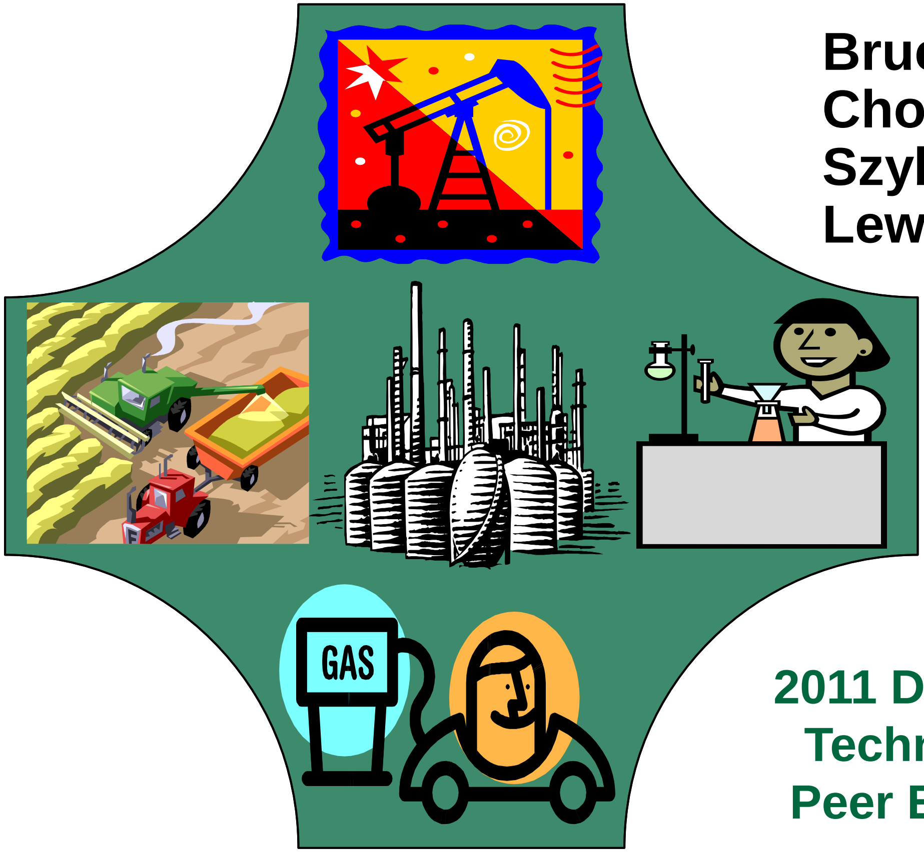
FT001 – Fuel and Lubricant Effects

Fuels Research, DOE agreements 13415, 13425



Bruce G. Bunting, Mike Bunce, Kukwon Cho, Jun Qu, Robert Crawford, Jim Szybist, Scott Sluder, John Storey, Sam Lewis, Robert Wagner

DOE management team:
Steve Goguen, Kevin Stork, Steve Przesmitzki, Dennis Smith

2011 DOE Hydrogen Program and Vehicle Technologies Annual Merit Review and Peer Evaluation Meeting, May 9-12, 2011

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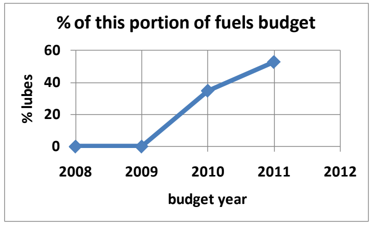
Outline

- **Overview**
- **Collaborations**
- **Objectives**
- **Milestones**
- **Approach**
- **Technical accomplishments and progress**
  - **Comparisons of fuels and engines (3 slides)**
  - **Statistics (1 slide)**
  - **Kinetic modeling (1 slide)**
  - **Ionic lubricants (1 slide)**
  - **Lube effects (1 slide)**
- **Future work**
- **Summary**
- **(Response to review comments)**
- **(Publications and presentations)**
- **(Critical assumptions and issues)**

Project overview

- **TIMELINE**
  - Started in 2004 with advent of APBF and NPBF projects
  - Work continues to evolve to new areas: new fuels, new engines, kinetics, statistical analysis, lubrication
  - Funding for APBF and NPBF now combined under ‘Fuels Science’
  - We have maintained our two presentation format (Bunting, Szybist)
- **BUDGET**
  - DOE funding of $935K (2011), $950K (2010), and $730K (2009)
  - Lubes now 50% of this portion of research



- **BARRIERS / TECHNICAL TARGETS**
  - Renewable fuels - technical and economic impact on infrastructure
  - Fuel effects on combustion and efficiency - inadequate data and tools
  - Lubricants – long term impacts on engines
- **PRESENT COLLABORATORS:**
  - Many, noted on next slide

Many collaborations, many areas

PARTNER / COLLABORATOR	AREA OF PARTNERING	ORNL CONTRIBUTION	PARTNER CONTRIBUTION
Reaction Design	Surrogate fuels, kinetic mechanisms, kinetic and CFD modeling	Engine and emissions data for fuels and surrogates	Access to MFC consortium and modeling tools, modeling of ORNL data
General Motors	Use of ionic liquids as engine lubricants	Formulation, bench, and small engine evaluation	Market requirements, bench evaluation, full engine evaluation
Univ. of Tennessee	Unique plant extracts as fuels, lubrication research	Advising, direction, experimental data	Graduate students, plant extracts, analysis
Univ. of Wisconsin	Use of hybrid kinetic mechanisms to study fuel effects	Funding, direction, experimental data	Modeling results, modeling tool development, joint publications
Massachusetts Institute of Technology	Lubricant effects on aftertreatment and engine durability	Work-in-kind, engine and aftertreatment data	Research direction by Durable Engine and Aftertreatment Consortium
University of Maine	Fuel effects, cellulosic derived biofuels	Advice, experimental data, data analysis	Samples of fuels, chemistry, data analysis
Pacific Northwest National Lab	Fuel chemistry, property, performance, and fit-for-use	Engine results, joint program direction, advice, fuels	Other results, joint program direction, analysis, fuels
C/e-Solutions	Fuels derived from municipal sewage processing	Engine results, advice	Surrogate fuels, process information
AVL Powertrain, AVL North America	Combustion analysis, statistics, engine design modeling	Use of equipment and methods in research	Training, assistance in setting up, access to software (and they sell us stuff, too)
Robert W. Crawford	Statistical analysis, principal components analysis	Engine and fuels data, funding, direction	Statistical analysis
sp3h	On-board NIR fuel quality sensor	Engine results, fuel samples, analysis, advice	Sensor results, data analysis, prototype sensor
DOE office of biomass programs	Fungibility and compatibility of emerging biofuels	Experimental data for emerging fuels or bio-feed stocks	Funding for study of fungibility and compatibility

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 and lubricant effects on combustion and engine optimization**
- **ORNL PROJECT OBJECTIVES (covered in this talk)**
  - **Continue the study of properties, chemistry, engine performance, and fit-for-use of emerging renewable fuels**
  - **Determine and help develop ability of kinetic modeling to accurately reproduce fuel effects**
  - **Continue use of statistics**
  - **Study of lubricants as related to engine efficiency and durability**

Milestone chart by fuel type

	2004	2005	2006	2007	2008	2009	2010	2011
Conventional fuels	XXX	XXX	XXX		XXX	XXX	XXX	XXX
Heavy crude derived				XXX	XXX			XXX
Renewable fuels			XXX	XXX	XXX	XXX	XXX	XXX
Conventional gasolines	XXX				XXX	XXX		
Surrogate fuels		XXX	XXX		XXX	XXX	XXX	XXX
Lubricant research							XXX	XXX

2011 milestones are:

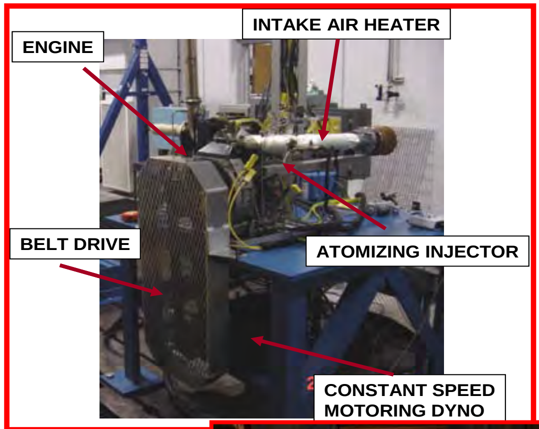
1) Evaluation of biofuels, fuels, and engines (in progress)
2) Supply engine data for Model Fuels Consortium (diesel engine installed with improved heat release measurement capability, fuels being blended)
3) Make statistical analysis routine (done, AVL Cameo™ combined with generalized PCA program)
4) Ability of kinetic mechanisms to mimic detailed fuel effects (in progress)
5) Further progress on ionic liquid lubes (meeting technical objectives)
6) Evaluate experimental oils for friction vs. viscosity in motored rig recommendations for improving rig (tests complete, improvements in progress)
7) ZDDP effects on friction and wear (equipment procured, plan developed, starting with new and used oil effects)

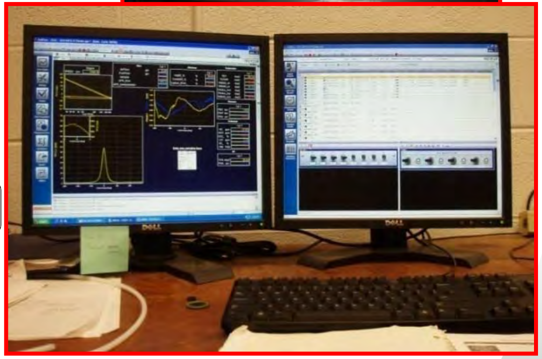
Approach

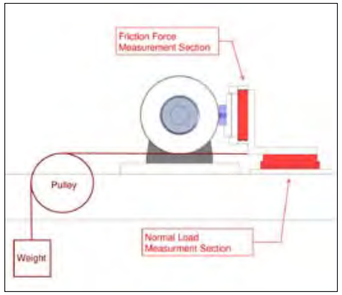
- Use a wide range of fully formulated fuels and surrogate blends to study effects of fuel properties and chemistry on advanced and conventional combustion engines, with emphasis on emerging fuels
- Use multiple research platforms and multiple collaborations to produce broadly applicable data
- Emphasis on fuel efficiency and system approach to understanding of engine, fuel, and lubricant effects
- Kinetic modeling and statistical analysis of results
- ORNL fuels talks split into two parts, but no longer by APBF and NPBF, second talk at 12:00 pm
  - Diesel, new biofuels, modeling, lubrication (this talk)
  - Gasoline, ethanol, efficiency, HCCI (12:00 pm)

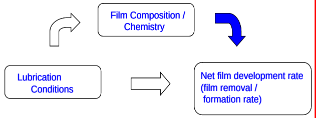
Multiple research platforms

- Single cylinder engine
  - Gasoline HCCI, PFI, intake heating
  - Diesel HCCI, PFI, intake heating
  - Conventional diesel, direct injection
  - Improved combustion analysis, precision energy balance
- Motored friction rig
- Bench friction rigs
- MIT friction rig

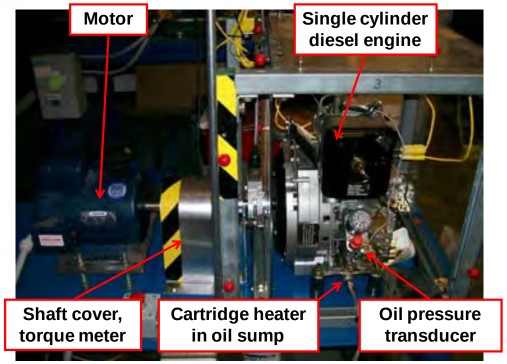




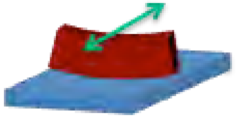


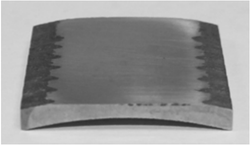


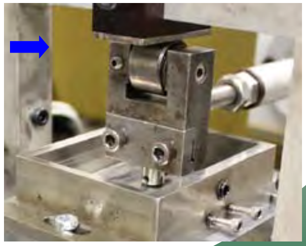
MIT friction-wear tribofilm test rig with controlled oil/additive flow-composition



Ring-on liner configuration (similar to ASTM G-181)







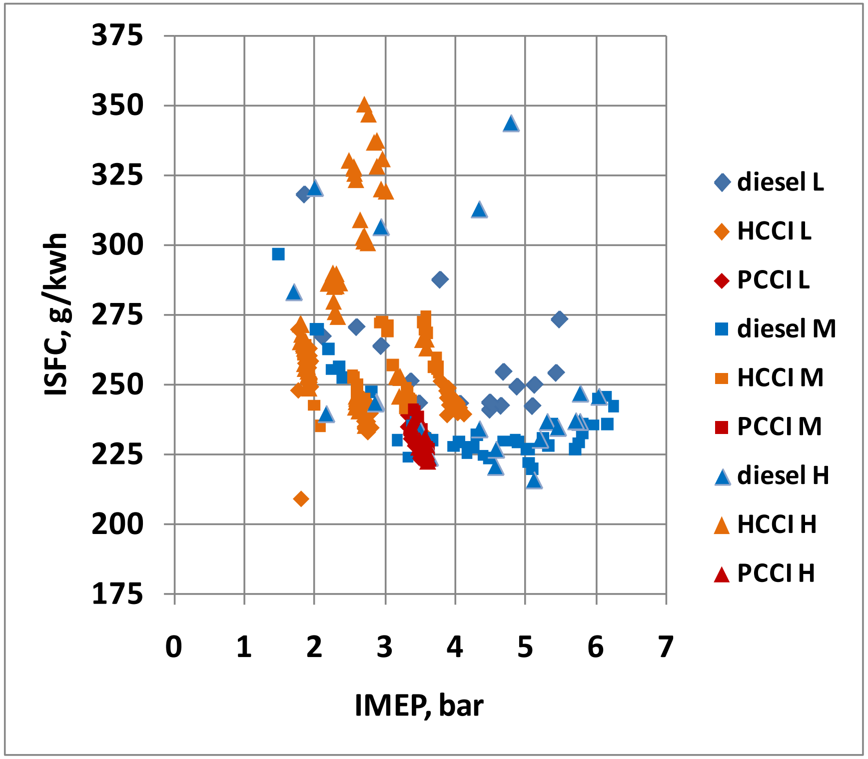
Fuels and combustion strategy comparison, 1

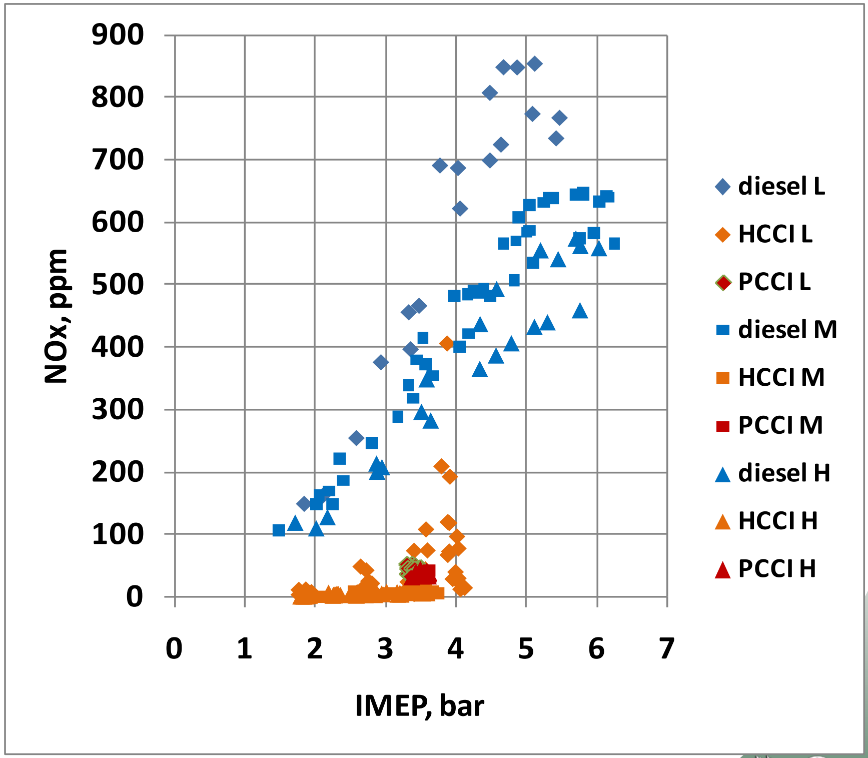
- **FACE diesel fuels, 3 combustion strategies, different engines, different test plans**
  - **Where timing sweeps were performed, best ISFC points were selected for plots**
  - **The following plots are only a small representation of comparisons which can be made**
  - **Results should not be extrapolated to other engines**

combustion style	engine	rpm	IMEP range, bar	injection	aspiration	varied in experiment	selection of plot points
diesel	Hatz single cylinder	1800	1.5 to 6.3	direct, mechanical, fixed timing	natural	fuel rate	all
HCCI	Hatz single cylinder	1800	1.8 to 4.1	port atomization	boosted, throttled	fuel rate, intake temperature, lambda	best ISFC
PCCI	GM 1.9 liter 4 cylinder	1500	3.1 to 3.4	direct, electronic	turbocharged	injection timing	best ISFC

Fuels and combustion strategy comparison, 2

- **Combustion strategy indicated by color, fuel cetane by shape, L=low=29 to 31, M=medium=44 to 46, H=high=49 to 55**
- **Diesel has wider operating range than HCCI (PCCI only evaluated at one IMEP)**
- **Fuel economy comparison difficult because of differing engine types**
- **Diesel produces more NOx than HCCI and PCCI, but HCCI will catch up at higher loads**





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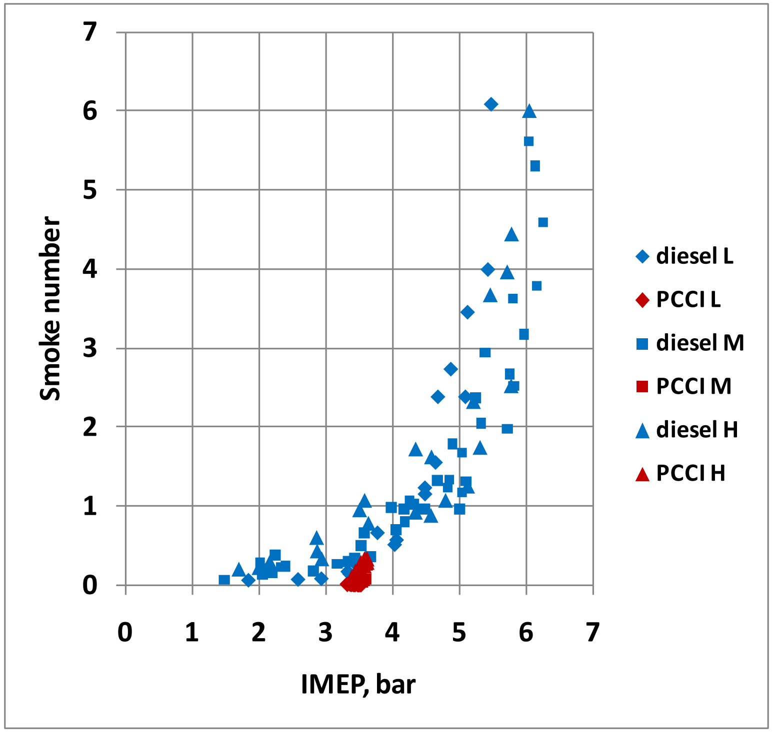
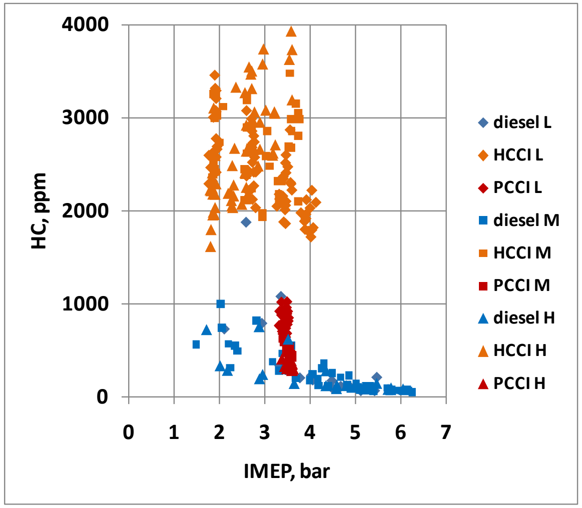
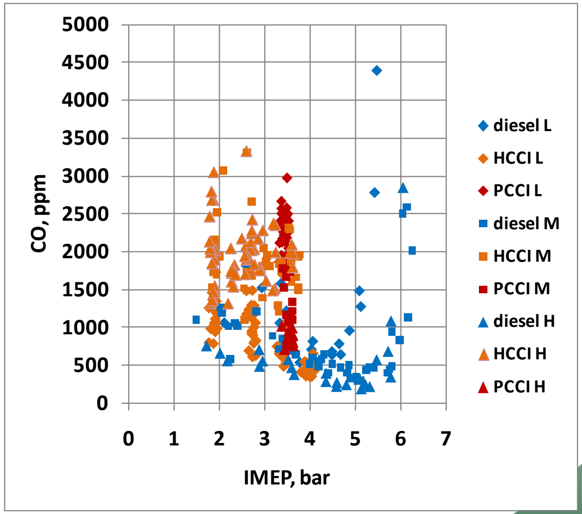
Fuels and combustion strategy comparison, 3

- Diesel appears to produce more smoke than PCCI
- Diesel and PCCI similar HC, HCCI much higher
- PCCI and HCCI produce more CO than diesel



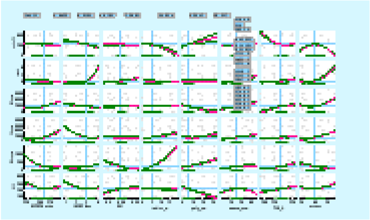


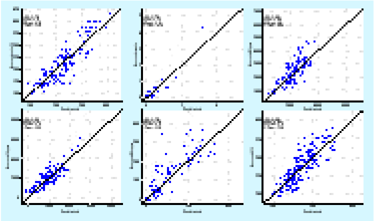


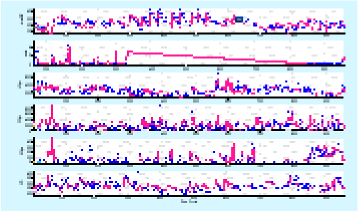
OVERALL TAKEAWAY: ENGINES WILL RESPOND DIFFERENTLY TO FUELS AND CONTROL STRATEGIES AND THESE SHOULD BE OPTIMIZED TOGETHER. THERE IS STILL A LOT OF RESEARCH TO BE DONE.

Making statistical analysis routine

- Funding stopped in 2011, some carryover from 2010
- Acquired AVL Cameo™ software for statistical analysis
- Developed generalized PCA module (design principal components, calculate vector values, resolve vector values back to chemistry and properties)
- Detailed studies completed for 'all diesel fuels', 'heavy crude derived fuels', and 'all biofuels' from ORNL data set of 100 fuels run during 2005 to 2011
- Key findings:







  - 4 to 7 fuel variables can resolve 'similar' fuels, but are not sufficient for global fuel studies
  - Properties and chemistry do about equally good job of describing fuels
  - Very important to track experimental design space – fuels are not orthogonal and have multiple internal correlations
  - PCA is a more efficient way to represent fuels for statistical analysis, but needs to be resolved back to properties and chemistry to understand trends and effects

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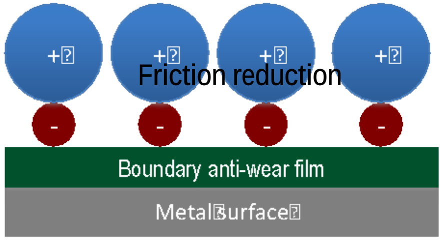
Ability of kinetic mechanisms to mimic detailed fuel effects

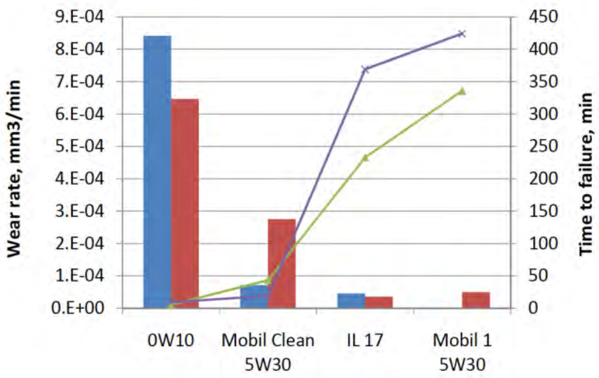
- **Reproducing detailed fuel effects in kinetic modeling requires complex surrogates to reproduce chemistry and physical properties of fuels**
  - **These complex surrogates result in kinetic mechanisms which can be too large for CFD modeling**
- **Two groups are developing hybrid mechanisms, with different approaches, that allows one model for physical properties (spray, mixing, and evaporation) and a second model for chemical processes (combustion)**
  - **Reaction Design and Model Fuels Consortium**
  - **University of Wisconsin Engine Research Center**
- **We are collaborating with both groups to evaluate methodologies, using mainly data run on Hatz diesel and HCCI engines for FACE diesel fuels**
- **Results are in progress and will be published later**

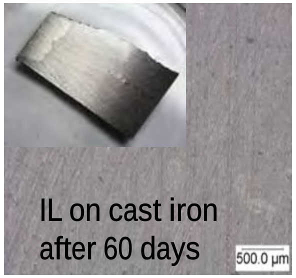
Ionic Liquid Lubricants, CRADA with GM

- Develop a new class of ionic liquid-based lubricants and demonstrate benefits as base stocks or additives for internal combustion engines.
- Team: ORNL: J. Qu, P.J. Blau, S. Dai, H. Luo, and B.G. Bunting
  GM: G. Mordukhovich and D.J. Smolenski
- Program timeline
  - Phase I. Design, Synthesis, and Characterization of ILs: 2/2010 (completed)
  - Phase II. Friction and Wear Bench Tests and Analysis: 2/2011 (completed)
  - Phase III. Single- and Multi-Cylinder Engine Tests: 2/2012 (in progress)
  - Phase IV. Full-Scale Multi-Cylinder Engine Tests: 2/2013
- Base stock approach: ILs have been developed with viscosity similar to 0W10 oil but wear protection comparable to 5W30 engine oil.
- Additive approach: Newly developed ILs are fully miscible with mineral and synthetic oils, non-corrosive, high thermal stability (>350 °C), excellent antiwear and friction reduction, and synergistic with ZDDP.

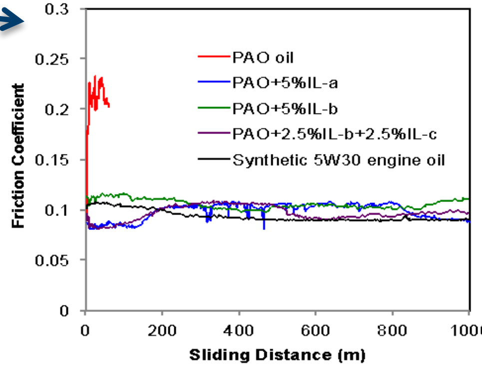


Friction and wear reduction mechanism of ionic liquids





Lubricant	Viscosity @ RT (cSt)	Wear rate (mm^3/N-m)	Wear reduction by IL additives
PAO-4 oil	35	$2.4x10^{-4}$	
PAO-4 oil + 5 wt% IL-a	37	$6.3x10^{-7}$	99%
PAO-4 oil + 5 wt% IL-b	36		
SAE 5W30 engine oil	140	$4.9x10^{-7}$	
SAE 5W30 engine oil + 5 wt% IL-a	151	$1.5x10^{-7}$	69%
SAE 5W30 engine oil + 5 wt% IL-b	150	$0.6x10^{-7}$	88%



Lube effects on friction and wear

- This is work-in-kind project with MIT Durable Engine and Aftertreatment Consortium
- Excellent opportunity because consortium includes 3 lube related companies, 4 engine related companies, and 2 aftertreatment related companies
- Our portion of research is being conducted as a UTK PhD project, with guidance from MIT group
- Key questions:
  - To what extent can a complex engine model (in this case, AVL Excite™) serve as a link between full engine performance and bench rigs, defining conditions and projecting results?
  - Can precision heat release and energy balance detect lube additive effects?
- First area of focus: new vs. used lube oils

Future work

- Obtain new fuels derived from oil shale, pyrolysis oil, and other fuels for engine, property, chemistry, and fit-for-use evaluation (joint effort with PNNL)
- Partner with other organizations to gain access to emerging biofuels
- Complete new series of fuels and surrogates on diesel engine for Model Fuels Consortium with detailed exhaust chemistry and particulate characterization
- Continue research to define kinetic mechanisms for modeling effects of wide range of complex fuels
- Begin engine evaluation of ionic liquid lubricants
- Complete set-up of equipment for MIT consortium project and begin research

Overall summary

- We have added another 30 fuels to our database this year, with more coming: plant extracts, cellulosic derived renewable and oxygenate fuels, oil shale, pyrolysis
  - New collaborations help us procure and understand these fuels
- The use of Hatz-based engines for research has expanded over the last several years: catalyst aging and poisoning, demonstration of HCCI, fuels evaluations, data for kinetic modeling, lubrication research
  - Major advantages; requires very little fuel, simple, robust, easy to modify, easy to model
- Use of statistical analysis and development of complete, kinetic mechanism research is continuing with focus on complex fuel effects
- Lubrication is an increasing part of fuels technology research and ORNL is well positioned to contribute