Shell Global Solutions

Application of detailed kinetic models to ignition processes, limitations

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Scope

- Introduction: industrial need
- Autoignition Temperature (AIT) =
  Minimum Ignition Temperature (MIT),
  Self-ignition Temperature (SIT),
- Minimum Ignition Energy (MIE)
- Some results (theoretical, experimental) based on EU project (Safekinex) and past work at Delft University of Technology
- Conclusions

Explosion prevention thus

Some of important explosion sensitivity indices are

Auto-ignition Temperature (AIT),

Determination modes: Shock tubes, Rapid compression machines, Constant volume bombs

Practical challenges τ, mixing, h

Minimum Ignition Energy (MIE)

Ample evidence these indices are affected e.g. by:

•Pressure ↑	AIT ↓	MIE ↓
•Temperature ↑	AIT NA	MIE ↓
•Heat loss ↑	AIT ↑	MIE ↑

(turbulence, apparatus conditions)

Can one relay on ambient conditions data?

Current status

Determination practice

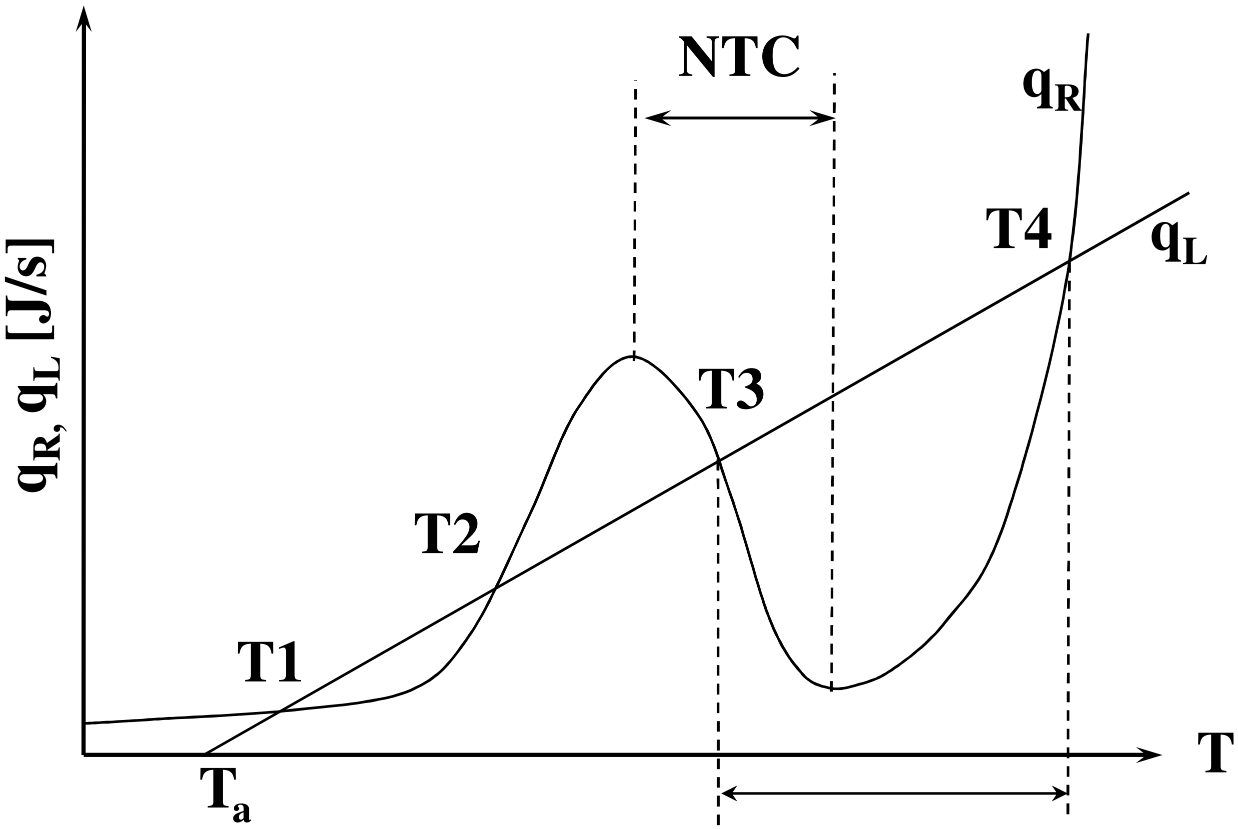
Standards exist for

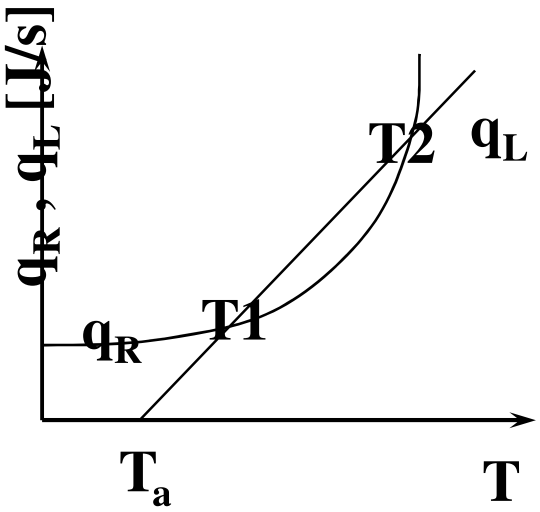
AIT, constant volume bomb only, ambient pressure

MIE, ambient pressure and temperature

Is that sufficient? !

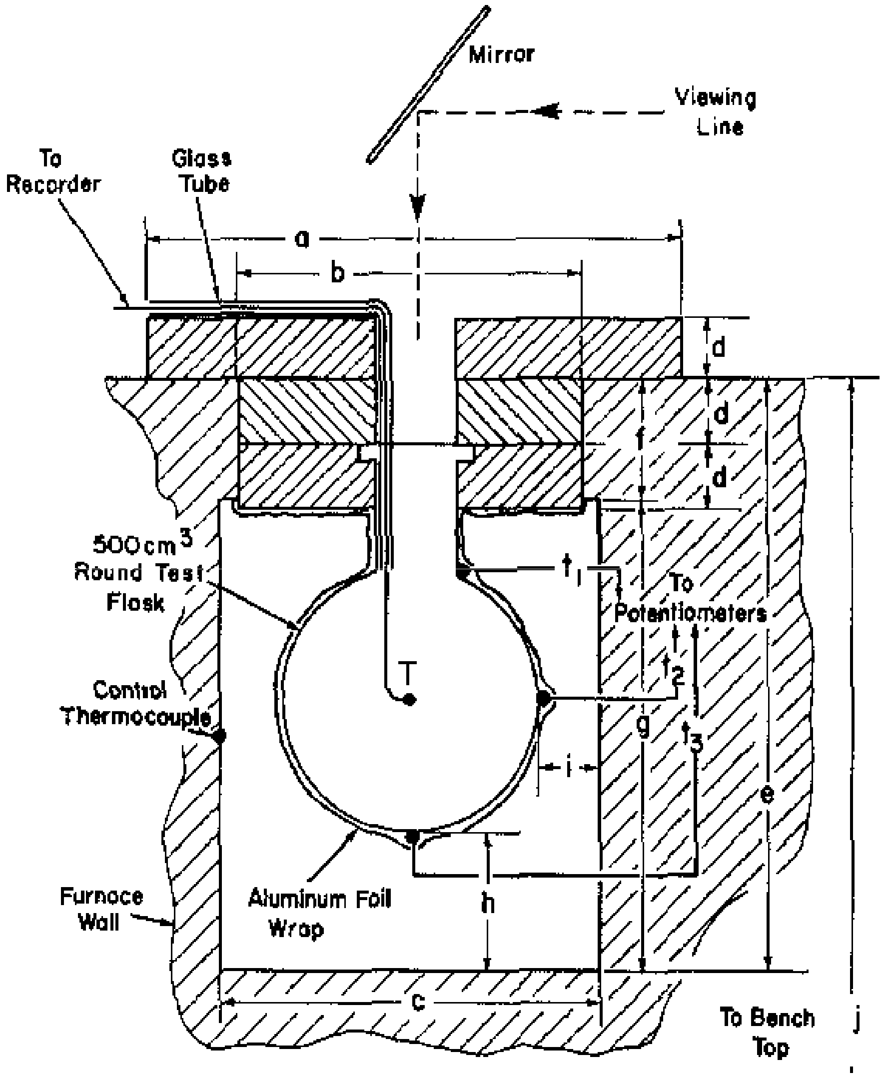
Inherent problem with AIT: heat loss





Extra safety margin ?

AIT Constant Volume Bomb ASTM E 659 – 78 (2005)

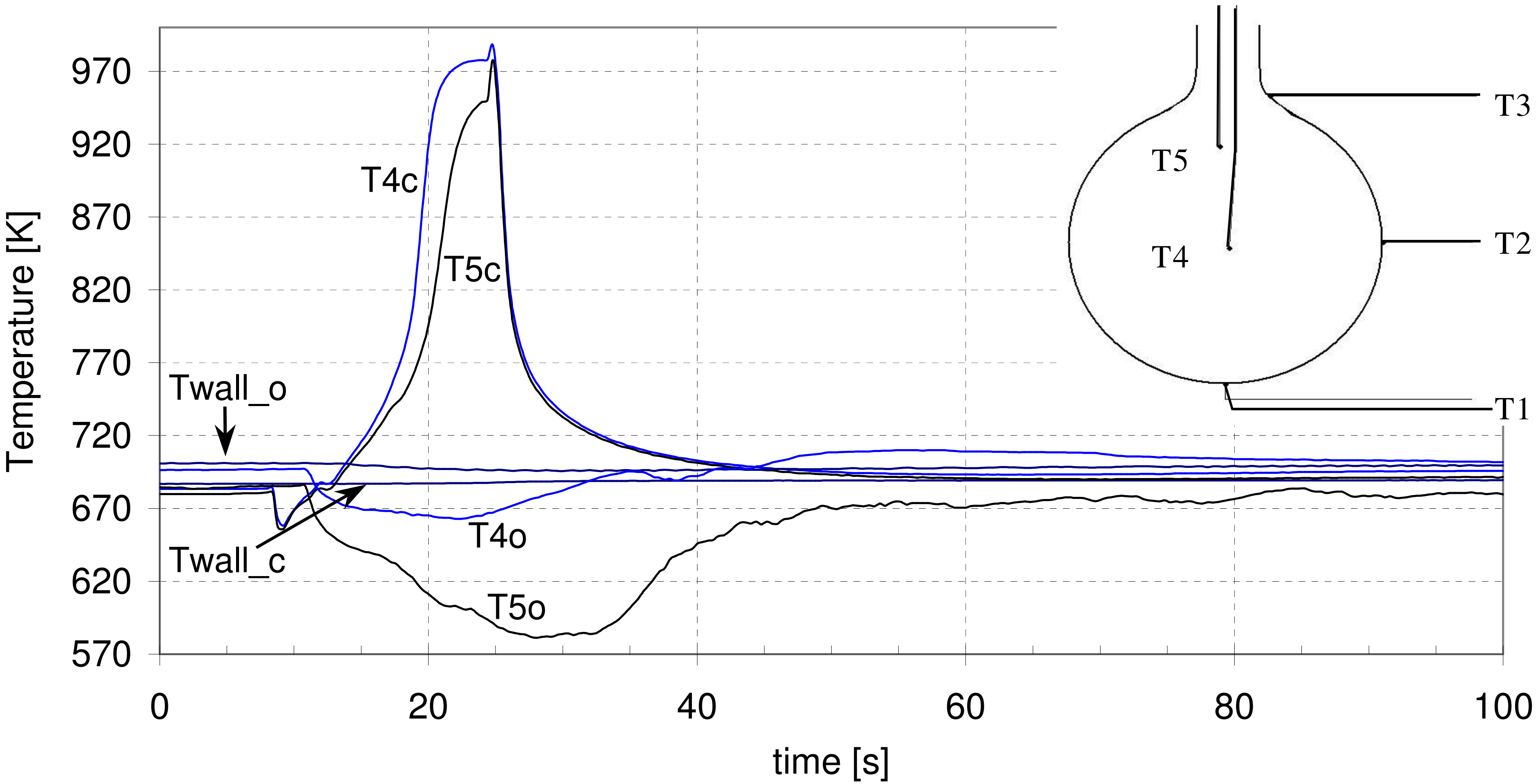


- Atmospheric pressure
- T max approximately 600℃
- 500 ml borosilicate glass
- 10 minutes observation
- Liquid samples
- Open vessel
- Ignition appearance of a flame accompanied by a sharp T rise

heat loss

natural convection induced

Open-closed flask CH4-C2H4-O2 mixtures



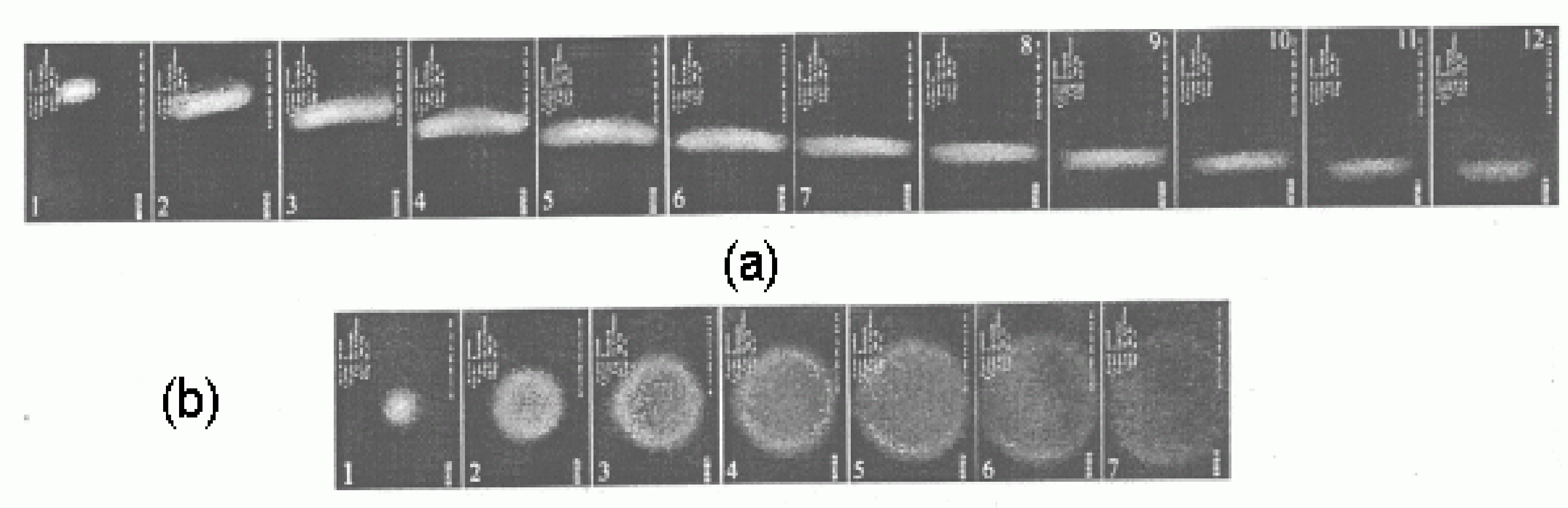
Clearly different combustion phenomena are observed depending on the closure mode of the vessel

Modes of heat transfer - Rayleigh Number (Ra)

$$Ra = g\beta r^3 C_p \rho^2 \Delta T / \lambda\eta$$

Ra < 600: conduction
600 < Ra < 10^4 : conduction and convection
Ra > 10^4 : convection

1g



(a)

~0g

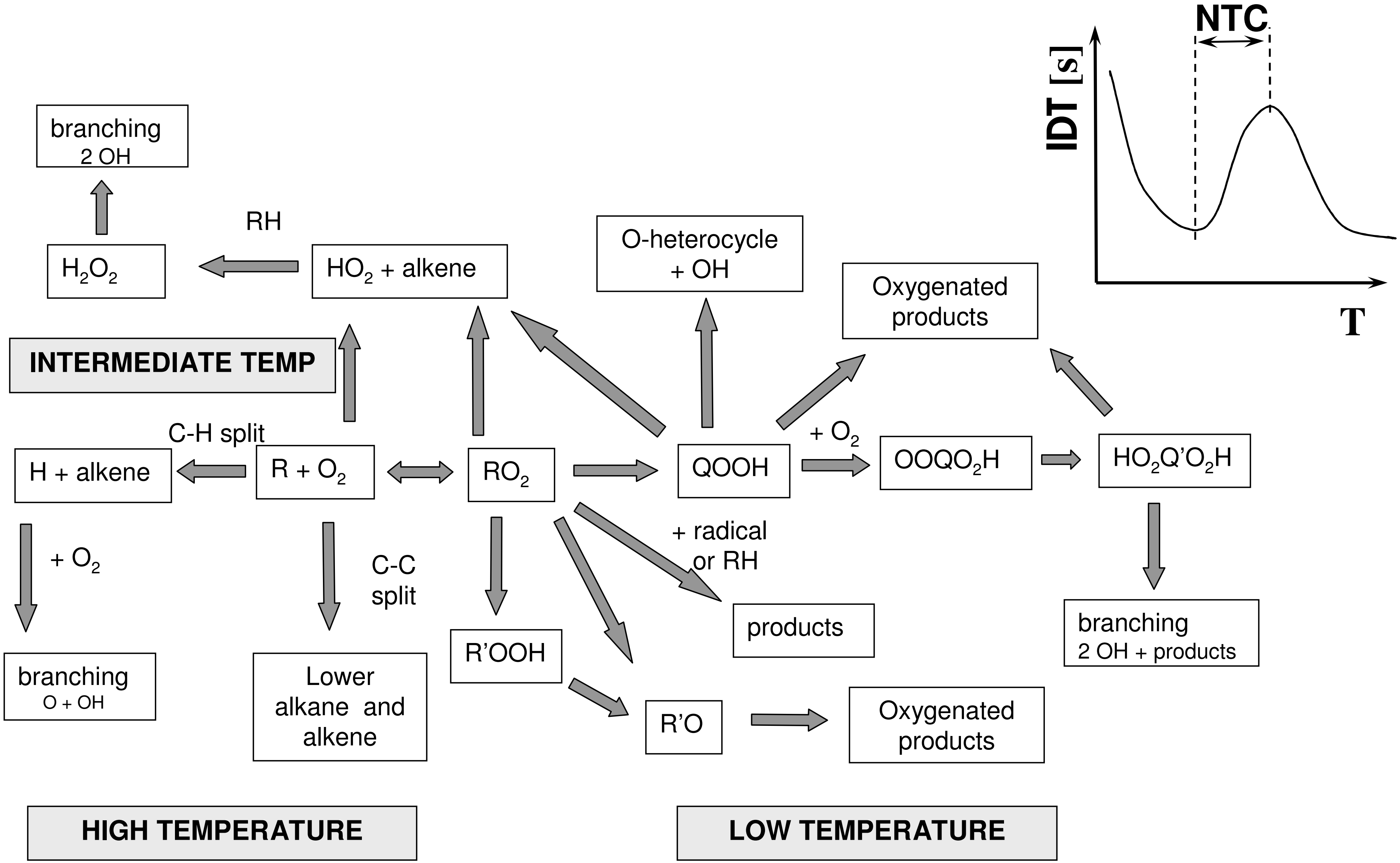
(b)

Natural convection assists laboratory SIT experiment: (1g) => importance assessment of timescales (chemical reaction, heat conduction, natural convection, heat diffusion del T) => complexity

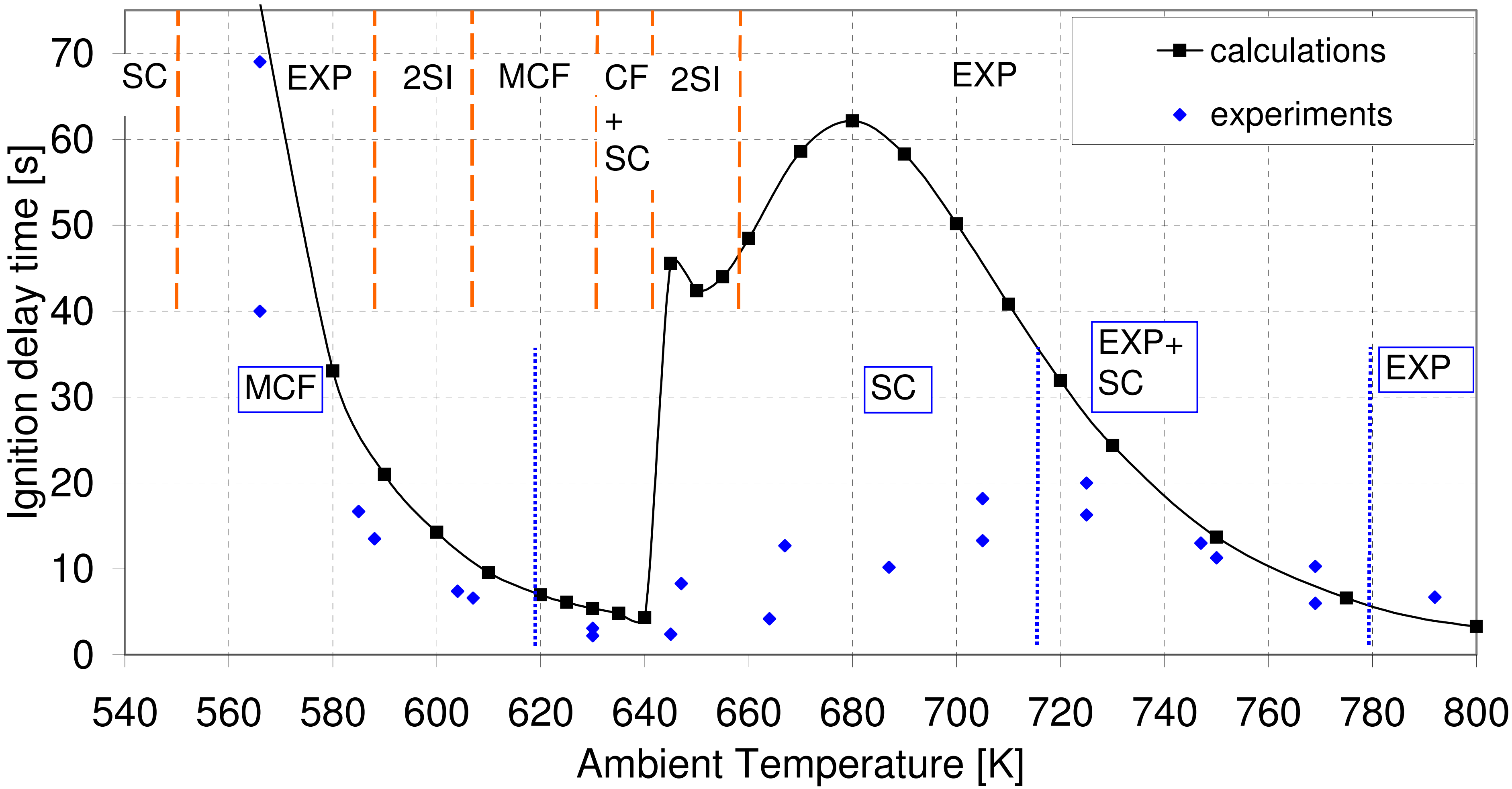
Work in progress

University of Cambridge under Dr S. Cardoso

Complexity of kinetic:Combustion kinetics with respect to T



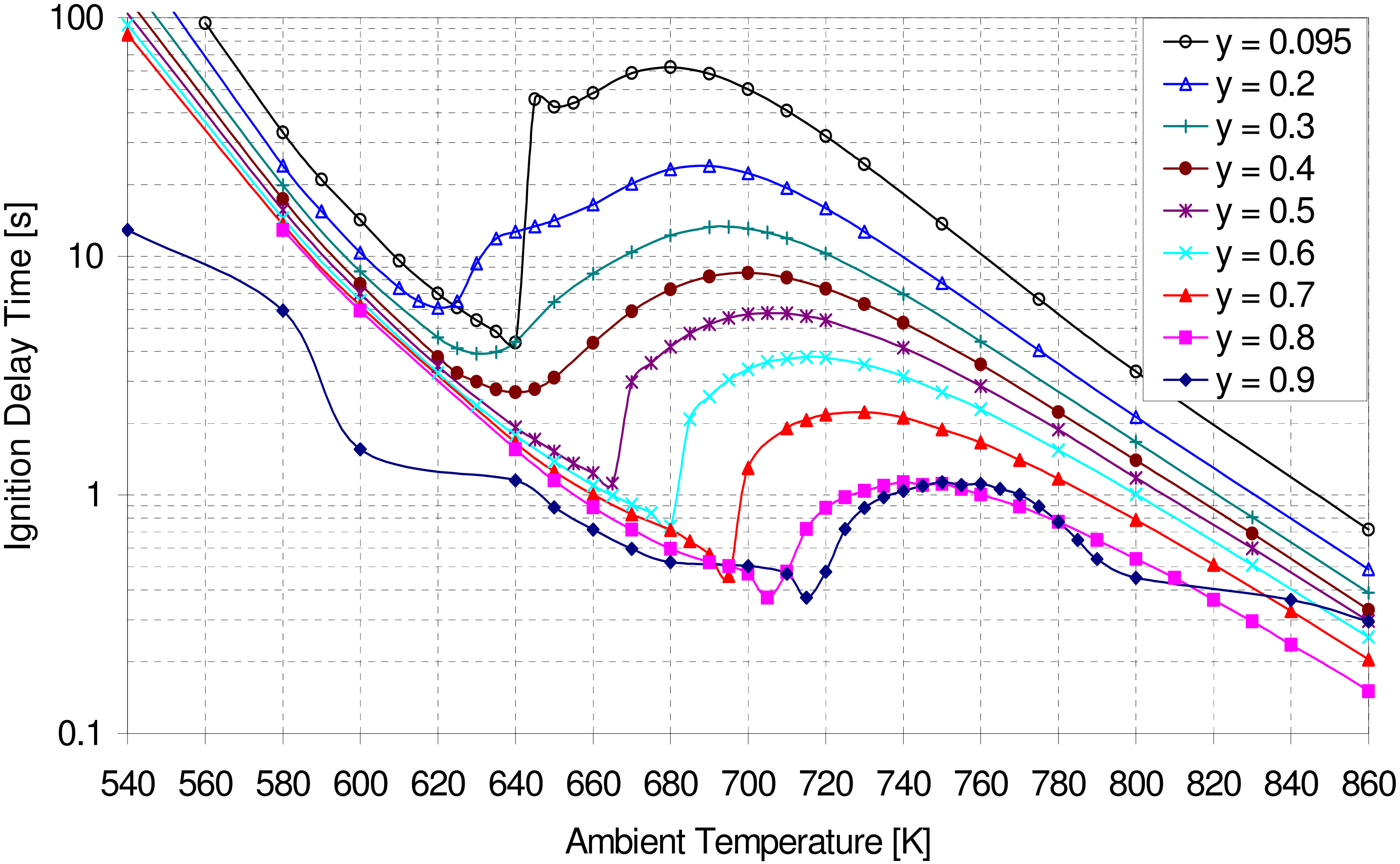
Comparison between experiments and numerical calculations; combustion phenomena



Difference in NTC => importance of interaction between physics and kinetic

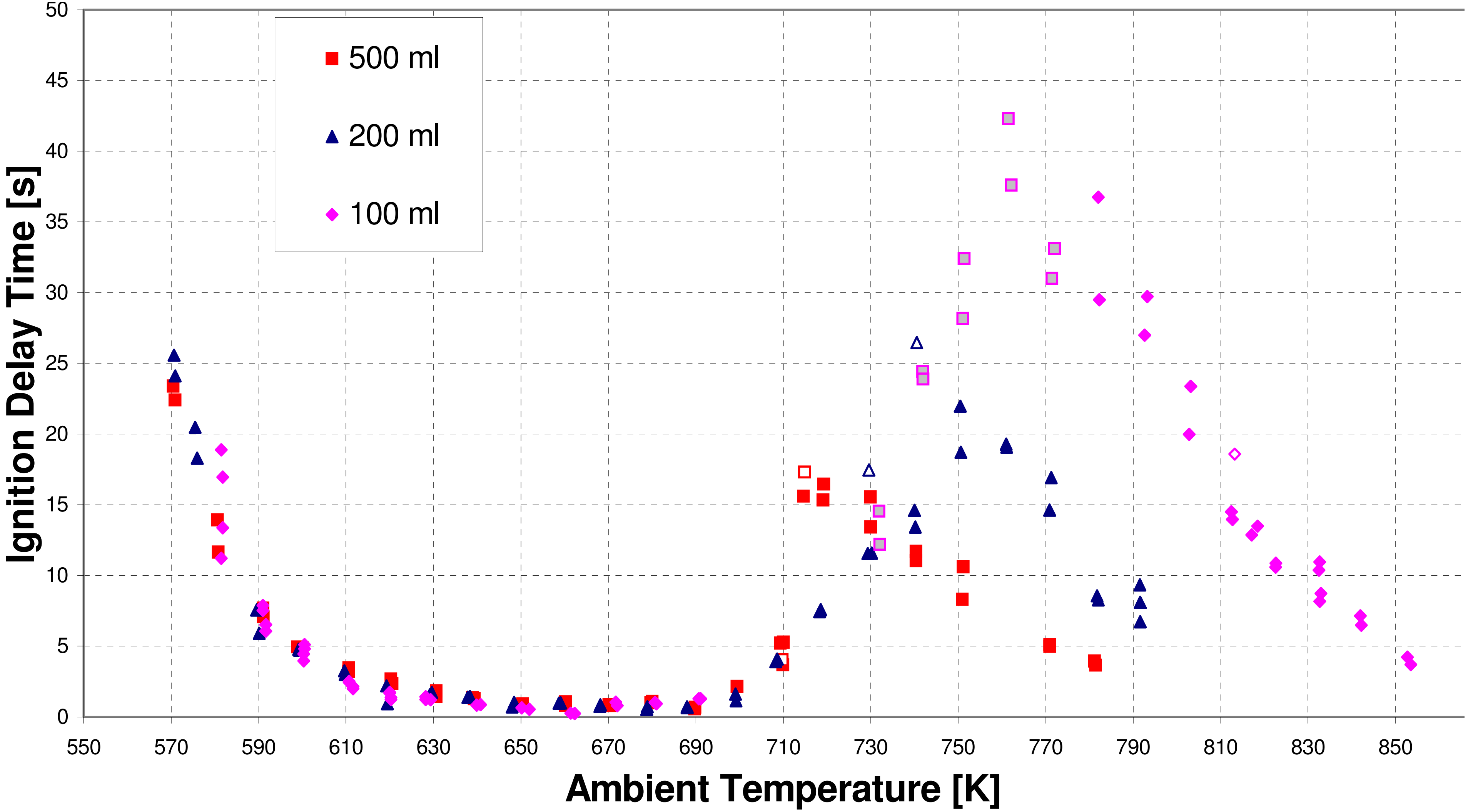
C4/air mechanism of CNRS Nancy

Effect of mixture composition on NTC



Logarithmic scale presentation of the negative temperature coefficient of various n-butane-air mixtures, P0= 1 bara, mole fraction of n-butane is in the legend, calculations.

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



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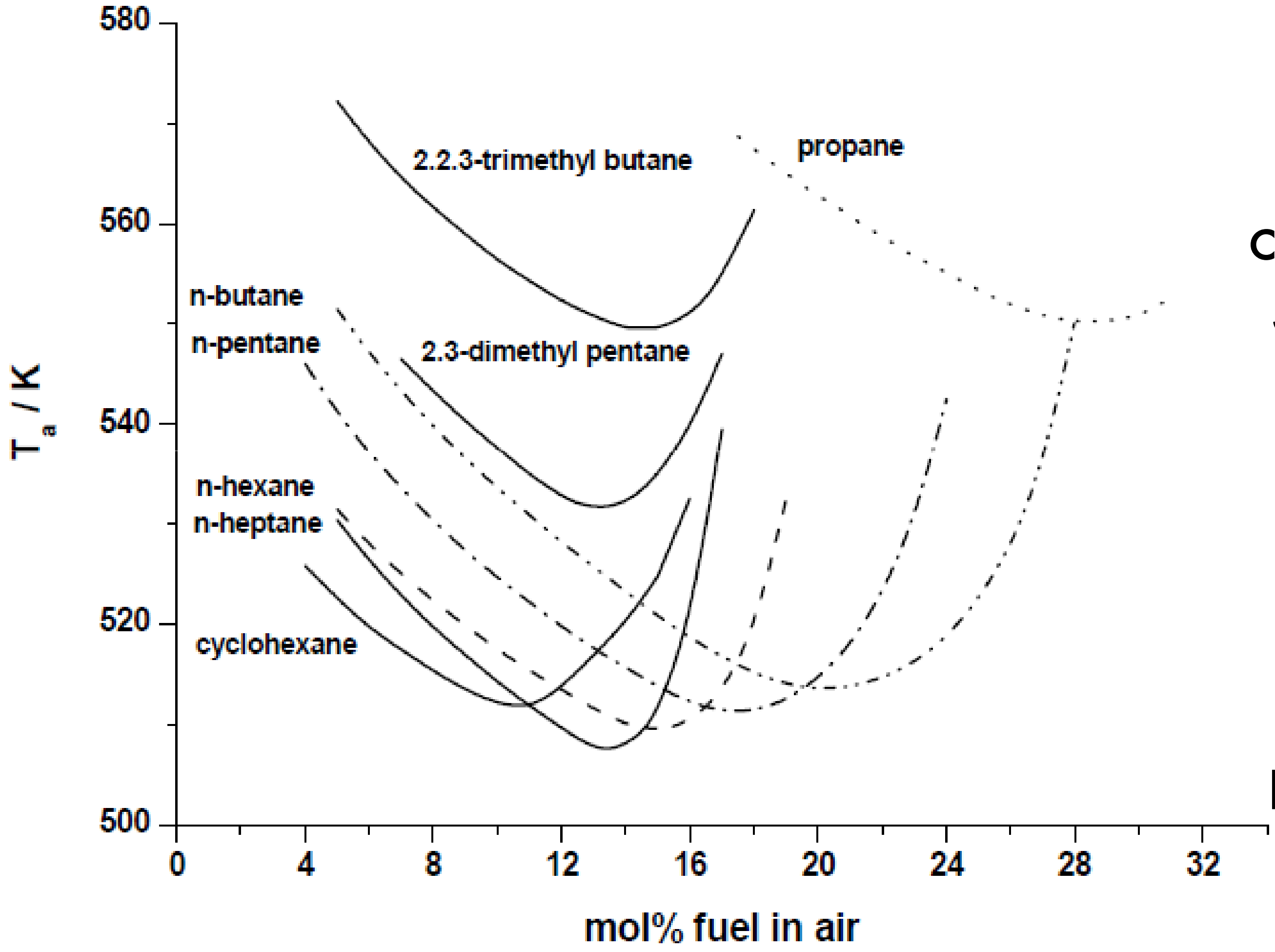
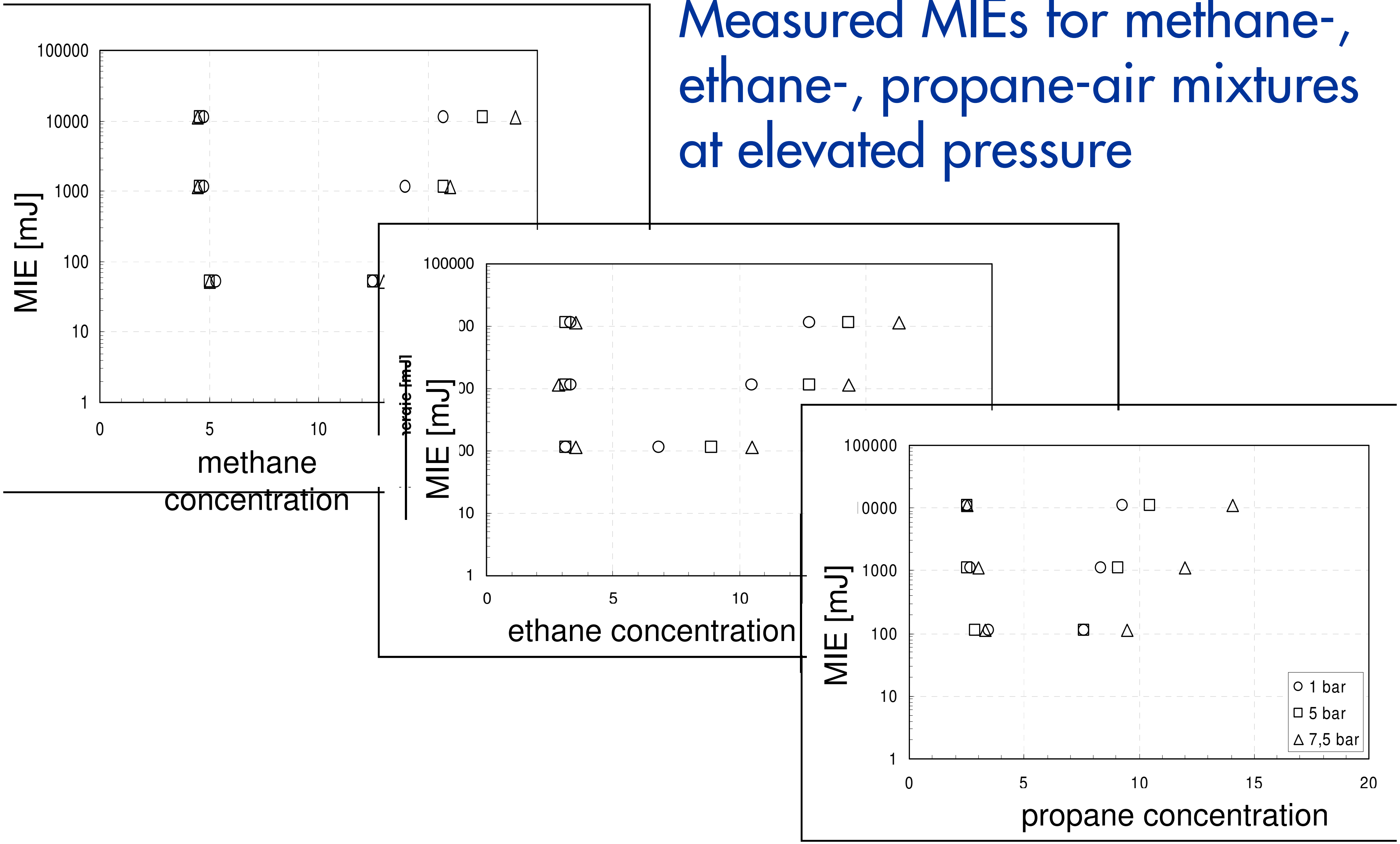


Theoretically calculated AIT and SIT using EXGAS input;

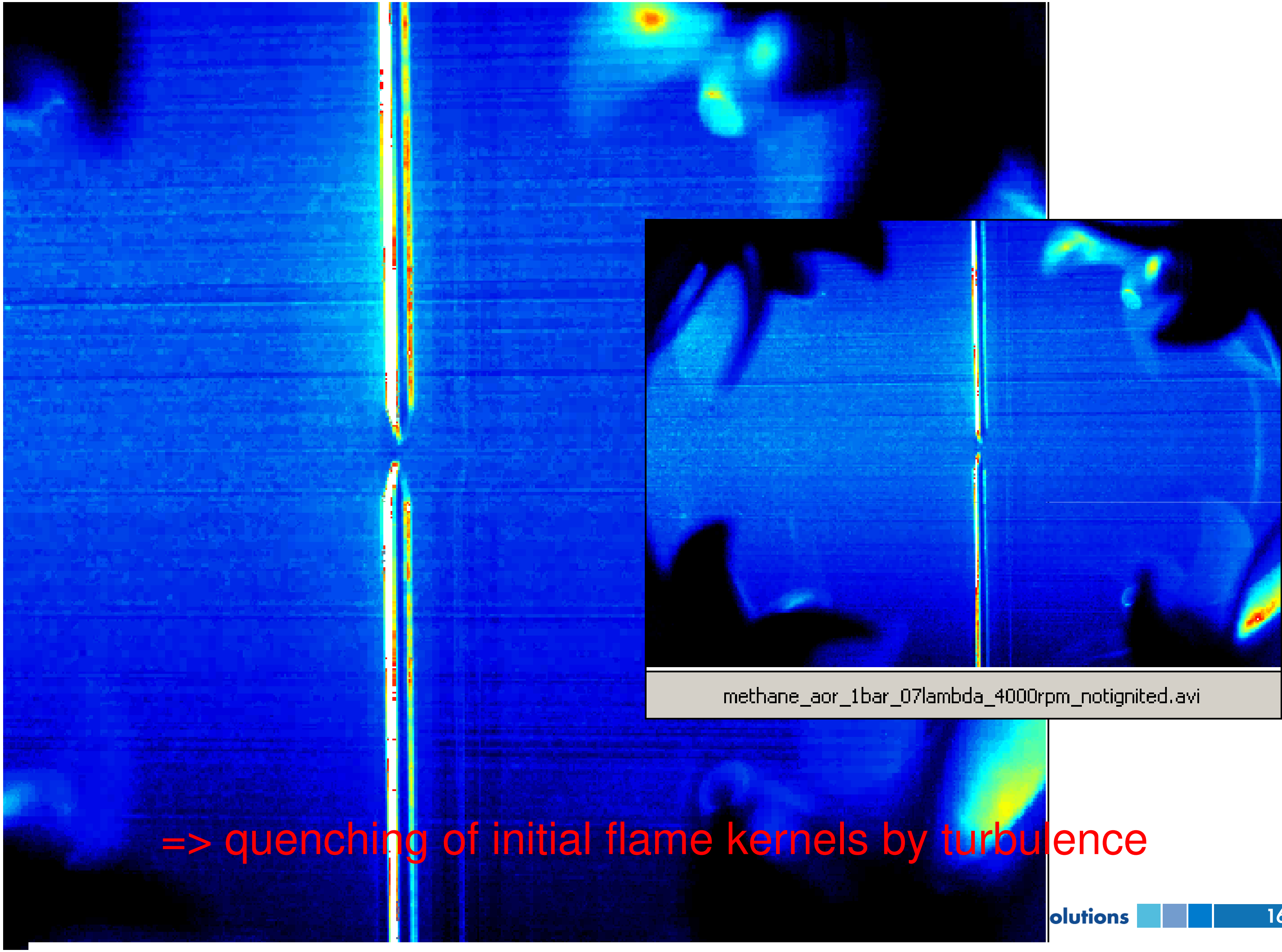
Source: Safekinex
Del. 38
Leeds University
Prof M. Fairweather
Prof J. Griffiths at al.

Minimun Ignition Energy

Measured MIEs for methane-, ethane-, propane-air mixtures at elevated pressure



Source: Universtiy Karlsruhe, Germany, dr **Max Weiß, Prof. N. Zarzalis**



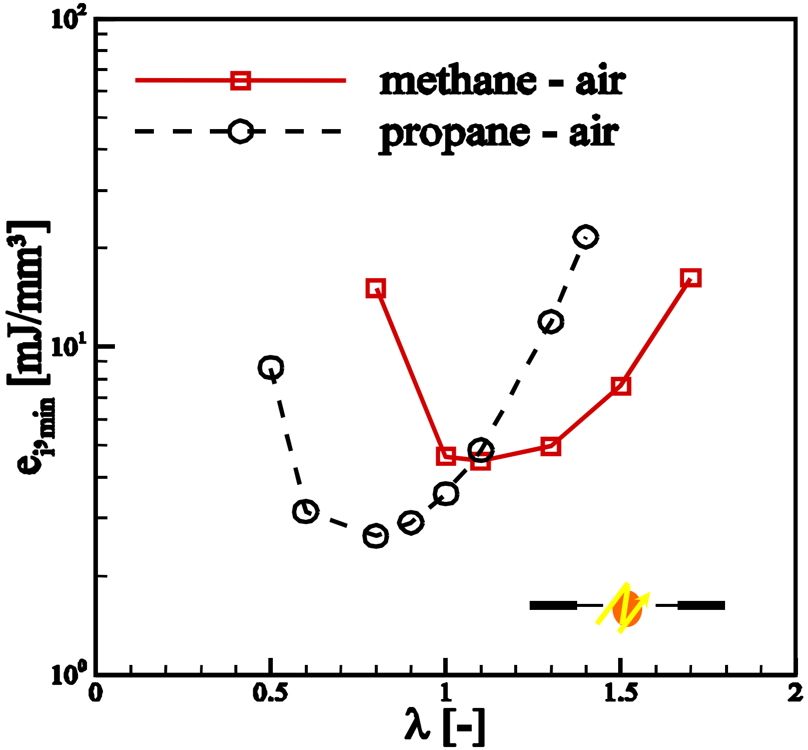
=> quenching of initial flame kernels by turbulence

Source: Universtiy Karlsruhe, Germany, dr **Max Weiß, Prof. N. Zarzalis**

Simulation Tool: INSFLA and COSILAB:

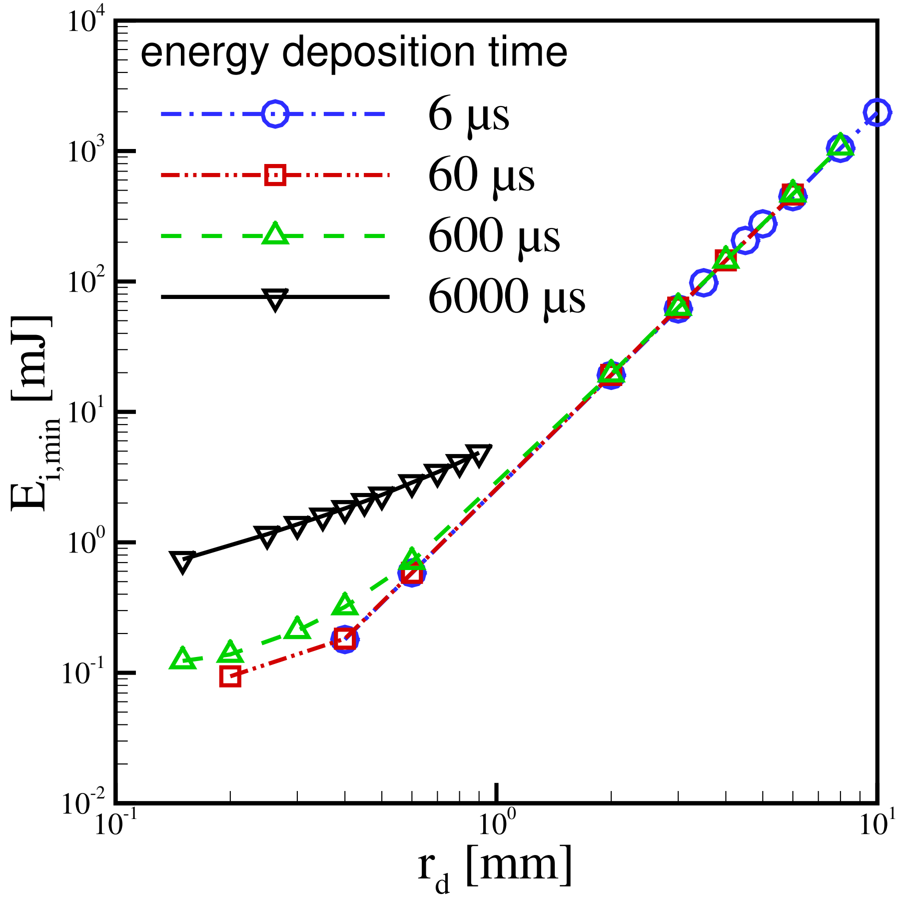
- one-dimensional
- solving unstead flames
- detailed kinetic scheme (HTOM)

Minimum ignition energy



Simulated MIEs for methane- and propane-air mixtures at atmospheric conditions

Influence of energy deposition time and radius on the MIE



energy deposition radius

Source: Universtiy Karlsruhe, Germany, dr **Max Weiß, Prof. N. Zarzalis**

Conclusions

1. Self-ignition phenomena in complex (realistic) conditions.
2. Measurement of AIT, MIE at elevated (process) conditions is a challenge
3. Better understanding
4. Good resolution on kinetic scheme or flow.

Thank you for your attention

Questions ?