



**Shell Global Solutions**



**UNIVERSITY OF LEEDS**

# **Kinetic Data Needs for Industry**

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**UKELG Meeting**

**10<sup>th</sup> September 2008**

**Loughborough University**

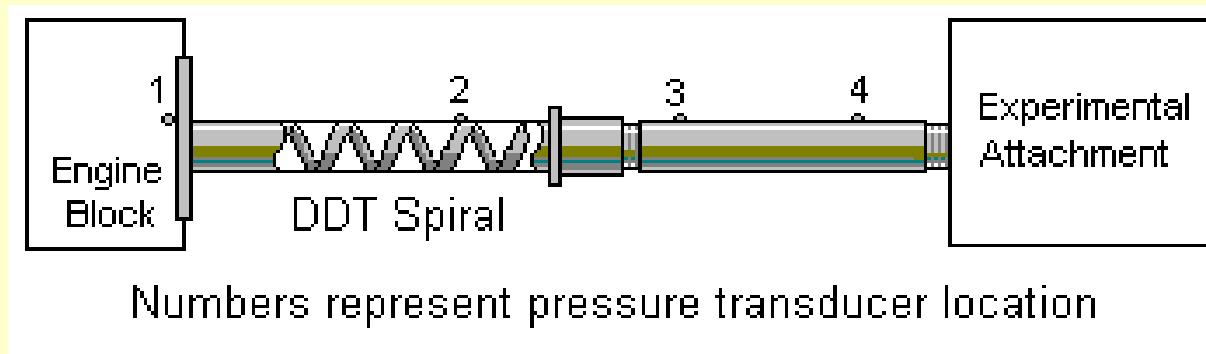
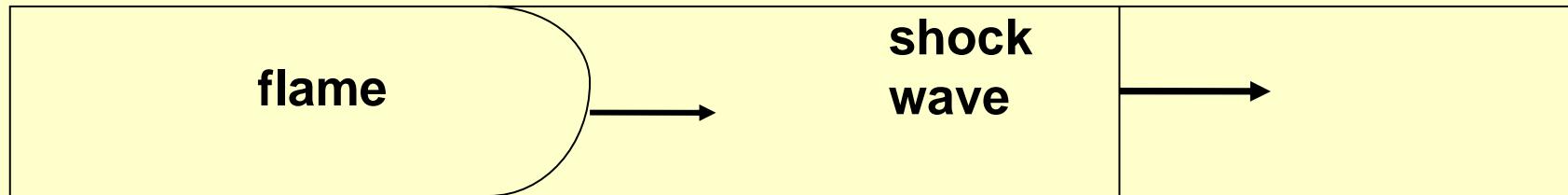
# Plan of Talk

1. Flammability limits.
2. Auto-ignition and its modes.
3. Measurement of autoignition delay times.
4. Apparatus for intermediate  $T$  and  $p$ .
5. Data limitations.

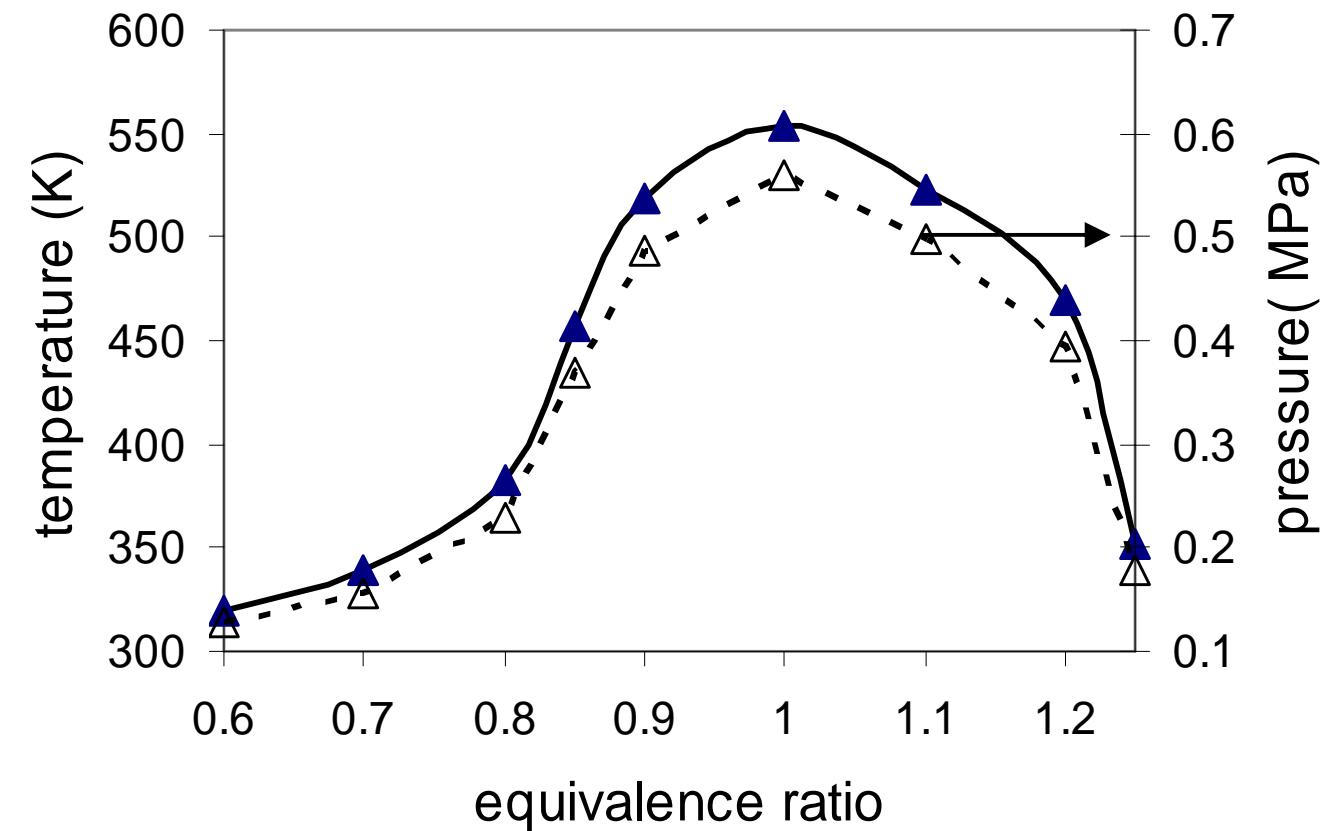
# Flammability Limits

- Mode of initiation must be satisfied.
- Initiation time,  $t_i$ , should be specified.
- Mixing time  $< t_i < \tau$  (auto-ignition delay time and aerodynamic time).

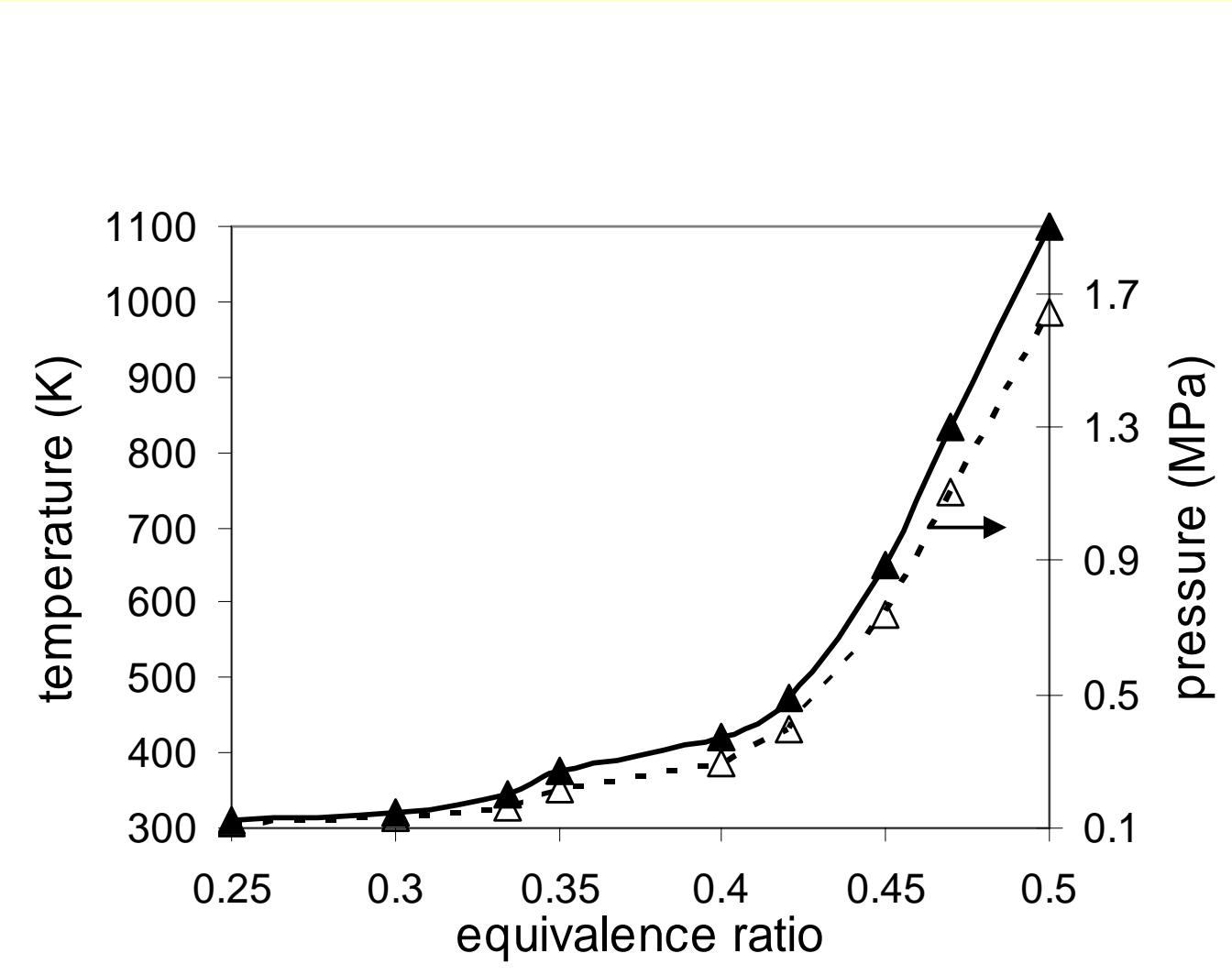
# Auto-ignition in Explosions



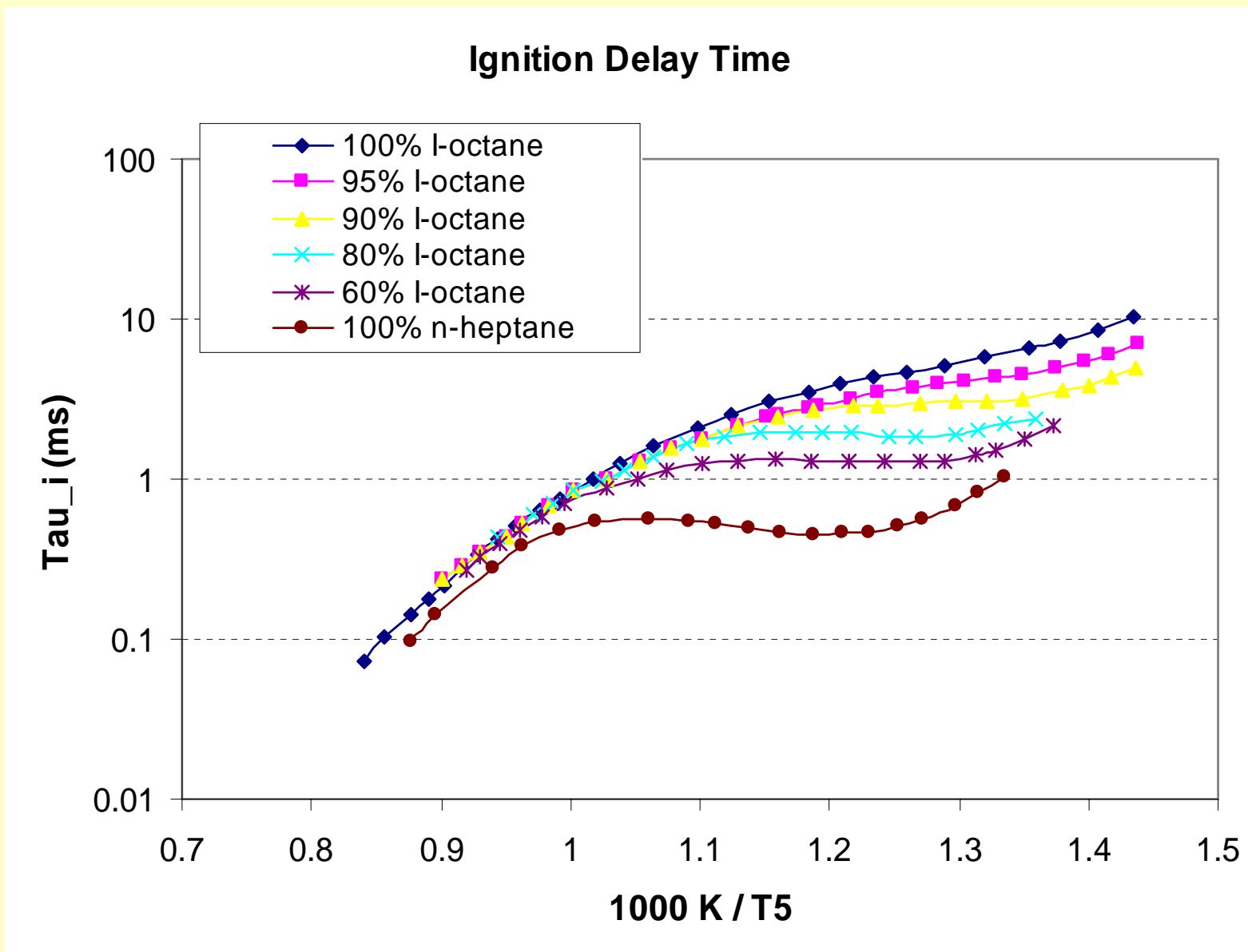
# $\text{CH}_4$ -air shocked temperature and pressure



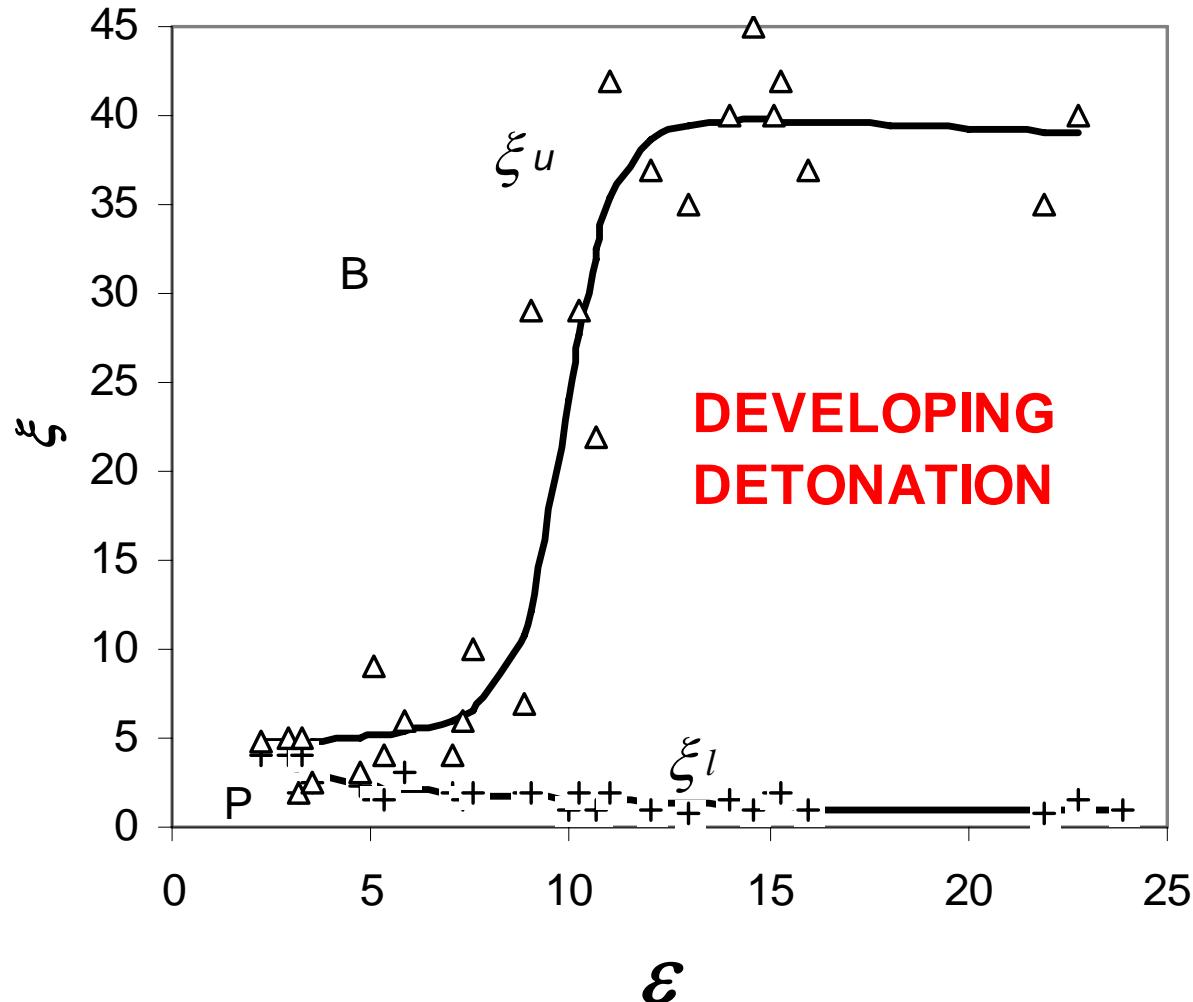
# $\text{H}_2$ -air shocked temperature and pressure



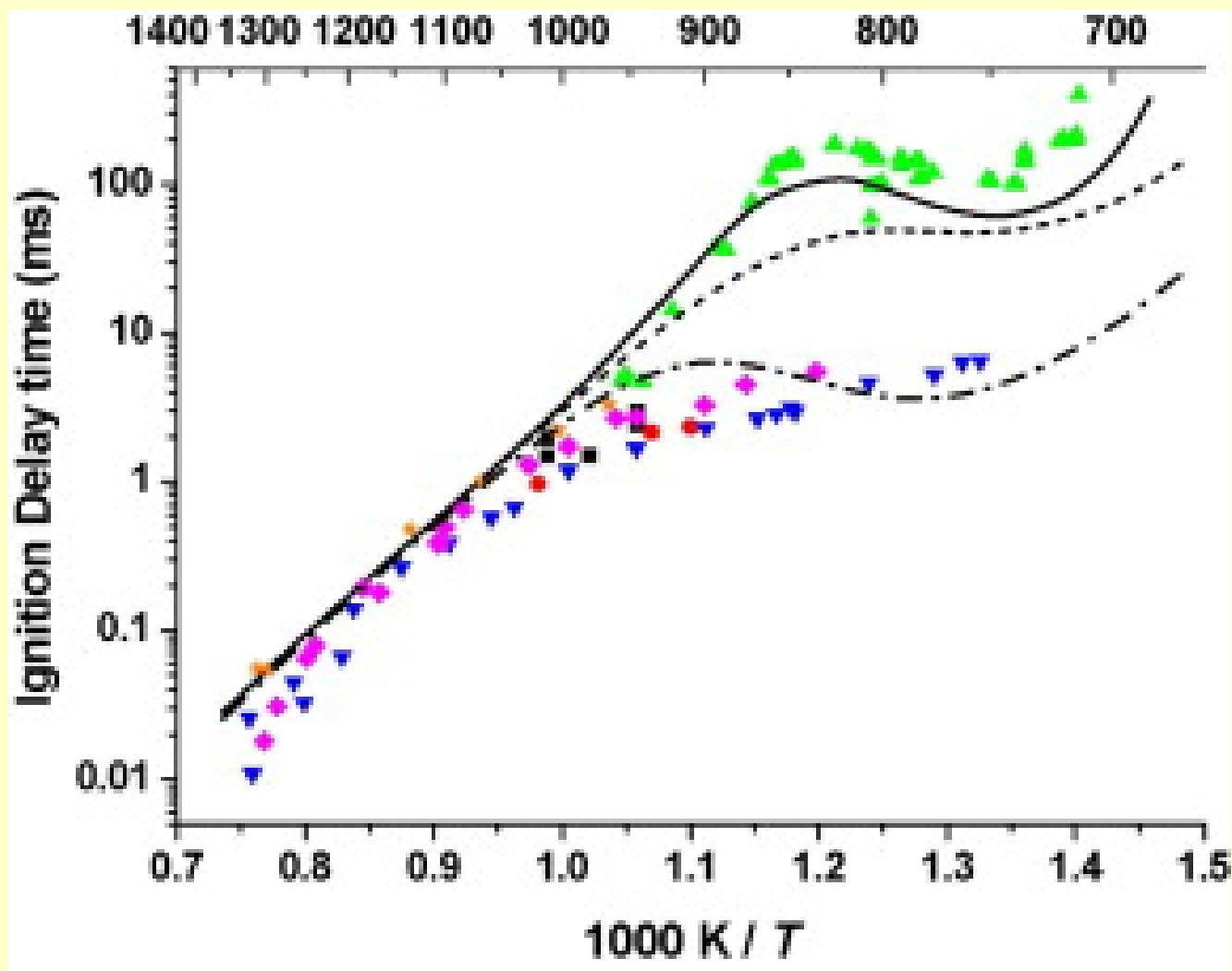
# Autoignition Delay Times, 4 MPa



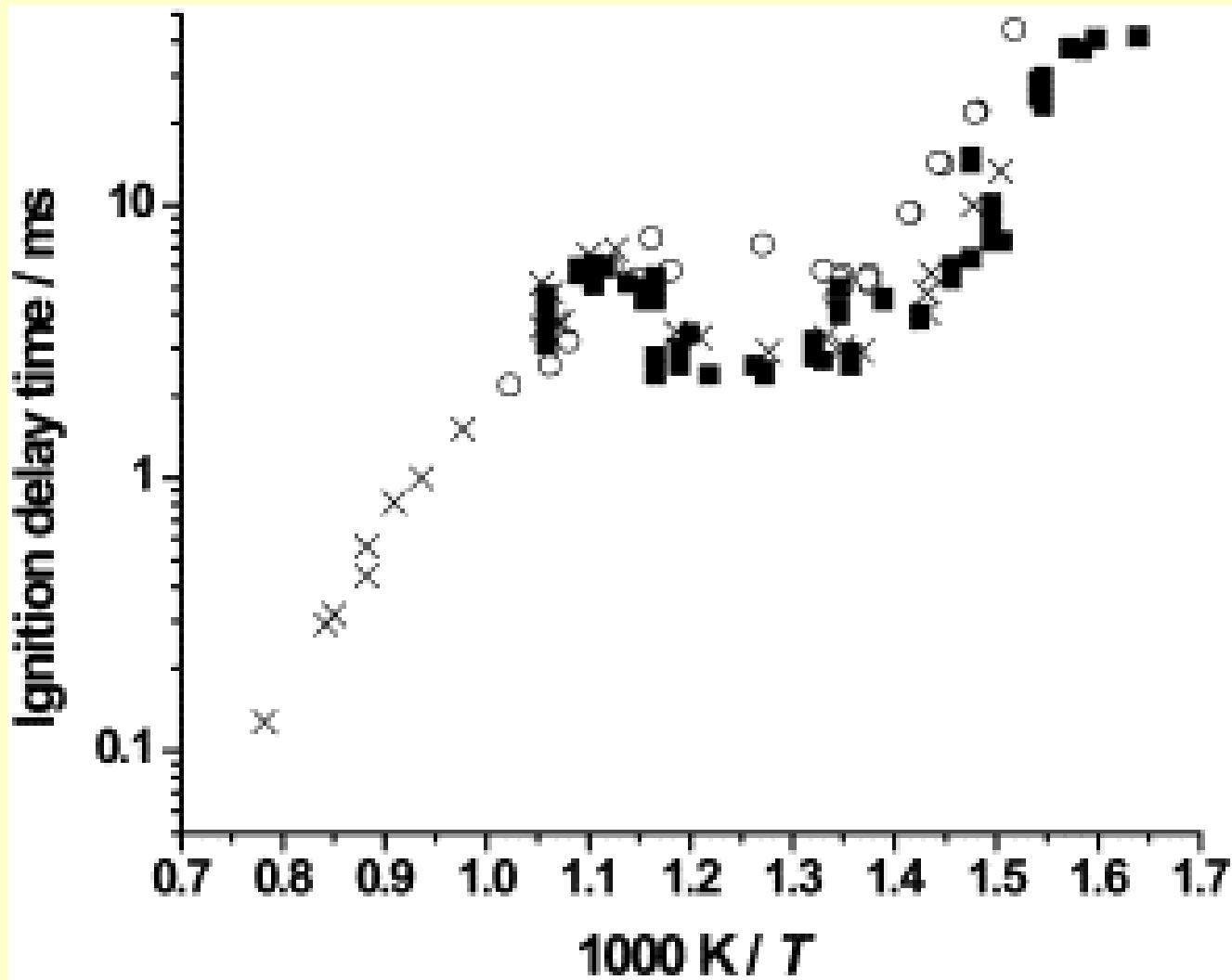
# Peninsula of Detonation at Hot Spots



# Propane-air Auto-ignition Delay Times $\phi = 0.5$ , p=30 atm.

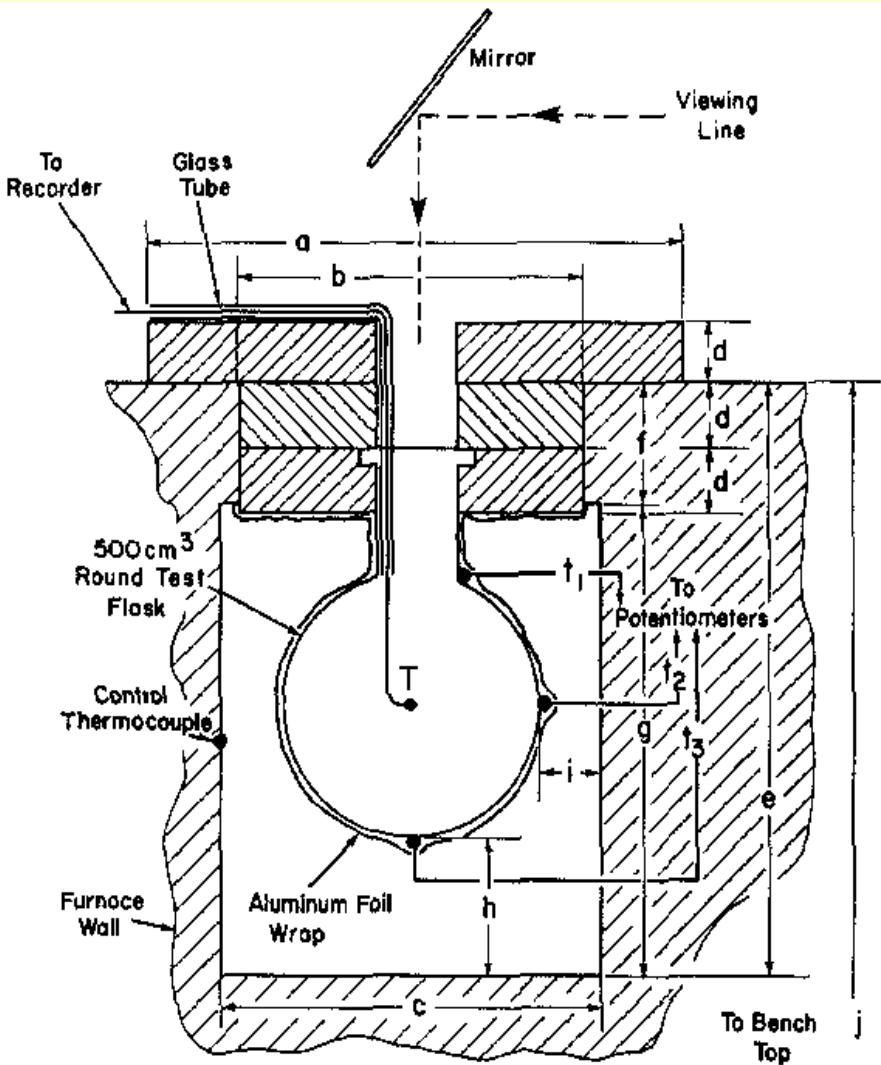


# *n*-heptane-air Auto-ignition Delay Times $\phi = 1.0, p = 10 \text{ atm.}$



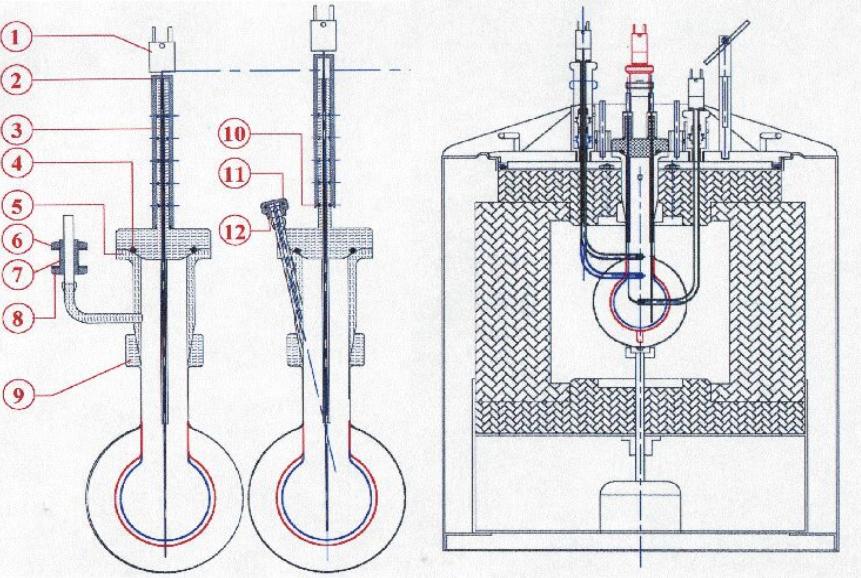
# Auto-ignition Temperature Bomb

## ASTM E 659 – 78 (2005)

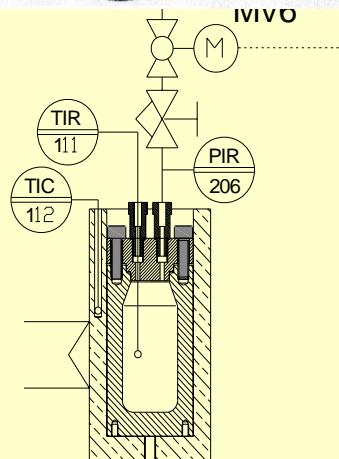


- Atmospheric pressure
- T max approximately 600°C
- 500 ml borosilicate glass
- 10 minutes observation
- Liquid samples
- Open vessel
- Ignition appearance of a flame accompanied by a sharp T rise

# New apparatus developed in (SAFEKINEX)

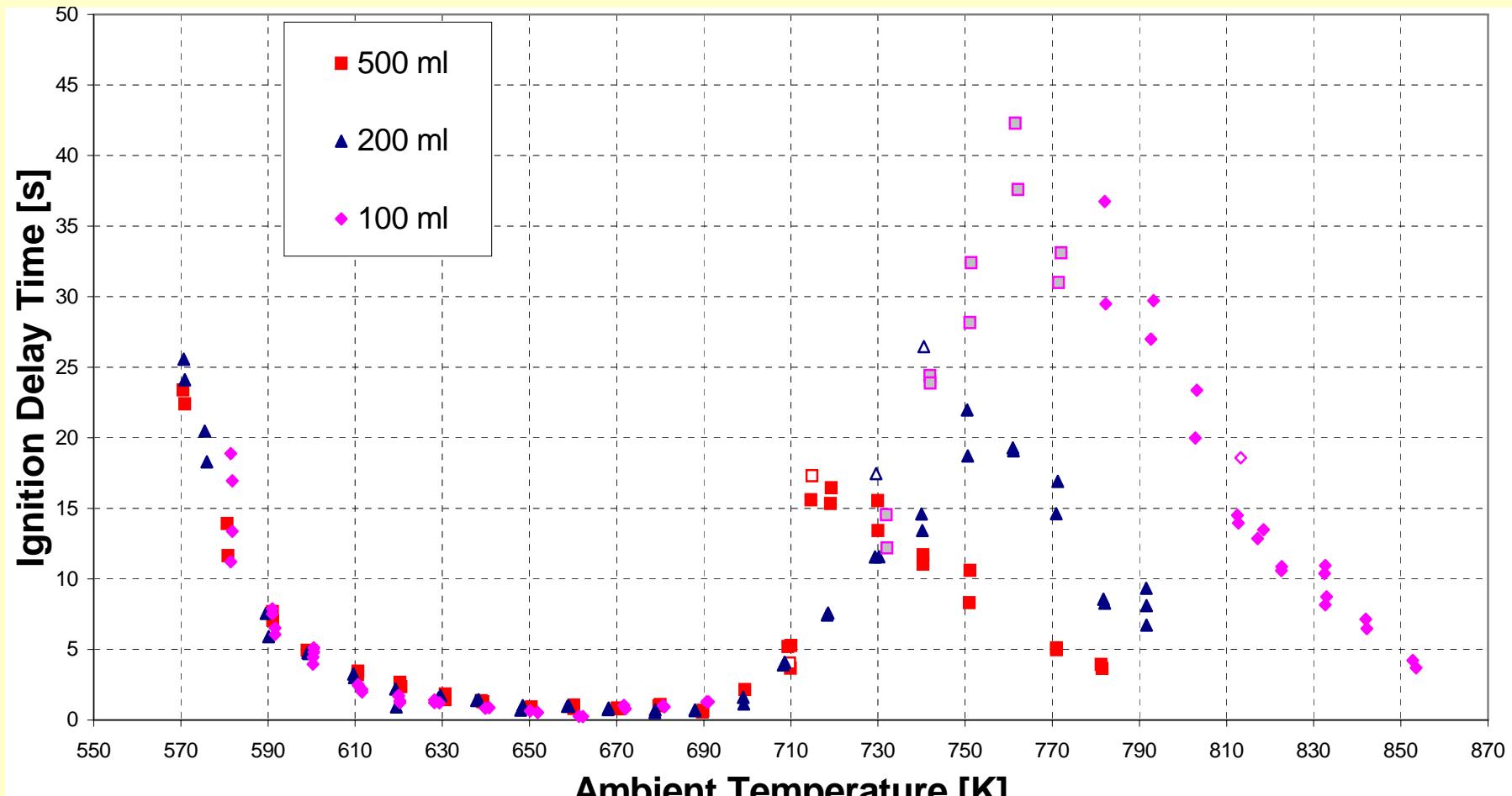


*TUD AIT vessel 100, 200, 500 ml,  
Semi-closed vessel, quartz,  
Two thermo- couples inside,  
steering possibility,  
Operation at (sub-)ambient pressure*



*BAM AIT vessel 200 ml,  
closed vessel, stainless steel,  
thermo- couple in the centre  
Operation at elevated pressure*

# Auto-ignition times for different volumes; 100, 200, 500 ml



# Problem of intermediate $T$ and $p$

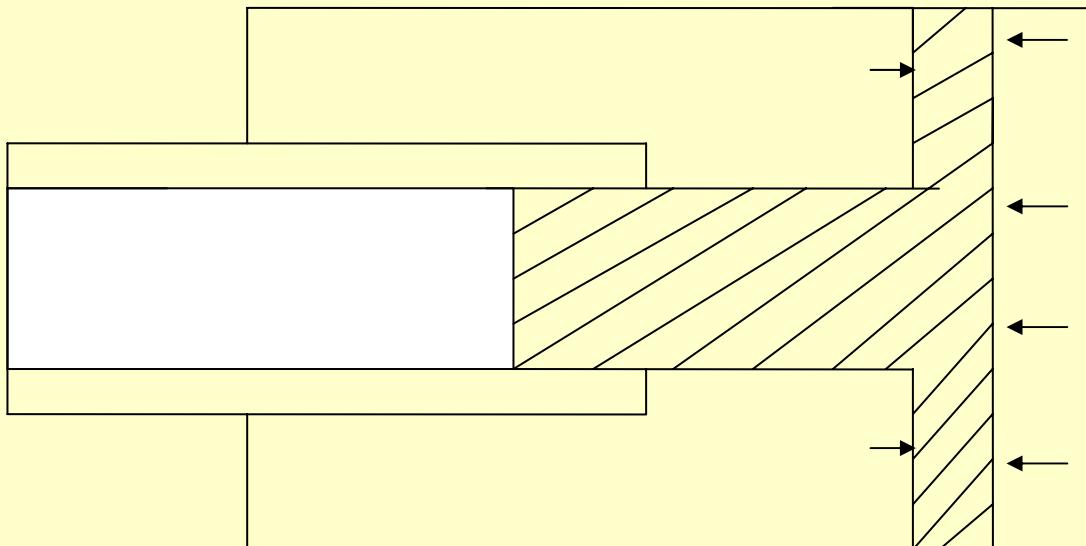
- Shock tube:  $\tau <$  shock duration
- RCM:  $\tau >$  compression time
- ASTM:  $\tau >$  mixing time

$\tau <$  aerodynamic time

- Proposed flying piston:  
 $\tau >$  compression time

# Proposed Flying Piston

Ensures  $\tau >$  mixing time  
All mixing at low  $T$



# Data Limitations

1. At high  $T$  and  $p$ :

Laminar burning velocity, Markstein numbers, Flame quench stretch rates.

2. At intermediate  $T$  and  $p$ :

Autoignition delay times.

3. Autoignition/detonation transition.

# References (1)

- Slides 4-6: D. Bradley, M. Lawes, Kexin Liu, "Turbulent flame speeds in ducts and the deflagration/detonation transition," Combust. Flame **154** (2008) 96-108.
- Slide 7: K. Fieweger, R. Blumenthal, G. Adomeit, "Self-ignition of S.I. engine model fuels: a shock tube investigation at high pressure," Combust. Flame **109** (1997) 599-619.
- Slide 8: D. Bradley, C. Morley, X. J. Gu and D. R. Emerson, "Amplified Pressure Waves during Autoignition: Relevance to CAI Engines", SAE paper 2002-01-2868, (2002), in SP-1718 "Homogeneous Charge Compression Ignition

# References (2)

- Slides 9 -10: S.M. Gallagher, H.J. Curran, W.K. Metcalfe, D. Healy, J.M. Simmie and G. Bourque, “A rapid compression machine study of the oxidation of propane in the negative temperature coefficient regime,” Combust. Flame 153 (2008) 316-333.
- Slides 11-13: H. Pasman, A. Pekalski, I. Kirillov, “Self-ignition in gaseous mixtures, still a great challenge to understand,” ISHPMIE Conference, St.Petersburg, 2008.
- Slide 15: M. Pöschl and T. Sattelmayer, “Influence of temperature inhomogeneities on knocking combustion,” Combust. Flame 153 (2008) 562-573.

# The End

