Integrating Fundamental and Applied Combustion Research

VERIFI Workshop

November 12, 2014

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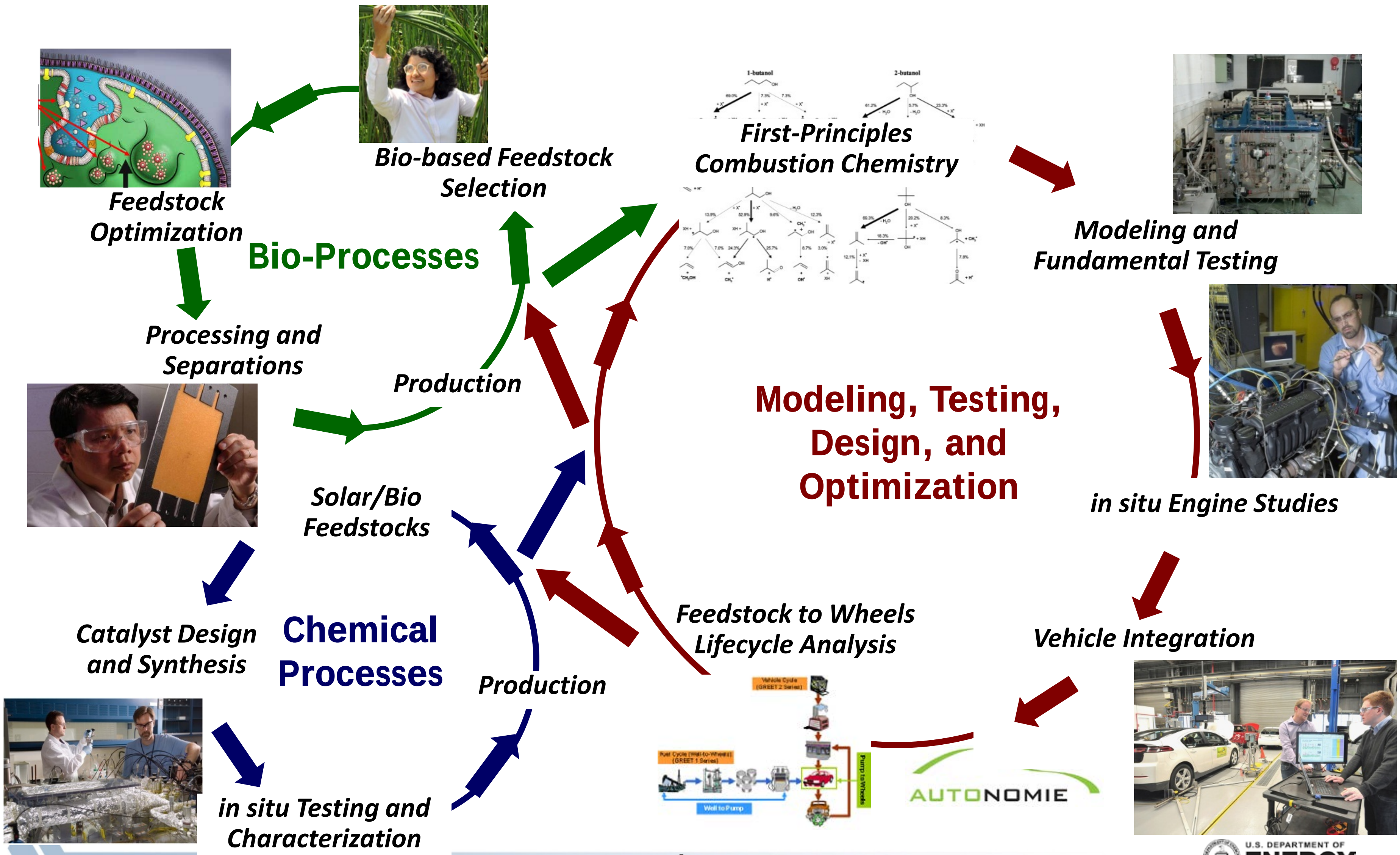
- EERE Vehicle Technologies
- Basic Energy Sciences
- Advanced Scientific Computing Research

VERIFI Fuels Work

VERIFI Enables Integrated Development of Fuels and Engines

Approach: a system-level, iterative feedback loop – new feedstocks, processing, combustion science, modeling, real-world testing, optimization, and life-cycle analysis



Fuels that have been explored via the VERIFI Integrated Process

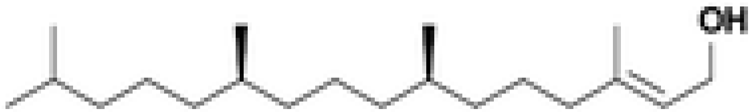
- Fatty Acid Methyl Ester Biodiesels from the following feedstocks
  - Soybean
  - Cuphea
  - Jatropha
  - Karanja
- Alcohols
  - Ethanol – C2
  - Propanol – C3
  - Butanol – C4
  - Pentanol – C5
  - Hexanol – C6
  - Phytol – C20
- Dual Fuel Combinations
  - Diesel / Natural Gas
  - Diesel / Gasoline
  - Diesel / Ethanol
  - Biodiesel / Ethanol
- Fuel Additives
  - EHN

Creating a new, alcohol fuel, Phytol

- Metabolic engineering efforts at Argonne have designed strains that can be produced in large quantities by photosynthetic bacteria eventually producing a (***really***) heavy alcohol called Phytol ($C_{20}H_{40}O$)
  - Biological process from bench level work is sugar based (no specific feed-stocks have been assessed)

Phytol ($C_{20}H_{40}O$)

tetramethyl-2-hexadecen-1-ol

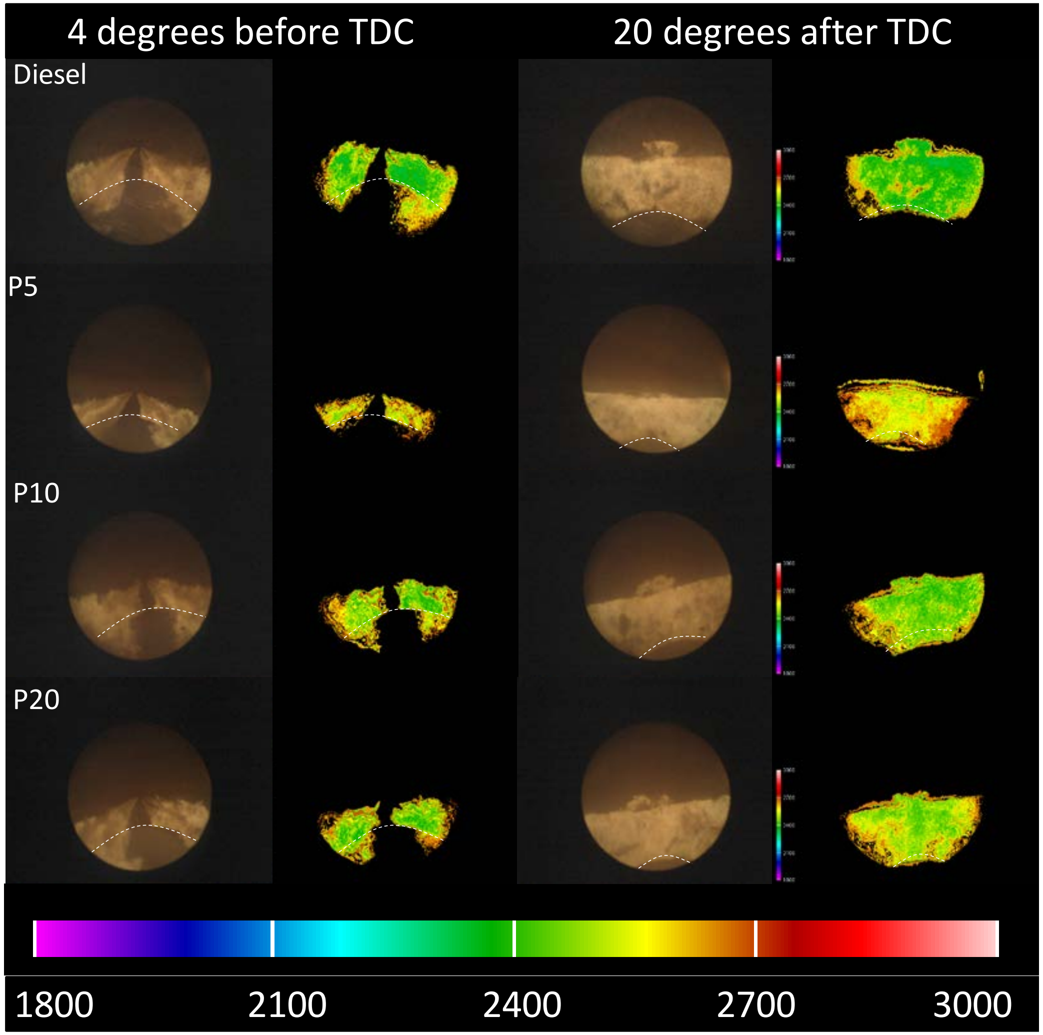


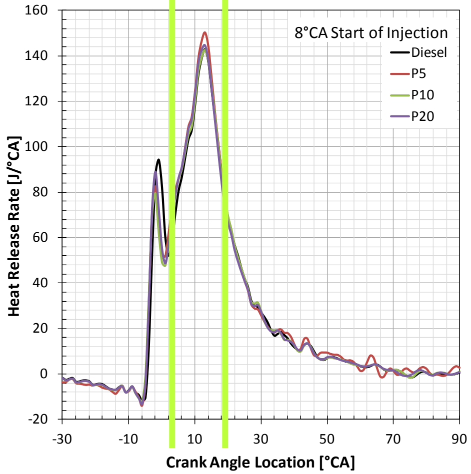
- The physical and chemical properties such as density, cetane number and heat of combustion are close to that of diesel fuel
- P5, P10, P20 blends of Phytol and diesel were made (by volume) and compared against baseline diesel experiments highlighted above

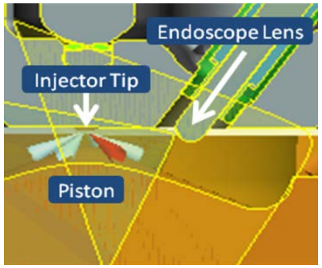
Phytol Fuel Properties

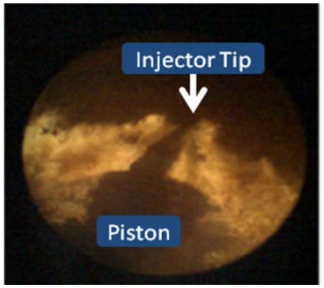
Fuel Property	Diesel	Phytol
Carbon content [wt%]	86.64	80.62
Hydrogen content [wt%]	13.01	13.5
Oxygen content [wt%]	0	6.05
Molecular weight [g/mole]	~170	296.54
Sulphur content [ppm]	11.2	< 10
Heat of combustion [kJ/kg]	44,463	43,584
Cetane number	47.7	45.9
Density @ 25°C [kg/m³]	849.2	850.9
Vapor pressure @ 25°C [Pa]	1000	< 1
Heat of vaporization [kJ/kg]	361	130
Viscosity @ 25°C [cSt]	3.775	63.54
Boiling point [°C]	320 (T_{90})	203

Biofuel engine experiments with "Precious" fuel (low quantities)



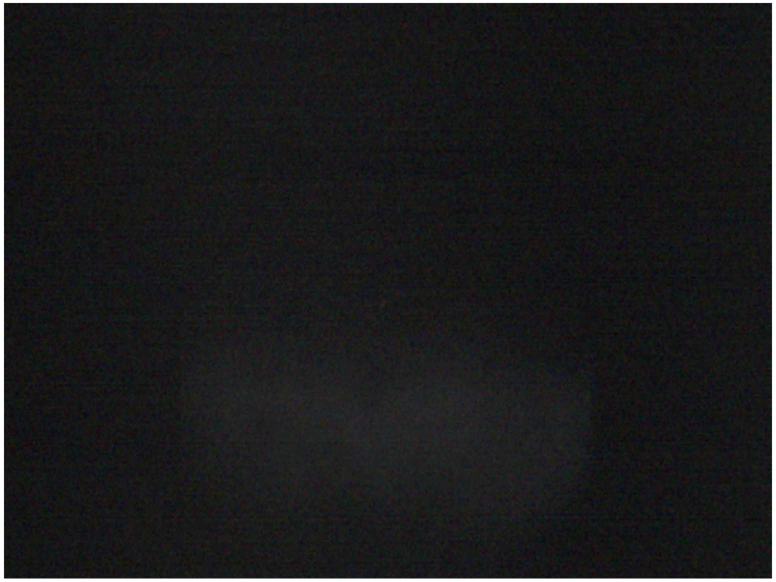






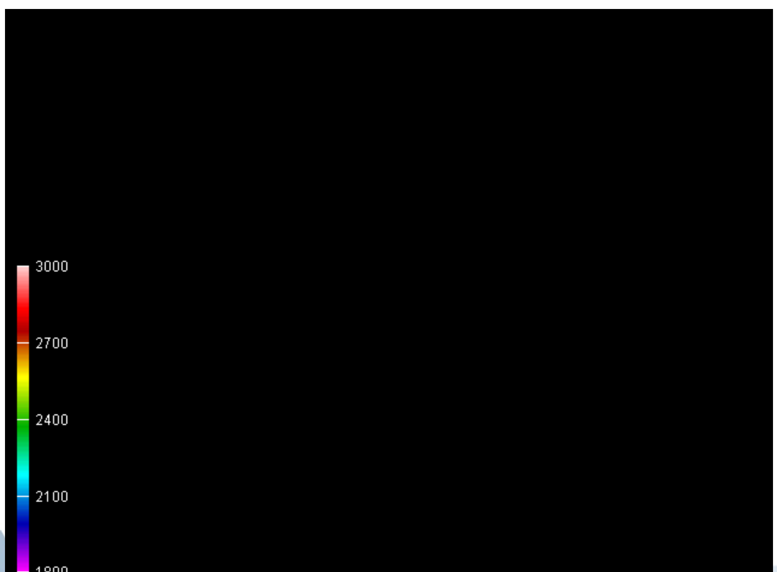
Diesel

P10

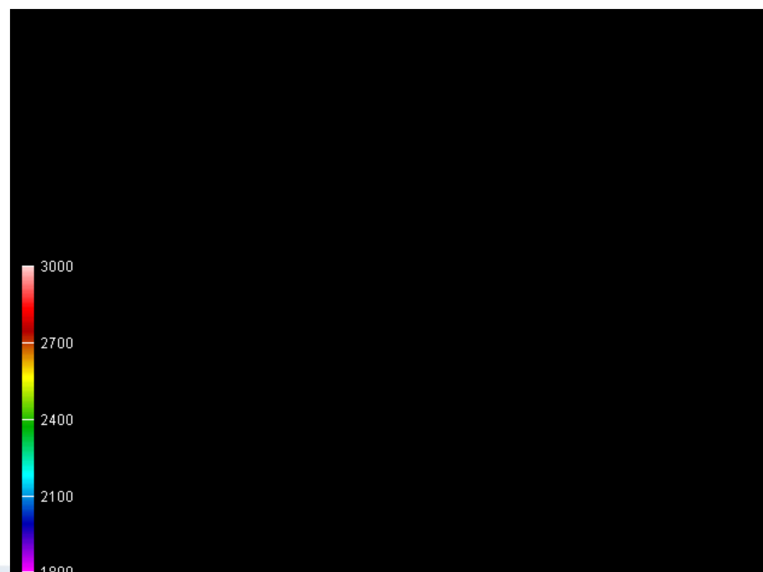


-8.0 deg CA, Rep 0
24oil100inj8deg100ers1500rpm

-8.0 deg CA, Rep 0
p1024oil100inj8deg100ers



-8.0 deg CA, Rep 0
24oil100inj8deg100ers1500_T1



-8.0 deg CA, Rep 0
p1024oil100inj8deg100ers_T

Biodiesel Fuel Mechanism Reduction Methodology

Computational time: $N^2 \sim N^3$

Detailed Mechanism (from LLNL)
3329 species, 10806 reactions

↓

DRG

↓

Isomer lumping

↓

DRGASA & Error Cancelation

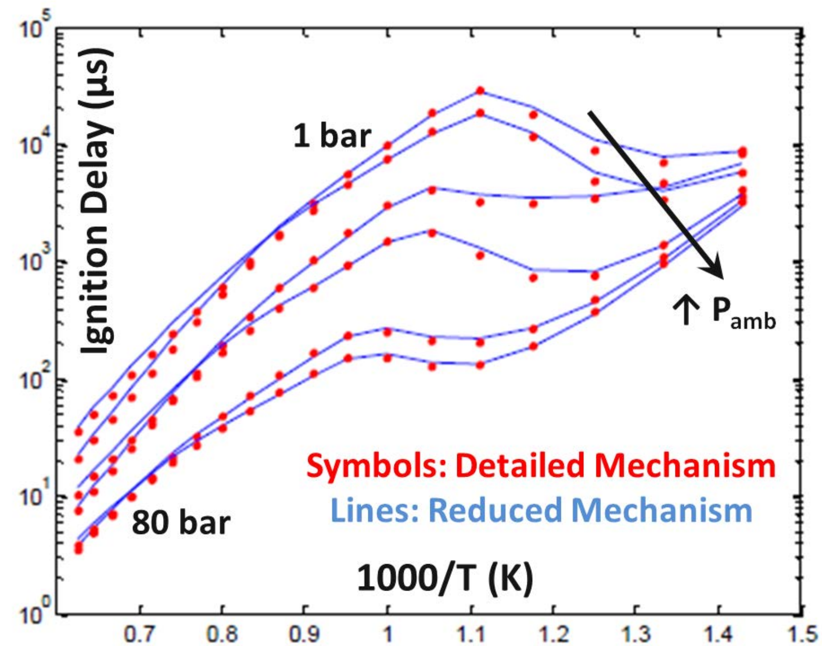
↓

115 species, 460 reactions[1]

~ 30 times reduction

Range of operation:

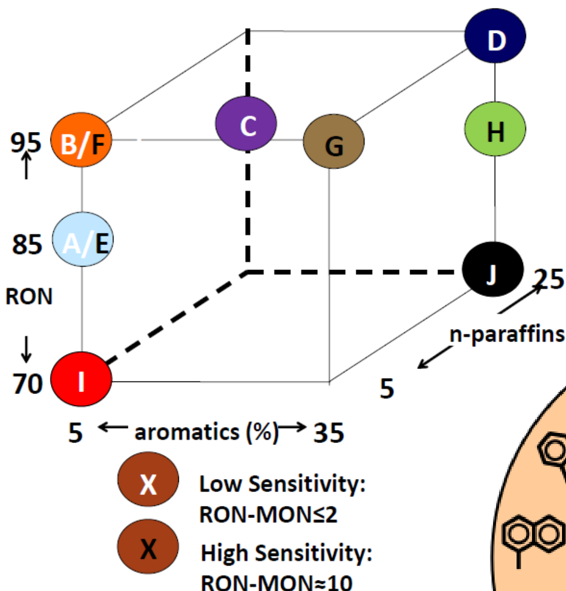
- ✓ Pressure: 1-100 atm
- ✓ Equivalence ratio: 0.5-2.0
- ✓ Initial temperature: 700 – 1800 K

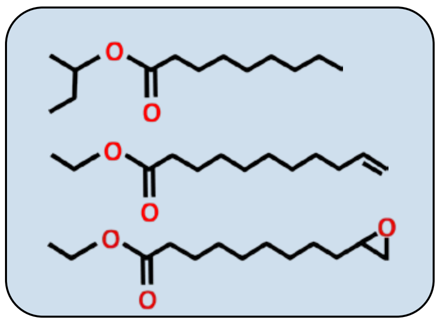


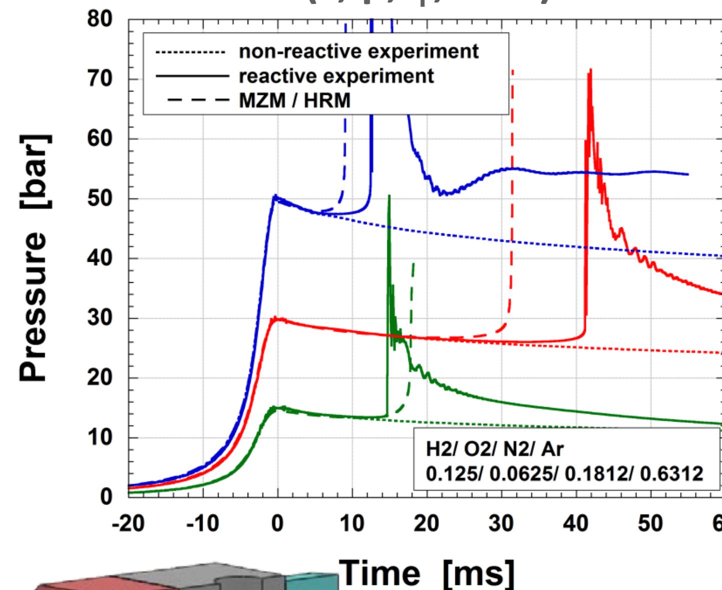
Z Luo, M Plomer, T Lu, S Som, DE Longman, SM Sarathy, WJ Pitz. *US National Combustion Institute meeting, March 2011*

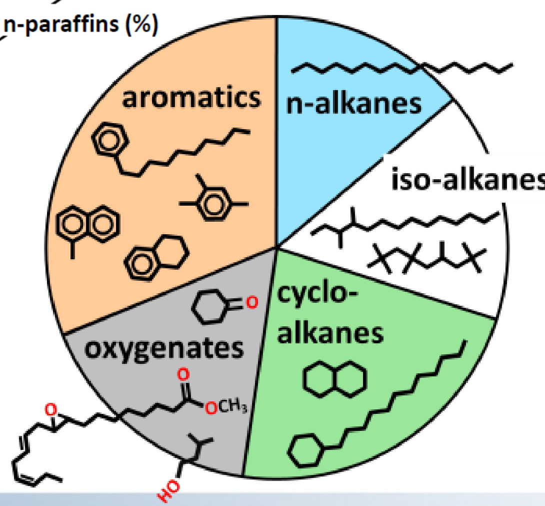
Rapid Compression Machine
Investigations of Fuel Chemistry / Autoignition

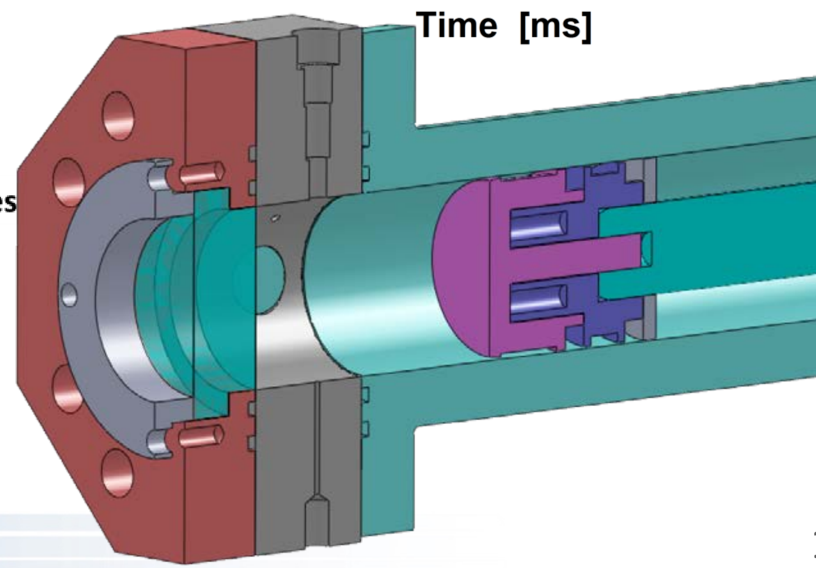
- Acquire fundamental data needed to understand fuel effects in future combustion engine validate chemical kinetic models at engine-relevant conditions (T, p, ϕ, EGR)
  - Gasoline (surrogates, FACE blends)
  - Diesel (surrogate components)
  - Biodiesel (molecular structure effects)











Fuel Design for LTC Engines

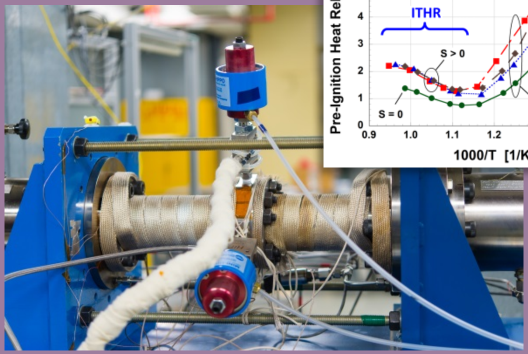
Need New Fuel Quality Metrics for Deployment

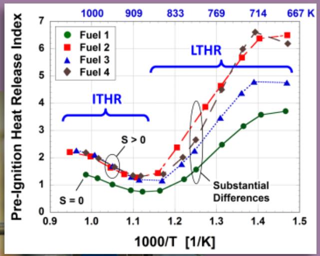
Argonne NATIONAL LABORATORY

Chevron

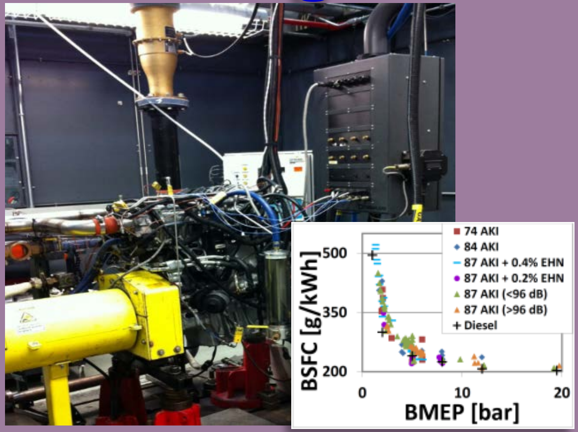
RON / MON are inadequate metrics

RCM

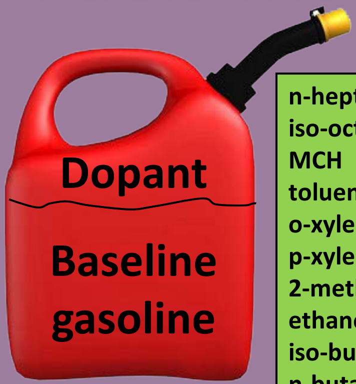




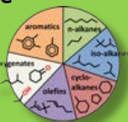
GCI Engine



Fuels Matrix

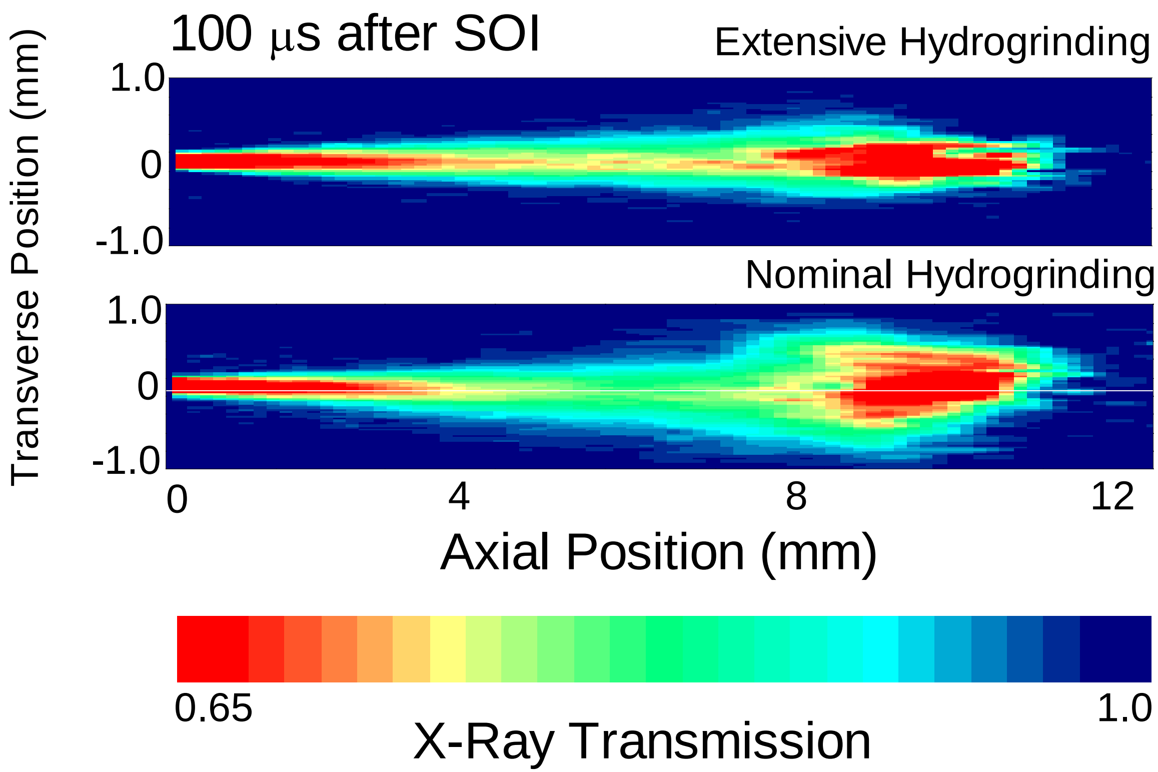


- n-heptane
- iso-octane
- MCH
- toluene
- o-xylene
- p-xylene
- 2-methyl, 2-butene
- ethanol
- iso-butanol
- n-butanol



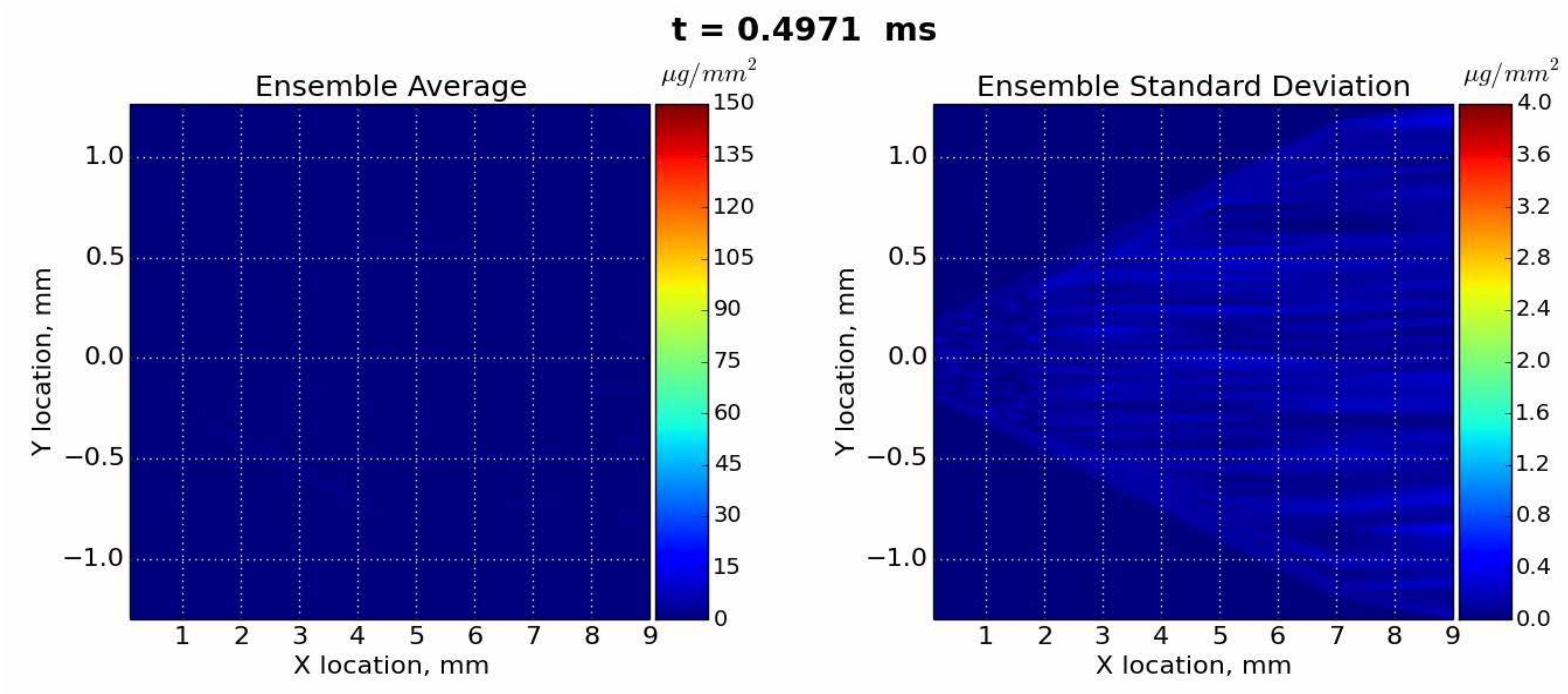
VERIFI X-Ray Experiment

Pioneering Fuel Spray Research at APS Provides Valuable Data to Manufacturers



- Images show mass distribution within sprays
- Provides quantitative near-nozzle data critical for accurate modeling

Quantifying Shot-to-Shot Variation in Sprays

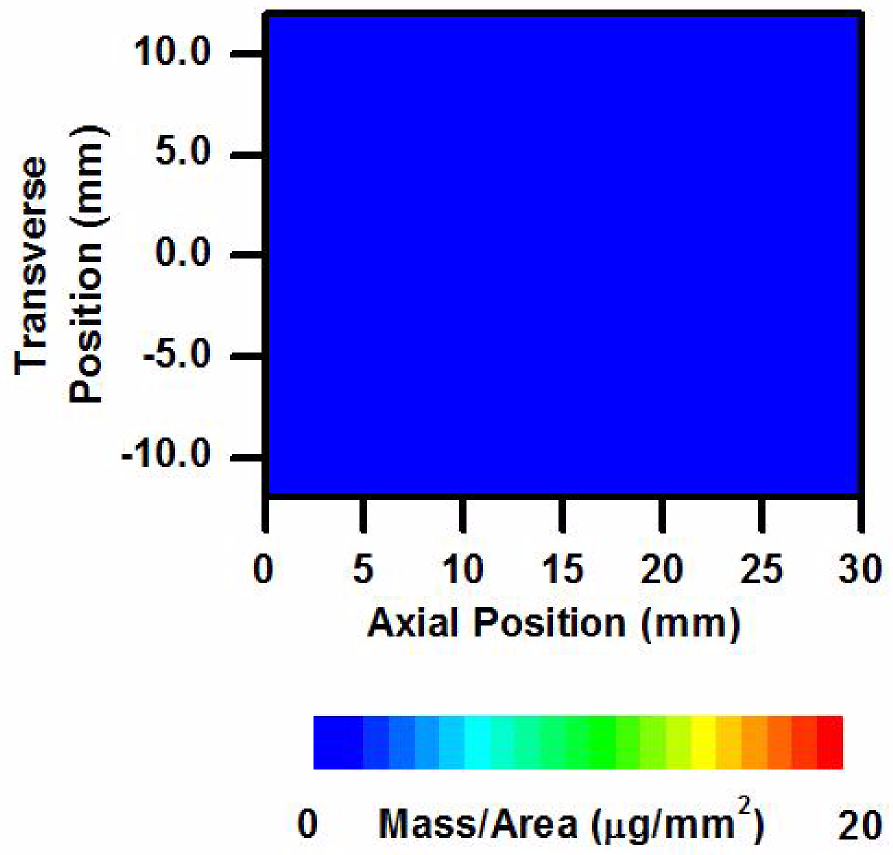


- Can quantify variability in fuel distribution in units of *mass*
- Used for model validation, injector evaluation

P_{inj}=500 bar
P_{amb}=20 bar
Ø 180 μm

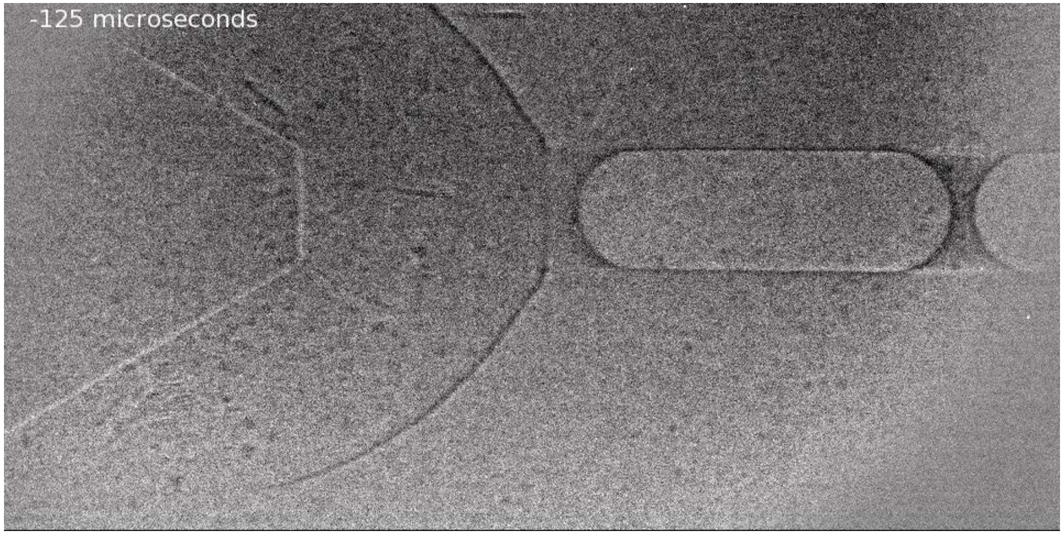
Investigating Natural Gas Injection

- Industrial collaborator (Westport Innovations) interested in improving their piezo DI natural gas injectors
- Quantitative measurements of gas jets difficult, density gradients cause refraction of visible light
- X-rays can quantify the gas density
- First measurements used argon gas
- Provides quantitative data never before available
- Being used for simulation development



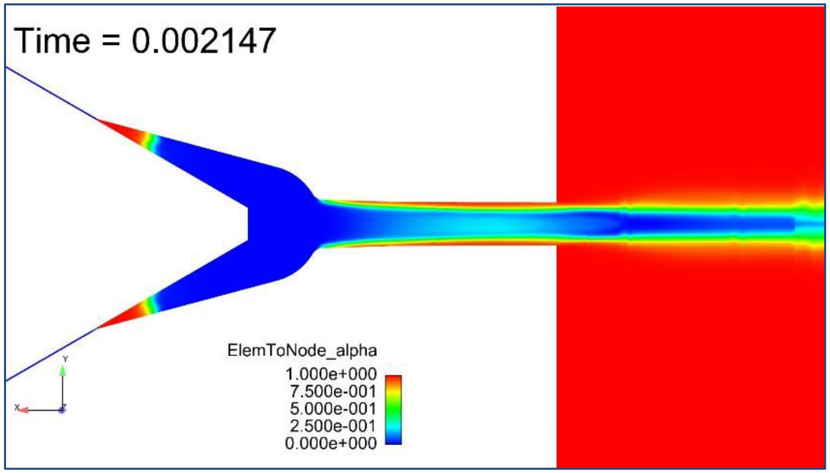
100 bar, 5 ms duration

X-ray Imaging of Fluid Flow Inside Diesel Injectors



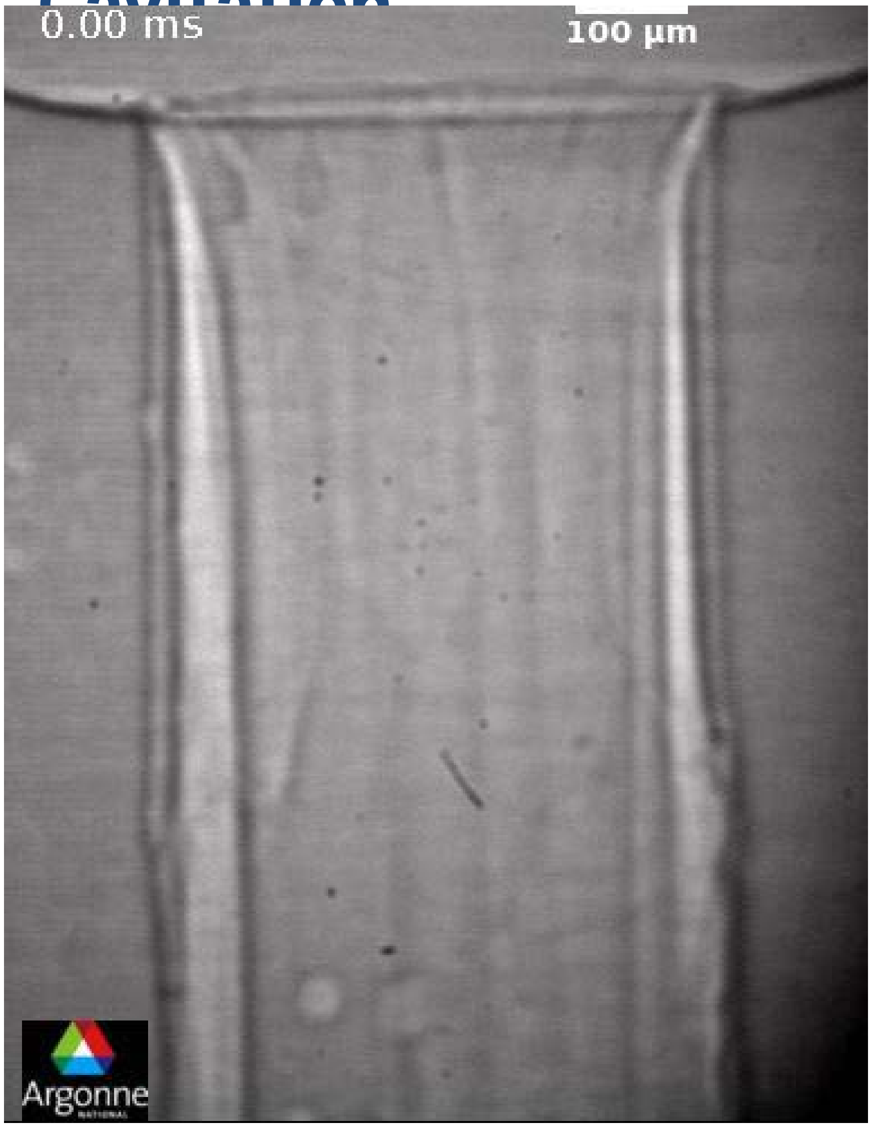
- Recently, we discovered that bubbles are pulled into the injector after the end of injection
- Simulations done at Argonne have helped to understand the mechanism

- These bubbles are important
- In an engine, they will be hot combustion products. May lead to injector damage
- As cylinder pressure falls, bubbles will expand. Fuel will be pushed into cold engine, causing emissions
- Additional simulations underway



Battistoni & Som, Argonne

Time-Resolved X-Ray Measurements of Cavitation



- Plastic Nozzle
- Partially degassed fuel
- Reveals gas along the walls
  - Cavitation or dissolved gas?
- Bubbles coming out of solution
  - Buoyant, 60 m/s in center of flow
- Collapsing bubbles cause pressure waves in fuel
- Trapped layer of fuel along wall

- Real fuel systems have **lots** of dissolved gas.
- Future measurements will attempt to distinguish vapor from dissolved gas