



# Opportunities for Innovation in Fuel-Engine Co-Optimization

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RON viscosity  
bulk modulus of compressibility volatility  
sensitivity Wobbe index  
soot precursor formation PMI  
cetane number heat of combustion  
C/H ratio flame stretch  
density strain sensitivity  
naphthene level specific  
T10 heat ratio  
exergy destruction olefin level  
energy density oxygenate level  
laminar burning velocity drivability index  
diffusivity aromatics level  
MON heating value  
cloud point  
flammability limits heat of vaporization  
smoke point surface tension  
ignition limits T50  
flash point sulfur level  
T90 Markstein length  
flame speed



# How do we characterize fuels?

## Fuels specifications are *Property* based

### SI Fuels (ANSI D4814):

- Vapor pressure
- Distillation curve (& driveability index)
- Distillation residue
- Corrosivity
- Gum content
- Oxidation stability

With the exception of sulfur, lead, benzene, and overall O<sub>2</sub> content, *details of the chemical composition of the fuel are not regulated\**



\* The Co-Optima fuel down-selection process is more rigorous

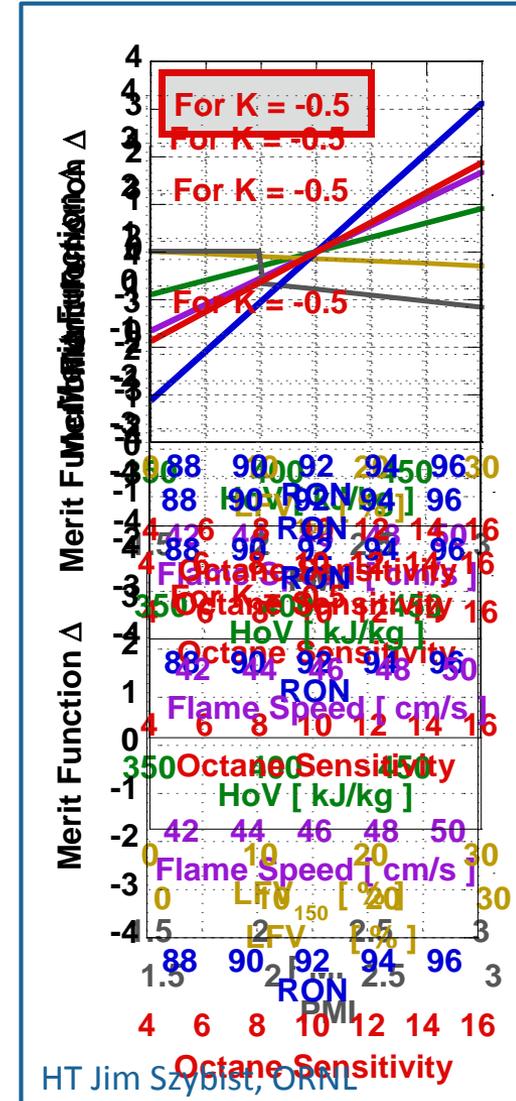


# What do engines want?

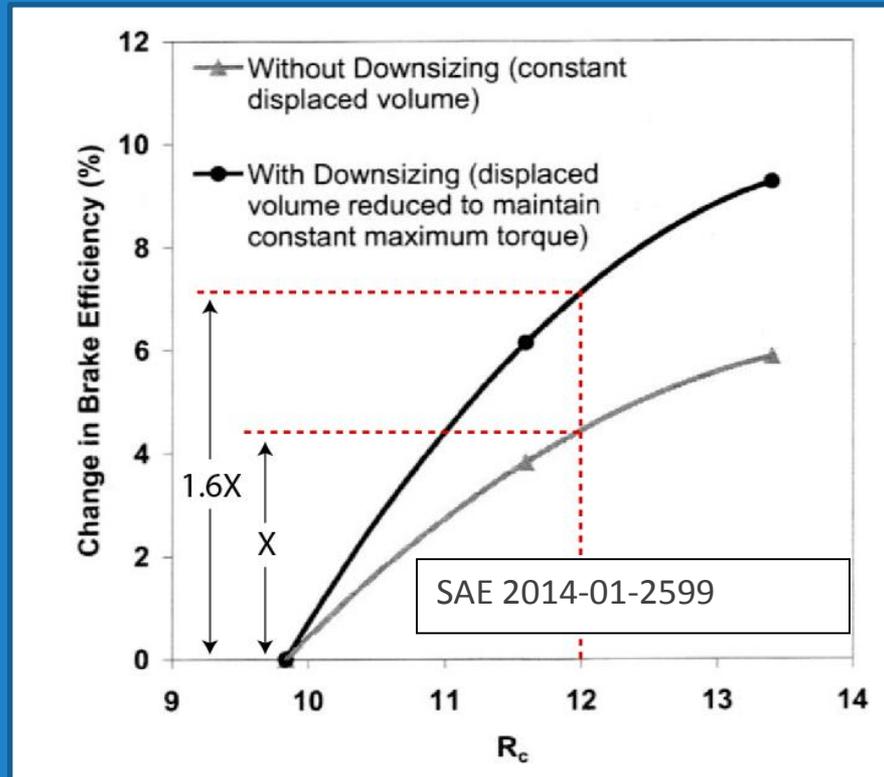
For conventional SI engines fuel effects on engine efficiency are well known –

$$\begin{aligned}
 \text{Merit} = & \sum \left[ \frac{\text{RON}_{mix} - 91}{1.6} - K \frac{\text{Octane Sensitivity} (S_{mix} - 8)}{1.6} + \frac{\text{Flame Speed} (S_{Lmix} - 46 [cm/s])}{3} \right. \\
 & + \frac{\text{Heat of Vaporization} (0.01[ON/kJ/kg](HoV_{mix} - 415[kJ/kg]) + (HoV_{mix} - 415[kJ/kg]))}{1.6} + \frac{(HoV_{mix} - 415[kJ/kg])}{130} \\
 & \left. - \text{Distillation } LFV_{150} - \text{Particulate Emissions } H(PMI - 2.0)[0.67 + 0.5(PMI - 2.0)] \right]
 \end{aligned}$$

Much work remains to understand fuel effects on advanced, Thrust II combustion modes...



# Efficiency Opportunities

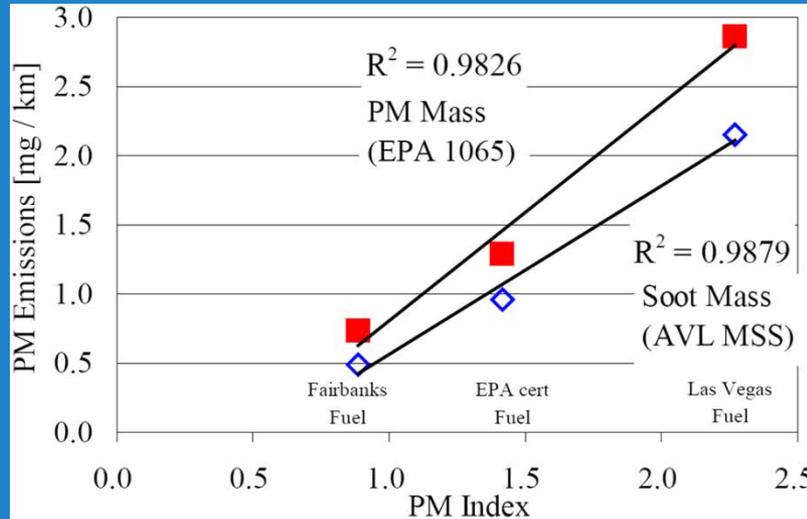
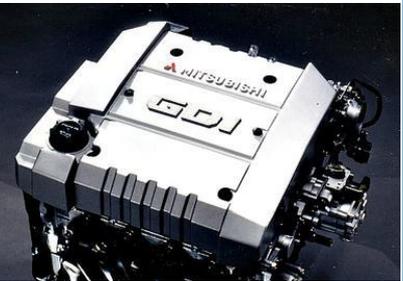


Increased auto-ignition resistance (RON, octane sensitivity) enables increased SI engine efficiency –

- Increased compression ratio  $R_c$
- More advanced timing
- No enrichment



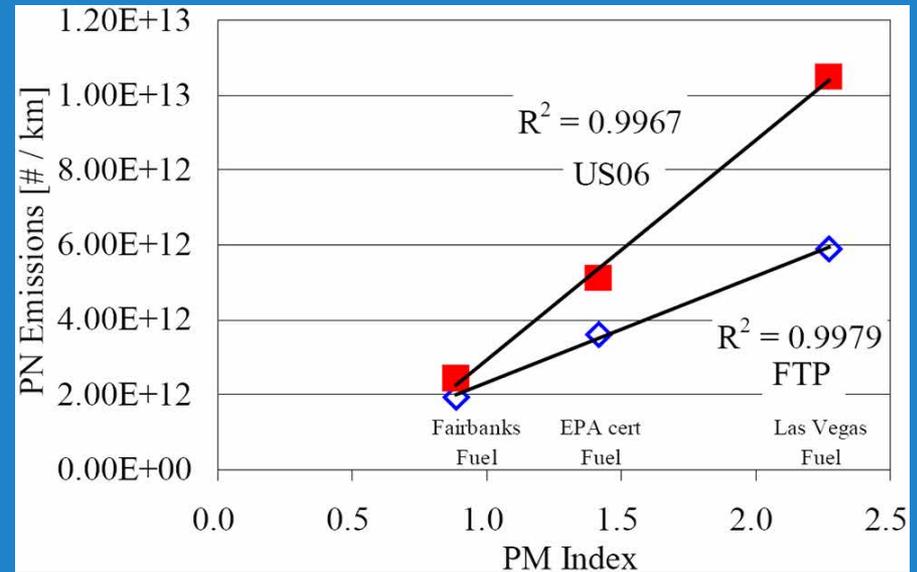
# Opportunities for improved emissions



Particulate mass

SAE 2010-01-2115

Particulate number

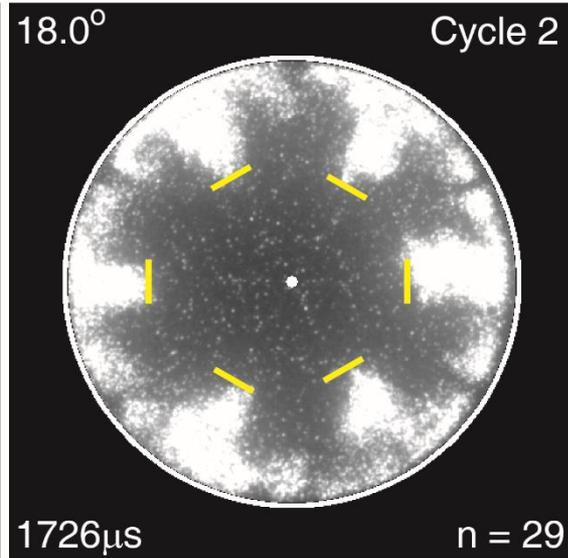
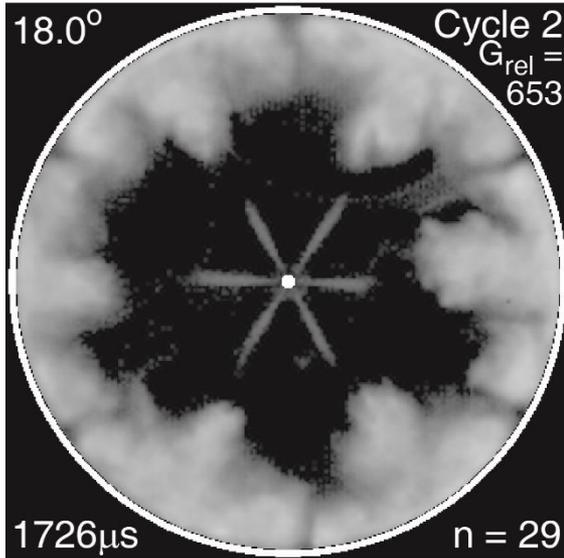




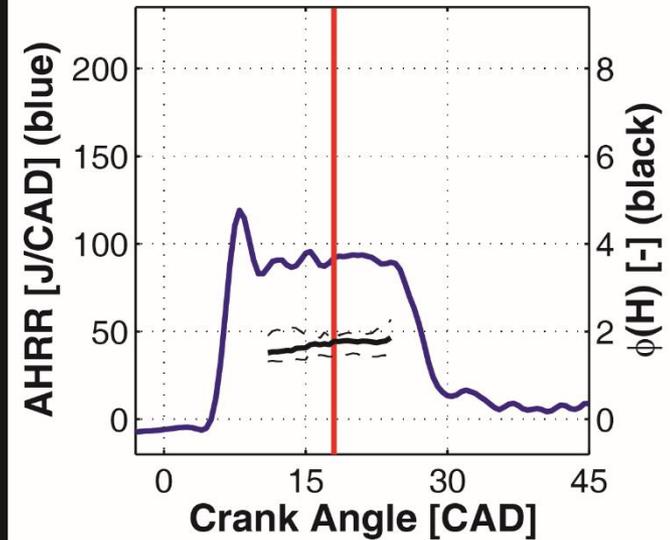
# Oxygenated fuels can enable advanced CI combustion modes

Natural Luminosity

OH\* Chemiluminescence



HT Chuck Mueller, SNL



- Moderate load, sustained “Leaner Lifted Flame Combustion” is achieved using a 50/50 volume % blend of diesel fuel with  $C_{10}H_{22}O_4$
- Promises highly efficient combustion with greatly reduced after-treatment needs



# Some fuels may be advantageous for both SI and advanced CI combustion

**Octane Index is often considered a measure of the true antiknock quality of a fuel:**

$$\text{OI} = \text{RON} - K * (\text{RON} - \text{MON}); \quad \text{Sensitivity} = (\text{RON} - \text{MON})$$

K is an empirical *engine* constant, independent of the fuel

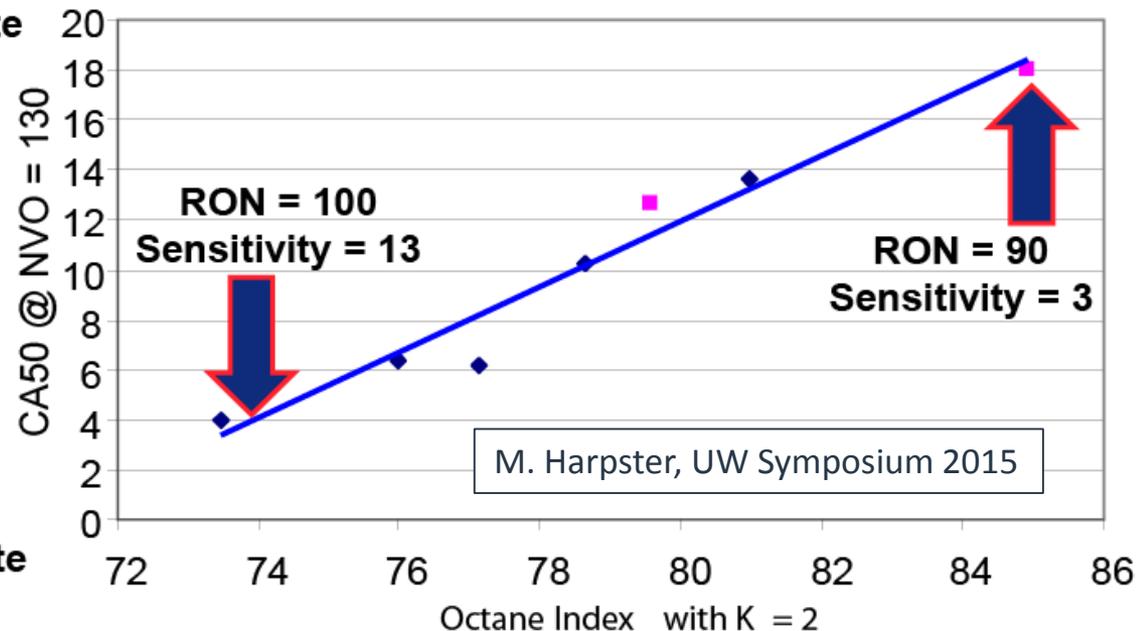
**Down-sized,  
boosted SI:  $K = -1$**

**Advanced CI:  $K = 2$**

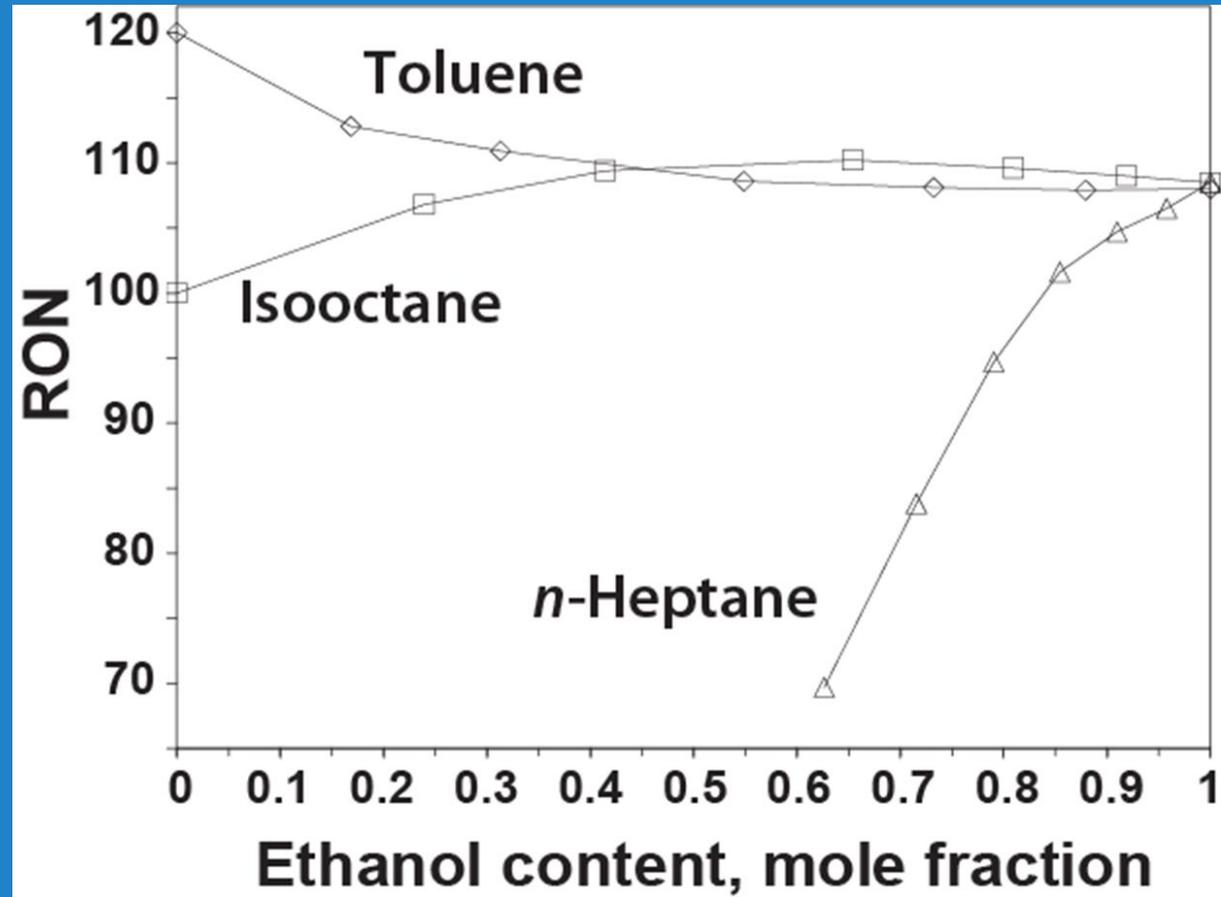
Hard to Ignite



Easy to Ignite



# Innovation Opportunities in Physical/Chemical Science

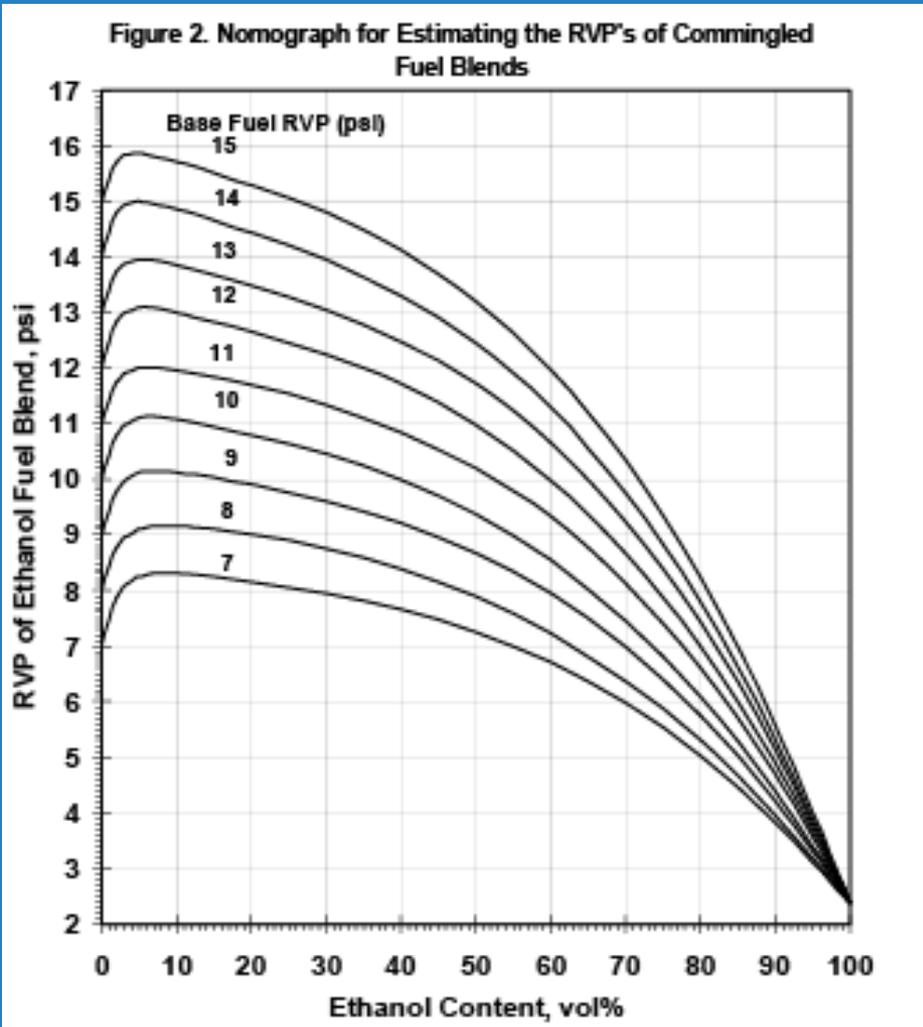


Auto-ignition kinetics of fuel blends



# Innovation Opportunities in Physical/Chemical Science

Science-based prediction of blend vapor pressure (a regulated quantity)





# Innovation Opportunities in Testing and Standards Development



Designation: D2699 - 13b



Designation: 237/87

Standard Test Method for Research Octane Number of Spark-Ignition Engine Fuel<sup>1</sup>



Designation: D4814 - 14a

Standard Specification for Automotive Spark-Ignition Engine Fuel<sup>1</sup>



Designation: E2071 - 00 (Reapproved 2015)

Standard Practice for Calculating Heat of Vaporization or Sublimation from Vapor Pressure Data<sup>1</sup>

This standard is issued under the fixed designation E2071; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last approval. A superscripted epsilon ( $\epsilon$ ) indicates an editorial change since the last revision or approval.

## 1. Scope

1.1 This practice describes the calculation of the heat of vaporization of a liquid or the heat of sublimation of a solid from measured vapor pressure data. It is applicable to pure liquids, azeotropes, pure solids, and homogenous solid solutions over the temperature range for which the vapor pressure equation fitted to the measured data is applicable.

NOTE 1—This practice is generally not applicable to liquid mixtures. For a pure liquid or azeotrope, composition does not change upon vaporization so that the integral heat of vaporization is identical to the differential heat of vaporization. Non-azeotropic liquid mixtures change composition upon vaporizing. Heat of vaporization data computed from this practice for a liquid mixture are valid only as an approximation to the mixture differential heat of vaporization; it is not a valid approximation to the mixture integral heat of vaporization.

1.2 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.3 There is no ISO standard equivalent to this practice.

1.4 This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.

## 2. Referenced Documents

2.1 ASTM Standards:<sup>2</sup>

D2879 Test Method for Vapor Pressure-Temperature Relationship and Initial Decomposition Temperature of Liquids by Isoteniscope

E1142 Terminology Relating to Thermophysical Properties

E1194 Test Method for Vapor Pressure (Withdrawn 2013)<sup>3</sup>

E1719 Test Method for Vapor Pressure of Liquids by Ebulliometry

E1782 Test Method for Determining Vapor Pressure by Thermal Analysis

## 3. Terminology

### 3.1 Symbols:

3.1.1  $A, B, C$ —Antoine vapor pressure equation constants ( $\log_{10} P$ , kPa, K), Antoine vapor pressure equation:

$$\log_{10} P = A - B/(T+C)$$

3.1.2  $P$ —vapor pressure, kPa.

3.1.3  $P_c$ —critical pressure, kPa.

3.1.4  $P_r$ —reduced pressure =  $P/P_c$ .

3.1.5  $T$ —absolute temperature, K.

3.1.6  $T_c$ —critical temperature, K.

3.1.7  $T_r$ —reduced temperature =  $T/T_c$ .

3.1.8  $V$ —molar volume,  $\text{cm}^3/\text{mol}$ .

3.1.9  $R$ —gas constant, 8.31433 J/mol-K; 8314330 kPa-cm<sup>3</sup>/mol-K.

3.1.10  $\Delta H_v$ —heat of vaporization, J/mol.

3.1.11  $\Delta Z_v$ —difference in compressibility factor ( $Z = PV/RT$ ) upon vaporization. Clapeyron equation:

$$\Delta H_v = -R\Delta Z_v [d(\ln P)/d(1/T)]$$

3.1.11.1 Discussion—The subscript “V” will be used throughout this practice to designate the vaporization of a liquid. If the vapor pressure data were measured for a solid, substitute the subscript “S” for the sublimation of a solid.

### 3.2 Definitions:

3.2.1 Specialized terms used in this practice are defined in Terminology E1142.

3.2.2 sublimation—transition from a solid phase to a gas-

- Need improved metrics and methods for autoignition testing
- Development of improved fuel specifications
- Improved property testing methods (Cu contaminants, Heat of Vaporization)

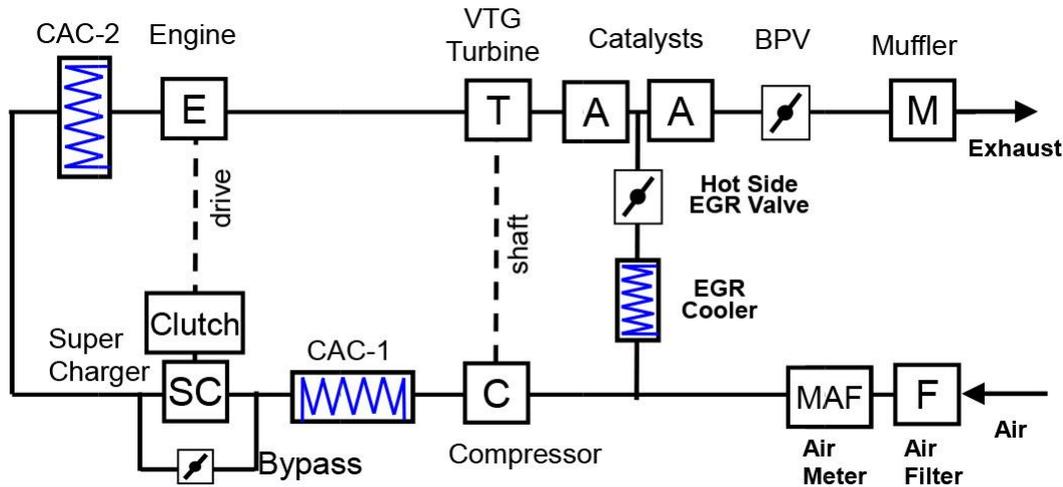


<sup>1</sup> This practice is under the jurisdiction of Committee E37 on Thermal Measure-



# Innovation Opportunities in Engineering & Design

## Delphi GCI air-handling system:



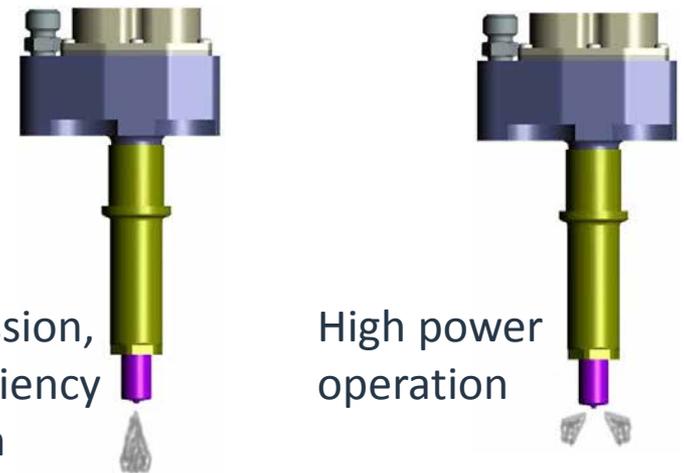
**Development of specialized air handling systems and components is needed**



## Fuel injectors:

- Dynamic geometry variation?
- Dual fuel?

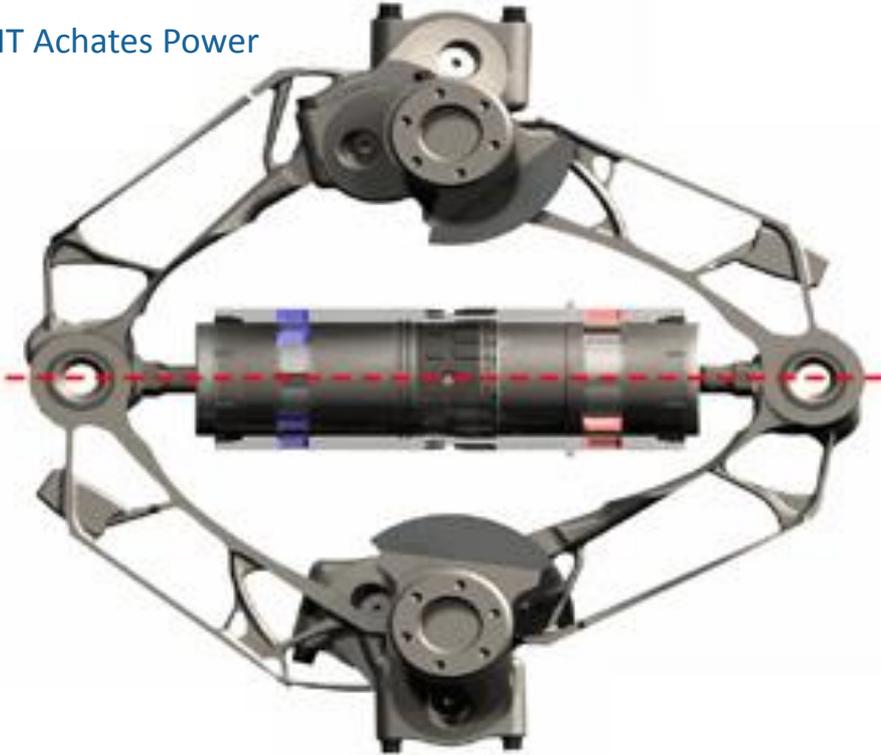
## Caterpillar mixed-mode injector concept





# Co-optimization opportunities offered by unusual architectures remain unexplored

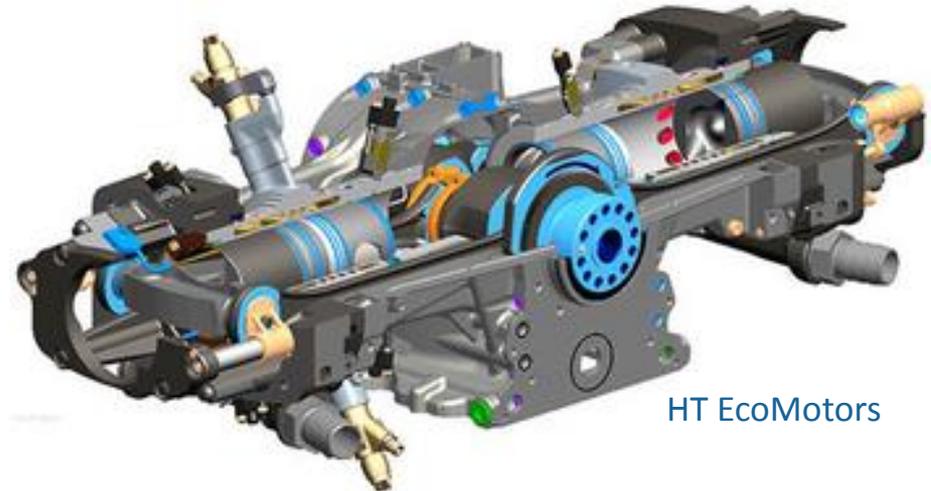
HT Achates Power



**Compatible with conventional and advanced combustion systems**



**Unique combustion chamber geometries offer opportunities & challenges for fuel-dependent mixture formation**



HT EcoMotors

Thank you!



Questions?