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The Effect of Fuel Volatility and Aromatic Content on Particulate Emissions

May 18 2012



Outline

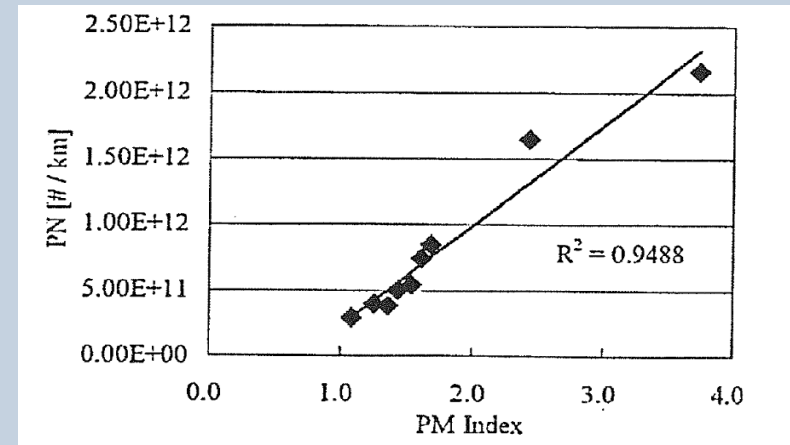
- **Introduction**
 - Honda paper
- **Fuel design**
 - Component selection
 - Raoult's law
 - UNIFAC
- **Experimental procedure**
 - Engine and operating point
 - Test points
- **Instrumentation**
- **Results**
 - Model fuels
 - EN228 Gasoline
 - EU5 Reference fuel
- **Conclusions**

What effect do aromatic content and fuel volatility have on particulate emissions?

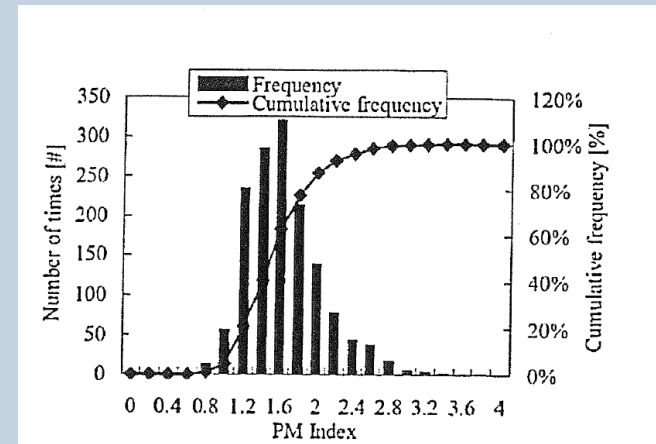
- SAE 2010-01-2115 paper “Development of a predictive model for gasoline vehicle particulate matter emissions” (Aikawa, Sakurai, & Jetter)
- Honda PM number index: $I(VP, DBE) = \sum_{i=1}^n \left[\frac{DBE_{i+1}}{VP_i} \right] W_{ti}$
- DBE: Double bond equivalent
 - A measure of how unsaturated a Hydrocarbon is
 - $DBE = \frac{2C - H - N + 2}{2}$
- No independent control of volatility and DBE. PFI engine only.
- Aim:
 - Verify index and extend to SGDI combustion system

Honda paper

- **Base fuel + 10% additives**
 - 2,2,4-Trimethylpentane
 - Dodecane
 - Ethylbenzene
 - 1,2,4-Trimethylbenzene
 - Ethanol
- **PM index range 1.01 – 3.86**
- **Range of worldwide fuels tested**



Relationship between PN (#/km) and PM index over NEDC (Aikawa, 2010)



Range of PM indexes of a selection of commercially available fuels worldwide (Aikawa, 2010)

Fuel composition

	T_b (K), 1.01325 bar	RON	BON
n-pentane	309.2	62	60
iso-octane	372.4	100	100
n-octane	398.8	-17	-19
75/25 io/no mix	379*	n/a	70*
Toluene	383.8	104	120
iso-decane	433.5	100	126
n-decane	447.3	-17	-41
24/76 id/nd mix	444*	n/a	-1*
1,3,5-Trimethylbenzene	437.9	n/a	161

Aromatic component selection based on BP and RON

* Linear average

Fuel design

Raoult's law

- Raoult's law relates the vapour pressure of an ideal solution to the vapour pressure of each of its chemical components by the molar fraction of each component present

- $y_i P = x_i P_{vpi}$ [Poling, Prausnitz, & O'Connell]

y_i : molar fraction of component i in vapour

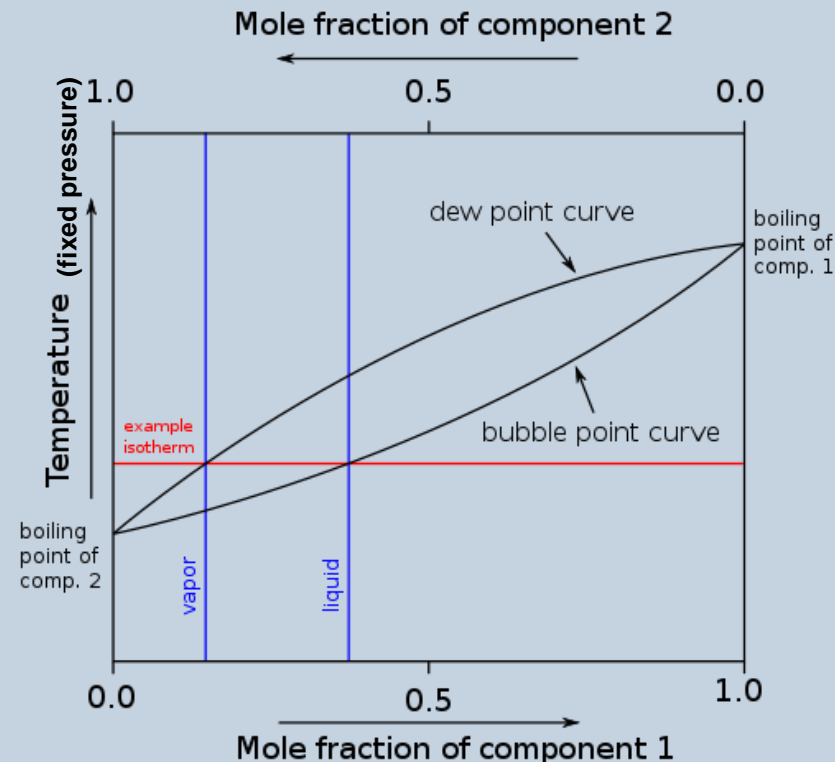
x_i : the molar fraction of component i in liquid

P_{vpi} : the vapour pressure of component i

P the partial pressure of the component.

- Assumptions:

- Neglect effect of surface tension and any external conditions (electric/magnetic field etc)
- Ideal mixing → linear relationship



Fuel design

UNIFAC*

- **UNiversal Functional Activity Coefficient (UNIFAC)**
- **Attempts to extend Raoult's Law to account for non-ideal mixing**
- **Semi-empirical model to predict non-ideal mixture behaviour based on molecular size and interactions**
- **Breaks molecules into functional groups to model interactions**
- **Cannot be used on electrolytes**

$$\ln \gamma_i = \ln \gamma_i^c + \ln \gamma_i^R$$

combinatorial residual

$$\ln \gamma_i^c = \ln \frac{\Phi_i}{x_i} + \frac{z}{2} q_i \ln \frac{\theta_i}{\Phi_i} + l_i - \frac{\Phi_i}{x_i} \sum_j x_j l_j$$

$$\ln \gamma_i^R = q_i \left[1 - \ln \left(\sum_j \theta_j \tau_{ji} \right) - \sum_j \frac{\theta_j \tau_{ij}}{\sum_k \theta_k \tau_{kj}} \right]$$

$$l_i = \frac{z}{2} (r_i - q_i) - (r_i - 1) \quad z = 10$$

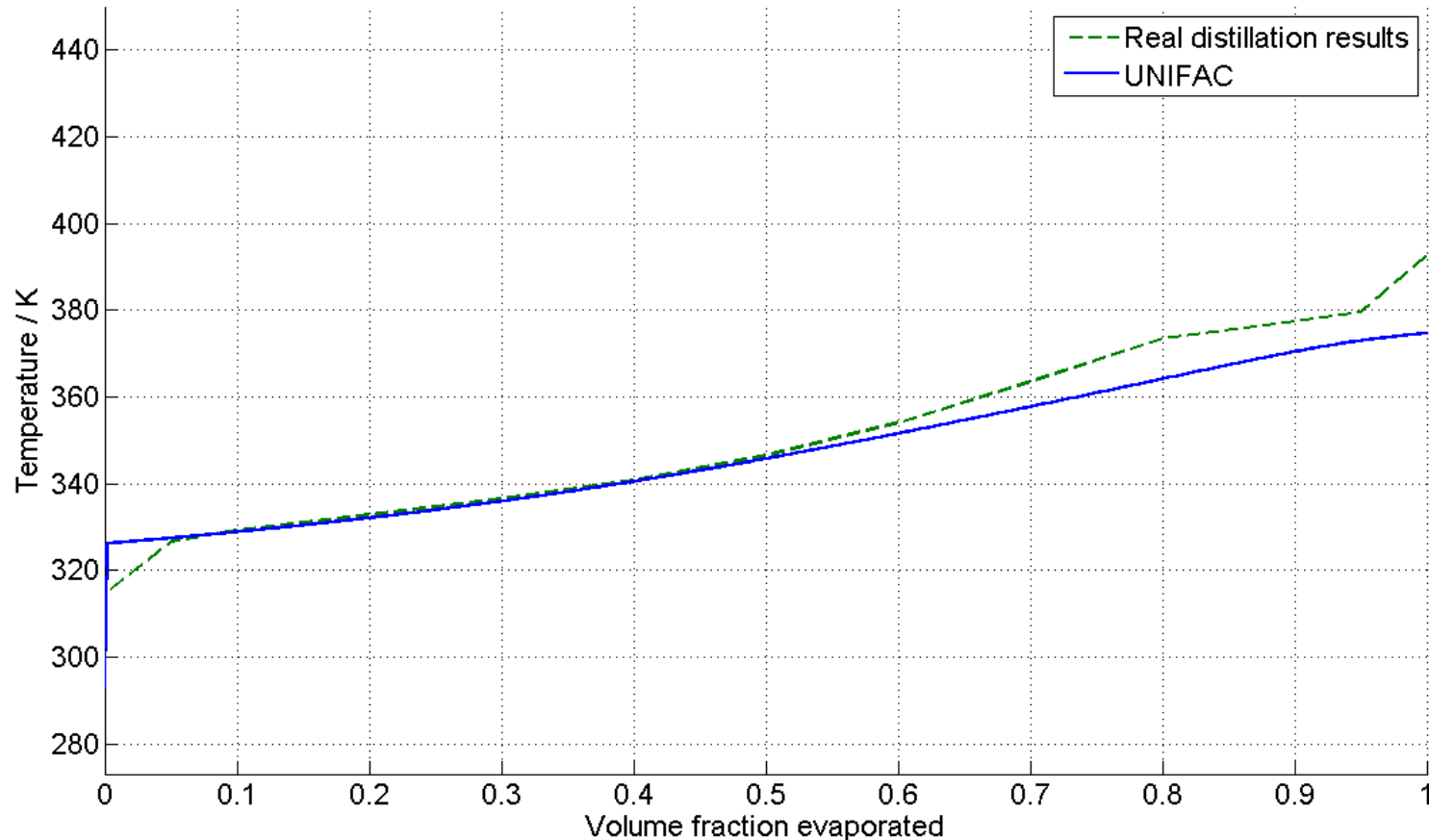
$$\theta_i = \frac{q_i x_i}{\sum_j q_j x_j} \quad \Phi_i = \frac{r_i x_i}{\sum_j r_j x_j} \quad \tau_{ji} = \exp \left(- \frac{u_{ji} - u_{ii}}{RT} \right)$$

UNIFAC equations (Poling et al 2000)

* Reid, R. C., J. M. Prausnitz, et al. (1987). The properties of gases and liquids. McGraw-Hill.

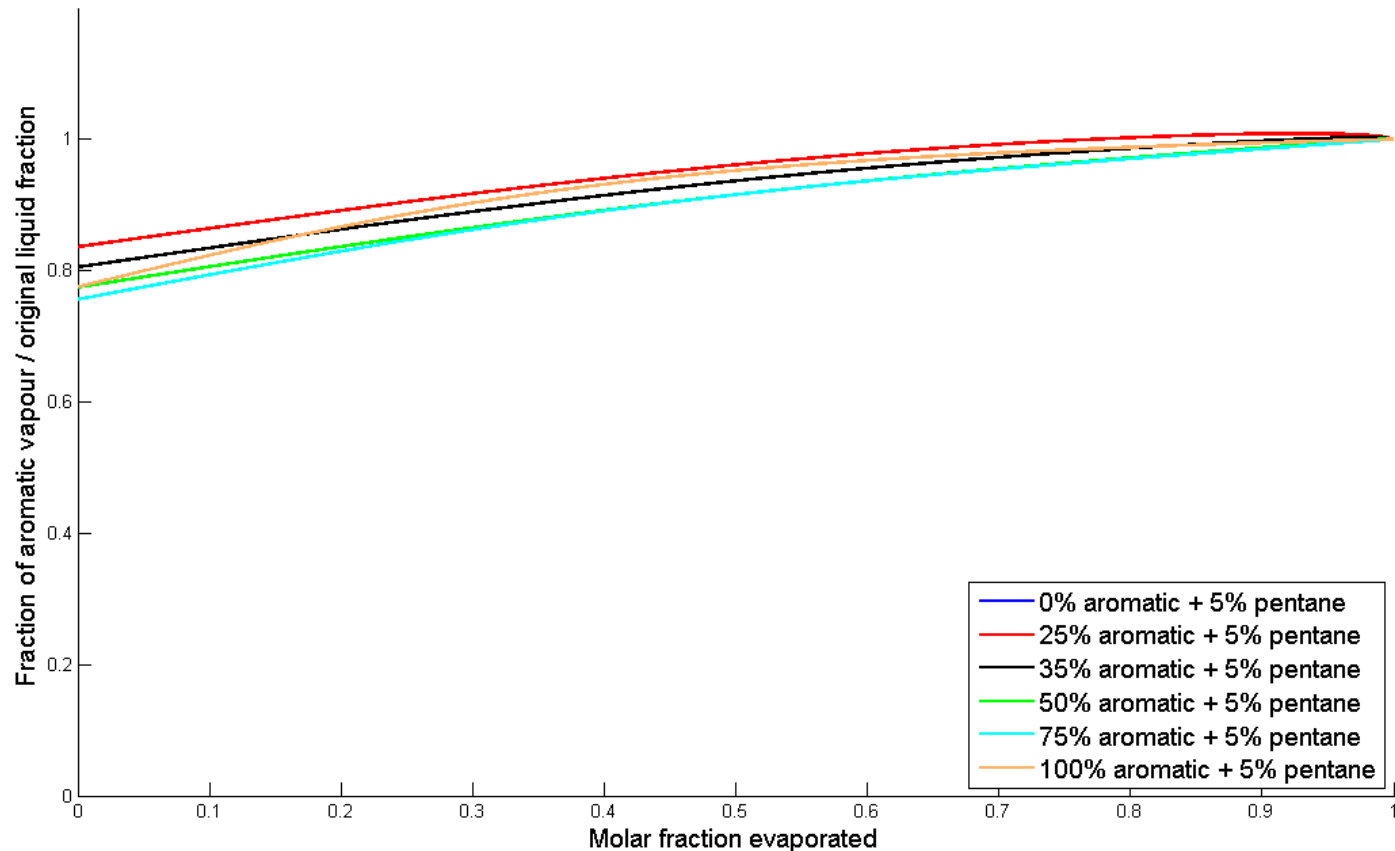
Distillation curve modelling

Comparison between UNIFAC model and real distillation curve for W10/83



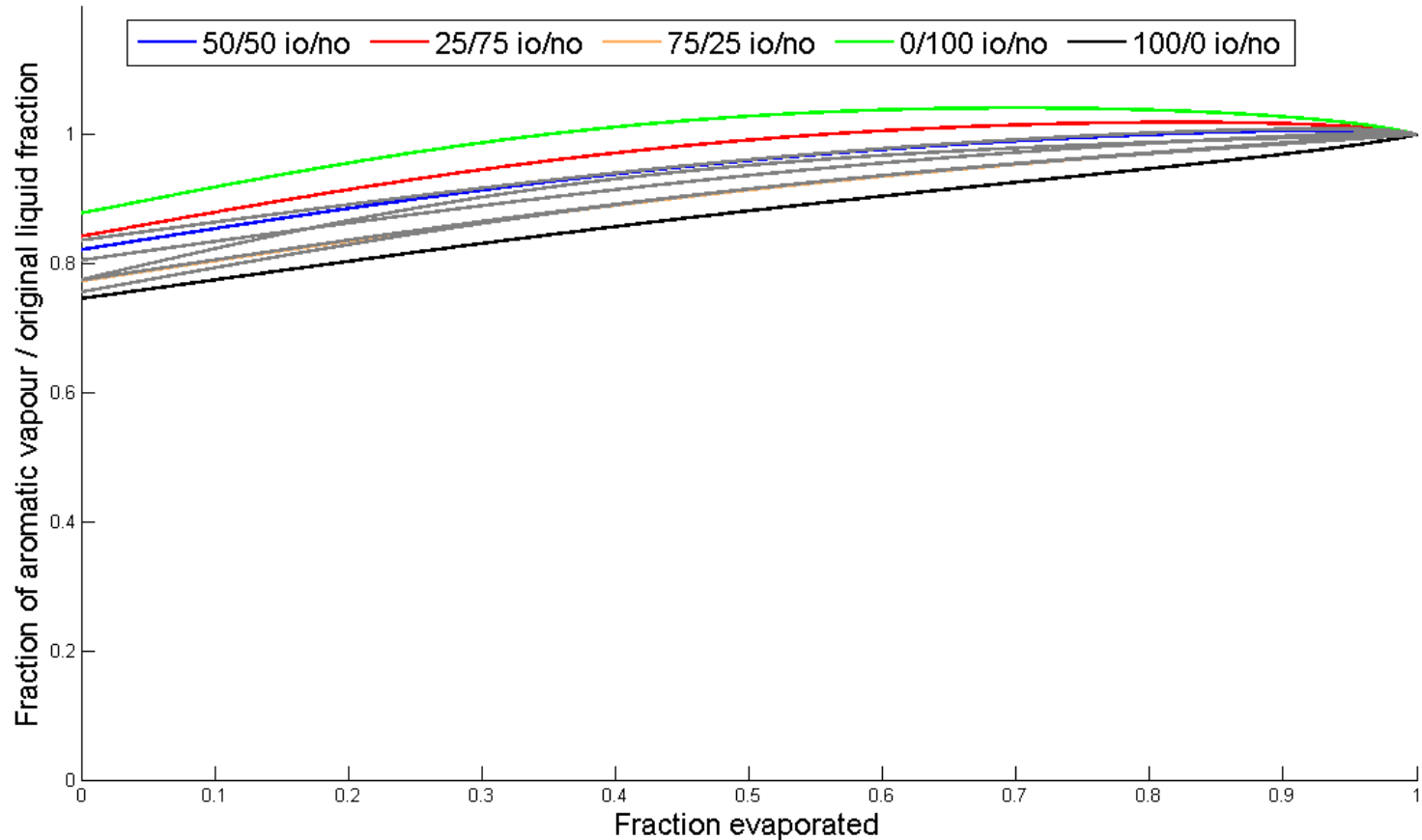
UNIFAC and Raoult's law results

UNIFAC + Raoult's law on mixes of octanes with varying aromatic content with 5% pentane



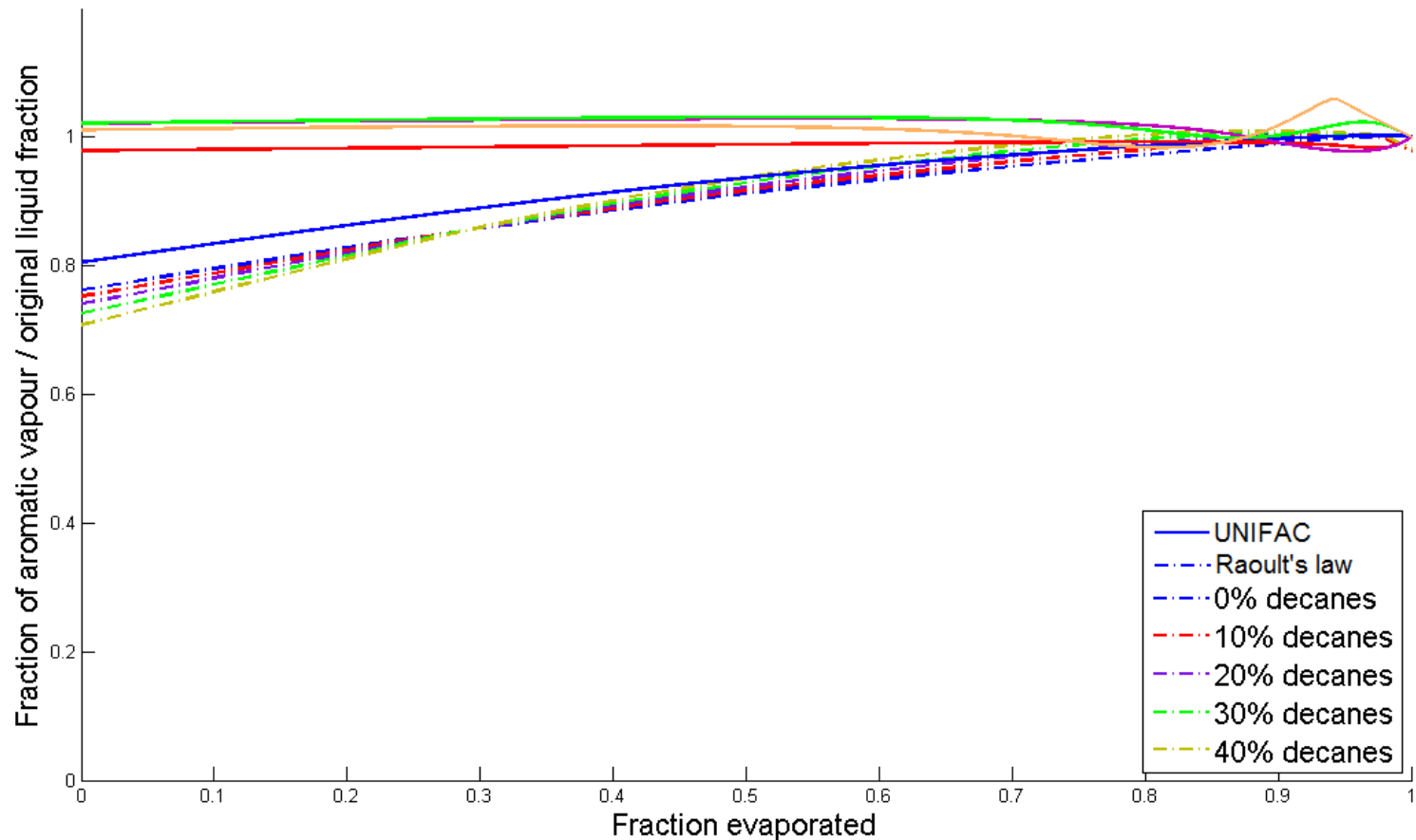
UNIFAC and Raoult's law results

UNIFAC + Raoult's law on varying io/no ratio with 50% toluene and 5% pentane



UNIFAC and Raoult's law results

Pure Raoult's Law on mixes with 35% aromatic content varying decane content with 5% pentane



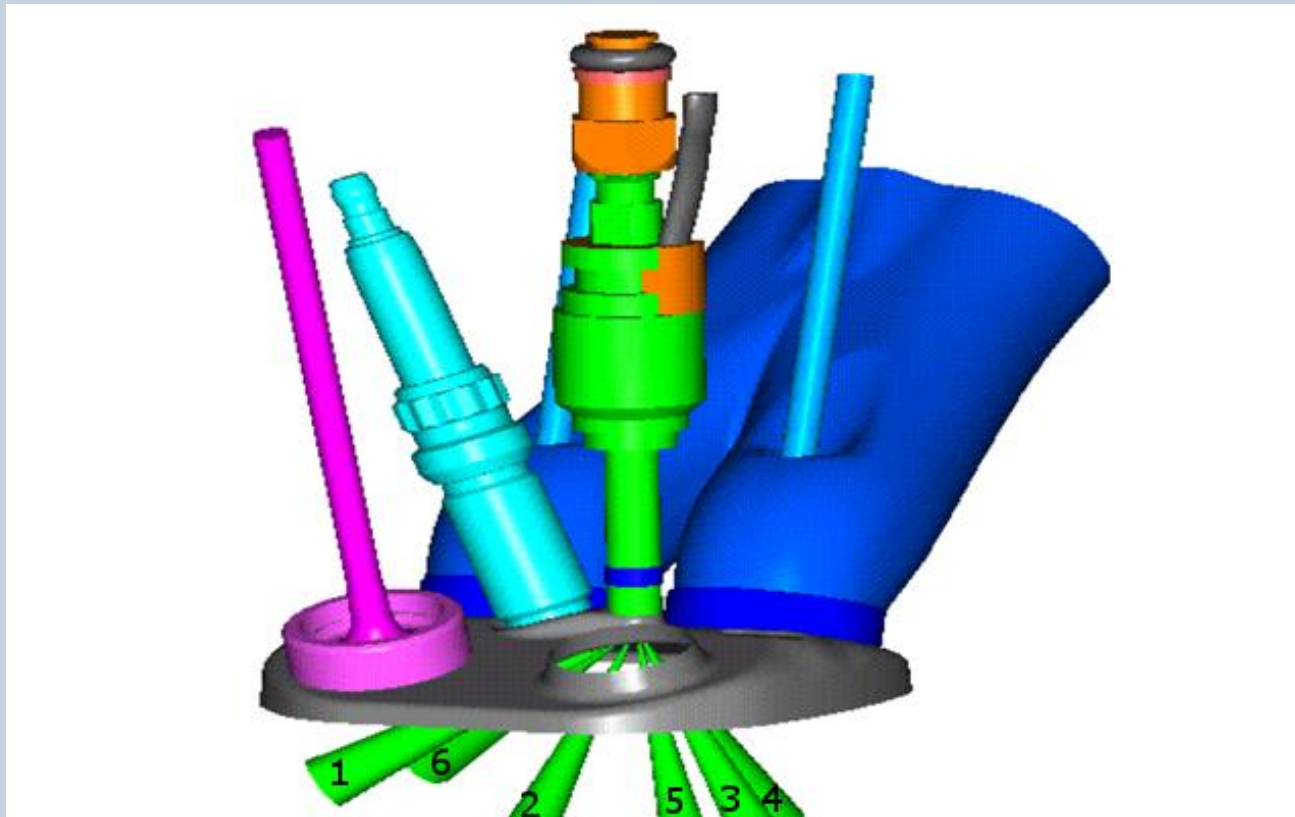
Jaguar AJ-V8 Gen III 5 Litres

- **Naturally Aspirated**
 - 283 kW (380 HP) and 515 Nm,
 - Compression Ratio: 11.5:1
 - Cam profile switching (CPS)
 - Variable geometry inlet manifold
- **Supercharged Version**
 - 375 kW (503 HP) and 625 Nm
 - Compression Ratio: 9.5:1
 - Eaton Supercharger
- **6 hole Bosch Injectors:**
 - 150 bar Injection Pressure
- **Inlet & Exhaust Variable Cam Timing**
- **Bore 92.5 mm, Stroke 93 mm**



© Jaguar Cars Ltd

AJV8 Gen 111 Fuel Injection Pattern



Malcolm Sandford, Graham Page and Paul Crawford, SAE 2009-01-1060

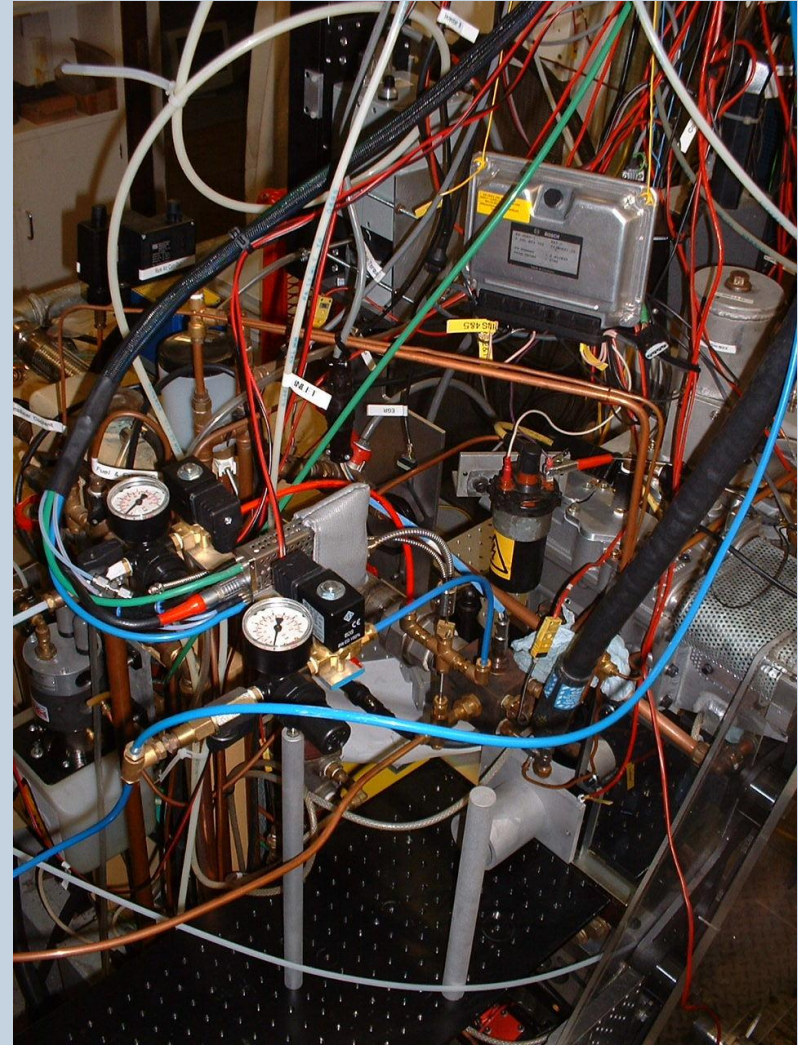
6 Fuel Jets

150 bar injection system

Single Cylinder Engine with Optical Access

- Bore 89 mm
- Stroke 90 mm
- Capacity 562 cc
- Compression Ratio 11.1
- Injection Pressure 150 bar

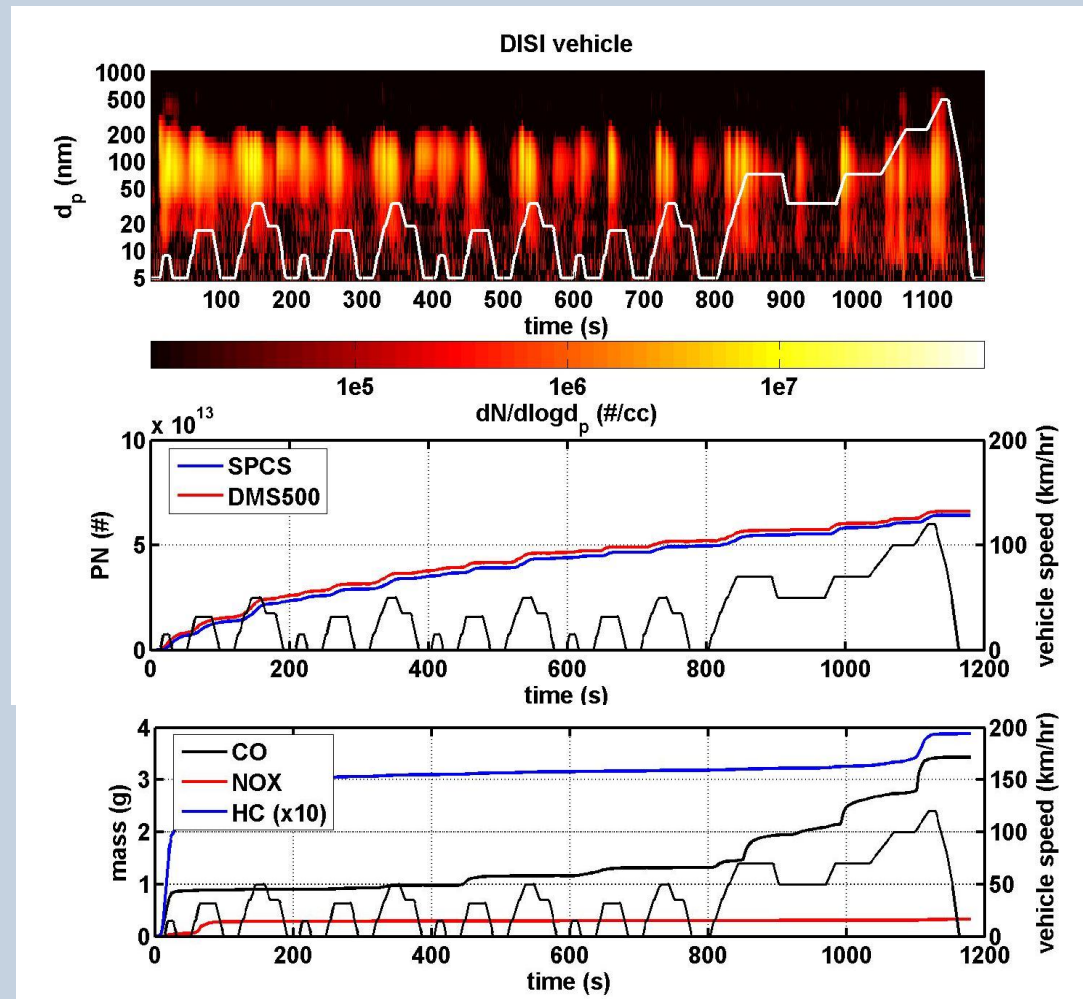
- GDI, PFI
- IMEP 1.8bar
- Mixture (air) inlet 40°C
- Coolant 60°C
- λ 0.9 and 1.01
- 1500 rpm



Particulate Matter Measurements

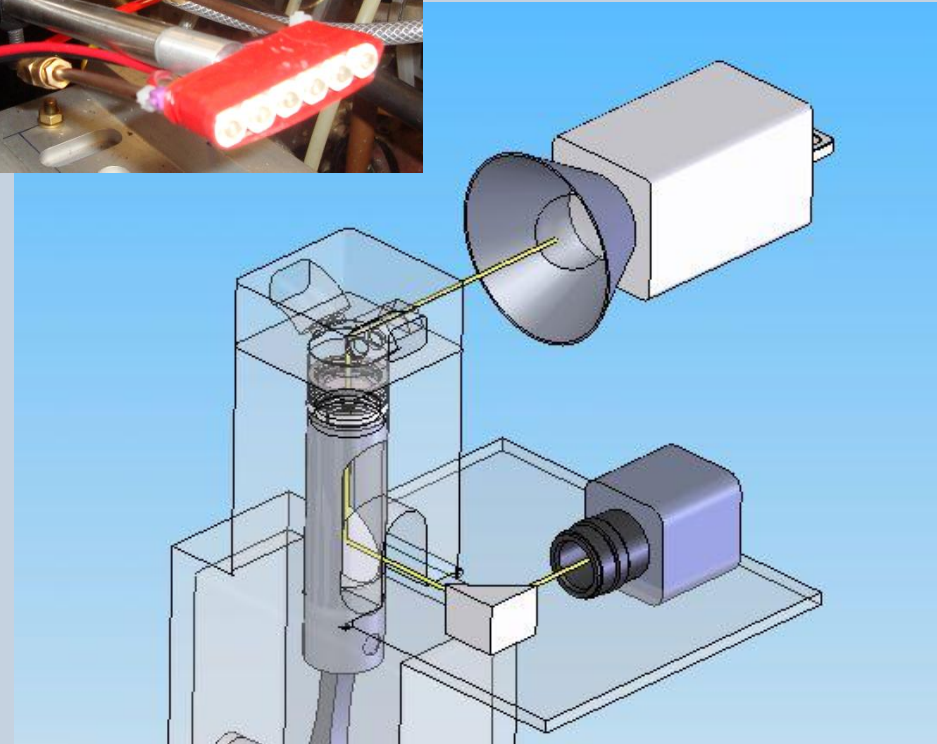
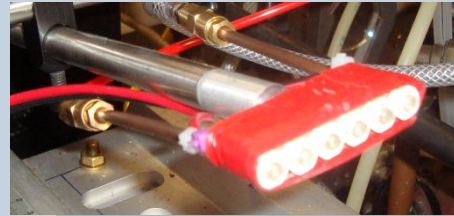
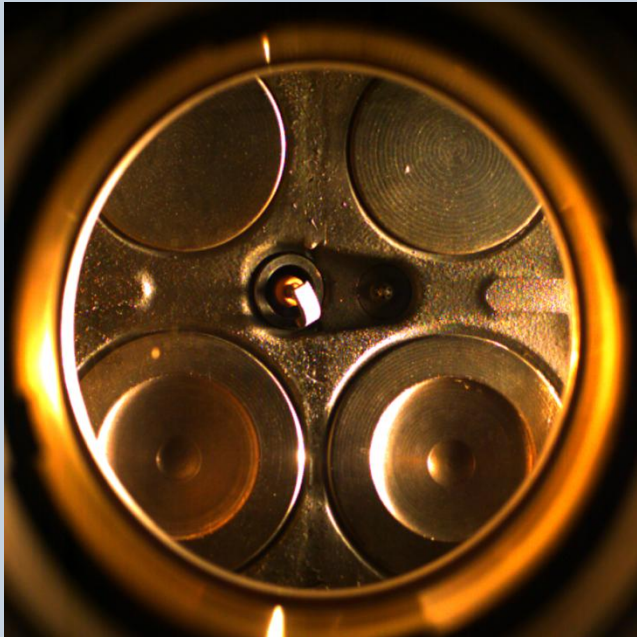
- EUDC
- PN Emissions are associated with Transients
- Gaseous Emissions are dominated by the Cold-Start

SAE 2010-01-0786



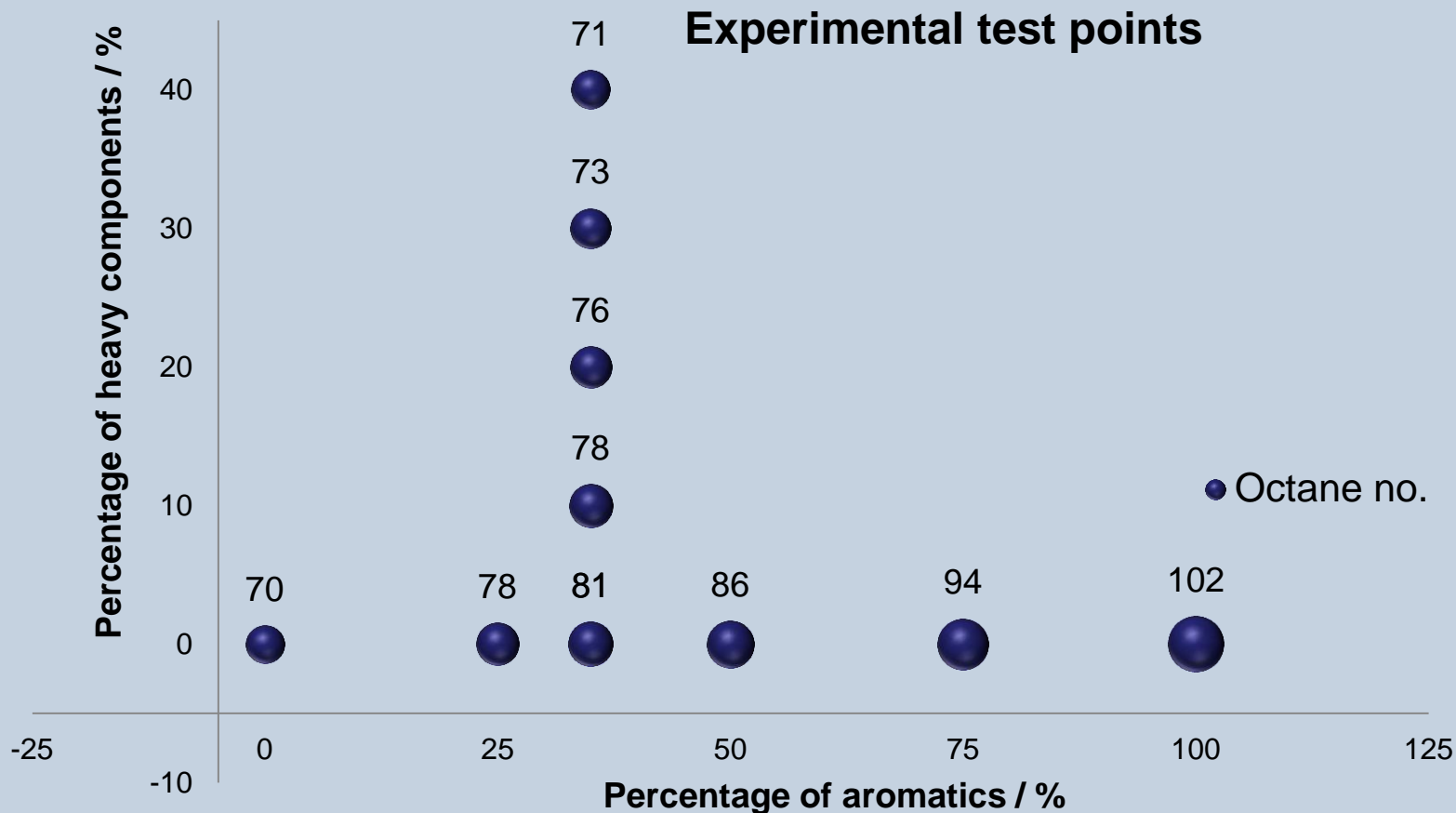
High Speed Imaging – Bowditch Piston

- Photron FASTCAM-1024PCI model
100K Colour Camera – 6000fps
- Resolution: 512 x 256 pixels



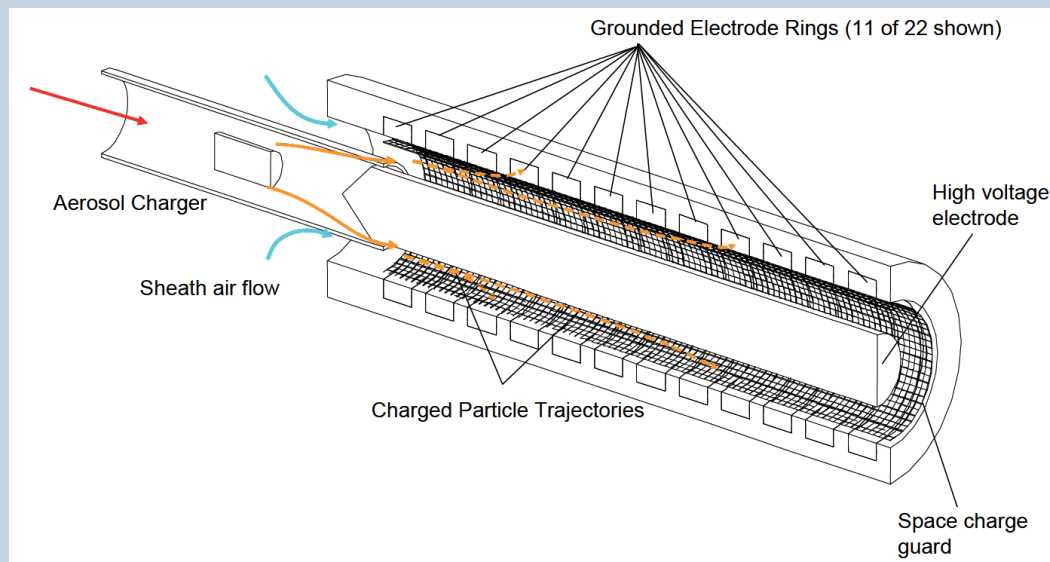
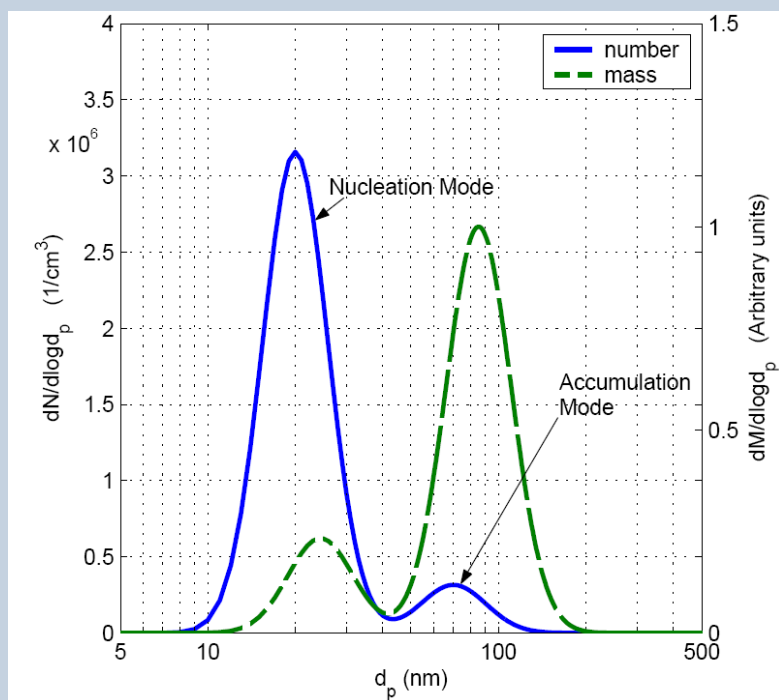
Experimental procedure

Test points



Particulate Matter measurements

Cambustion DMS500



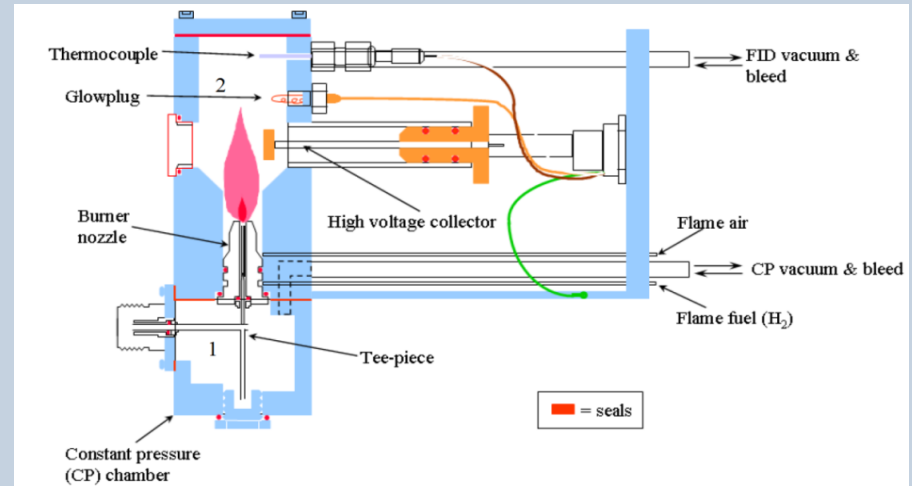
Reavell et al. SAE 2002-01-2714

Only accumulation mode used
Replicates PMP measurement protocol
[Braisher et al. SAE 2010-01-0786]

In-cylinder hydrocarbon sampling

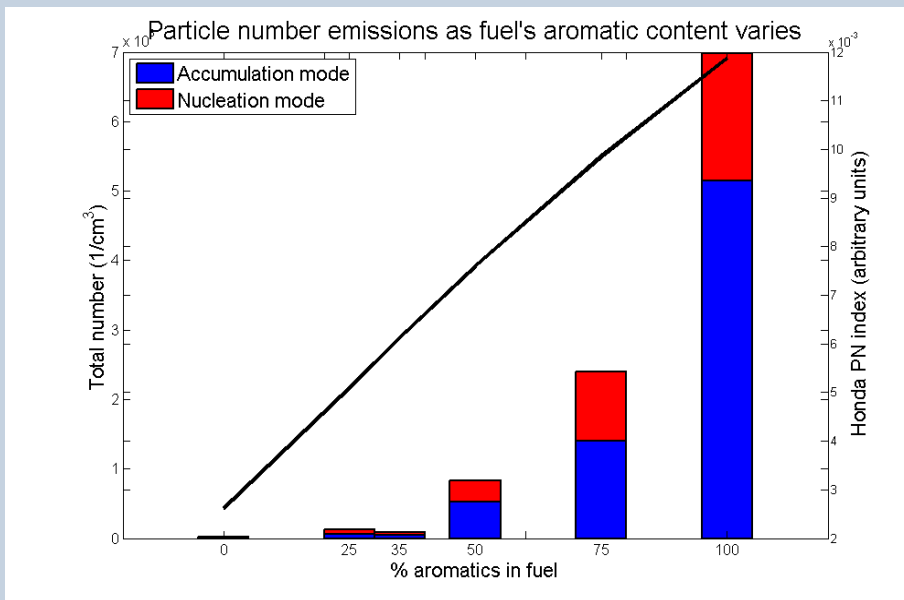
Cambustion HFR400 fast FID

- fFID measures hydrocarbon levels by chemi-ionization
- Response time ~ 4ms

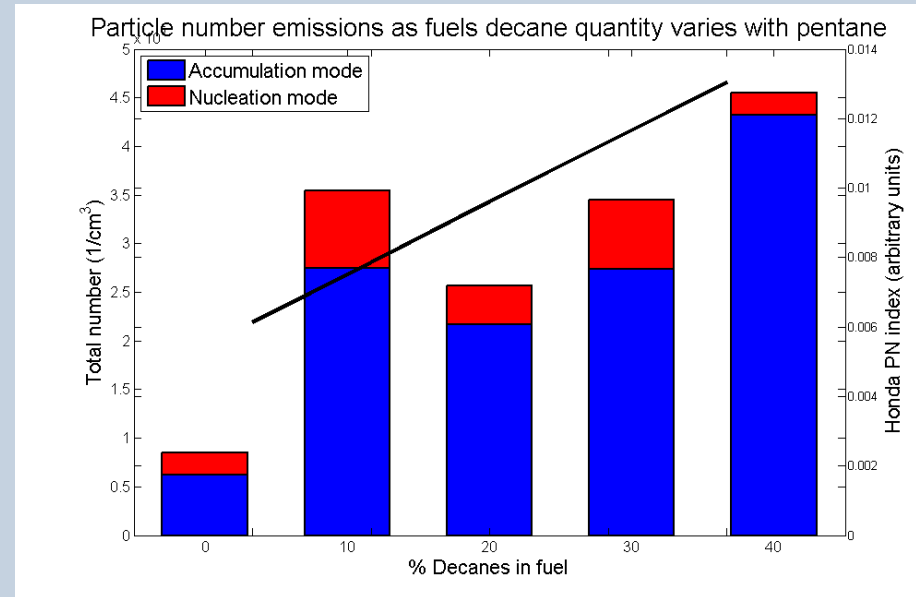


Results

- Clearest trends at $\lambda = 0.9$
- Clear agreement with index



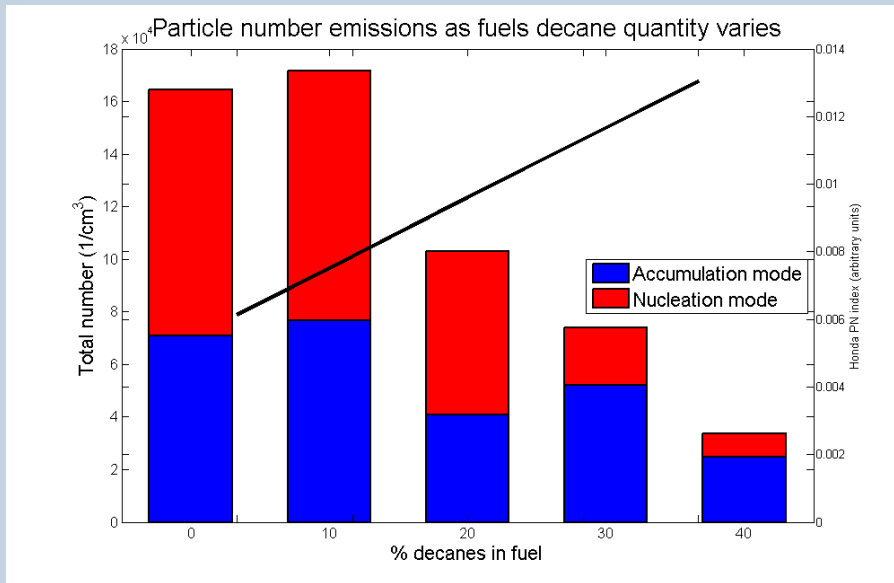
Aromatic sweep $\lambda=0.9$



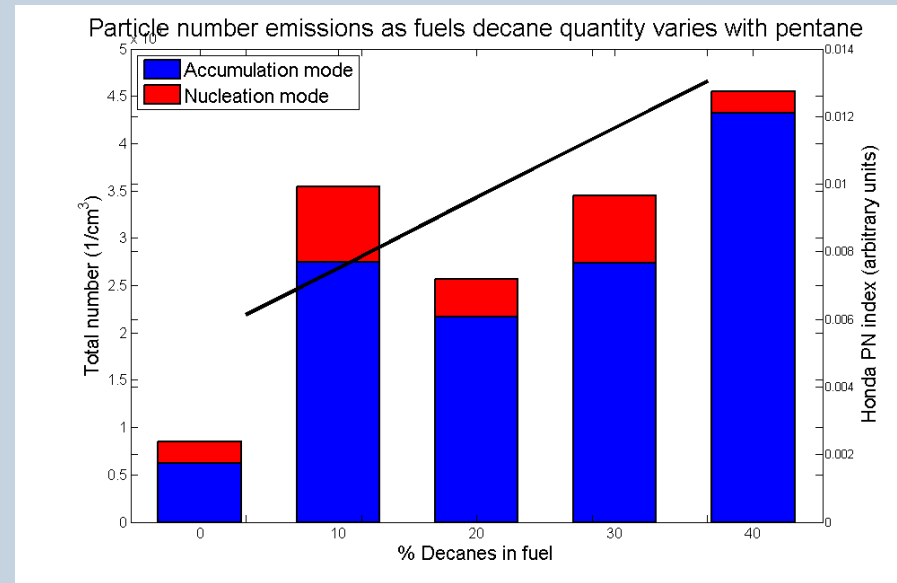
Volatility sweep $\lambda=0.9$

Importance of n-pentane

- Much better agreement between volatility sweep and Honda predictions
- Pentane mimics “light end” of commercially available ULG



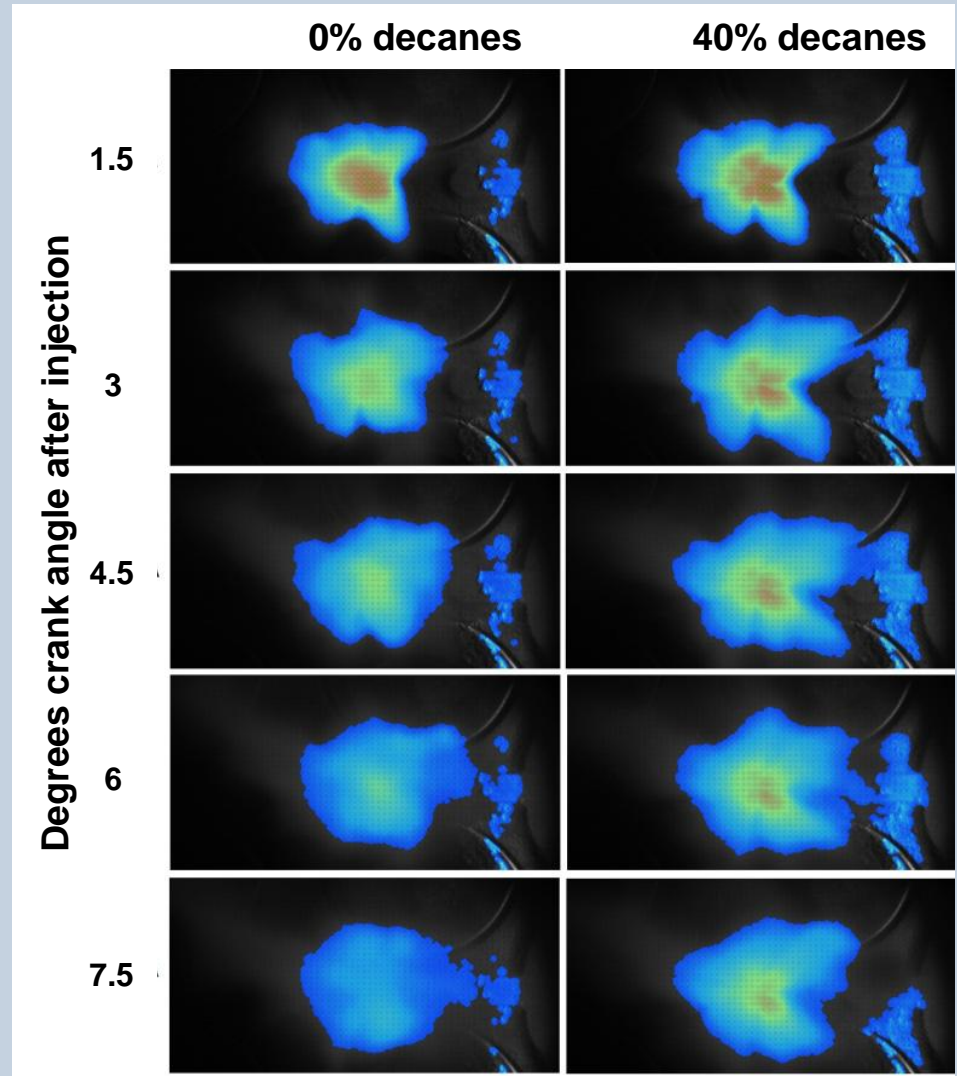
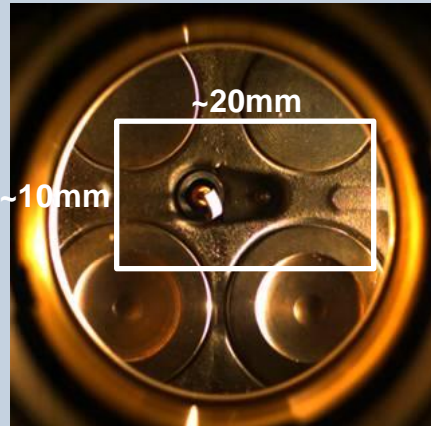
No pentane



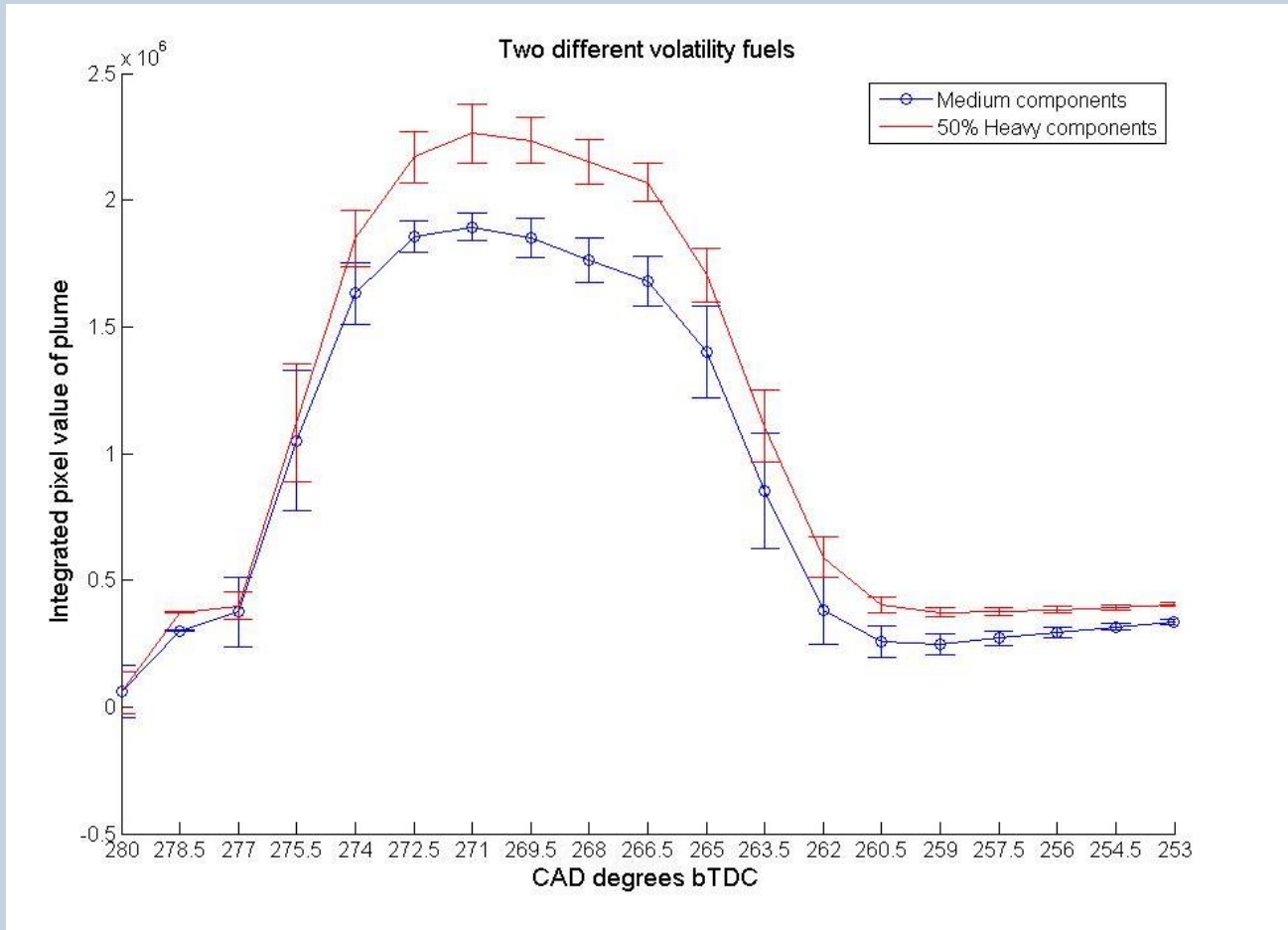
With pentane

Spray penetration

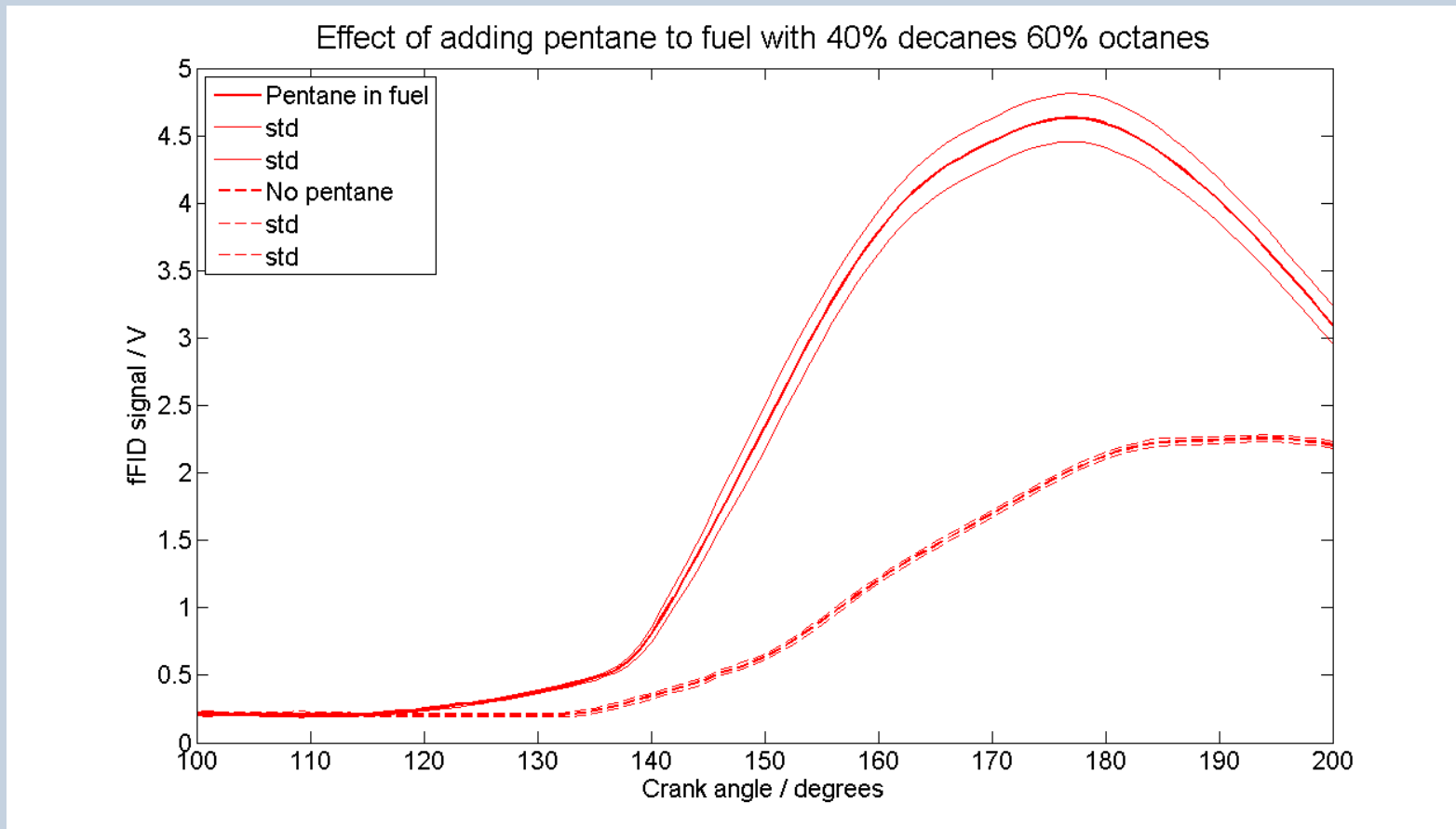
False colour images



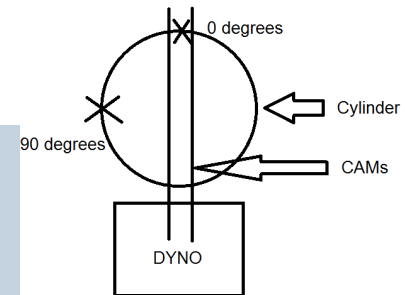
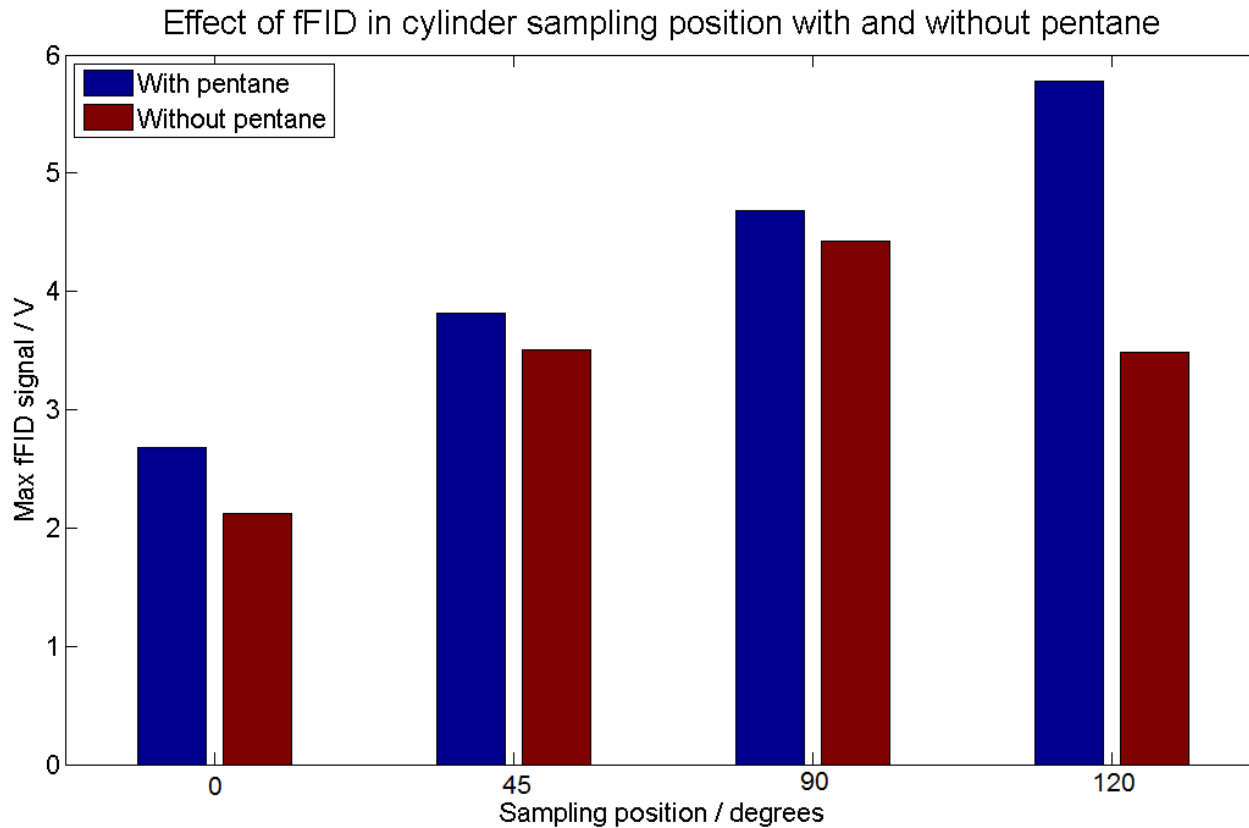
Spray penetration



In-cylinder hydrocarbon sampling showing effect of pentane in fuel (40% decanes, 60% octanes)

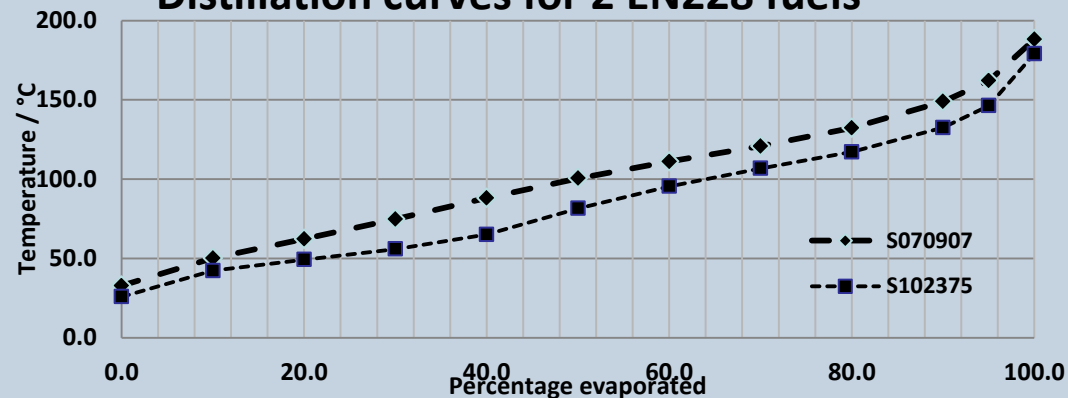


Effect of sampling position



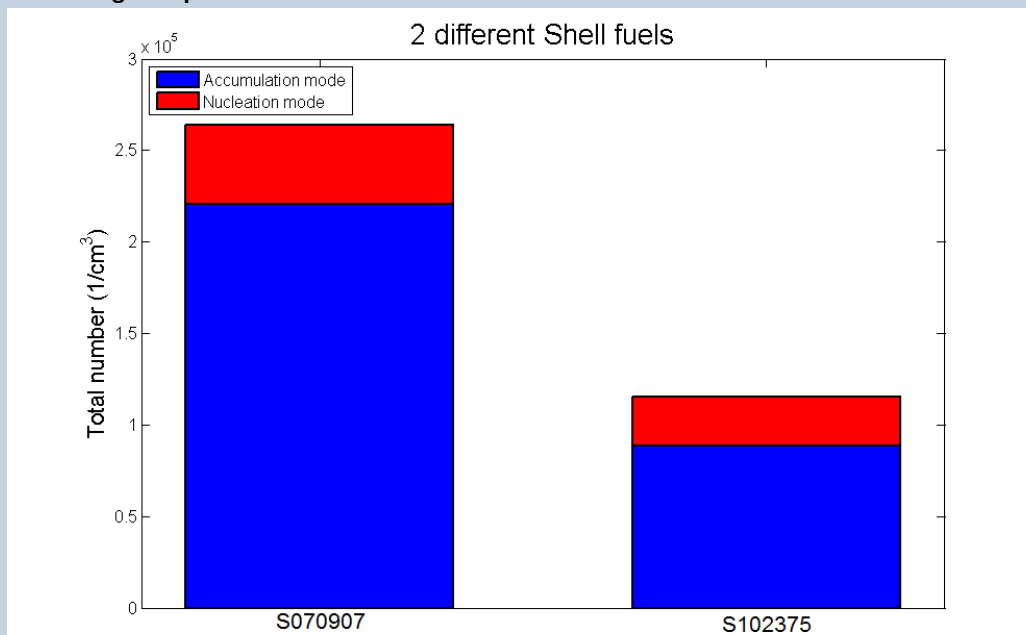
Application to real fuel

Distillation curves for 2 EN228 fuels



	S070907	S102375
RVP* (kPa)	70.6	88.6
DBE	1.58	1.25
FBP (°C)	188.1	179.0
PN Index	1.62e-2	9.77e-3

* Not same method as Honda paper



EU5 Reference Fuel

CEC RF-02-08 fuel specification

	Min	Max
RVP (kPa)	56.0	60.0
Olefins (% v/v)	3.0	13.0
Aromatics (% v/v)	29.0	35.0
Ethanol (% v/v)	4.7	5.3
FBP ($^{\circ}$ C)	190	210

	EU5 (Min I)	EU5 (Max I)
RVP* (kPa)	60.0	56.0
DBE	2.19	2.53
FBP ($^{\circ}$ C)	190	210
PN Index	2.74e-2	3.43e-2

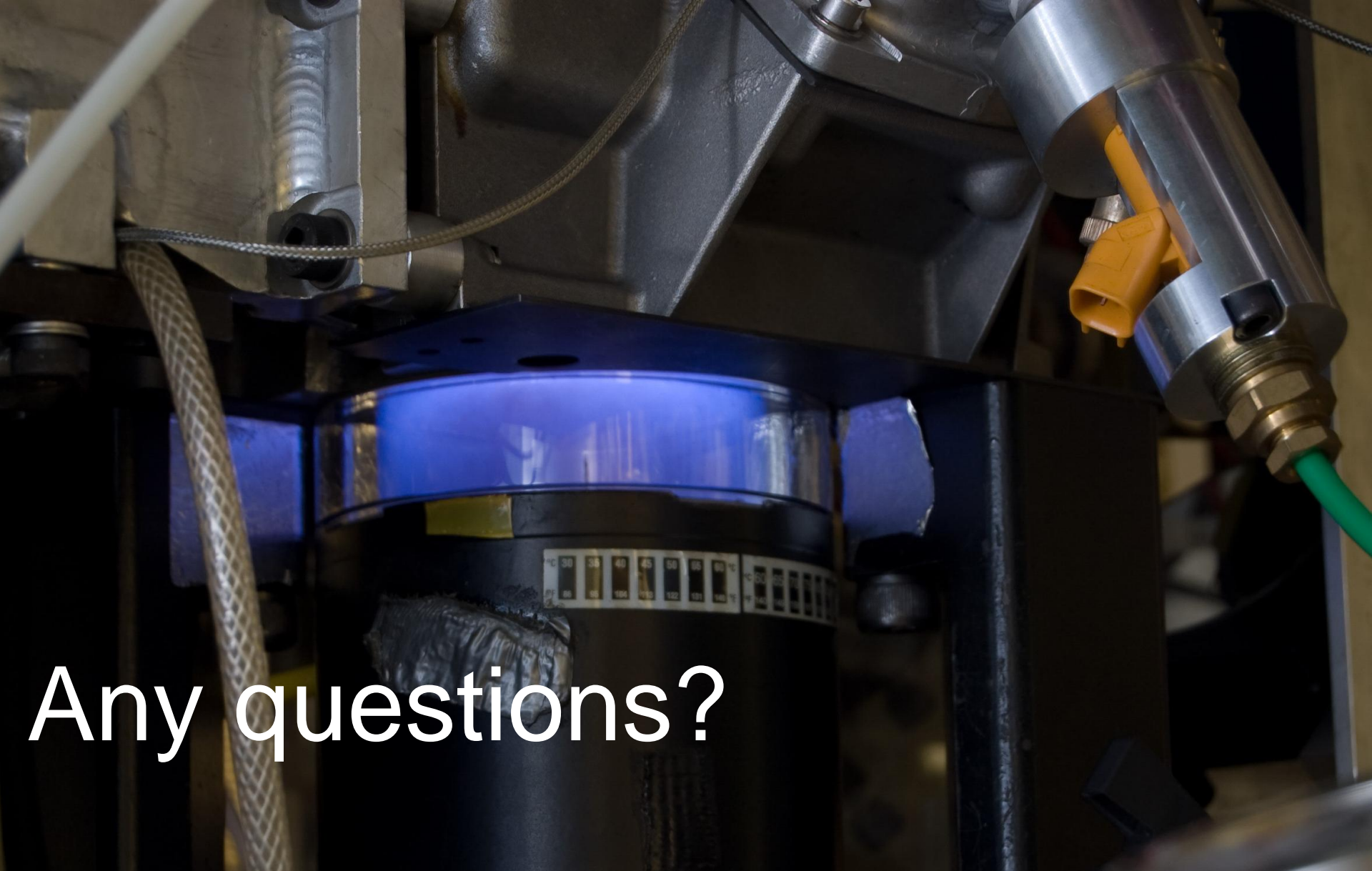
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Conclusions

- Fuels blends have been devised that have independent control of volatility and aromatic content
- UNIFAC needs to be used modelling co-evaporation of aromatics
- Effect of light components on Fuel spray is significant
- Trends reported by Honda replicated in SGDI engines using model fuels
- Trends also observed using real fuels in SGDI engine
- Implications for reference fuels



Any questions?

Fuel design

Selection of aromatic components

- Looking for similar boiling points to paraffin components
 - Octanes (~379K), decanes (~444K)
- Aromatics have high RON

	T_b (K), 1.01325 bar	BON*
Benzene	353.2	108
Toluene	383.8	120
1,2,4-Trimethylbenzene	442.5	123
1,3,5-Trimethylbenzene	437.9	161

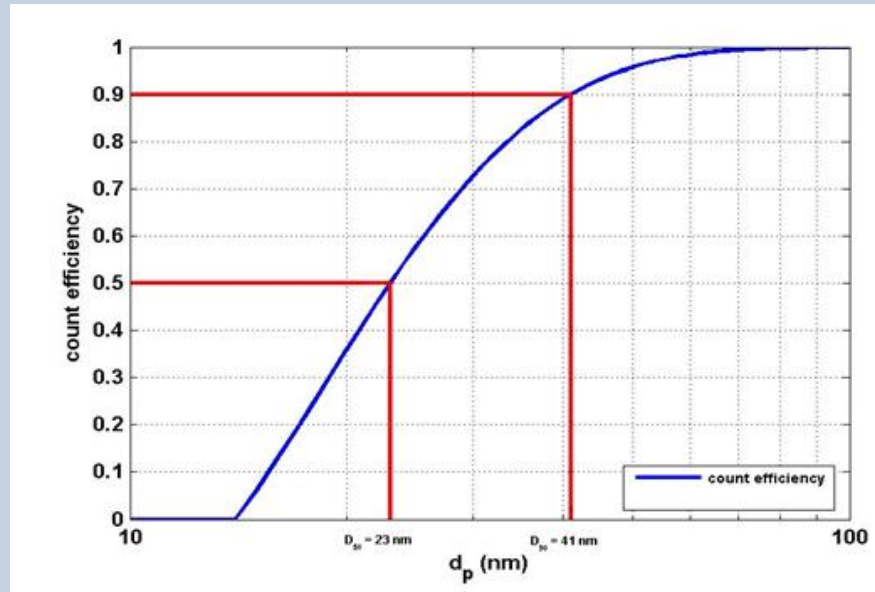
*BON (Blending Octane Number) – equivalent octane number when blended as 20% solution in a 60/40 iso-octane/n-heptane mix. Attempt to give more relevant number than RON when blended with other components. [Lovell 1948]

Digital filtering of low diameter PN

To replicate PMP measurement protocol

50% count efficiency: $D_{50} = 23$ nm

>90% count efficiency: $D_{90} = 41$ nm

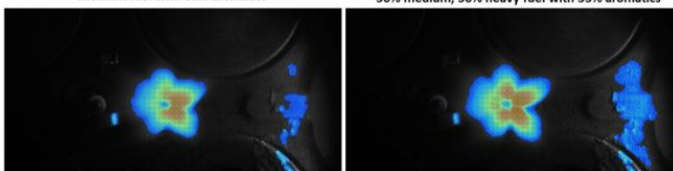


$$\text{Wiebe function: } f = 1 - \exp \left[-3.54 \left(\frac{d_p - 14}{40} \right)^{1.09} \right] \quad d_p > 14$$

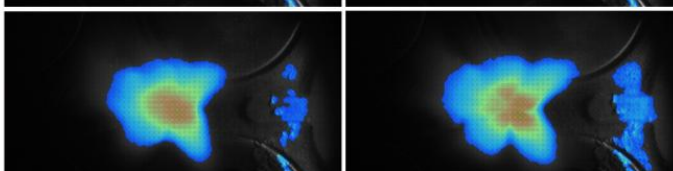
Medium fuel with 35% aromatics

50% medium, 50% heavy fuel with 35% aromatics

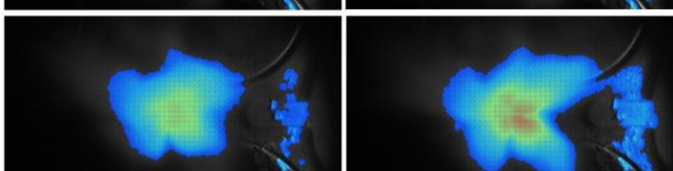
0° CA



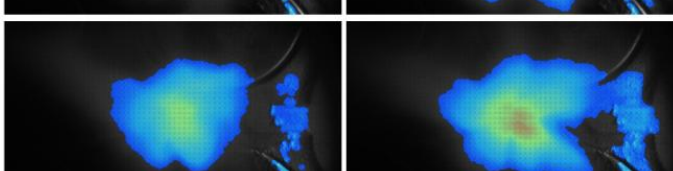
1.5° CA



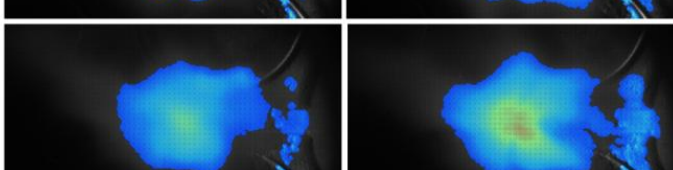
3° CA



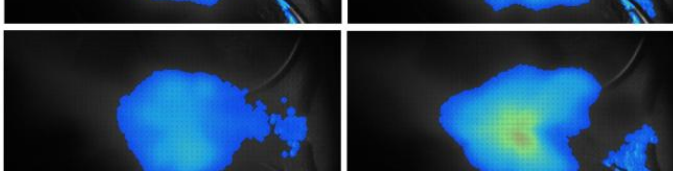
4.5° CA



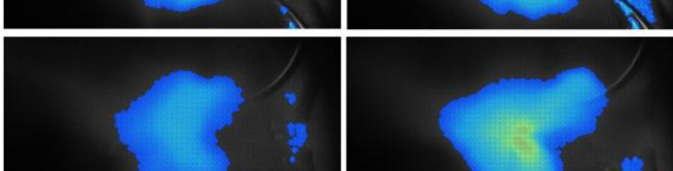
6° CA



7.5° CA



9° CA



10.5° CA

