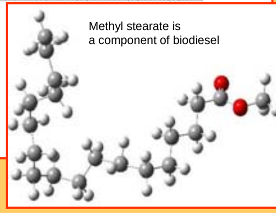
Efficient Combustion for Renewable Fuels

NSTD capabilities in combustion chemistry and high-performance computing are coupled with National Transportation Research Center strengths in experimental engine research to develop use of alternative fuels in energy efficient, environmentally sound transportation systems.

Biofuels present technical challenges when used in advanced combustion.

- Physical properties are different from standard diesel.
- Heating values are somewhat lower (Biodiesel is 33.3-35.7 MJ/L, Diesel is 36.4 MJ/L).
- High efficiency clean combustion shows promise to lower both soot and NO_X.
- But biodiesel combustion chemistry must be understood to understand impact on low temperature combustion.

Simulation coupled with experiment addresses these questions.



Biodiesel versus Tetradecane

property	Diesel*	Biodiesel*
Density [g/cm³]	0.7625	0.8837
vapor pressure [dyne/cm²]	22.244	0.00061 (0.01180)
surface tension [dyne/cm]	26.83	24.87
liquid viscosity [dyne-s/cm²]	0.0314	0.091
liquid thermal conductivity [erg/cm-s-K]	1.4430E+4	1.0020E+4
latent heat [erg/g]	3.6E+9	3.379E+9**
vapor specific heat [kcal/mol-K]	0.1536#	0.2026#
vapor diffusion coefficient [cm²/s]	8.50E-2	9.441E-3
vapor viscosity [dyne-s/cm²]	1.00E-4#	1.21E-4**#
vapor thermal conductivity [erg/cm-s-K]	4344.7#	2601.9#
liquid specific heat [J/g-K]	2.270182	2.0128153

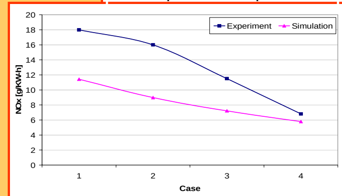
Fuel physical properties are needed for accurate prediction of thermochemical behavior

- Critical properties for biodiesel and olefin fragments not measured experimentally
- Were determined from molecular structure calculations
- Properties used in prediction of physical behavior in multicomponent spray models

Emissions were predicted using chemical kinetic simulations

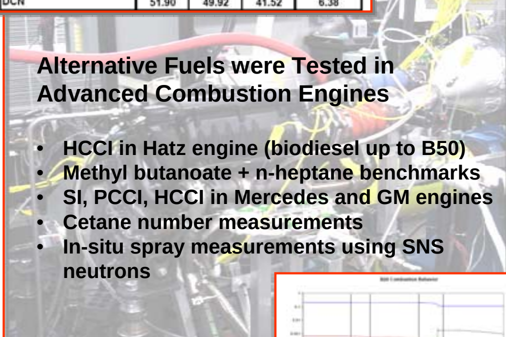
- Used derived physical properties to determine heat release
- 1500 reaction mechanism reduced to a couple hundred reactions by sensitivity analysis
- Implemented heat transfer and multizone model
- Developed parallel software, XCHEMKIN, for automated mechanism reduction

NOx Predictions from ERC-Bio Reproduce Experiment



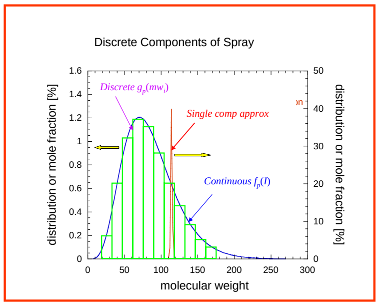
Properties and compositions of surrogate fuels used for simulation

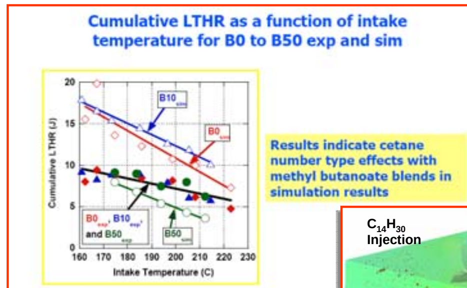
	$B0_{sim}$	$B10_{sim}$	$B50_{sim}$	Methyl Butanoate
Wt% methyl butanoate	0.00	4.02	19.64	100.00
Wt% C	83.90	82.89	78.97	58.80
Wt% H	16.10	15.85	14.88	9.87
Wt% O	0.00	1.30	6.20	31.33
A/F_{stoich}	15.12	14.87	13.88	8.77
LHV (MJ/kg)	44.40	43.40	39.18	25.97
DCN*	51.90	49.92	41.52	6.38



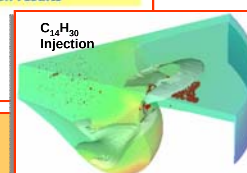
Alternative Fuels were Tested in Advanced Combustion Engines

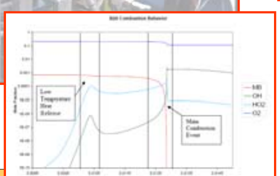
- **HCCI in Hatz engine (biodiesel up to B50)**
- **Methyl butanoate + n-heptane benchmarks**
- **SI, PCCI, HCCI in Mercedes and GM engines**
- **Cetane number measurements**
- **In-situ spray measurements using SNS neutrons**





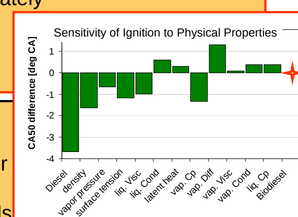
Results indicate cetane number type effects with methyl butanoate blends in simulation results





Engine Simulations Were Aligned with Model Validation

- Accurate meshes for GM, Mercedes and Hatz engines, Bosch nozzle
- Predictions were improved using new multicomponent spray model that handles discrete biodiesel components
- Effects of chemistry and physical properties were evaluated separately
- Homogeneous charge compression ignition and Premixed charge compression ignition both modeled

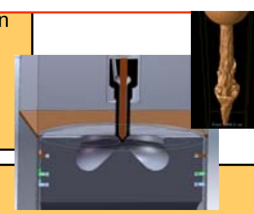


Support of Education

As reported in the *Oak Ridger*, September 13 2007, activities at Oak Ridge High School caught the attention of Rep. Zach Wamp, seen here in a photo with Ms. Benita Albert and her senior math class. Two of the students, KC Cushman and Refuyat Ashen, are working on chemical kinetic modeling of biodiesel and ethanol fuels in HCCI engines. They have submitted a paper to the prestigious Siemens competition. A Farragut senior student, Timm Moon, will be modeling the properties of long chain olefins and methyl esters using electronic structure calculations.

Future Opportunities

- Collaboration with universities and other national labs
- Biofuels development (weeds-to-wheels)
- KIVA simulations of advanced combustion
- Droplet formation by interface tracking
- CFD model development
- Collaborations with industry on advanced simulation and fuel development



Papers

- SAE 2007-01-4010 (Szybist et al.) **Simulation of Biodiesel Blends HCCI in a Modified Hatz Diesel Engine**
- SAE 2007-01-4030 (Chakravarthy et al.) **Differences in physical properties of soy bio-diesel and n-heptane : Implications for use of bio-diesel in diesel engines**
- SAE 08-PFL-944 (Ra et al.) **Effects of Fuel Physical Properties on Diesel Engine Combustion using Diesel and Bio-diesel Fuels**
- SAE 08-PFL-945 (Brakora et al.) **Development and Validation of a Reduced Reaction Mechanism for Biodiesel Fueled Engine Simulations**

Participants

Joanna McFarlane, Valmor de Almeida (NSTD)
Johney Green, Kalyan Chakravarthy, Stuart Daw (ESTD)

- Bruce Bunting, Tom Briggs, Zhiming Gao, Sam Lewis, Scott Sluder, Jim Szybist, Robert Wagner (ESTD), Bill Steele (NSTD),
- Jessica Brakora, Youngchul Ra, Rolf Reitz – University of Wisconsin
- Wurigen Bo, Jim Glimm, Xiaolin Li, Xingtao Liu – SUNY Stony Brook
- David Torres – Los Alamos National Laboratory
- Jelani Griffin – Georgia Institute of Technology
- Stanton Elseroad – Vanderbilt, Gokhan Yesilyurt – U. Michigan
- K.C. Cushman, Refuyat Ashen – Oak Ridge High School
- Timm Moon – Farragut High School

Research sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory (ORNL), managed by UT-Battelle, LLC for the U. S. Department of Energy under Contract No. DE-AC05-00OR22725