Laminar burning velocity correlation for H_2 ICE modeling

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H_2 ICE session

Problem

- Support H_2 ICE development through modeling
- Modeling turbulent combustion of H_2 requires data on laminar burning velocity u_l
- u_l: propagation speed of planar flame front in a premixed, quiescent mixture
- Literature:
  - insufficient data on H_2/air
  - hardly any engine-like conditions
  - no data on effect of residuals (EGR!)
  - limited data taking account of stretch effects

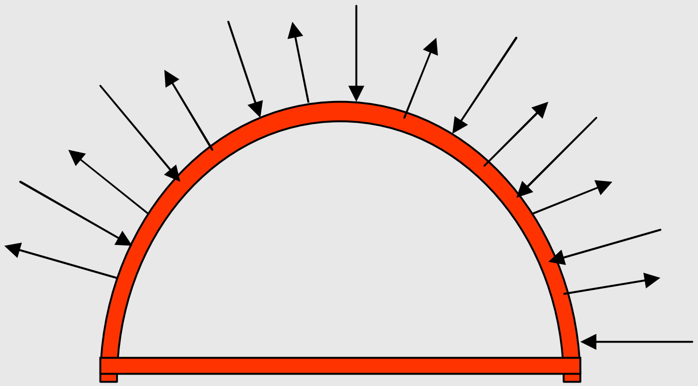
Solution?

- Calculation of u_l with 1D chemical kinetics code. Straightforward? Unfortunately not:
  - Reaction mechanism OK at atmospheric, severe doubts at high p and T
  - Calculations seem to break down for lean mixtures and elevated p
  - Limited use (e.g. effect of residuals)
- Measurement of u_l
  - At engine-like conditions
  - Taking account of stretch effects
  - However: experimental difficulties…

Stretch

Stretch: affects the balance between diffusion of unburned gas to the flame front and heating of the unburned by the flame front

Heat flux from flame front to unburned, ~ D_T



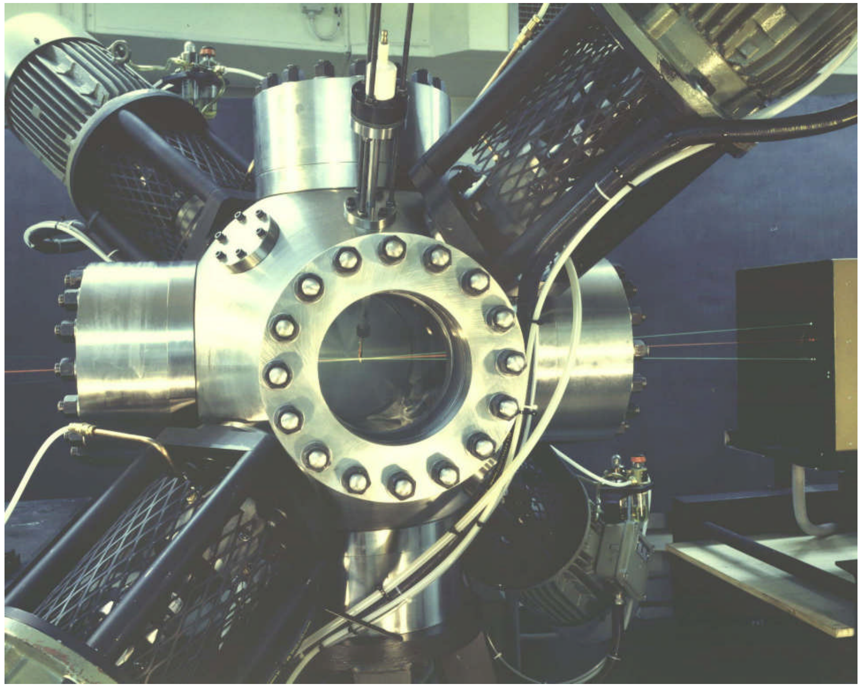
Mass diffusion of unburned to flamefront, ~ D_M

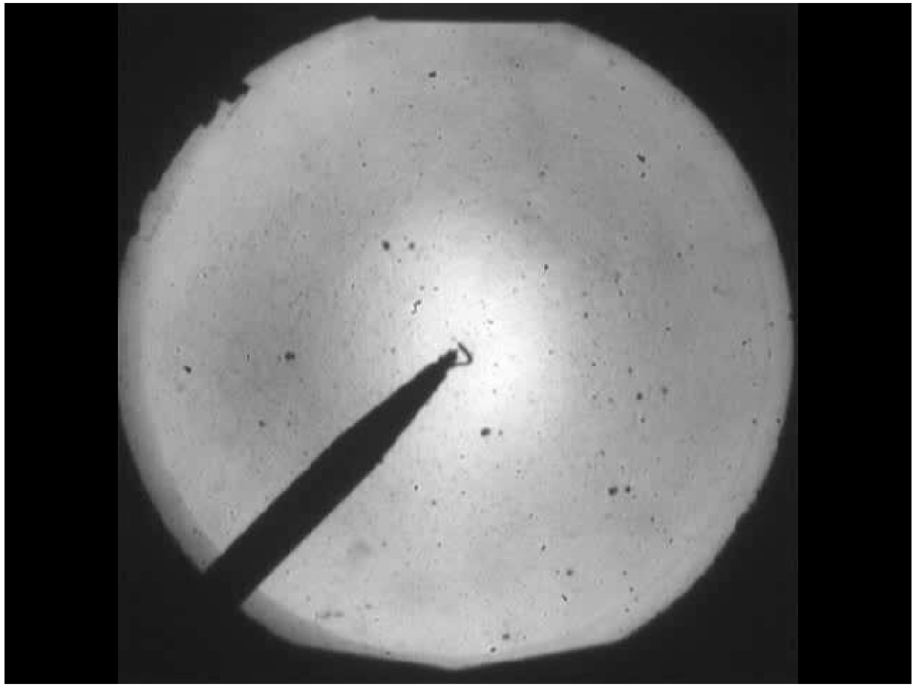
Thus: affects flame speed!

Any experimental set-up: deviation from steady, non-stretched planar geometry

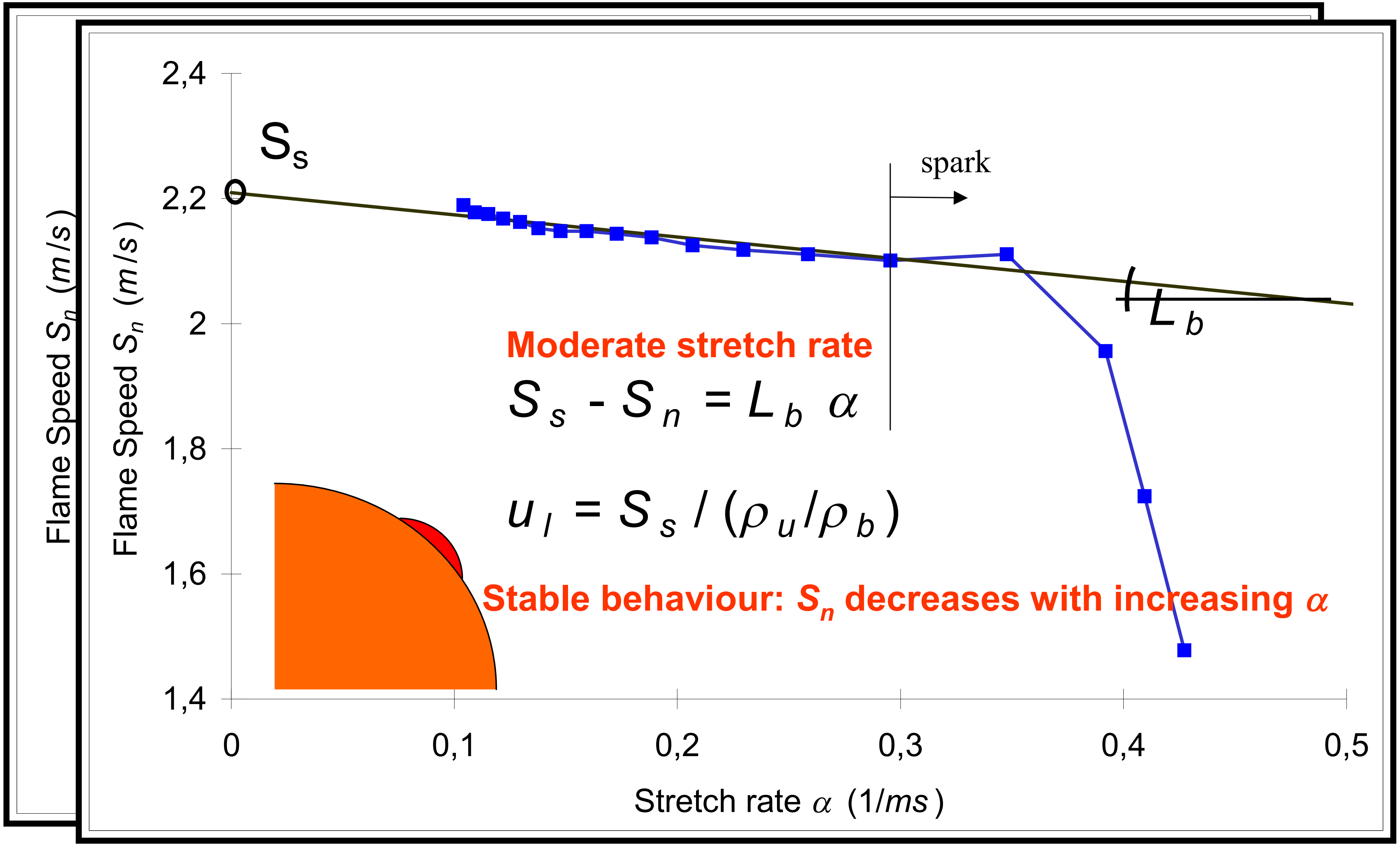
Stretch rate α=1/A dA/dt, relative change of flame area element

Measurement of u_l





CH_4/air, $\phi = 1$, 300 K, 1 bar



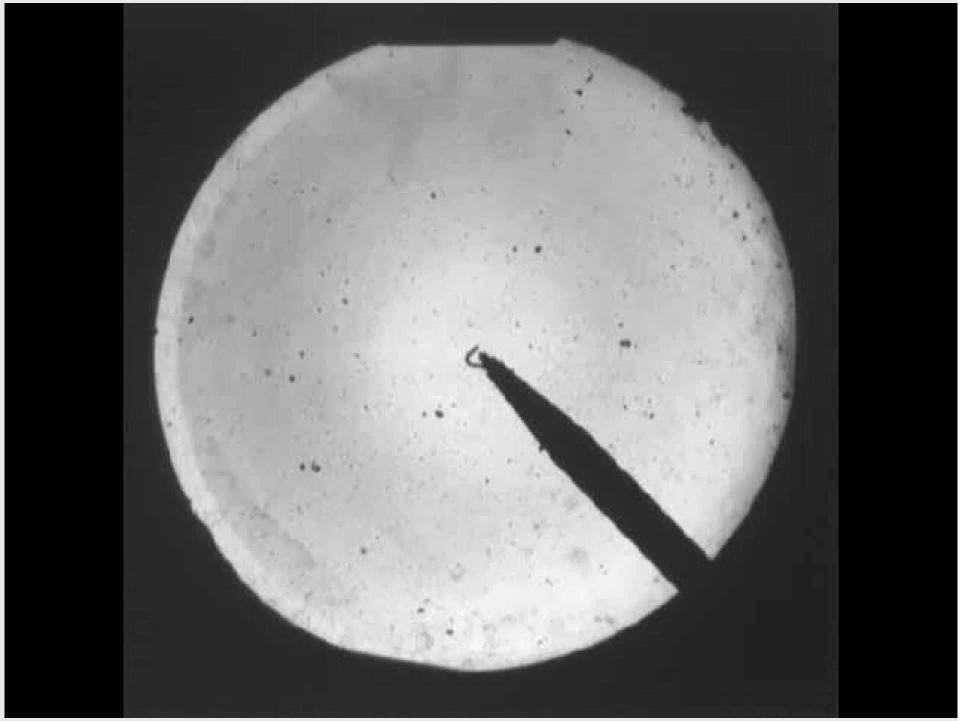
Stretch and instabilities

Dependent on mixture properties:

- flame is insensitive to flame stretch rate
- flame speed decreases for positive flame stretch (stable)
- flame speed increases for positive flame stretch (unstable)

Lean hydrogen mixture: unstable, develops cells and accelerates

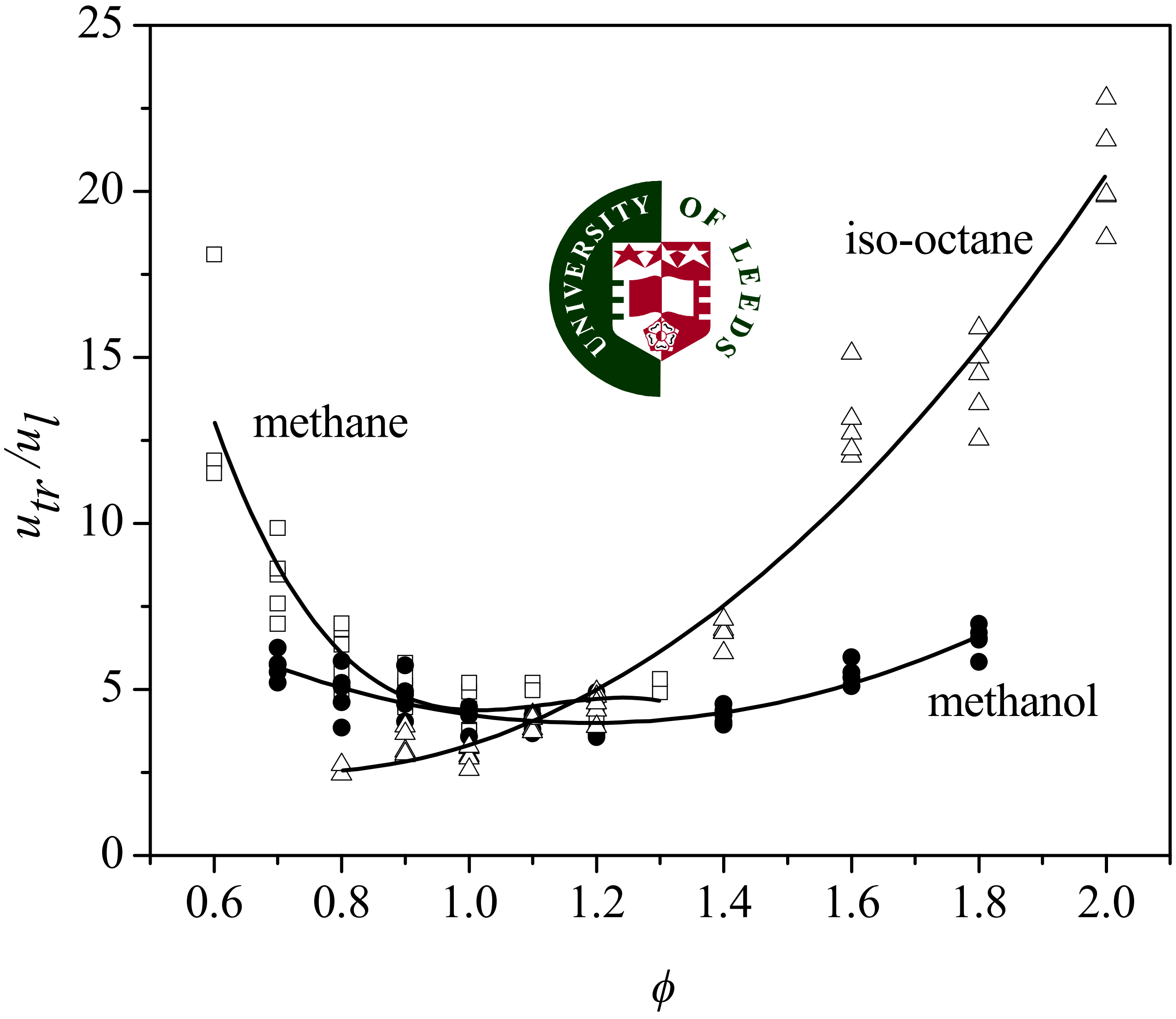
Flame observation: prerequisite to determining correct burning velocity!



Stretch and instabilities

Relevance to engine combustion:

- Flames get increasingly unstable for higher pressures
- Existing u_l correlations mostly pressure-derived, thus influenced by stretch! e.g. iso-octane/air correlations of Metghalchi&Keck
- It is very likely that for all practical fuel/air mixtures, the laminar flames are unstable at engine conditions
- But: a number of turbulent combustion models assume the turbulent motion 'erases' the flame instabilities, so that these have no effect on the turbulent burning velocity
- Others assume the effect of instabilities is only important at low u' / u_l



Lawes, Ormsby, Sheppard, Woolley, CS&T 177:1273-1289

Database u_l H_2 mixtures

Measurements of H2/air/residuals u_l's at:

- 300, 365 and 430 K
- 1, 5 and 10 bar
- Residual concentrations up to 30 vol%
- Equivalence ratios ϕ between 0.25 and 1.0

However, at 5 and 10 bar: no u_l's!

Methodology: use of $u_{n,10mm}$ to determine trends

- Indication of burning velocity
- Fixed condition, repeatable
- 10 mm: compromise ignition – cellular acceleration
- Parallel work: stability analysis (see later)

u_l correlation for engine code

$$u_n = u_{n0}\left(\frac{T}{T_0}\right)^{\alpha_T}\left(\frac{p}{p_0}\right)^{\beta_p}\left(1-\gamma f\right)$$

- Based on measurements of cellular flames at elevated pressure
- Effects of residual gas: new, can be added to other correlations
- Compared with existing correlation (Iijima&Takeno, C&F1986) in engine code
  Result: nonphysical results with existing correlation, good results with ours

Refs: - PhD Verhelst, http://hdl.handle.net/1854/3378
- Verhelst, Woolley, Lawes, Sierens, 30th Comb Symp p209-216

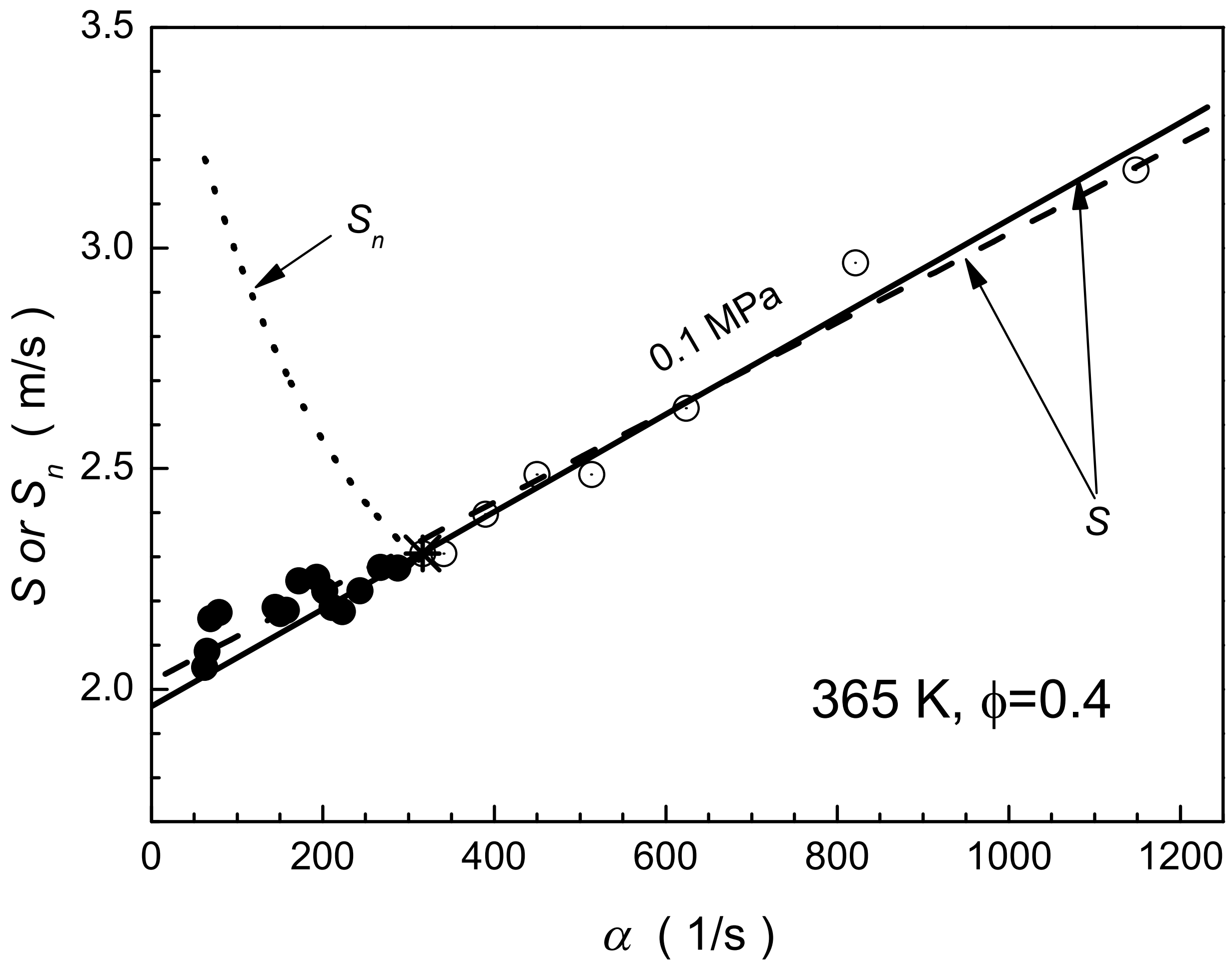
Extension

- Correlation is for stoichiometric to lean mixtures
- Current interest in H_2 DI engines: also data on rich mixtures needed
- Correlation was extended by IFP in the framework of the EU HyICE programme
  - Used by BMW and IFP

Refs: Proceedings 1st Int Symp on H_2 ICEs
- Gerke, Boulouchos, Wimmer p94-106
- Benkenida, Colin, Jay, Knop p195-206

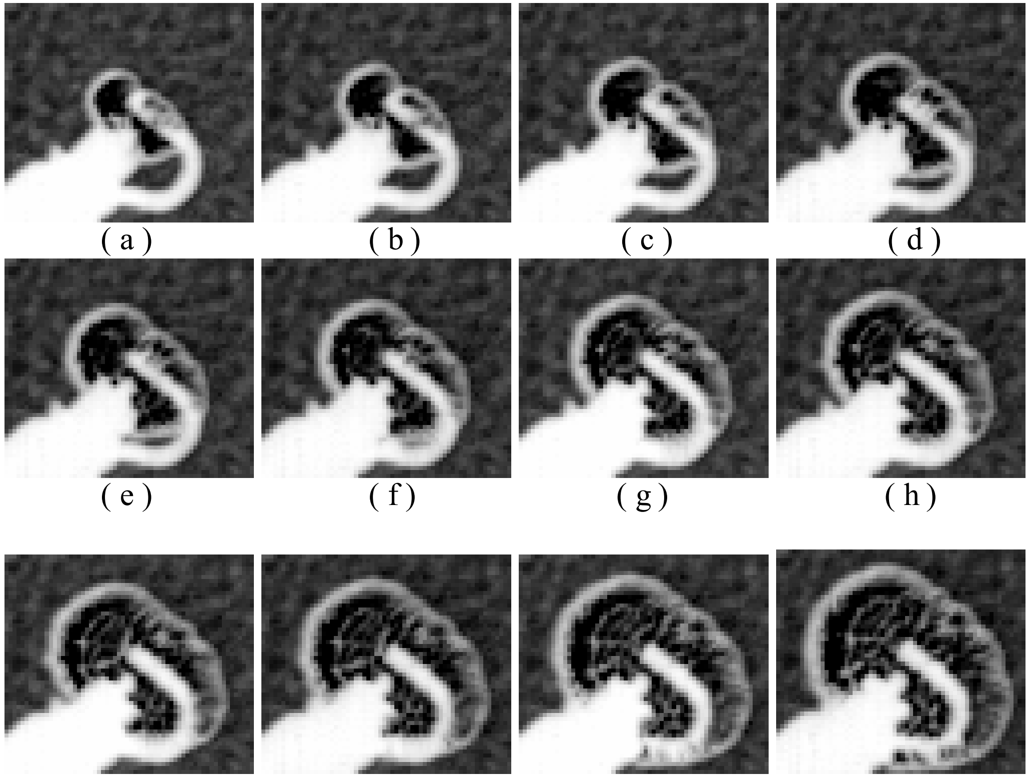
Stability analysis

- Ideally: $u_n = I_0\ u_l$ in engine code, I_0: stretch model
  However: currently impossible, u_l? I_0?
- Cellularity = ordered, reproducable
  - Use fractal considerations to determine surface of smooth flame from surface of cellular flame, ratio of flame speeds of cellular flame to 'smooth' flame equals ratio of flame areas
  - Determine inner and outer cutoff scales from range of wavelengths inducing instability
    Inner cutoff: given by start of cellularity
    Outer cutoff: flame size



Bradley, Lawes, Liu, Verhelst, Woolley, C&F 149:162-172

Experimental difficulties keep haunting us…



(a) (b) (c) (d)

(e) (f) (g) (h)

(i) (j) (k) (l)

p=0.5 MPa, T=365 K, ϕ=0.6, time interval 0.04 ms (25000 fps)

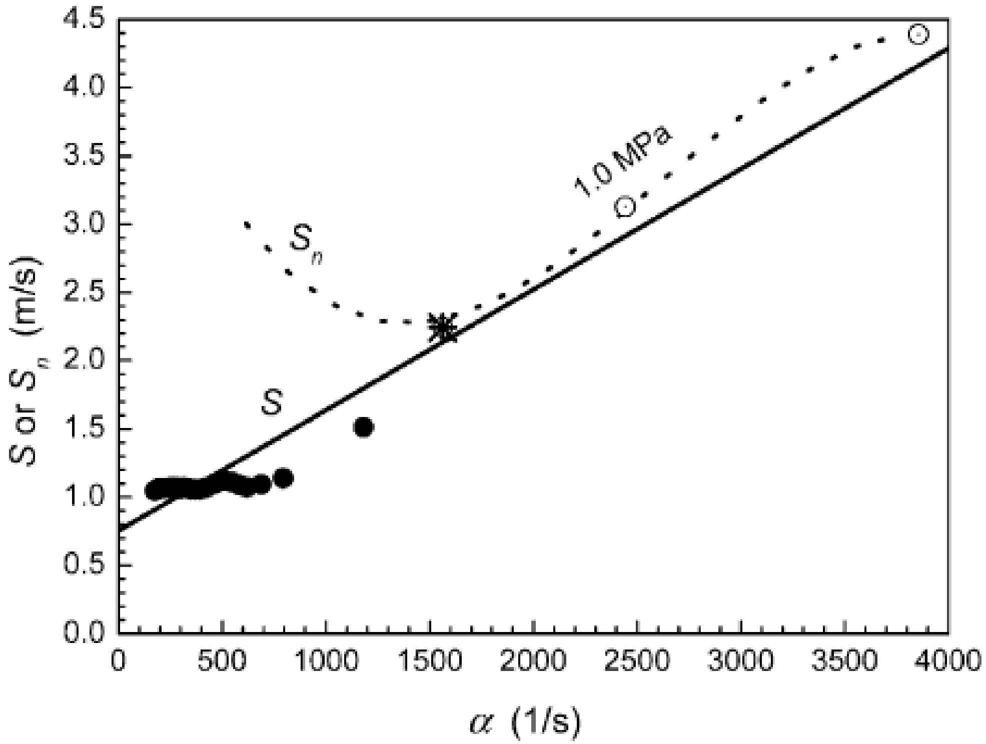
Bradley, Lawes, Liu, Verhelst, Woolley, C&F 149:162-172

Experimental difficulties

- Implications primarily for determination of Markstein numbers:

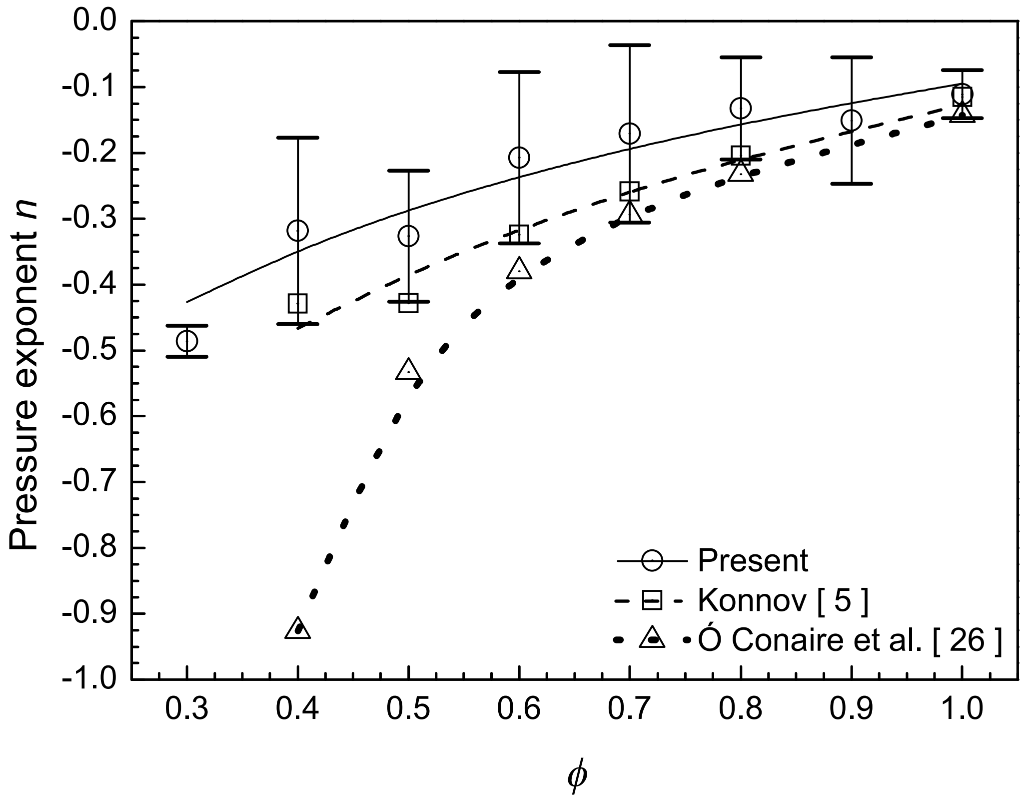
$$\frac{u_l - u_{nr}}{u_l} = K_s Ma_{sr} + K_c Ma_{cr}$$

- Large uncertainties on Markstein numbers
- l_0 model would require data on Ma
- High p: determination u_l also problematic



Encouraging results

- Pressure exponent
  $u_l \sim p^n$



- Uncertainty on kinetics:

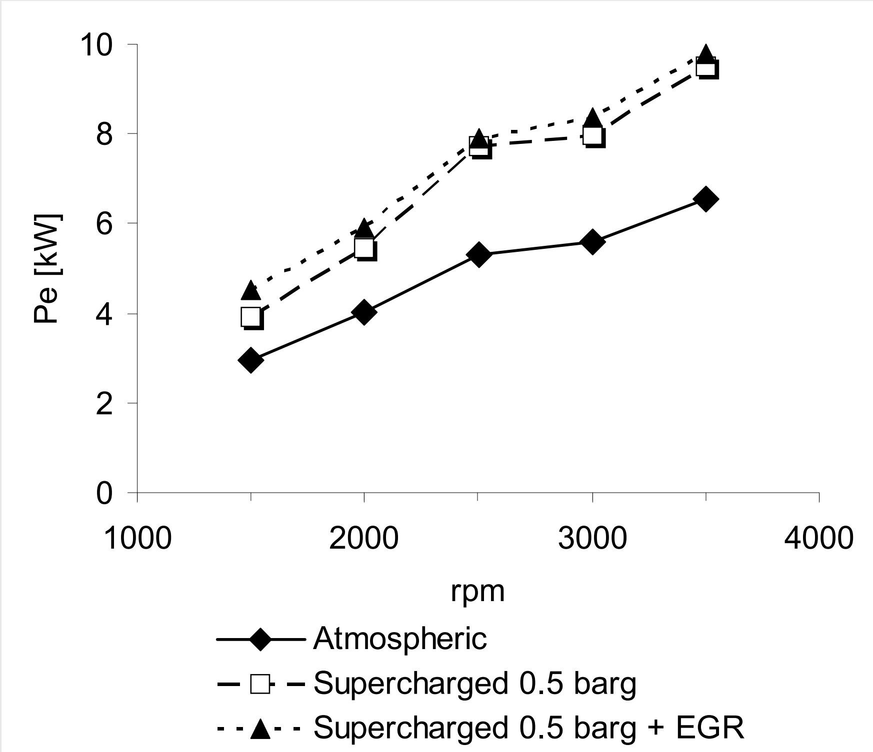
$$H + O_2 \rightarrow OH + O.$$

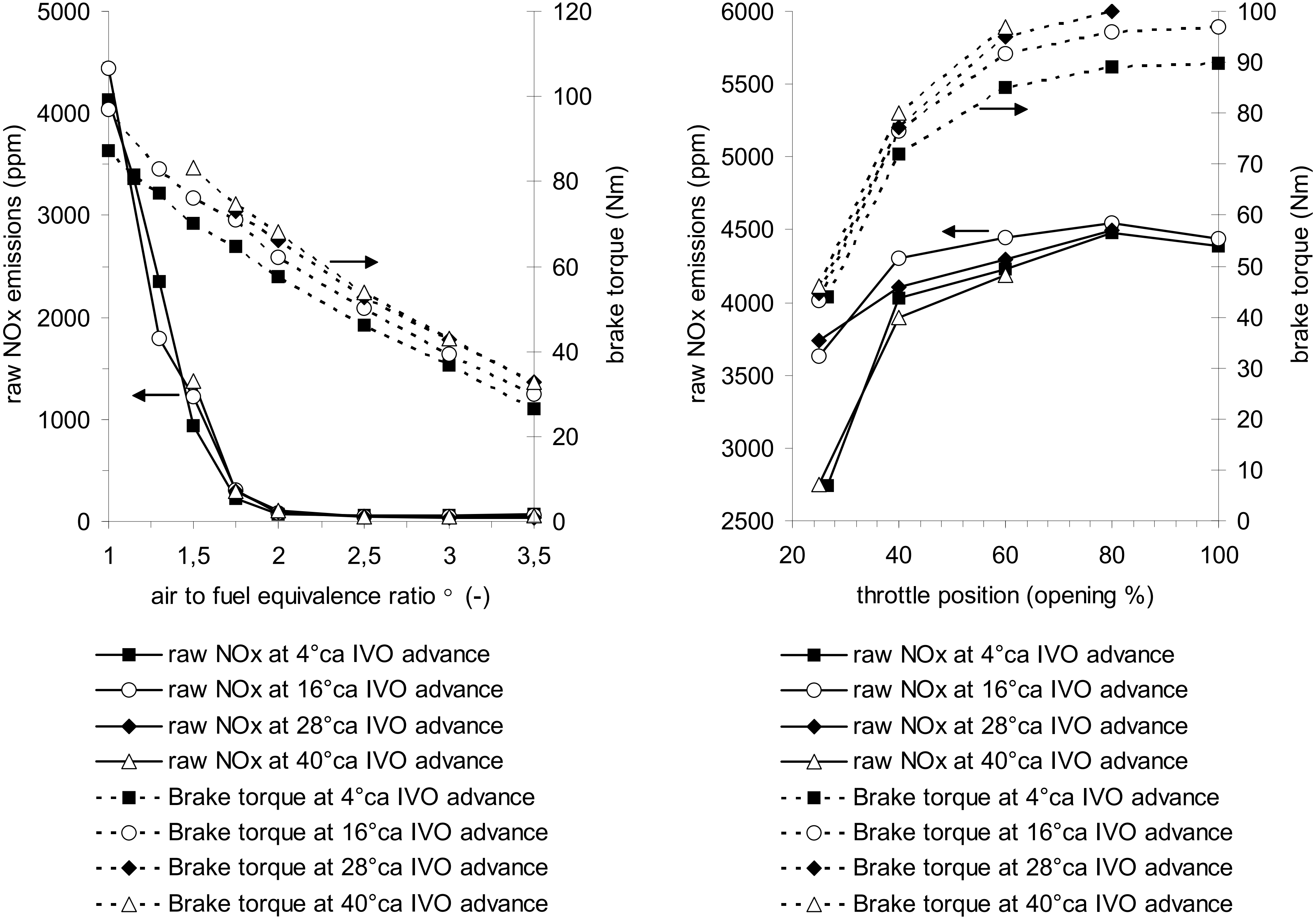
Rate constant	Pressure		
	0.1 MPa	0.5 MPa	1.0 MPa
$k_2/1.6$	2.63 m/s	2.19 m/s	
k_2	2.87 m/s	2.52 m/s	2.16 m/s
$1.6k_2$	3.04 m/s	2.79 m/s	2.46 m/s

C&F 149:162-172

Other work

- Numerical: H_2 ICE code (quasi-dimensional) – see PhD
- Experimental
  - Supercharging+EGR on single cylinder engine
  - Variable valve timing on four cylinder engine
  - SAE World 2008 paper





5000
4000
3000
2000
1000
0
raw NOx emissions (ppm)
120
100
80
60
40
20
0
brake torque (Nm)
1
1,5
2
2,5
3
3,5
air to fuel equivalence ratio ° (-)
raw NOx at 4°ca IVO advance
raw NOx at 16°ca IVO advance
raw NOx at 28°ca IVO advance
raw NOx at 40°ca IVO advance
Brake torque at 4°ca IVO advance
Brake torque at 16°ca IVO advance
Brake torque at 28°ca IVO advance
Brake torque at 40°ca IVO advance
6000
5500
5000
4500
4000
3500
3000
2500
raw NOx emissions (ppm)
100
90
80
70
60
50
40
30
20
10
0
brake torque (Nm)
20
40
60
80
100
throttle position (opening %)
raw NOx at 4°ca IVO advance
raw NOx at 16°ca IVO advance
raw NOx at 28°ca IVO advance
raw NOx at 40°ca IVO advance
Brake torque at 4°ca IVO advance
Brake torque at 16°ca IVO advance
Brake torque at 28°ca IVO advance
Brake torque at 40°ca IVO advance

Thank you!

Further information:

See www.FloHeaCom.UGent.be/H2

By the way: BMW Hydrogen 7 comes to Ghent University tomorrow at 2 pm!