_6O_4S_8V$

Mol. Wt.: 5989.94

Courtesy of Prof. Murray Gray, Univ. of Alberta

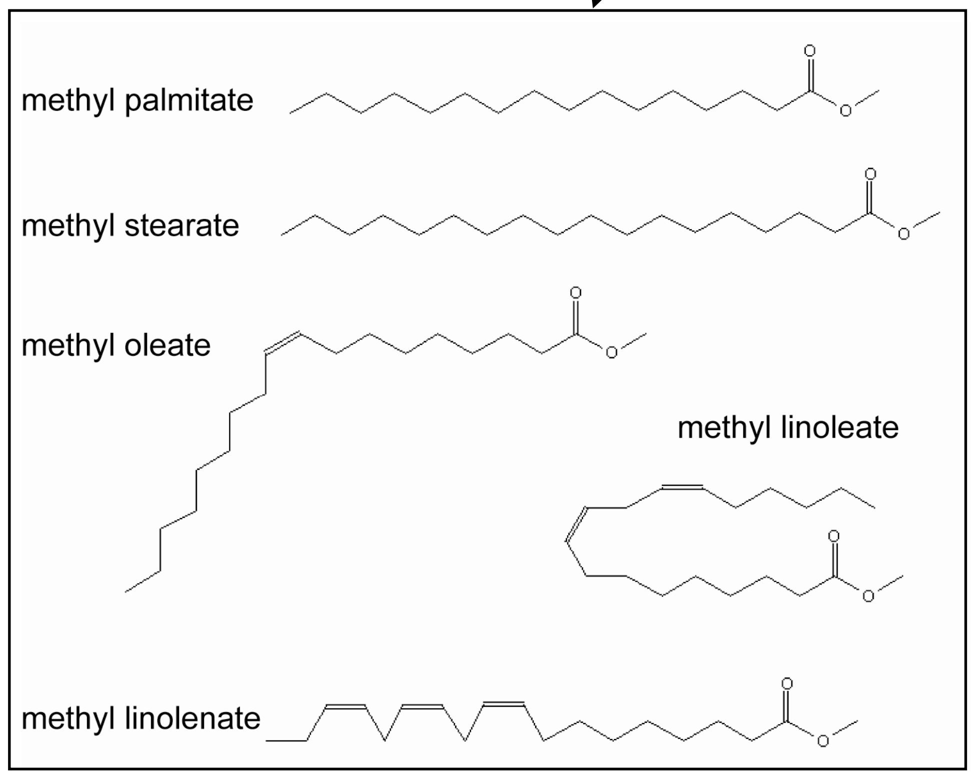
New Fuels Can Be Very Different from Conventional Fuels, and Burn Differently

Conventional diesel



Source: Farrell et al., SAE 2007-01-0201

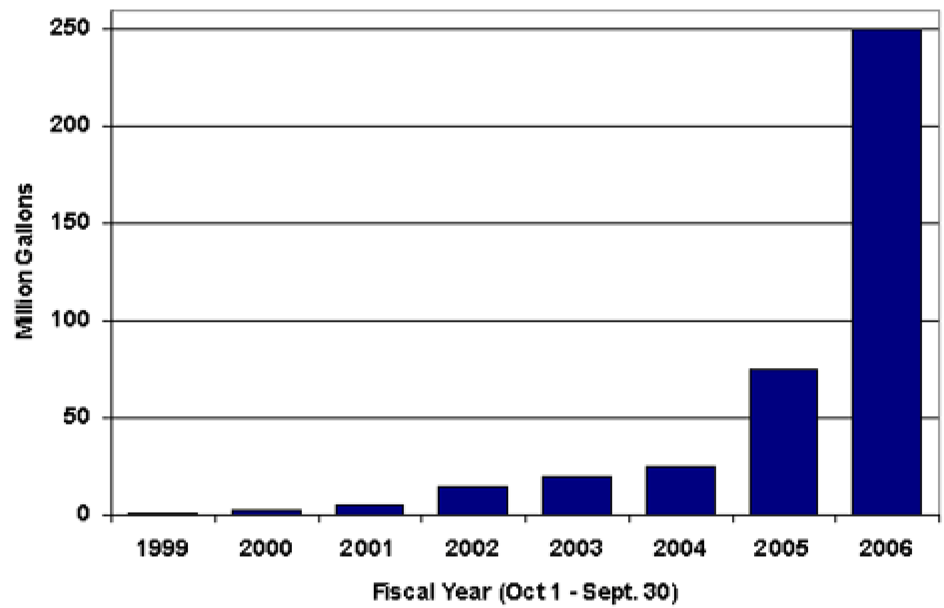
Biodiesel
(soy methyl esters)



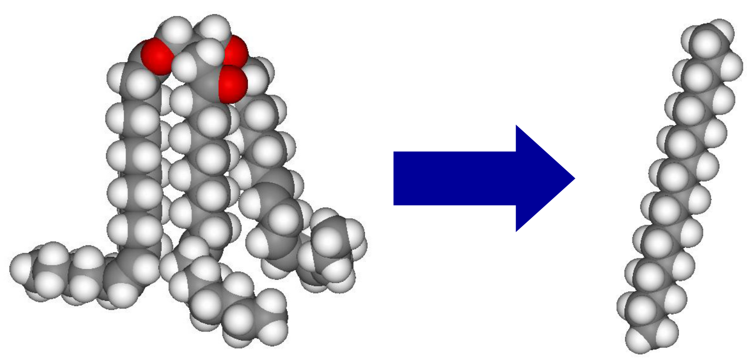
Source: Mueller, CRF News, May/June 2006

Biodiesel and Renewable Diesel

- Biodiesel
  - 250 million gal/yr = 0.016 Mbpd
  - Algal production could increase per-acre yield by 40x
  - NO_x emissions ↑ and stability are concerns
- Renewable diesel = fats/oils run through a refinery hydrotreater (to saturate molecule and remove oxygen)
  - $1/gal tax credit for refiners soon may be repealed



Source: National Biodiesel Board



Take-Home Message #2

The diversity of fuel streams will continue to increase.

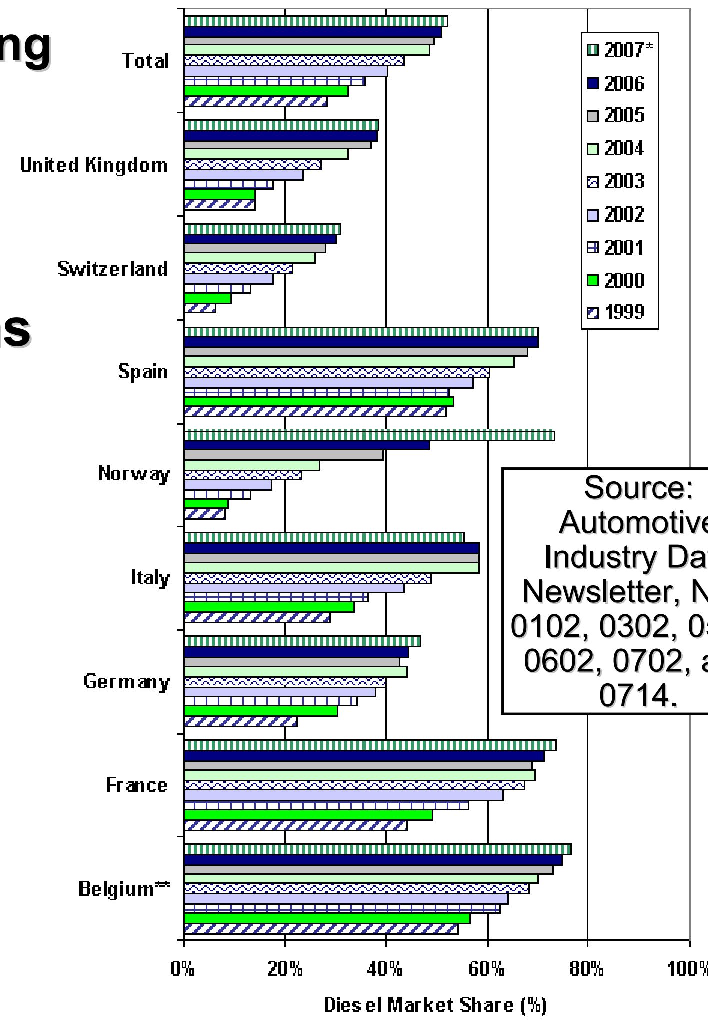
Since future fuel streams will require extensive processing, it is in our best interest to understand fuel effects on combustion so that we can produce optimal fuels.

High-Efficiency, Clean-Combustion (HECC) Engine Technologies

Why Compression-Ignition (CI) Engines?

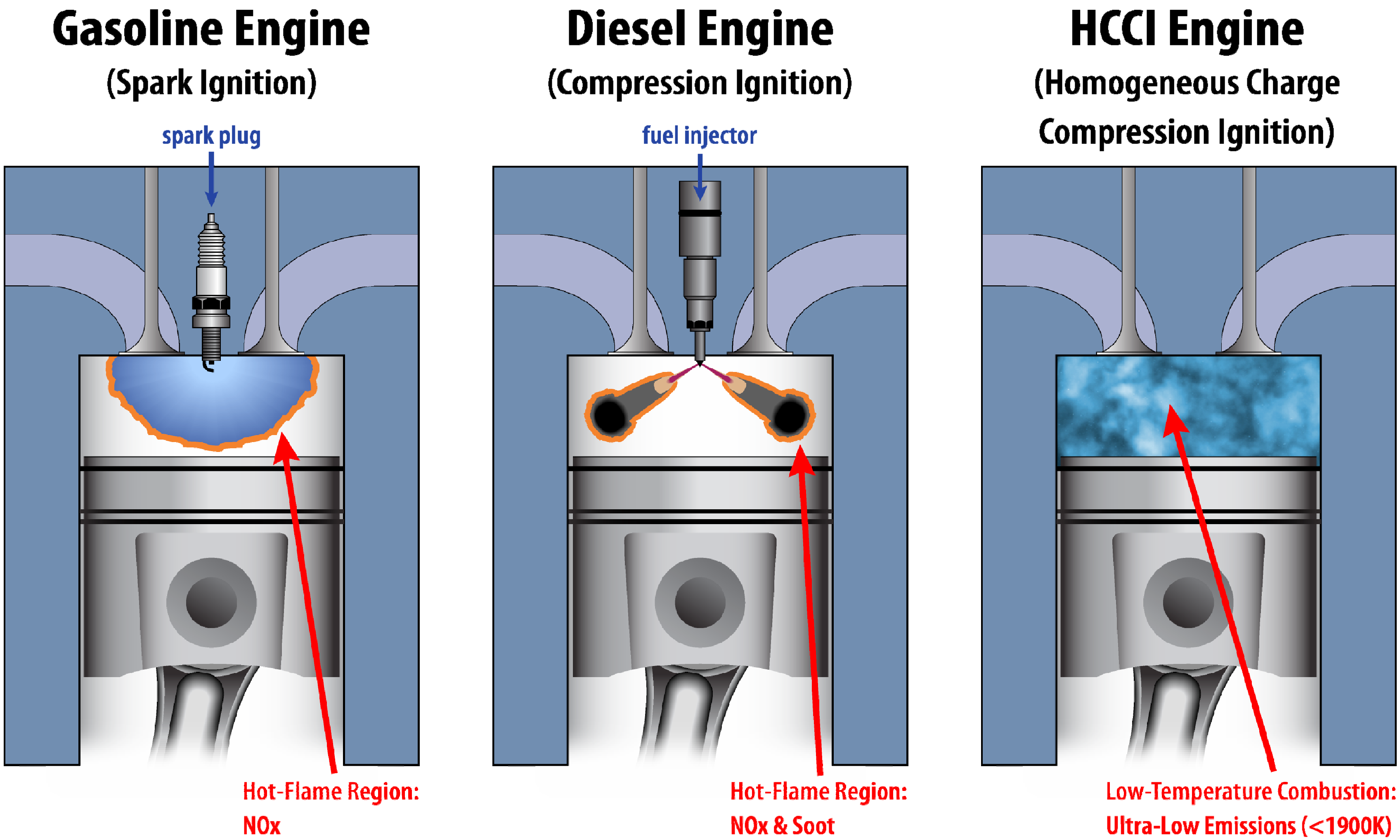
- **Higher efficiency**
  - **Higher compression ratio, no throttling**
  - **~25-40% ↑ *vs.* spark-ignition (SI)**
  - **Enhances energy security, cuts greenhouse-gas emissions**
- **Historical barrier of higher emissions is being surmounted**
- **They're fun to drive!**
  - **Higher torque at low speeds than SI**
  - **Much quieter and more reliable than US diesels of the 1980s**

New Diesel Car Sales in W. Europe



Source: Automotive Industry Data Newsletter, Nos. 0102, 0302, 0501, 0602, 0702, and 0714.

Comparison of Conventional SI and CI Modes to One HECC Strategy



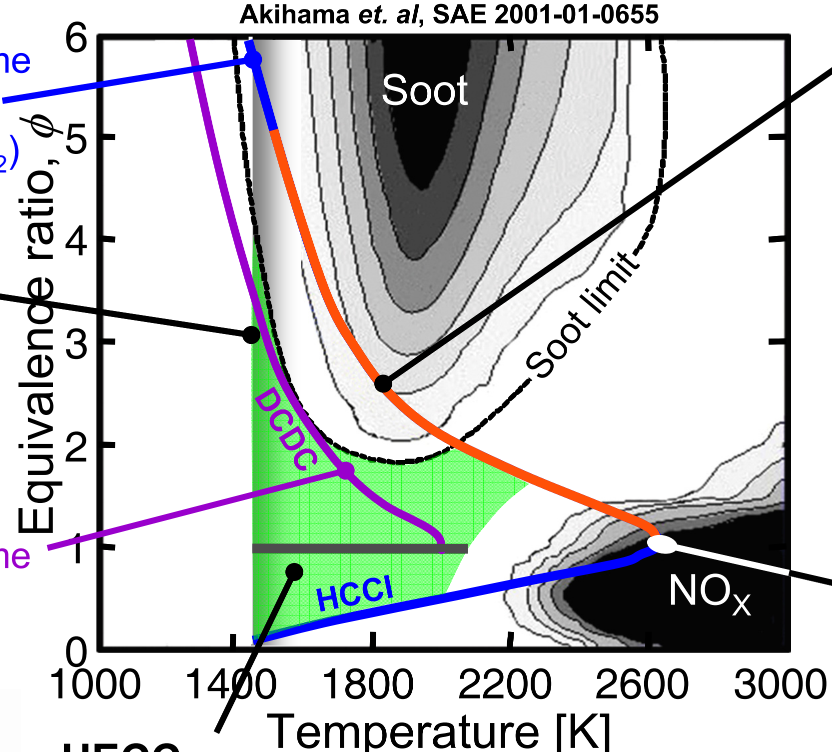
Graphical Summary of SI, CI, & HECC Modes

Akihama *et. al*, SAE 2001-01-0655

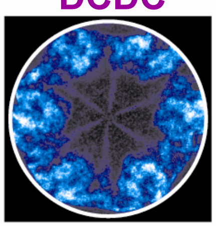
Adiabatic flame temperature in air (21% O_2)

CO to CO_2 conversion diminishes

Adiabatic flame temperature 10% O_2

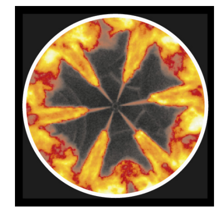


DCDC



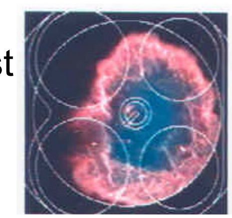
Diesel (CI) combustion

- Controlled heat release (mixing)
- Controlled combustion timing
- Wide load range
- High efficiency (relative to SI)
- **NO_x and PM emissions**



Spark ignition (SI) combustion

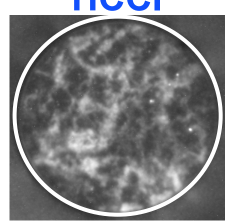
- Controlled heat release (flame propagation)
- Controlled combustion timing
- Wide load range
- Three-way catalyst
- **Low efficiency** (relative to diesel)



HECC

- High efficiency (high CR, no throttle)
- Low NO_x and PM emissions
- **Load range?**
- **Combustion timing?**
- **Heat release rate?**
- **Transient control?**
- **Fuel?**

HCCI



Take-Home Message #3

Diesel and gasoline engines are converging to a common configuration:

- ***Unthrottled***
- ***CI (perhaps with ignition assist)***
- ***Partially premixed charge***
- ***Exhaust gas recirculation***
- ***Compr. ratio higher than today's SI***

Recent Results from the Sandia Advanced Fuels Laboratory

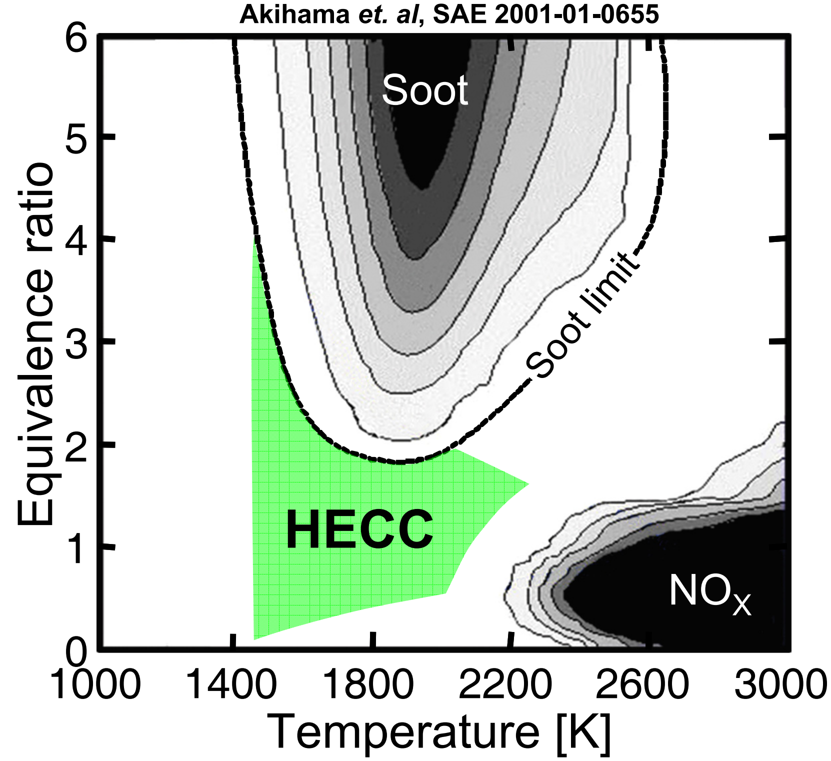
How to Quantify Stoichiometry with Oxygen-ated Fuels or Once Reactions Have Begun?

- **Answer: The oxygen equivalence ratio, ϕ_Ω**

$$\phi_\Omega \equiv \frac{2n_C + \frac{1}{2}n_H}{n_O}$$ **, neglecting atoms bound in CO_2 and H_2O**

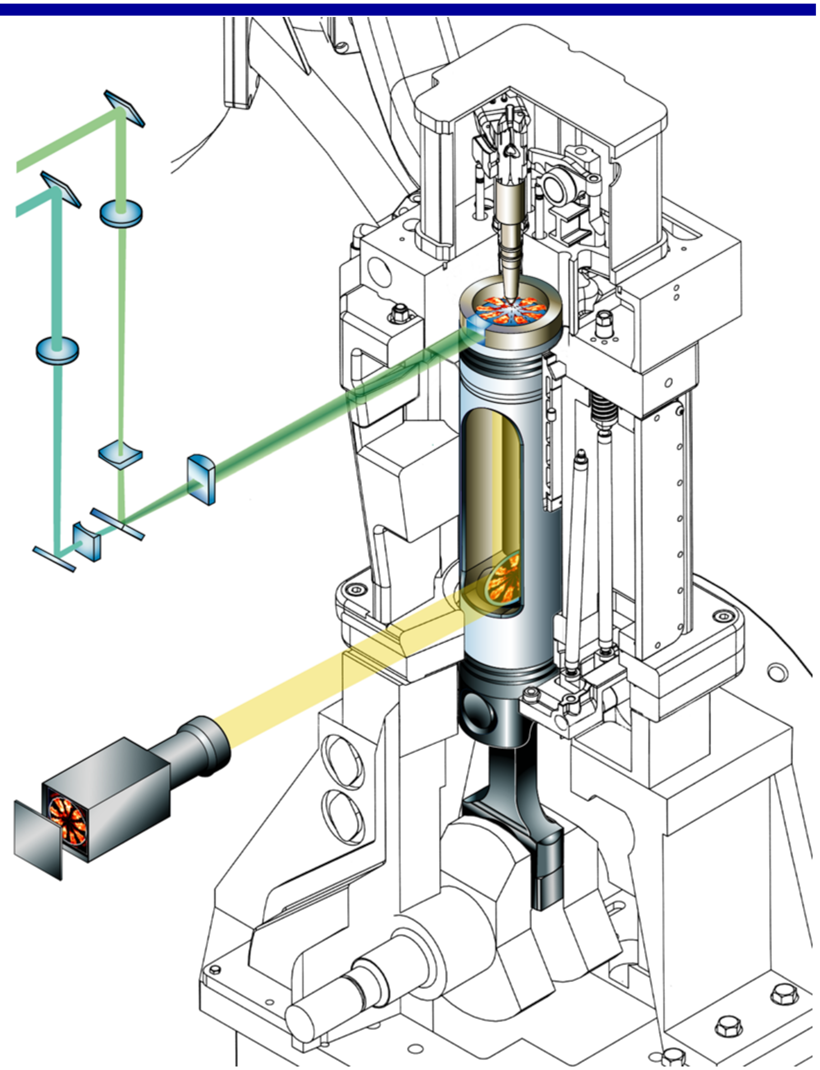
- **Important when oxygenated fuels are used (*e.g.*, biodiesel, ethanol, ethers, …)**
- **Important for tracking reaction progress in (ϕ,T) space**
- **Same as traditional ϕ definition before reactions have begun**
  - **As long as fuel not oxygenated**
  - **General relationship between ϕ and ϕ_Ω provided in SAE 2005-01-3705**

Akihama *et. al*, SAE 2001-01-0655



Optical Engine Specifications and Schematic

Research engine	1-cyl. Cat 3176
Cycle	4-stroke CIDI
Valves per cylinder	4
Bore	125 mm
Stroke	140 mm
Conn. rod length	225 mm
Conn. rod offset	None
Piston bowl diameter	90 mm
Piston bowl depth	16.4 mm
Squish height	1.5 mm
Swirl ratio	0.59
Displacement per cyl.	1.72 liters
Compression ratio	11.3:1
Simulated compr. ratio	16.0:1



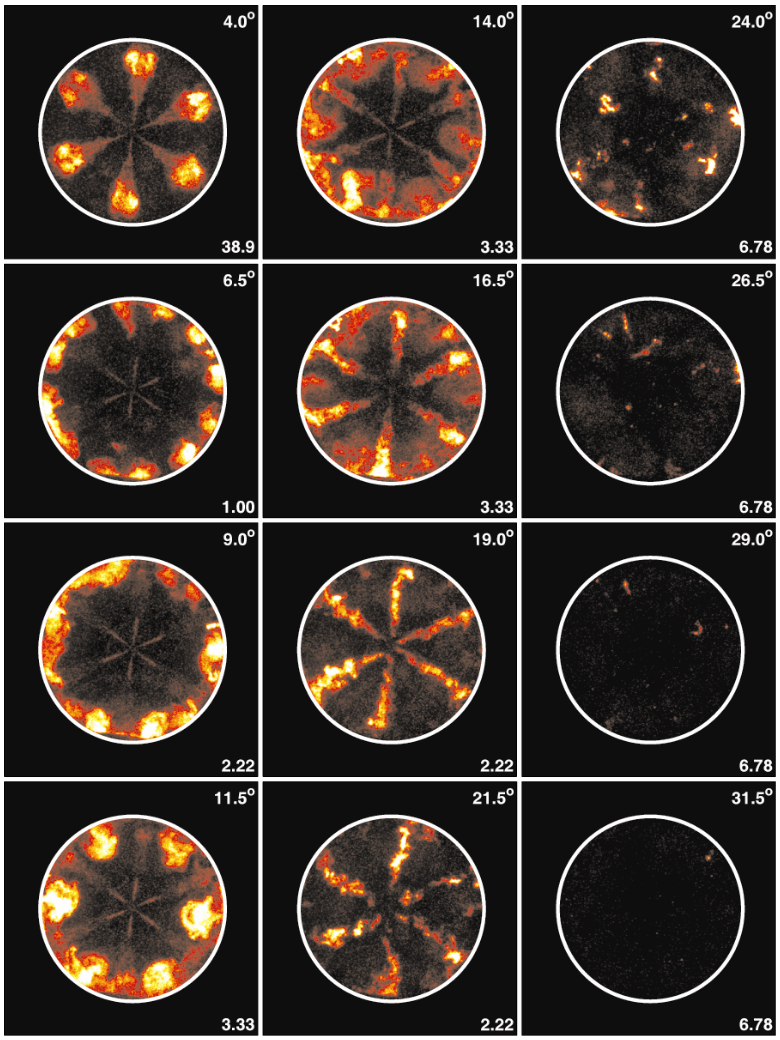
Quartz windows in piston and upper periphery of cylinder liner enable optical access

Dilute Clean Diesel Combustion (DCDC) Using Emerging Fuels

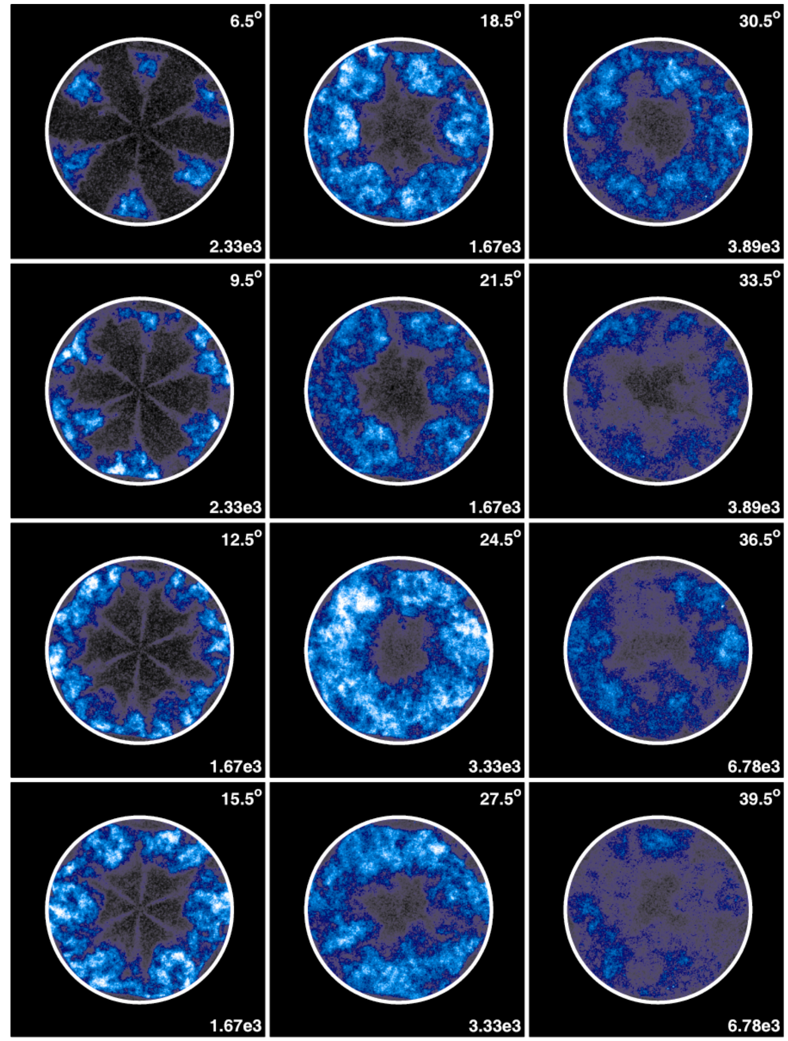
Test conditions for all results:

- **1200 rpm, 6.7 bar IMEP**
- **1450 bar peak injection pressure**
- **6 x .163 mm x 140° nozzle**
- **EGR simulated with N_2 addition**

Natural Luminosity Imaging of Undiluted and Highly Dilute Combustion (DGE Fuel)



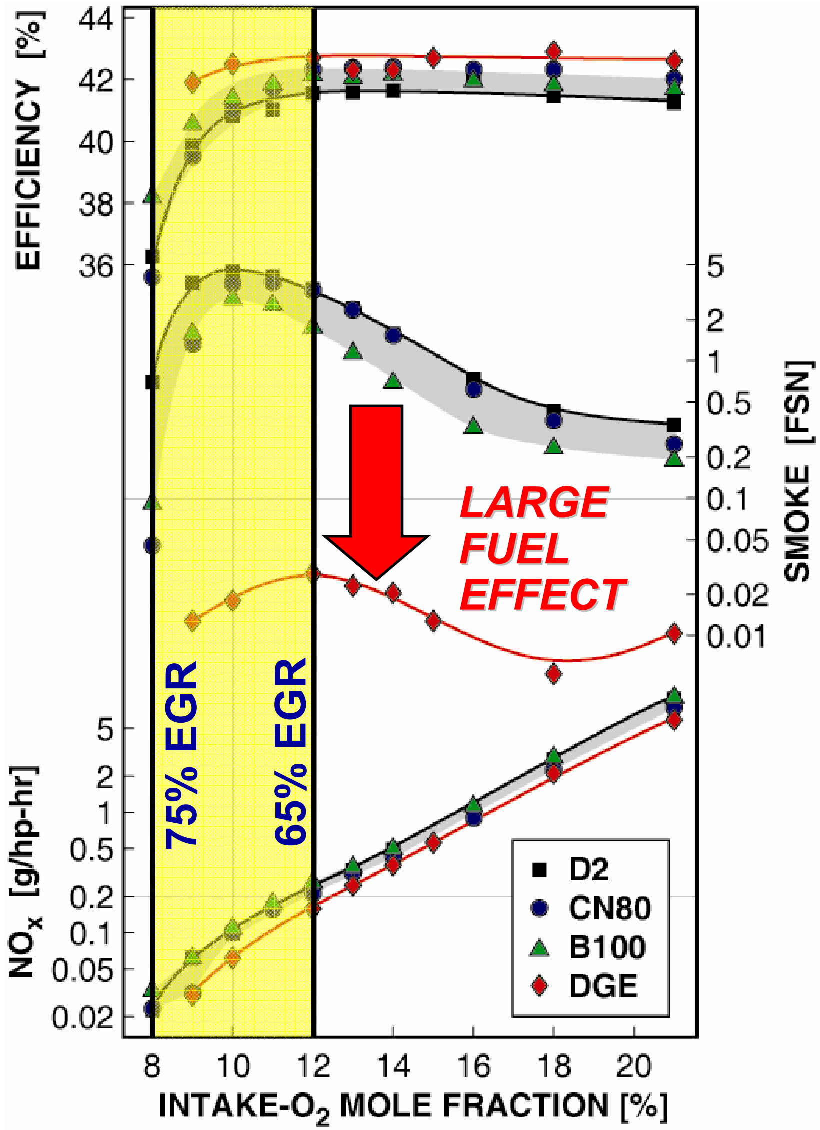
Undiluted



9% Intake-O_2 Mole Fraction

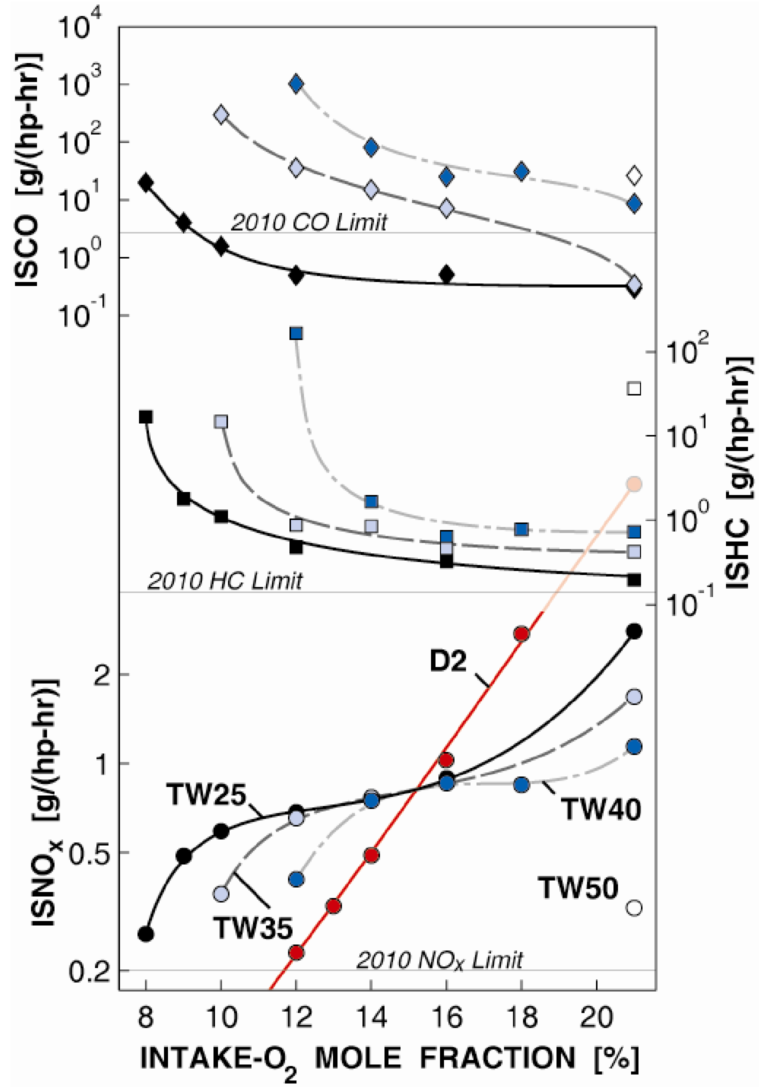
To What Extent Is DCDC Possible with More-Conventional Fuels?

- **Answer: With near-term fuels, smoke emissions become ~50X too large at required EGR levels**
  - **Efficiency drops before compliant smoke emissions obtained**
  - **Highly oxygenated fuel can remove this barrier**
- **Very high levels of cooled EGR required for NO_x compliance**
  - **Leads to high levels of heat rejection, burden on air-handling systems**
  - **Is there a better way to introduce diluent?**



Are Fuel-Water Mixtures a Viable Alternative to EGR for NO_x Control?

- **Answer: Yes, potentially**
  - Studied blends of tri-propylene glycol methyl ether with 25 to 50 vol% water
  - Stable blends pass corrosivity tests for ferrous metals and copper
  - Ignition delay ≈ 40-50 cetane #2 diesel
  - Can lower NO_x by ~10x without using EGR (relative to #2 diesel)
  - Surprisingly, NO_x doesn't decrease as rapidly as expected with simulated EGR
  - HC and CO compliance possible with oxidation catalyst
  - Exceedingly low in-cyl. soot and engine-out smoke



Take-Home Message #4

Dramatic fuel changes enable efficiency and emissions targets to be met without costly aftertreatment, but there is still much work to be done to meet the targets with minimum incremental cost.

Research Needs

- **See "Basic Research Needs for Clean and Efficient Combustion of 21st Century Transportation Fuels": http://www.sc.doe.gov/bes/reports/files/CTF_rpt.pdf**
- **My wish list:**
  - **Non-intrusive (optical?), 2-D or 3-D diagnostics for quantitative measurement of relevant combustion scalars *at high pressure and in the presence of multiple interferences* (*e.g*., soot, liquid fuel, oxygen, dirty windows, stratified T and species, …)**
  - **Quantitative diagnostics for liquid fuel films on in-cylinder surfaces (mass, distribution, composition)**
  - **Validated, reduced chemical-kinetic mechanisms for ignition and combustion of real fuels to enable computational engine/fuel system optimization, including accurate prediction of all relevant emissions (soot, NO_x, HC, CO, aldehydes, …)**
  - **Novel efficiency-improvement strategies (thermodynamic analyses, thermoelectrics, improved turbocharging, other waste-heat recovery strategies, …)**

Summary

- We must increase transportation system efficiency while continuing to improve air quality
- The diversity of fuel streams will continue to increase;
  - Since future fuel streams will require extensive processing, it is in our best interest to understand fuel effects on combustion so that we can produce optimal fuels

  meanwhile, diesel and gasoline engines are converging to a common configuration
  - Unthrottled
  - CI (perhaps with ignition assist)
  - Partially premixed charge
  - Exhaust gas recirculation
  - Compr. ratio higher than today's SI
- Dramatic fuel changes enable efficiency and emissions targets to be met, but much work remains to be done to meet the targets with minimum incremental cost

Summary

- **We must succeed, and advancements in our understanding of combustion – from fundamentals to applications – will play a critical role**

Questions???

Acknowledgments

Dr. Glen C. Martin – *post-doc*

Dr. Ansis Upatnieks – *former post-doc*

Prof. A.S. (Ed) Cheng – *collaborator*

Advanced Engine Combustion, FACE, Diesel Surrogates – *working groups*