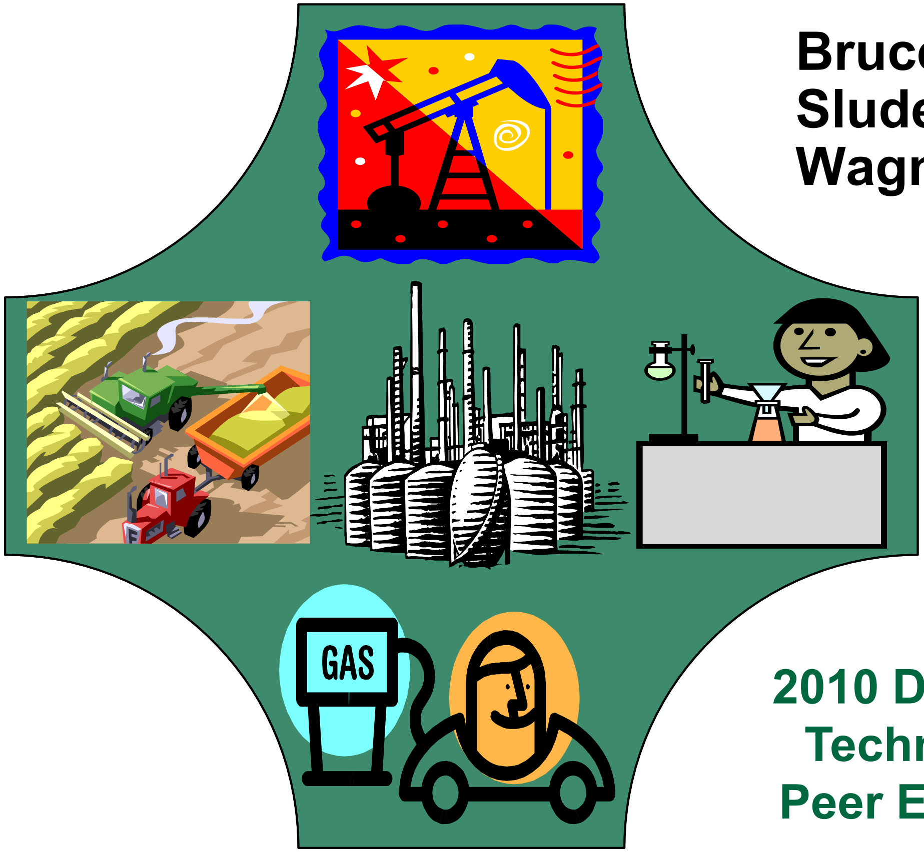
FT001 – APBF Effects on Combustion
(advanced petroleum based fuels, DOE project # 18546)



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2010 DOE Hydrogen Program and Vehicle Technologies Annual Merit Review and Peer Evaluation Meeting, June 7-10, 2010

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Outline

- **Overview**
- **Objectives**
- **Milestones**
- **Approach**
- **Technical accomplishments and progress**
- **Future work**
- **Summary**
- **(Response to previous year's review comments)**
- **(Publications and presentations)**
- **(Critical assumptions and issues)**

Project overview

- **TIMELINE**
  - Started in 2004 with advent of APBF and NPBF projects
  - Work has continued and evolved to new areas
    - New fuels, new engines, kinetics, statistical analysis
  - Future of APBF unknown for 2011
- **BUDGET**
  - DOE funding of $950K (2010) and $730K (2009)
  - On related projects, industry funding of $50K to $150K per year
- **BARRIERS / TECHNICAL TARGETS**
  - Determine fuel characteristics enabling emission compliant, high efficiency engines
  - Enable more effective use of LTC and HCCI combustion strategies
- **PARTNERS, PAST AND PRESENT**
  - Cummins, 3 major oil companies, algae/biodiesel processor, Reaction Design, U. Wisconsin, MIT, Michigan State, U. Tennessee, CRC

Objectives

- **VEHICLE TECHNOLOGIES PROGRAM GOALS**
  - **Improve energy security, energy options, and energy efficiency**
  - **Develop cost-competitive fuel options which displace petroleum**
  - **Develop data and predictive tools for fuel property effects on combustion and engine optimization**

- **ORNL PROJECT OBJECTIVES**
  - **Determine how fuel chemistry and properties interact with conventional and advanced combustion engines to produce optimal performance**
    - **Study wide range of conventional and emerging fuels on multiple research platforms**

Advanced petroleum based and Non-petroleum based fuels research

- **APBF and NPBF overlap in many areas and projects have moved from one to the other as budgets and priorities evolve**
  - **Catalyst aging and poisoning has shifted to NPBF support, with a new emphasis on biodiesel effects**
  - **Most fuels research includes both APBF and NPBF fuels**
  - **Kinetic modeling and advanced statistics are funded by NPBF, but used in both APBF and NPBF programs**
- **APBF also now includes GM ionic liquid lubrication CRADA**
- **Currently, there is more interest and emphasis on NPBF**

Milestone chart by fuel type

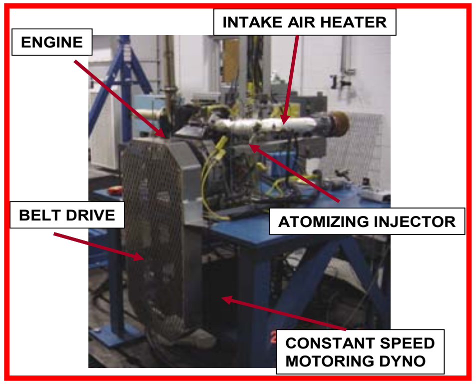
	2004	2005	2006	2007	2008	2009	2010	2011
Conventional diesel fuels		XXX	XXX					
FACE diesel fuels					XXX	XXX	XXX	
FACE gasoline fuels							XXX	XXX
Oil sands derived				XXX				
Oil shale derived					XXX			
Biodiesels			XXX	XXX	XXX		XXX	XXX
Conventional gasolines	XXX				XXX	XXX		
Gasoline surrogates		XXX	XXX		XXX	XXX	XXX	XXX
Diesel surrogates					XXX		XXX	XXX
EtOH + other alcohols / blends					XXX	XXX	XXX	XXX
Fungible, compatible biofuels								XXX

- **2010 milestones are:**
  - **follow up study of FACE diesel fuels in GM 1.9 liter engine**
  - **Run 4 additional fuel series in HCCI and PCCI**
  - **Both will be completed this year**

Approach

- Use a wide range of fully formulated fuels and surrogate blends to study effects of fuel properties and chemistry on advanced combustion engines
- Use multiple research platforms (single cylinder, multi-cylinder gasoline, and diesel advanced combustion engines) to produce broadly applicable data
- Emphasis on fuel efficiency, system approach to understanding of engine and fuel, and on fuel robustness of engines
- Statistical analysis and kinetic modeling of results
- Collaborations with industry, other labs, and universities to leverage capabilities and disseminate results
- APBF fuels include conventionally derived hydrocarbon fuels with normal and modified properties and chemistry for improved operation
  - Separate talk at 1:45pm will cover NPBF fuels

Multiple research platforms



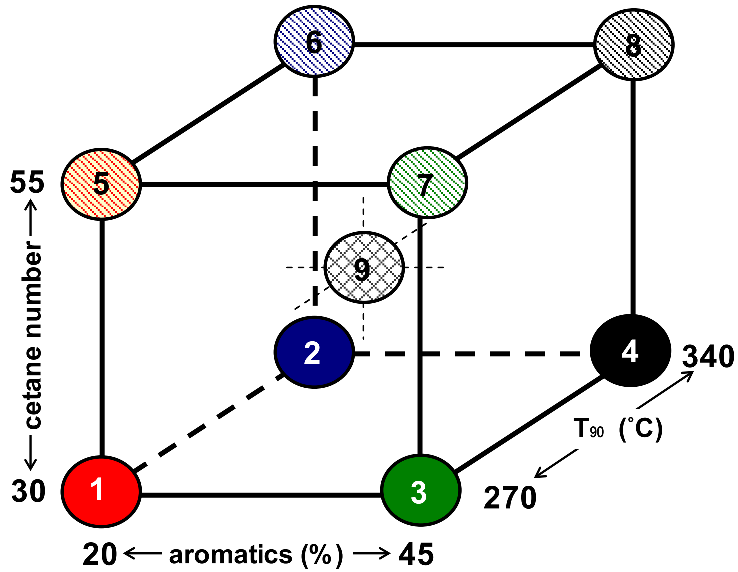
- HCCI single diesel / gasoline
  - Existing engine
  - PFI, intake heating
- GM 1.9 liter 4 cylinder diesel
  - Existing engine
  - Full authority control
- GM Ecotec gasoline
  - New engine
  - Operates as single cylinder
  - Hydraulic valve actuation
  - GDI and PFI capable

New work since 2009 merit review

- FACE fuels
  - HCCI vs. HECC results
- Gasoline and diesel surrogate blends
  - Detailed HCCI exhaust chemistry
  - Multi-zone kinetic modeling study
- Combustion kinetics studies (in NPBF)
  - New project on kinetic mechanism reduction (with U Wisc.)
  - Reaction Design Model Fuels Consortium CRADA continuing
- Statistical analysis of fuel and engine results (in NPBF)
  - CRC AVFL 13C project (funds in project)
  - Currently evaluating 2 statistical analysis software packages
- Engine control research
  - Combustion stability modeling study (with LLNL)
- Ionic liquid lubrication CRADA with GM

FACE diesel fuels run on two engines

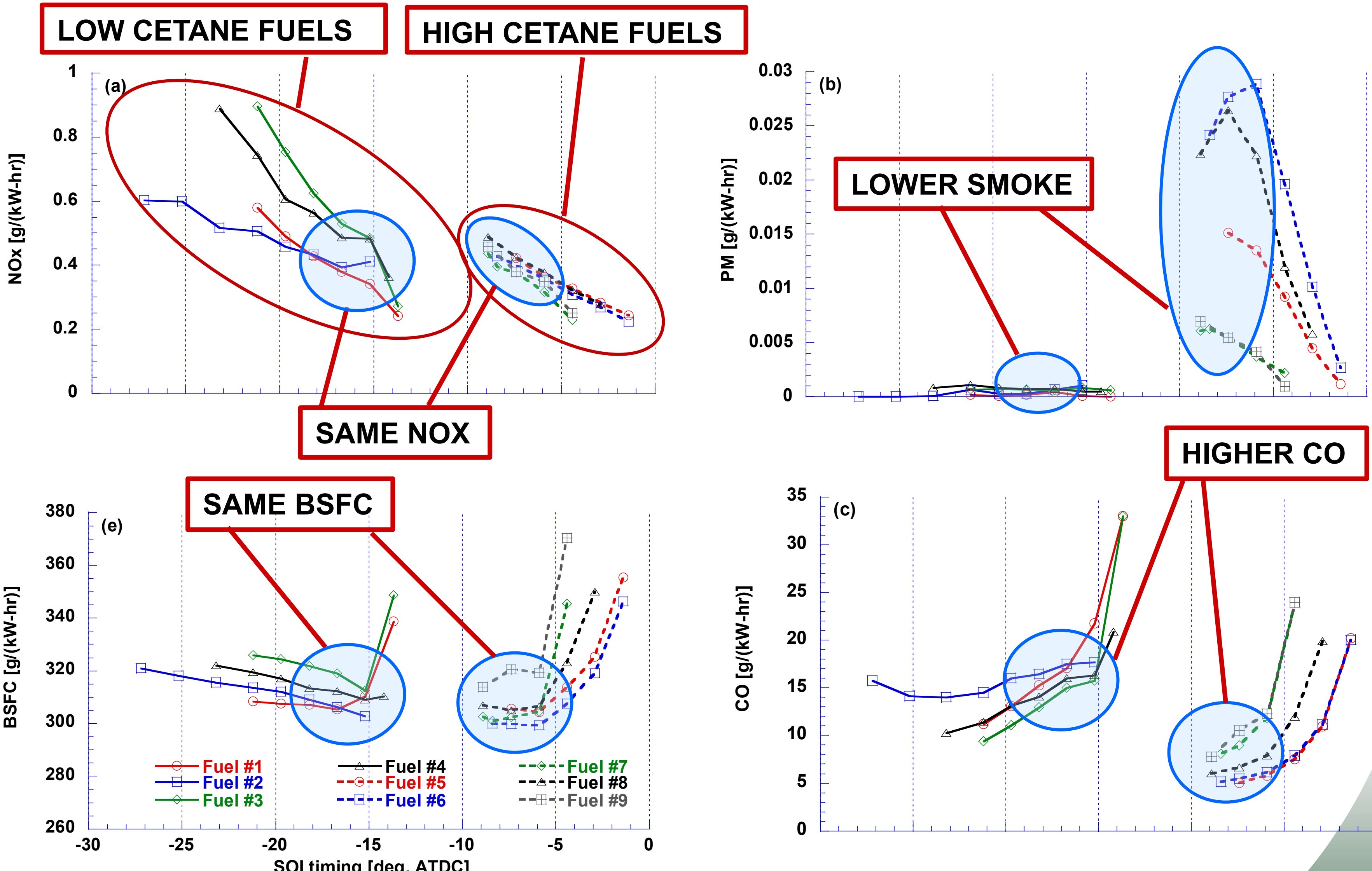
- **HCCI single cylinder engine**
  - **Mixing controlled in intake manifold, fairly constant**
  - **Combustion phasing controlled by intake temperature**
  - **Combustion quenching at lower intake temperatures**
- **GM 4 cylinder diesel engine operated in PCCI**
  - **With single injection, combustion phasing and mixing are both controlled by injection timing and ignition delay**



Performance differences between engines

- HCCI engine
  - Definitely prefers low cetane fuels for best ISFC
    - Higher intake temperatures reduces cylinder quenching
- PCCI engine
  - Achieves same BSFC and NOx with high and low cetane fuels
    - Higher cetane fuels required later injection
      - Less mixing time
      - Higher smoke, lower CO and HC
    - Lower cetane fuels required earlier injection
      - More mixing time
      - Lower smoke, higher CO and HC

GM 1.9 engine, FACE diesel fuels, low vs. high cetane fuels



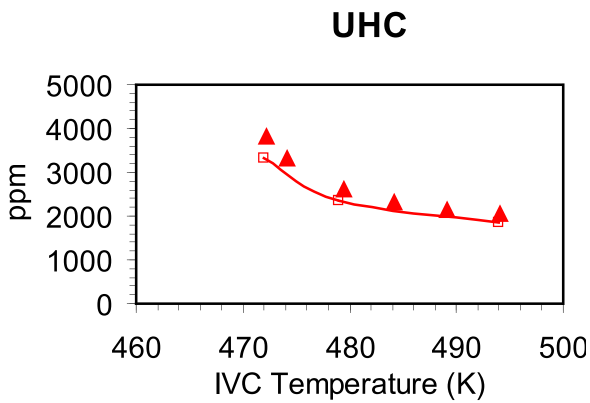
Detailed exhaust chemistry for HCCI engine

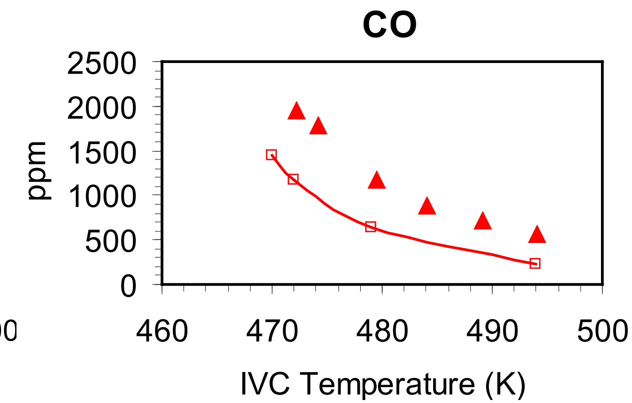
- Two series of surrogate fuels
  - Gasoline surrogates
    - 87 RON PRF (non-aromatic blend)
    - 87 RON TRF (aromatic blend)
    - 87 RON PRF + 30% ethanol (i-blend)
  - Diesel surrogates
    - FACE 9 (baseline)
    - 44 cetane n-hexadecane + 1-methylnaphthalene
      - Sooting fuel
    - 44 cetane n-hexadecane + heptamethylnonane
      - Non-sooting fuel
- Fixed speed and fuel rate

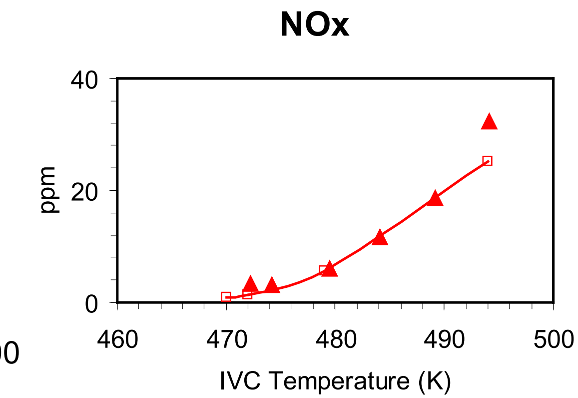
Major conclusions – detailed HCCI exhaust chemistry

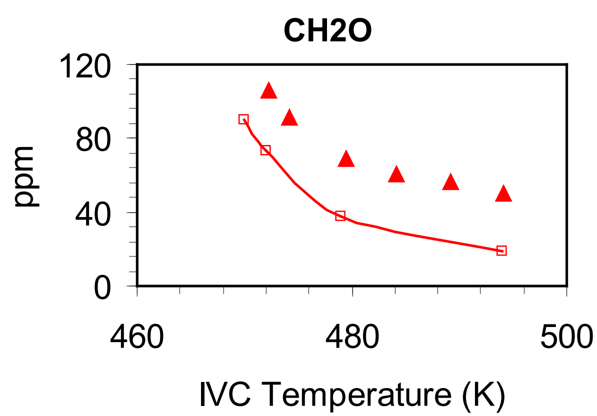
- **About 90% of HC emissions are unburned fuel, with fuel chemistry profile maintained in exhaust**
- **Combustion intermediates can be measured in exhaust**
  - **Major species are formaldehyde (40 to 120 ppm), acetaldehyde (20 to 80 ppm), butadiene (2 to 14 ppm)**
  - **Other species such as benzaldehyde and benzoic acid are present if fuel contains aromatics**
  - **These species can be reproduced with CFD kinetic modeling**
- **Particulates from engine are mainly volatile condensation particles, not representative of diesel soot**

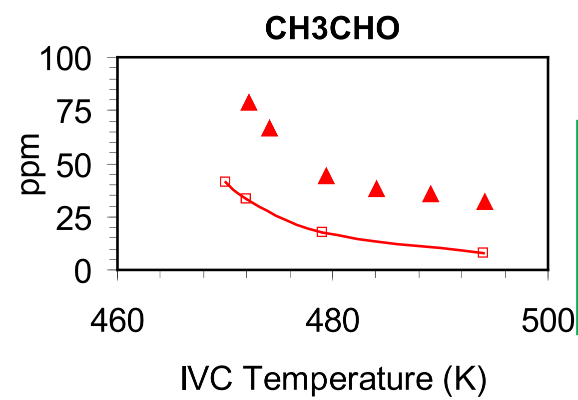
HCCI CFD modeling, particulate characteristics





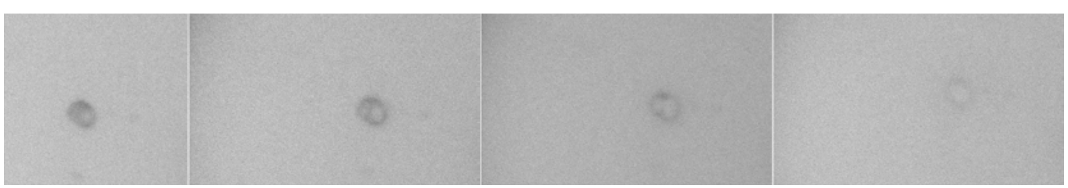






▲ **Data** —□— **Model**

SAE 2010-01-0362
Reaction Design MFC reduced mechanism
428 species, 2378 reactions
Reaction Design Forte CFD
53,800 cells at TDC



TIME IN BEAM ⇒

TEM image of HCCI exhaust particulate
- **10-20 nm diameter**
- **indistinct**
- **evaporate in microscope**

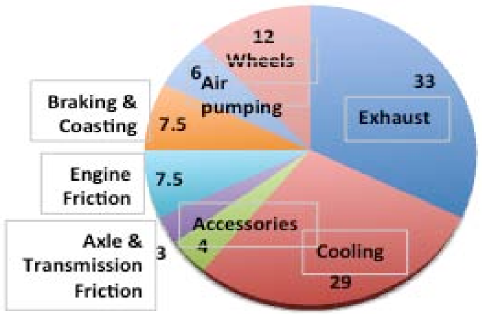
CRADA with GM: Ionic Liquid Lubricants

- **Goal: develop new class of lubricants based on ionic liquids and demonstrate benefits for internal combustion engines**
  - **As base stock or blending stock**
  - **As lubricant additive**
- **Team: ORNL: J. Qu, P.J. Blau, S. Dai, H. Luo, and B.G. Bunting**
  GM: G. Mordukhovich and D.J. Smolenski
- **Program timeline: 5/09 - 2/13 (45 months)**
  - **Phase I. Design, Synthesis, and Characterization of Candidate Ionic Liquids**
  - **Phase II. Friction and Wear Bench Tests and Analysis**
  - **Phase III. Instrumented Single- and Multi-Cylinder Engine Tests**
  - **Phase IV. Full-Scale Multi-Cylinder Engine Tests**

Ionic Liquids as Lubricants and/or Lubricant Additives (ORNL-GM CRADA)

STATUS QUO

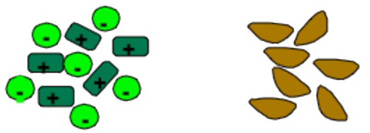
In an automobile, ~10% of energy is lost to friction



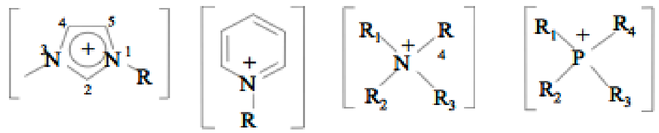
Distribution of energy consumption in car

NEW INSIGHTS

Ionic Liquids – A new class of more effective, environmentally friendly lubricants or lubricant additives could potentially leads to huge energy savings



Molecular structures



1-alkyl-3-methyl-imidazolium | *N*-alkyl-pyridinium | Tetraalkyl-ammonium | Tetraalkyl-phosphonium ($R_{1,2,3,4}$ = alkyl)

(a) Common cations

$[PF_6]^-$, $[(CF_3SO_2)_2N]^-$, $[BR_1R_2R_3R_4]^-$

$[BF_4]^-$, $[CF_3SO_3]^-$

$[CH_3CO_2]^-$, $[CF_3CO_2]^-$, $[NO_3]^-$, Br^-, Cl^-, I^-, $[Al_2Cl_7]^-$, $[AlCl_4]^-$ (decomp.)

(b) Common anions

Unique properties

- Inherent polarity
- Higher thermal stability
- Reduced volatility
- Can be non-flammable
- High flexibility of molecular design

Superior lubricating characteristics compared to fully-formulated engine oils

- Up to 50% friction reduction
- Up to 55% wear reduction

Projected cost <$5/L with scale-up

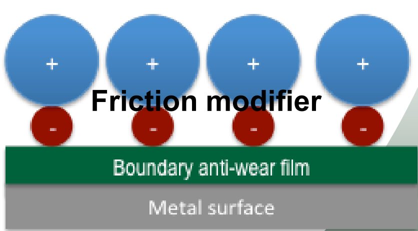
Output

As base stock:

- Friction and wear reduction
- Operating temperatures up to 500 °C
- Non-flammable
- Tailor to special applications

As oil additive:

- Multi-functions possible: friction, wear, detergent
- Potentially reduction or elimination of ZDDP (catalyst poisoning)
- Easier penetratrion into current market.



ILs as multi-function additives

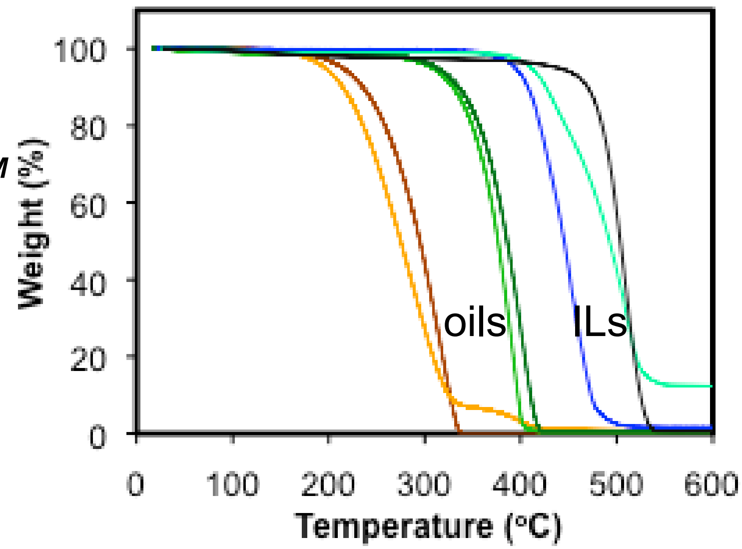
Patent: J. Qu, J.J. Truhan, S. Dai, H. Luo, P.J. Blau, "Lubricants or Lubricant Additives Composed of Ionic Liquids Containing Ammonium Cations," U.S. Patent, published on Mar. 20, 2008, Publication# US-2008-0070817-A1.

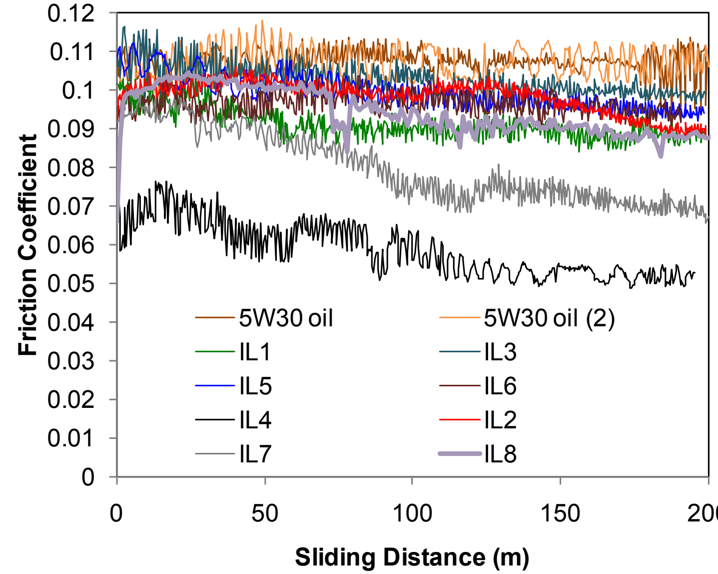
OAK RIDGE National Laboratory

Technical Progress and Plan

Progress

- **Ionic liquids as neat lubricants** (**vs.** ***Mobil 1™ 5W-30 fully-formulated engine oil***)
  - Higher thermal stability (350-470 °C vs. 230-250 °C)
  - Friction reduction up to 50% in bench tests
  - Most are much less corrosive than water for cast iron
- **Ionic liquids as oil additives** (***5% mixed with Mobil 1™ 5W-30 fully-formulated engine oil***)
  - Required development of oil-soluble ILs
  - Wear reduction up to 30% in bench tests
  - Partnering with Chevron for supply of partially-formulated engine oils for blending studies





Plan for FY10-11

- Tailoring and optimization of molecular structures
- Tribological bench tests - investigation of lubricating mechanisms
- Single cylinder engine evaluation
- Prepare for multi-cylinder engine evaluation

Future work

- FACE gasoline fuels will be evaluated when available
  - Stoichiometric, spark-assisted HCCI with ORNL GDI HVA engine
    - Operation up to 7.5 bar IMEP
    - Focus on operating range, efficiency, and emissions
  - Dilute, premixed HCCI
    - Focus on kinetics, property and chemistry effects
- FACE diesel fuels will be evaluated a second time on GM diesel with more complex PCCI control strategies and at multiple speeds and loads
- Surrogate blends will be prepared and evaluated for comparison to FACE gasoline and diesel fuels
  - Evaluations in support of CRC AVFL18 project (diesel surrogates)
  - Evaluations in support of Reaction Design CRADA (NPBF)
- Mining of past data using statistics to determine common responses between fuels and engines and determine common, controlling fuel characteristics (NPBF)

Overall summary

- Cetane number remains a major fuel variable for advanced combustion engines
  - Advanced combustion engines respond differently to fuels based on how mixing and ignition are controlled
- Fuel studies have been expanded to include detailed exhaust chemistry, kinetic modeling and statistical analysis of trends
- Ionic liquids represent a new class of lubricants or lubricant additives with potential to reduce engine friction and wear