



University of Illinois at Urbana-Champaign's GATE Center for

Advanced Automotive Bio-Fuel Combustion Engines

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Overview

Timeline

•Start: October 2005 •Finish: September 2012 •80% Complete

Budget

•Total Project Funding •DOE: \$592,350 •UIUC:\$157,179 •Funding received •FY09:\$123,326 •FY10:\$123,161

Barriers

Educational and research challenges

- •Bio- vs. -fuels: currently an educational disconnect
- •Biofuel automotive combustion with high efficiency and low emissions is not a direct extrapolation of current automotive practices
- •Biofuel properties relevant to automotive combustion remain an almost uncharted area

Partners Local and International

- •Energy Biosciences Institute
- •University of Salento, Italy
- •National Technical University of Athens, Greece
- •Volkswagen, Europe
- •Gamma Technologies
- •Ford, USA

- •Cummins
- Quantlogic
- •Caterpillar
- •Deere & Company •BP
- Incobrasa Industries
- Tetravitae







Objectives

- Set up a comprehensive syllabus that will enrich the technical expertise of graduate students of thermal/automotive sciences in agricultural/biological issues related to biofuels and vice-versa.
- Provide a channel through which well established theoretical, computational, and experimental methodologies can be focused so that the potential of biofuels for automotive combustion is fully explored.
- Develop state-of-the-art techniques for automotive R&D with a particular emphasis on laser diagnostics, modeling, and multidimensional computations.
- Establish a mutually beneficial strong link with both the automotive and agricultural industry.





Milestones

GATE Center of Excellence on Advanced Automotive Bio-Fuel Combustion Engines



Phase II: September 2007 – September 2010

Fully investigate potential of biofuels for automotive combustion, provide group of highly skilled scholars and engineers to develop new technology, and transfer knowledge on novel and environmentally friendly fuels and on advanced engine designs to industry

Month/Year	Milestone		
Oct. 2009	Student society engagement (SAE, Pi-Tau-Sigma charter is advised by GATE co-PI)		
Jan. 2010	Identification of novel fuels for investigation (butanol, baelene, and algae biodiesel)		
Jan. 2010	Establish collaboration with international partners (in China, Greece, and Italy)		
Nov. 2010	Active involvement of the Industrial Advisory Board		
Ongoing	Knowledge transfer to industry via collaborations, meetings, conferences and industrial internships. Technology transfer to bio- fuel production industry (EBI, Tetravitae)		
Ongoing	Fundamental and applied research projects on biofuel properties and combustion		





Overall Approach

Establish a high-quality interdisciplinary program at the M.S. and the Ph.D. level that will bridge the current educational disconnect between mechanical and biological aspects of biofuel technology and will integrate educational initiatives and collaborative research projects

- An interdisciplinary curriculum that provides comprehensive, advanced training on automotive biofuel combustion to students that approach the subject both from both Mechanical Engineering and Agricultural/Biological Engineering backgrounds has been set up.
- Seminal research projects of current interest have been identified by the PIs and have been assigned to GATE fellows The input of the Industrial Advisory Board will be crucial for the determination of future research directions.
- Industrial internships that will constitute a required program component.





Technology

and

Environment

ENTROPMENT

Overall Approach



- In-Cylinder Diagnostics
- Emissions Reducing Technologies
- Biofuels in micro-combustion



GATE

GATE Center of Excellence on Advanced Automotive Bio-Fuel Combustion Engines

- Performance measures
 - Comparison with proposed milestones
 - Student participation and evaluation
 - Research productivity (publications, presentations)
- The project is on time with respect to Phase II tasks
 - Establishment of interdisciplinary curriculum
 - Research projects and thesis work (ongoing)
 - Students participate in industrial internships (Caterpillar)
 - Active involvement of the advisory board (ongoing)
- 46 students involved in the seminar series, 20 enrolled in new class, numbers above campus averages.
- 28 archival journal publications, 14 peer-reviewed refereed conference papers,

16 conference presentations, 7 theses, two book chapters and one book by the 3 co-PIs and the 9 supported students in the fourth year.

- GATE co-PIs elected Fellow of SAE and Associate Fellow of the AIAA in recognition of GATE-related research activity.
- The Technical Meeting of the Central States Section of the Combustion Institute was organized on-campus in the University of Illinois in March 2010.





Accomplishments - Educational

• All 46 students involved in the program so far participated in the seminar class ME 598/ABE 598: "*Automotive Bio-energy*". The students were required to investigate a wide range of bio-fuel related issues (mechanical, agricultural, chemical, economical, legal) and give half-hour presentations.

• Weekly sessions with typically two student presenters. Students supported on GATE fellowships gave 1 hour-long presentations of their research.

• Fifteen External speakers from industry, academia, and national laboratories. Matthew Hall (U. Texas, Austin), Joseph Katz (Johns Hopkins Univ.), David Kassoy (U. Colorado Boulder), Donghui Qi (Xian University), Lance Schideman (UIUC), Reginald Mitchell (Stanford Univ.), Ronald Adrian (Arizona State Univ.) (twice), Angela Violi (Univ. Michigan), Nasib Qureshi (USDA), Gustavo Dassori (ADM), Mitchell Smooke (Yale Univ.), Clancy Rowley (Princeton Univ.), Gang Chen (MIT), Jacqueline Chan (Sandia National Laboratories)

• Six Ph.D. GATE students (to NASA, Huntsville, Hellenic Petrol, Creative Thermal Solutions, TSMC, Bosch, Jilin Univ.) and five M.S. GATE students (to Sandia National Lab, Caterpillar (2), Saudi Arabian Oil Company, UIUC Ph.D. Program) graduated.

• GATE student participation in the Energy and Sustainability Engineering (EaSE) graduate option program formalized at the University of Illinois.

• First five students enrolled in the MS program with Energy Concentration in August 2010.





Accomplishments – Educational

Fundamentals

Core Specialty

Electives

- ME 404 Intermediate Thermodynamics
- ME 501 Combustion Fundamentals (Modified course)
- ABE 436 Renewable Energy Systems
- ME 403 Internal Combustion Engines
 ABE 466 Engineering Off-road Vehicles
- ME 503 Design of Internal Combustion Engines
- ME 598 Laser Diagnostics for Thermal/Fluids Engineering
- TAM 537 Experimental Methods of Fluid Mechanics
- ABE 488 Bioprocessing Grains for Fuels
- ME 498 Optics: Theory and Application (New course)
- <u>New Course: ME 498 Optics: Theory and Application:</u> Intended as a rigorous introduction of optics and laser diagnostics. This course will provide a practical understanding of light to engineering and science students who are non-specialists.
- <u>Modified Course: ME 501 Combustion Fundamentals</u>: The syllabus of the course was modified by a new instructor in order to include topics such as: Combustion Waves (Rankine-Hugoniot relations, ignition, extinction and flammability limits, intrinsic combustion instabilities, turbulent combustion, spray combustion





Accomplishments – Research Properties of Next Generation Biofuels for Diesel Engines

Next generation fuels that include bio-butanol and algae-derived biodiesel should be able to meet ASTM standards to ensure compatibility with existing diesel engine technology
Blends of bio-butanol, biodiesel and diesel fuel can be formulated to achieve properties that meet most of the requirements of the ASTM specification

•Algal oils contain higher quantities of polyunsaturated fatty acids that are more prone to oxidation and will have a shorter shelf life

Degree of Unsaturation	Algae	Soybean	Rapeseed	Coconut	Palm
1	20-40%	22-34%	10-15%	5-8%	40-52%
2	5-50%	50-60%	50-60%	1-3%	2-11%
3	5-50%	2-10%	10-20%	none	none
≥4	0-40%	none	none	none	none



Number of Carbon Atoms

Saturated methyl esters have cetane numbers that are 10-50% lower than for straight chain alkanes and are similar to the cetane numbers for 1-alkenes
Higher order alcohols have cetane numbers similar to biodiesel and alkenes, but their high melting points may hinder use in internal combustion engines







Water Emulsified Biofuel Combustion in a Constant-Volume Combustion Chamber

How water emulsified fuel looks like

W5, W10, W15, W20 (by water volume percentage)

- The spray and combustion characteristics of water emulsified fuels with different water content were studied in the constant volume chamber under various ambient conditions.
- Different laser diagnostic techniques were applied to investigate the liquid jet penetration, natural flame luminosity and soot formation
- Both liquid jet penetration and flame luminosity images suggest the enhancement of atomization most likely due to the microexplosion phenomena



W20 @ 800K.



D100 @ 800K.









Combustion and Soot Formation of Biodiesel/Diesel Blends under Different Ambient Oxygen Concentrations





- The INFL decreases with reduced oxygen concentration for biodiesel at ambient temperature from 800 K to 900 K, then increases at the ambient temperature of 1000 K and 1200 K.
- Biodiesel combustion reduces soot emission dramatically compared to diesel combustion at all conditions. At 800 K ambient temperature, there is nearly zero soot emission for biodiesel combustion at 21 % oxygen concentration, and the soot emission for biodiesel at 1200 K ambient temperature is comparable to the soot emission for diesel at 800 K low temperature combustion.





Spray of Butanol/Biodiesel/Diesel Blends and Micro-Explosion





- Spray jet penetration is shorter with higher ambient temperature, due to faster liquid evaporation. Adding butanol to the binary mixture of biodiesel-diesel also reduces spray penetration due to the higher volatility of butanol
- Adding butanol to biodiesel-diesel blend induces micro-explosion under certain initial ambient temperature conditions.
- Droplet micro-explosion can be modelled up to four components
- There exits an optimal ambient pressure for micro-explosion
- The optimum composition for microexplosion is B50S50. With a fixed butanol content, increasing biodiesel favours microexplosion.



Goal

V6 DI diesel engine fueled with biodiesel and its blends.

To study performance and emissions of a common-rail



Common-Rail V6 Engine Fueled with Diesel and Biodiesel Blends









<u>Approach</u>

- A configurable ECU, coupled with ETAS INCA software is capable of changing all engine parameters.
- An independent PID control system is used to vary intake pressure and temperature.
- EGR ratios and injection strategies are adjusted to see their independent effects.

<u>Results</u>

- Default ECU calibrations will change engine parameters like injection timings and EGR when using biodiesel.
- The EGR and injection strategy need to be optimized for biodiesel combustion.
- NOx emissions increased by about 10% at higher loads; soot decreased by 20%.





Application of Variable Cone Angle Injection in Biofuel Engines

- To study the effects of spray angle on flow patterns and pollutant formation
- Narrower tip angle provides longer span with spray lying in the bowl region
 - More flexibility in injection strategies
 - Spray enters the squish region with earlier timing for larger tip angle
 - Spray is confined in the bowl region with narrower tip
- Better fuel economy with variable cone angle spray
 - Fuel injected during 1st injection sees better combustion due to faster evaporation of fuel
 - Fuel will not combust for very early conventional injection





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Bio-Butanol Fuel Utilization Technologies

I. Electrostatic atomization: Butanol e-sprays are amenable to electrostatic manipulation. Stable butanol electrosprays were achieved within a narrow region of low flow rates. Possible causes of polydispersion were the e-spray menisci oscillations, the instabilities initiating the droplet break-up, the inertia effects and finally the degree to which butanol electric conductivity was constant can contribute.

II. Combustion: Pure butanol flames were found to be more vulnerable to extinction than methane and butanol-methane mixture flames with the same φ and total combustion heat release but they showed higher resistance to extinction than ethanol. A monotonic behavior of the extinction strain rate was observed with increasing heat release, both in pure butanol and in butanol-methane mixture cases.





G100 B25G75

Emissions Characteristics of Neat Butanol Fuel Using a Port Fuel-injected, Spark-Ignition Engine

- The goal is to determine for a given engine torque output, how does load (characterized by intake MAP) change with the addition of butanol?
- Adjustments of engine load to match brake torque show no definitive trend for 25 percent butanol

 Looking at the emissions results (UHC, NOx, CO), it appears that blending gasoline with 25% n-butanol by:

 Unburned hydrocarbon emissions are reduced by 18 percent at 900 rpm and up to 34 percent at 1500 rpm

 Carbon monoxide emissions are increased by 3 percent at 900 rpm up to almost 17 percent at 1500 rpm Nitrogen oxide emissions are lower by approximately 10 percent at 900 rpm and 1500 rpm but the same as G100-3 at 1200 rpm



ntake MAP (kPa) 58.0 56.0 54.0 52.0 50.0 900 1200 1500 Engine speed (rpm)

Engine load

62.0

60.0

Carbon monoxide emissions





Engine speed (rpm)





D.C. Rokamaklin or ALI Energy Conversion and Monage

Bio-butanol Blending Effects on Diesel Engine Performance and Emissions

- International collaboration with the National Technical University of Athens, Greece.
- Soot was significantly reduced for butanol–diesel fuel blends in comparison to neat diesel fuel.
- NOx emissions were slightly reduced with this reduction being higher the higher the percentage of butanol in the blend.
- CO emissions were reduced.
- UHC were increased
- A slight increase in specific fuel consumption was observed with increasing butanol content along with a corresponding slight increase of brake thermal efficiency and a slight decrease of exhaust gas temperature.







Collaborations/ Partnerships/ Technology Transfer

- GATE student internships with industrial partner Caterpillar (four interns).
- MS and Ph.D. graduate placement secures technology transfer to related industry and national laboratories (Creative Thermal Solutions, TSMC, Bosch, Sandia National Lab, Caterpillar, Cummins, Gamma Technology, NASA, Bosch, Wright-Patterson).
- Industrial partners provides valuable inputs on research direction of the center and provides research funding, e.g., funding from Ford, John Deere, Quantlogic leads to new technology.
- Collaboration on the University of Illinois campus with the BP-funded Energy Biosciences Institute and the Center for Advanced Bioenergy Research.
- Presentations to National Land Improvement Contractors of America, National Soybean Research Laboratory, Sandia National Laboratory, and auto. companies.
- Standing collaboration with Prof. Rakopoulos's group at NTU-Athens (Greece) has led to a series of publications on automotive combustion of bio-butanol.
- Visiting Professor Qunxing Huang from Zhejiang University provided an insight in related technologies and tools of scientific research used for similar efforts in China.
- Interactions with TetraVitae (Dr. Jay Kouba CEO), which has already licensed technology for the anaerobic production of bio-butanol on the possibilities of duel usage of n-butanol and iso-butanol.



Future Work

Activities for Next Fiscal year

- Initiate Phase III of the proposed project with the objective to establish a permanent Center that will provide a steady supply of highly-skilled engineers that will promote the science and technology of bio-fuel combustion.
- Involve actively the Industrial Advisory Board of the Center and implement their suggestions as to syllabus improvement.
- Solicit feedback from the first generation of graduates under the prism of their current employment in industry/government.
- Complete technology transfer through active collaborations: EBI, Tetravitae interested in biobutanol related technologies.
- Continue research work and expand towards new directions:

Algae-derived fuels and higher alcohols: physical properties, spray, combustion and engine experiments, modeling of in-cylinder combustion.

Fundamental calculations of chemical kinetics of bio-butanol with recently proposed kinetics.

Electrostatic manipulation of combustion by acting on the plasma generated by the flame either with the electrostatic field of the charged fuel or with external fields.



Summary

- In its fourth year of operation, the GATE Center on Advanced Automotive Bio-Fuel Combustion Engines at UIUC supported the research of 9 Ph.D. candidates and involved 46 students in an interdisciplinary curriculum that offered instruction on agricultural, biological, chemical, mechanical and economical aspects of emerging bio-fuel technologies.
- The first generation of Ph.D. completed their studies and have been placed to industry and the National Laboratories (12 Ph.D. and 12 M.S. graduates)
- The research activity of GATE Fellows and involved faculty produced 42 archival publications, 30 conference papers, 7 theses, two book chapters and one book.
- The GATE syllabus was enriched with a new class that was made available to GATE-affiliated students and fellows and 15 external speakers from the academia, government, and industry delivered seminars on bio-fuel related topics.
- Technology transfer has been initiated (bio-butanol, property determination)
- •Center participation in an Energy and Sustainability Engineering (EaSE) Graduate Option program as well as MS-Energy Concentration Programs.





Support Research Slides







Experimental and Computational Investigation of Combustion Phenomena in Mesoscale Ducts

- Established oscillatory phenomena of repeated extinction/ reignition in small scale tubular reactors that can be used for autonomous power generation.
- For methane-oxygen flames, the flame behavior is primarily a function of equivalence ratio. For propane-oxygen flames, Reynolds number is also a major factor. Oscillating flames are most stable in short ducts, and become more prone to extinction as the duct length increases. A duct with low thermal conductivity is necessary to produce stable oscillations, at least when no external heating is provided.
- A high temperature region exists near the duct exit that can provide heat for re-ignition during oscillations. Oscillating flames are capable of producing a nearly uniform temperature throughout the duct.
- The extinction-ignition cycle of oscillations does not lead to leakage of fuel or combustion intermediates. Complete combustion occurs during oscillations.
- A computational model using high-level mechanisms succeeded in capturing all experimentally observed flame behaviors, including oscillations. However, more detailed mechanisms may be necessary in order to accurately predict the locations of the boundaries between behavioral regimes.







Computation vs. Experiment

- Similar regime layouts
 - Blowout at high ϕ , stationary flames and oscillations at lower ϕ
 - Stationary flames at higher Re than oscillations
- Similar φ limit for oscillations: ~2.25 for computations, ~2.4 for experiments
 - Similar limit for full-tube oscillations as well
- Propagation depth of oscillations increases with decreasing ϕ
- Regime boundaries
 - Nearly independent of Re for experiments, but computations show Re dependence
- Additional extinction regime
 - High ϕ , low Re extinction regime of computations not observed in experiments
- Different wall temperature distributions likely a factor in all discrepancies
 - I: Blowout
 - II: Oscillations over part of tube length
 - III: Stationary flame front/ oscillations over part of tube length
 - IV: Oscillations over full tube length
 - V: Extinction



- Blowout
- Stationary flame front in tube
- Oscillation: partial tube length propagation
- Oscillation: full tube length propagation
- \times Extinction
- ⊠ Indeterminate







Algae Biodiesel Combustion in a Constant-Volume Combustion Chamber



Microalgal biomass recovered from the culture broth at Cyanotech Corporation, Hawaii, USA.





Growth of the cells of *C. protothecoides* under autotrophic(left, green) and heterotrophic (right, yellow) conditions. (Miao X and Wu Q, 2006)

Crop	Oil yield (L/ha)	Land area needed (M ha) ^a	Percent of existing US cropping area ^a	
Com	172	1540	846	
Soybean	446	594	326	
Canola	1190	223	122	
Jatropha	1892	140	77	
Coconut	2689	99	54	
Oil palm	5950	45	24	
Microalgae ^b	136,900	2	1.1	
Microalgae ^c	58,700	4.5	2.5	(Chisti Y, 200

<u>Motivation</u>

Oil crops cannot significantly contribute to replacing petroleum fuels since their high demand of land. This scenario changes if microalgae are used to produce biodiesel. Between 1 and 3% of the total U.S. cropping area would be sufficient for producing algal biomass that satisfies 50% of the transport fuel needs

<u>Approach</u>

•A constant volume chamber will be utilized to simulate the engine combustion at specific environment condition, including ambient temperature, pressure and oxygen density, injection timing and pressure.

 Both spray and combustion flame could be analyzed through laser diagnostic and natural flame luminosity.





Diesel Power Generator Fueled with Hydrous *n*-Butanol-Diesel Blends Goal

 Studying the performance and emissions of a single cylinder power generator by using non-dehydrated normal butanol-diesel blends.
 Approach



- The engine speed was fixed at 2000 rpm while the electrical output power were varied form idling (0 kW), 1.6, and 3.2 kW.
- Water contents were fixed at 0.5 and 1.0%wt of overall diesel blend, while the butanol adding ratios were varied from 5 to 10, 15, 20, and 25 wt%.

Preliminary Results

- SFC increased with *n*-butanol addition and water content tended to retard it.
- NOx went up with BT addition to a critical point and further reduced 15, 6, and 22% at three loads by using BT25W1.
- PM decreased with higher butanol content and shows 60, 43, and 50% reduction at three loads by using BT25W1.





Butanol Combustion under Various Ambient Conditions





Flame LuminositySoot FormationFlame LuminositySoot Formationat 1000K Ambient Temperatureat 1200K Ambient Temperature

• Different oxygen concentrations (21%, 16%, 10.5%) and ambient temperatures (800, 1000, 1200K) were investigated to simulate the real engine cylinder environment.

•The oxygen concentration has little effect on the autoignition between 16% and 10.5% at 800K-1200K.

•The dilution from inert gas results in larger flame volume and a higher total soot mass and distribution.

•The total soot mass are sensitive to the ambient temperature at 10.5% oxygen concentration.





0.03

30.02

0.01

0.04

0.03

(a) 0.02

0.01



Droplet Evaporation Model with Continuous Thermodynamics

- Continuous thermodynamics describes a mixture using a probability distribution function
 - Only three equations are needed to be solved for a mixture
 - Computational efficiency is embedded in model formulation
 - It provides a more efficient approach
- Formulated a new zero-dimensional droplet evaporation model using continuous thermodynamics
 - Allowing multiple distribution functions
 - Accounting the preferential vaporization and finite diffusion effects
- Representation of fuel affects the predicted evaporation behavior



