Why the Lewis number seems to have an unexpected importance even in highly turbulent flames !

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with support from
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S.P.R. Muppala, Kingston University, London

Premixed Flame Workshop - Montreal - 09. August 2008

Flamelet-Ansatz für Vormischflammen

Flamelet-Idee:

- Gefaltete laminar-ähnliche Flamme
- Flamme beschrieben durch mittleren Reaktionsfortschritt $\overline{c}$

  $\overline{c}$ = Wahrscheinlichkeit, verbranntes Gas zu finden
- 1 Transportgleichung für mittleren Reaktionsfortschritt (statt *N* Speziesgleich.)

$$\frac{\partial}{\partial t}\left(\overline{\rho}\,\overline{c}\right)+\frac{\partial}{\partial x_i}\left(\overline{\rho}\,\overline{u}_i\overline{c}\right)=\frac{\partial}{\partial x_i}\left(\overline{\rho}\,\frac{\nu_t}{Sc}\,\frac{\partial\overline{c}}{\partial x_i}\right)+\overline{w}_c$$

- Reaktionsrate wie im laminaren Fall x Faltungsfaktor Σ

$$\overline{w}_c=\rho_u\,s_L\,I_0\,\Sigma$$

Korrektur (Flammenkrümmung)

Aber Modell für Σ nötig ...

Turbulent Flame Speed Closure (TFC) Modell

Ansatz: (Zimont, Lipatnikov, 1995)

$$\overline{w}_c = \rho_u s_L \; I_0 \; \Sigma$$

$$\hat{s}_T \cdot \left|\nabla \overline{c}\right|$$

Turbulente Brenngeschwindigkeit

Ort der Reaktionszone (statistisch gemittelt)

$$\hat{s}_T = f(\mathrm{Re}_t, u', s_L, \ldots)$$

Turbulenzeinfluss modelliert mit algebraischer Beziehung

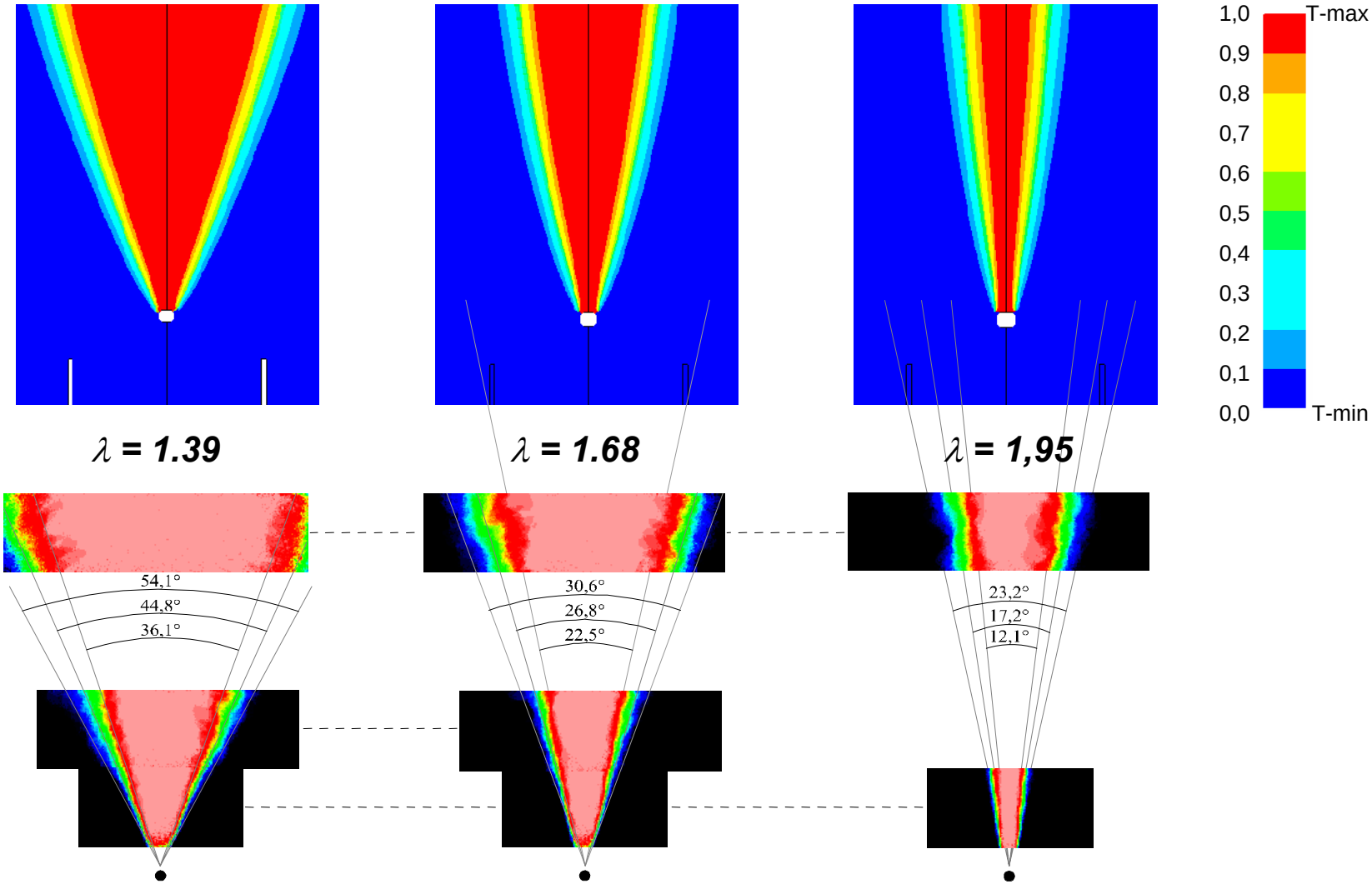
Lösung als Subroutine mit Standard-CFD-Programm (Fluent)

Testfall: V-Flame

Mittlere Temperatur

Simulation

(S. Hölzler)



Experiment

2-dim. Rayleigh-Thermometry (A. Soika)

$\dot{m} = 18$ kg/h

Dinkelacker, Hölzler, Comb. Sci. Techn. 158, 321 (2000)

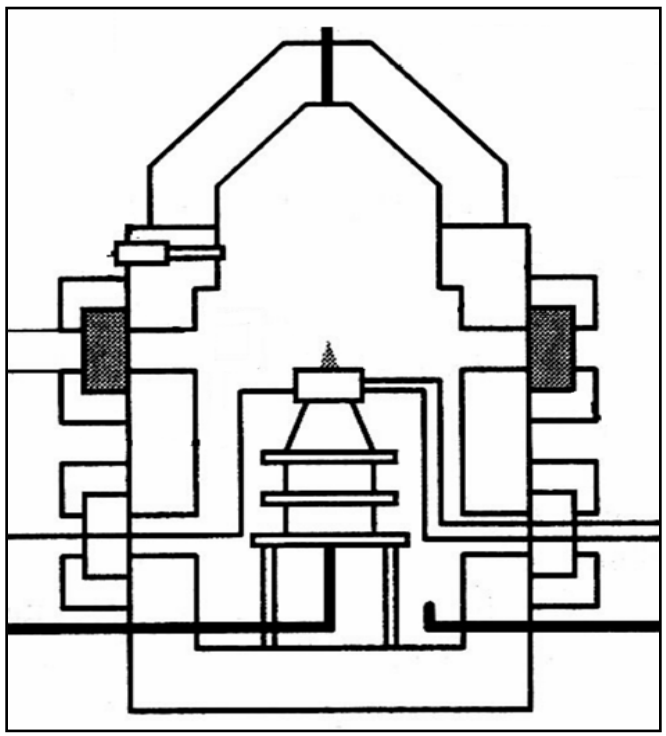
Test Data Series (Kobayashi)

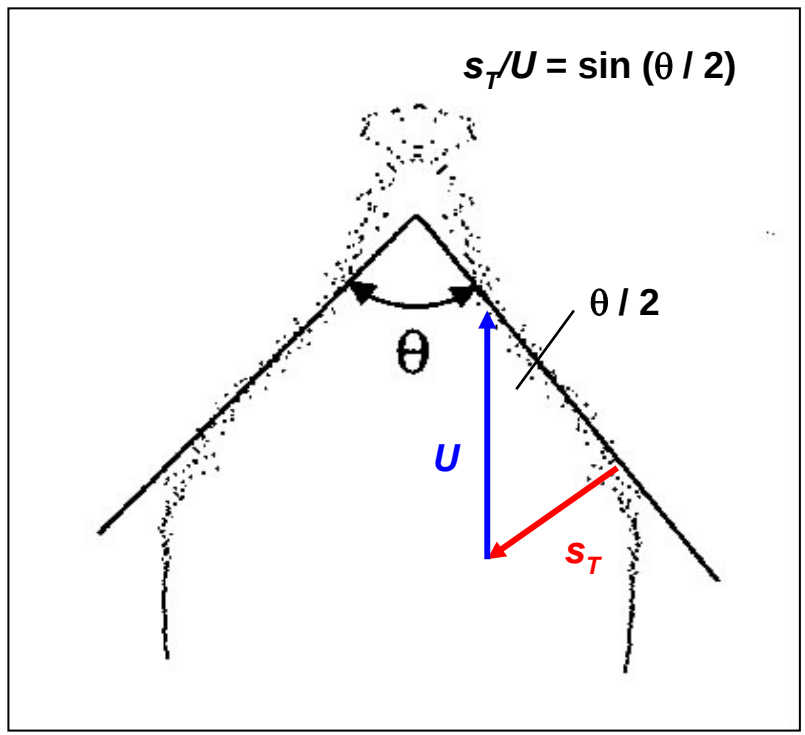
Bunsen Flame, Premixed

p = 1 - 10 (30) bar
D = 20 mm
U = 2 ... 4.6 m/s
Re = 2 500 ... 50 000
u', l_x measured (centre of inlet)

Methane/Air	Φ	= 0.9
Ethylene/Air	Φ	= 0.5, 0.7, 0.9
Propane/Air	Φ	= 0.9

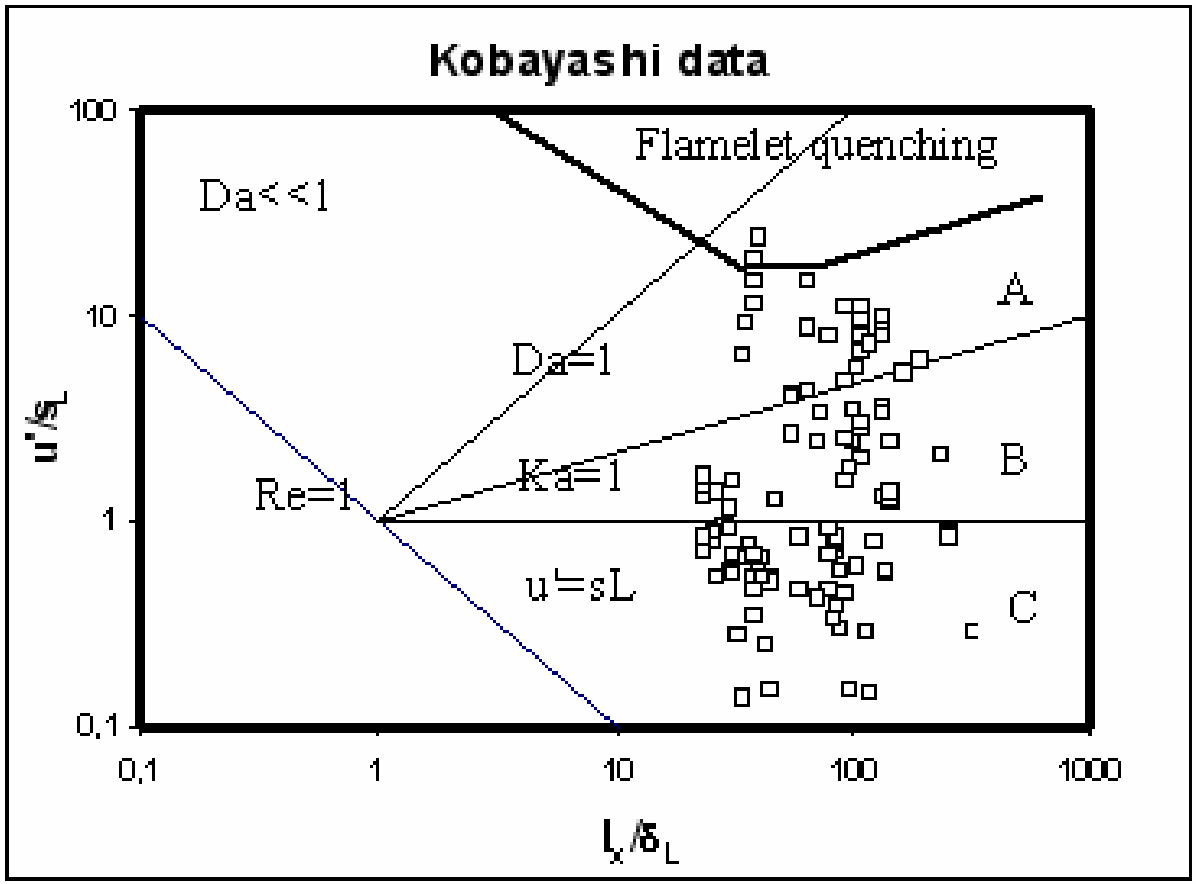
Data of 101 different flames





Test Data Series (Kobayashi)

fills broad range in Borghi-Peters Regime diagram

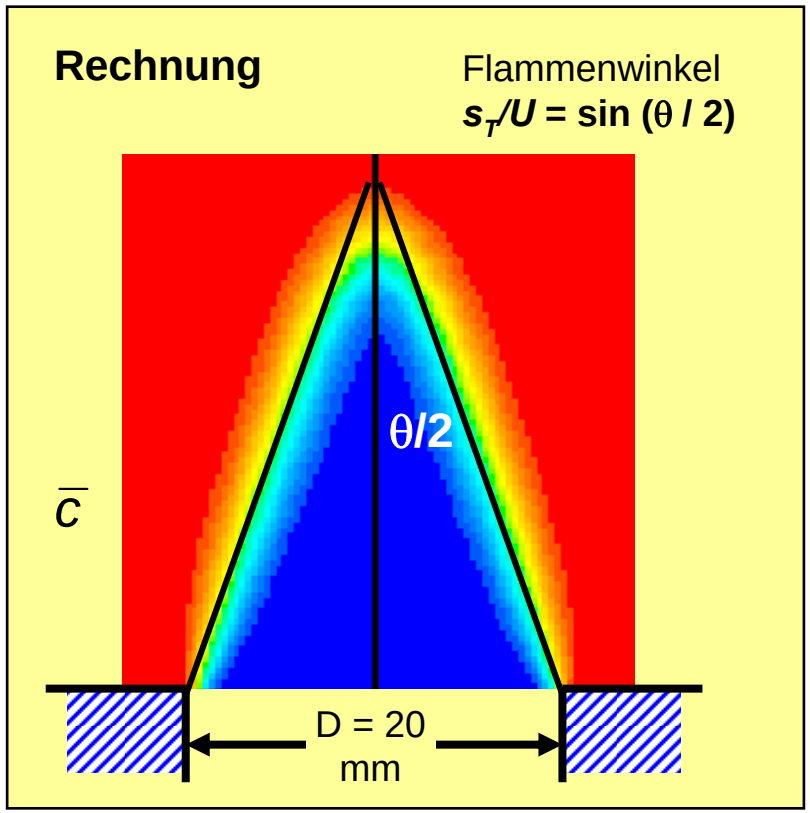


Data of 101 different flames

p = 1 - 10 bar

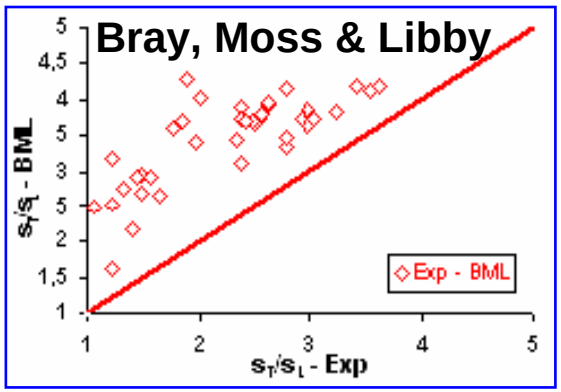
Methane/Air	Φ	= 0.9
Ethylene/Air	Φ	= 0.5, 0.7, 0.9
Propane/Air	Φ	= 0.9

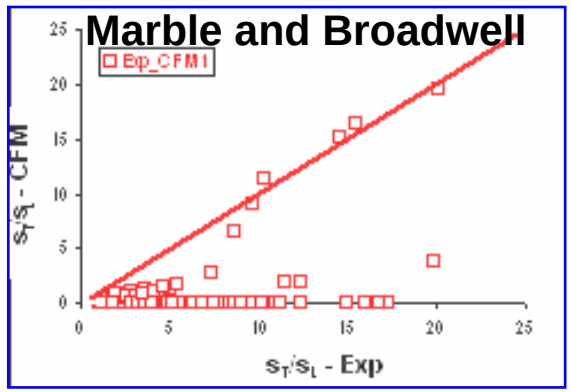
Modellierung des Druckeinflusses

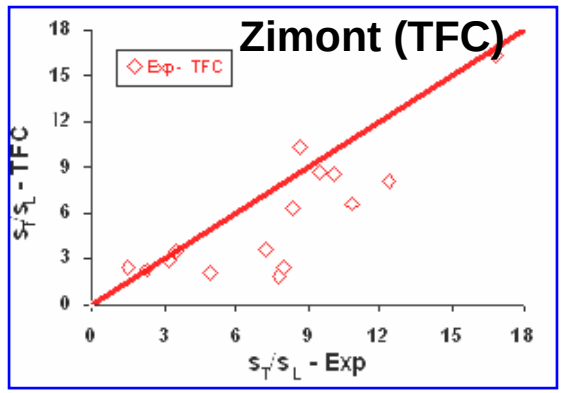


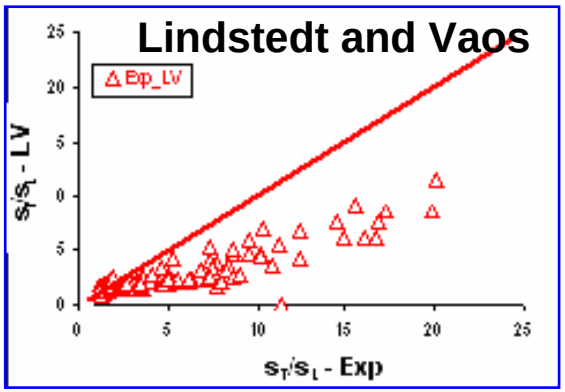
Calculation with different models

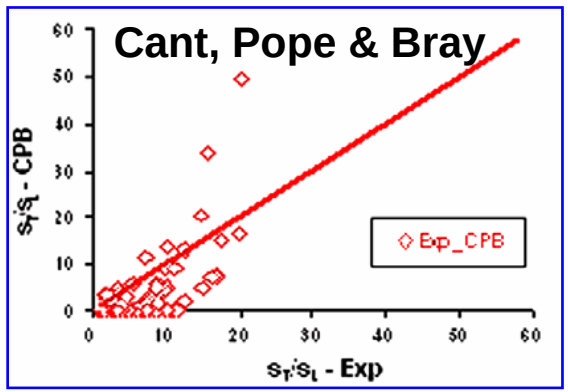
Calculated Flame Angle vs. measured Flame Angle (each dimensionless)









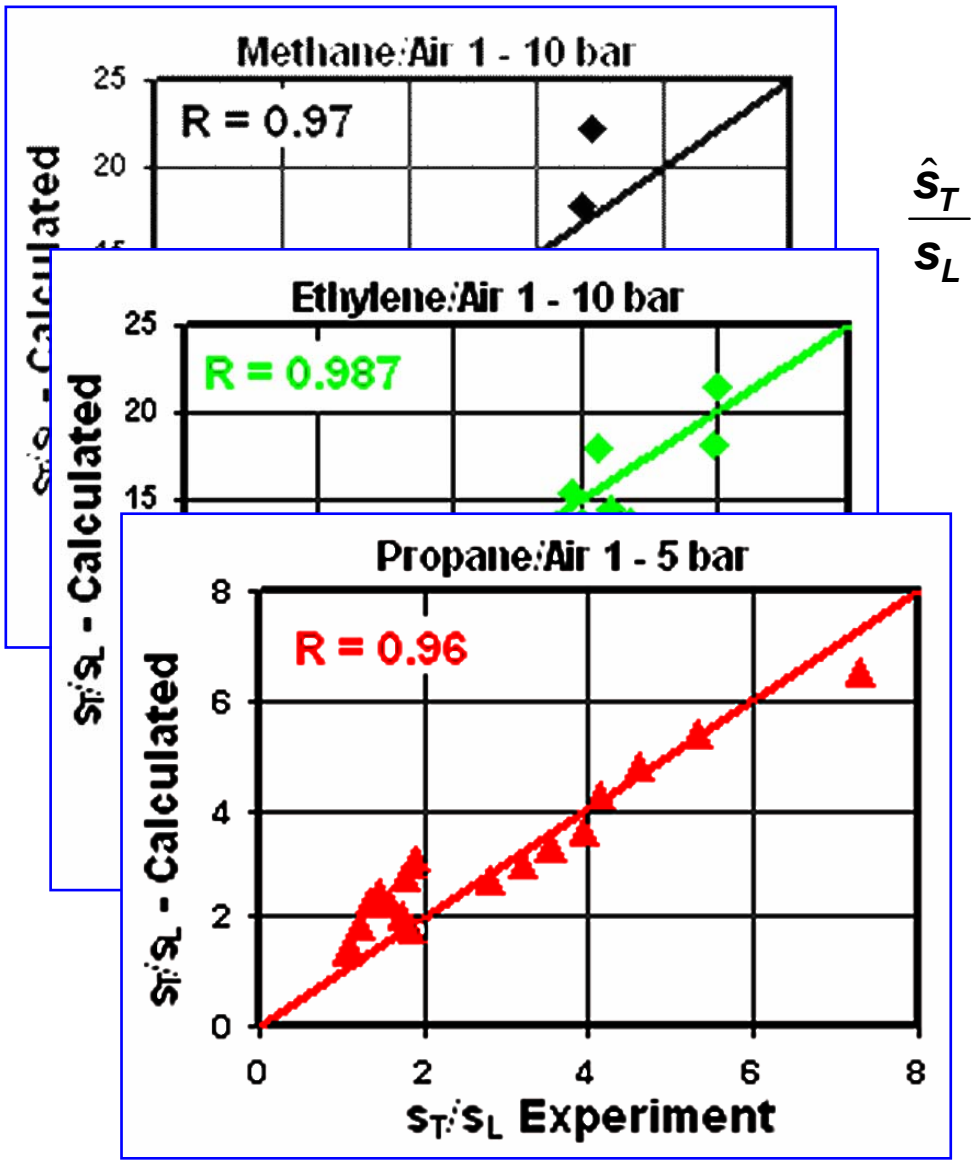


Algebraic BML-like models

Flame surface density models

Algebraic gradient approach model

Modelling of Pressure Influence



Methan-Luft, 1 - 10 bar, 17 Flammen

$$\frac{\hat{s}_T}{s_L} = \frac{A_T}{A_L} = 1 + 0.46 \cdot \mathrm{Re}_t^{\,0.25} \cdot \left(\frac{u'}{s_L}\right)^{0.3} \cdot \left(\frac{p}{p_0}\right)^{0.2}$$

Ethylen-Luft, 1 - 10 bar, 64 Flammen

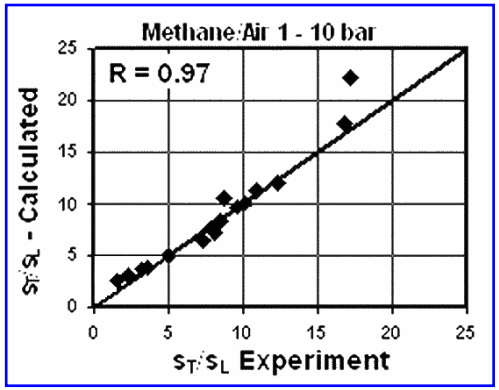
$$\frac{A_T}{A_L} = 1 + 0.39 \cdot \mathrm{Re}_t^{\,0.25} \cdot \left(\frac{u'}{s_L}\right)^{0.3} \cdot \left(\frac{p}{p_0}\right)^{0.2}$$

Propan-Luft, 1 - 5 bar, 20 Flammen

$$\frac{A_T}{A_L} = 1 + 0.28 \cdot \mathrm{Re}_t^{\,0.25} \cdot \left(\frac{u'}{s_L}\right)^{0.3} \cdot \left(\frac{p}{p_0}\right)^{0.2}$$

Muppala et al., Comb. Flame 140, 257 (2005)

Modelling of Pressure Influence

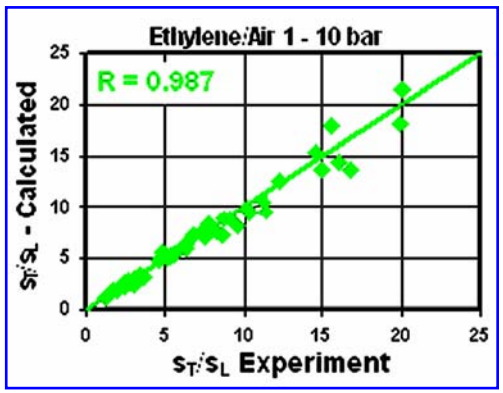


Le = 1

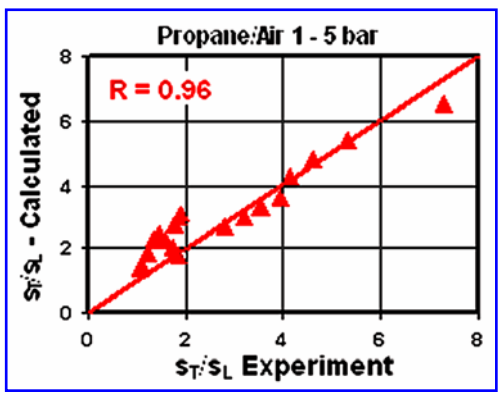
Universell, für magere Methan, Ethylen, Propan-Flammen (1 - 10 bar)

$$\frac{A_T}{A_L} = 1 + \frac{0.46}{Le} \cdot \mathrm{Re}_t^{\,0.25} \cdot \left(\frac{u'}{s_L}\right)^{0.3} \cdot \left(\frac{p}{p_0}\right)^{0.2}$$

Lewis Zahl (*Le = a / D*)



Le = 1.2



Le = 1.62

Muppala et al., Comb. Flame 140, 257 (2005)

Lewis Number

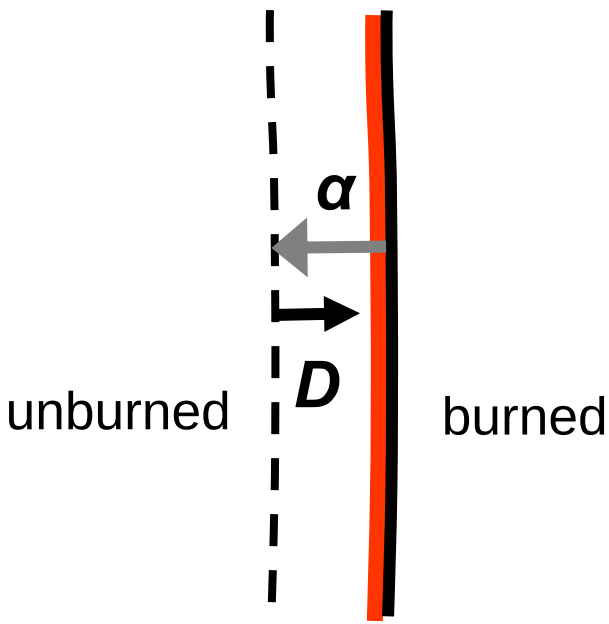
$$Le = \frac{\alpha}{D} = \frac{\text{thermal diffusivity}}{\text{mass diffusivity (fuel)}}$$

- **Why such a big influence of the Lewis number ?**
- **Molecular diffusion.**
- **Known for laminar flame instability - but why for highly turbulent combustion ?**

Lewis Number

$$Le = \frac{\alpha}{D} = \frac{\text{thermal diffusivity}}{\text{mass diffusivity (fuel)}}$$

Laminar plane flame



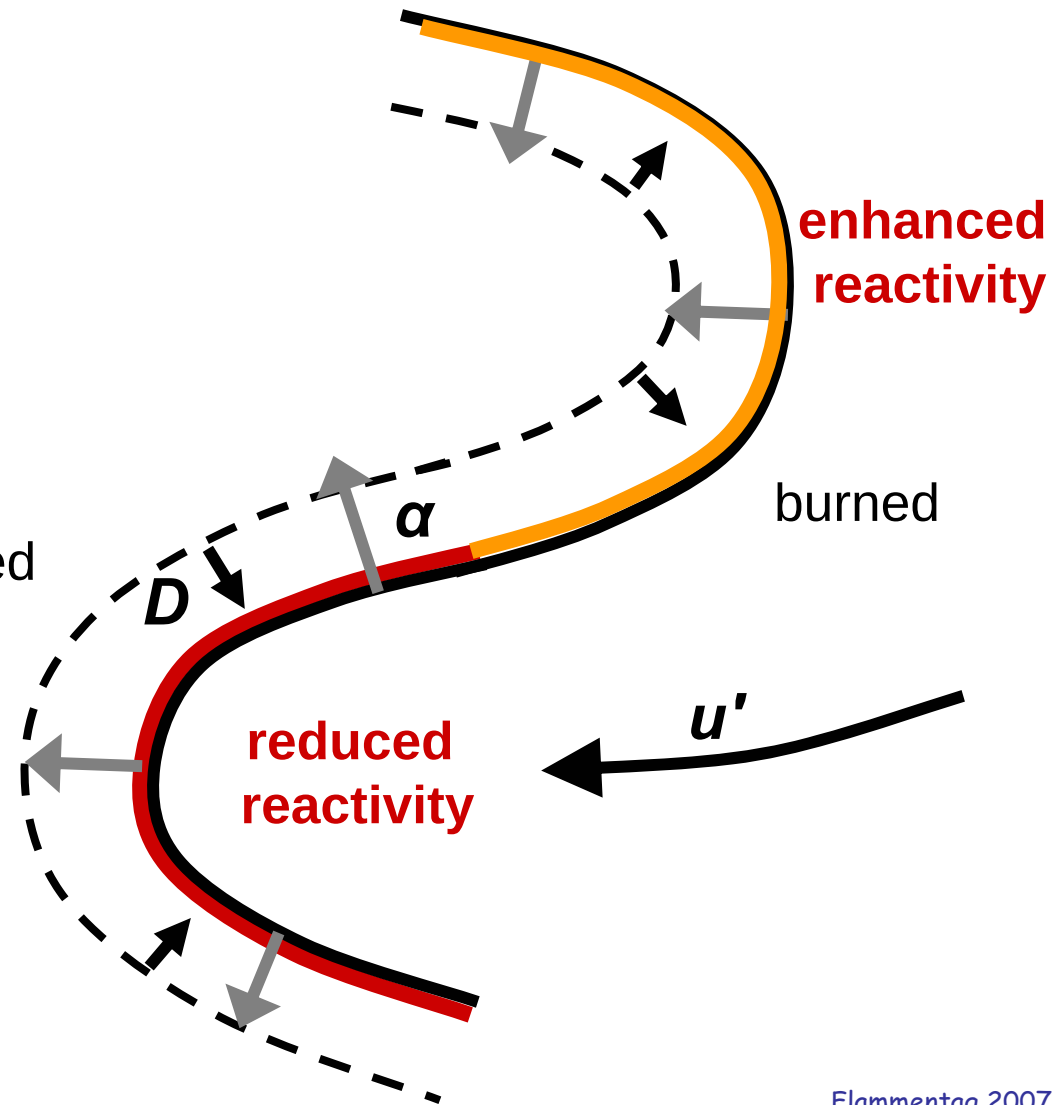
Dinkelacker et al., Dt. Flammentag (2007)

Lewis Number

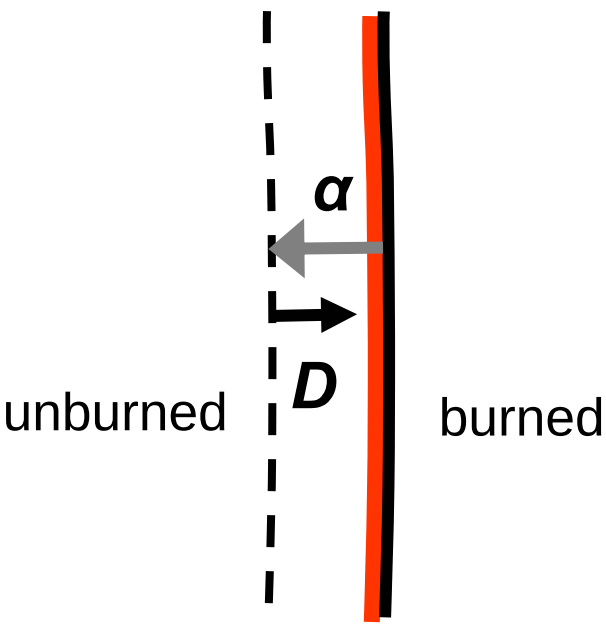
$$Le = \frac{\alpha}{D}$$

Example
Le > 1
(Propan)

Turbulent flame



Laminar plane flame



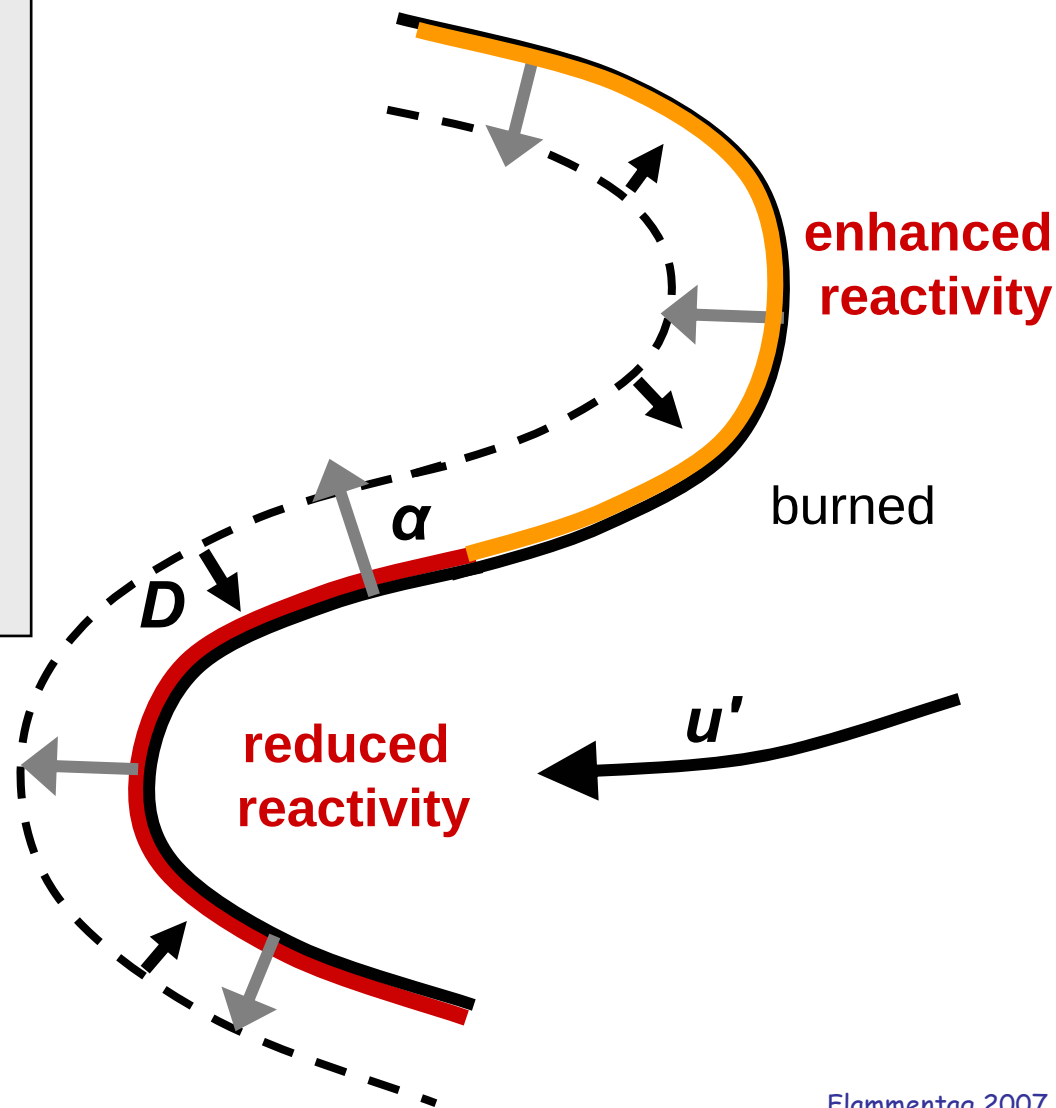
Dinkelacker et al., Dt. Flammentag (2007)

Lewis Number

Is there Le-influence on "average" reaction rate ???

- **Highly turb. flames: pos. and neg. curvature is equally distributed !**
- **So in first order no Le-influence expected !**

Turbulent flame



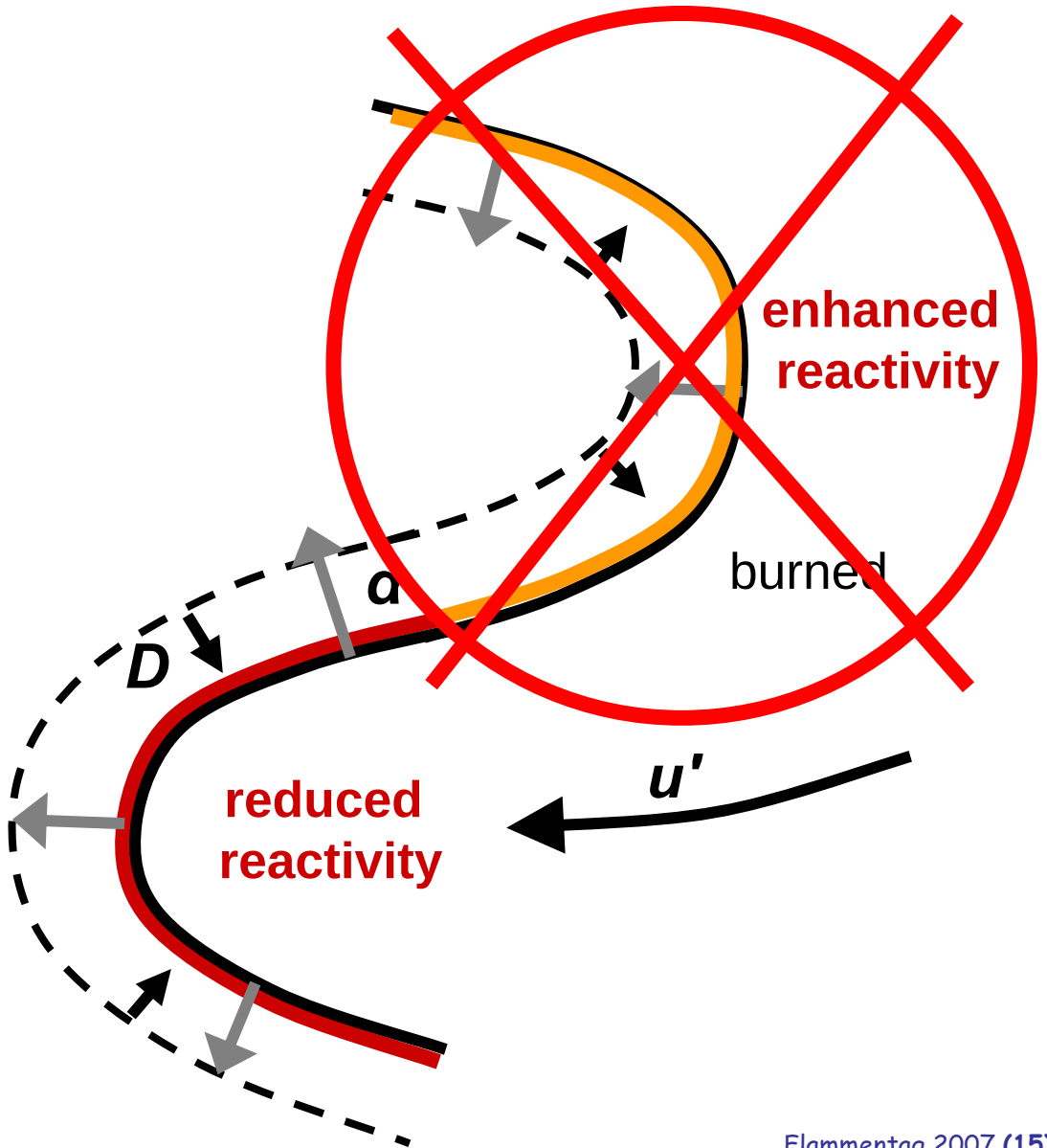
Dinkelacker et al., Dt. Flammentag (2007)

Leading Edge Concept (Zel'dovich, Lipatnikov, Chomiak)

Leading Edge (positive curved part) dominates the flame propagation
(≅ mean reaction rate)

Here fuel diffusion and thermal diffusion eventually unbalanced

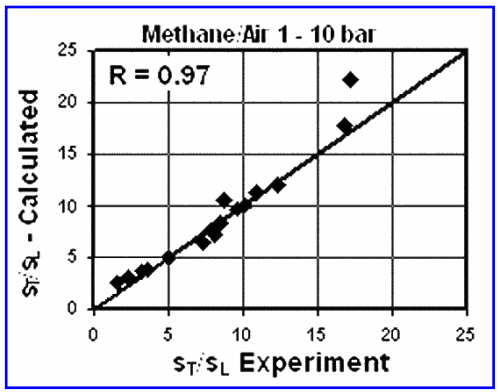
Rear part is "only" follow up



Le > 1 (Propane):
less reactive as
Le = 1 (Methane)

Dinkelacker et al., Dt. Flammentag (2007)

Modellierung des Druckeinflusses

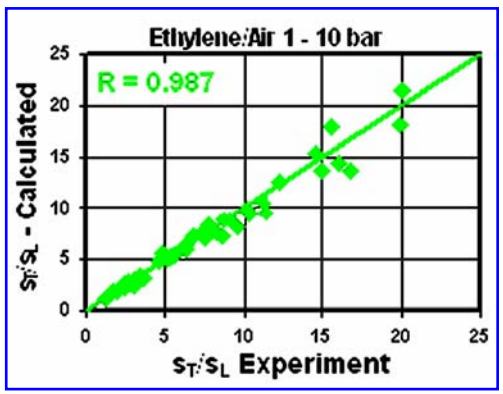


Le = 1

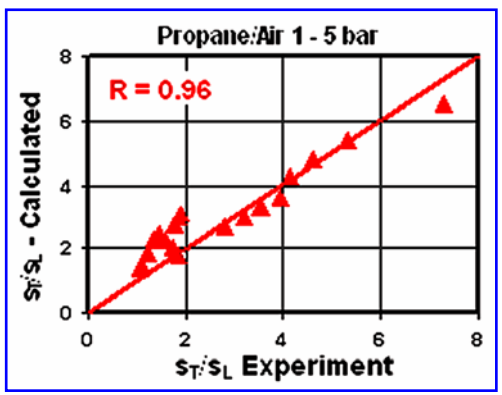
Universell, für magere Methan, Ethylen, Propan-Flammen (1 - 10 bar)

$$\frac{A_T}{A_L} = 1 + \frac{0.46}{Le} \cdot Re_t^{0.25} \cdot \left(\frac{u'}{s_L}\right)^{0.3} \cdot \left(\frac{p}{p_0}\right)^{0.2}$$

Lewis Zahl (*Le = a / D*)

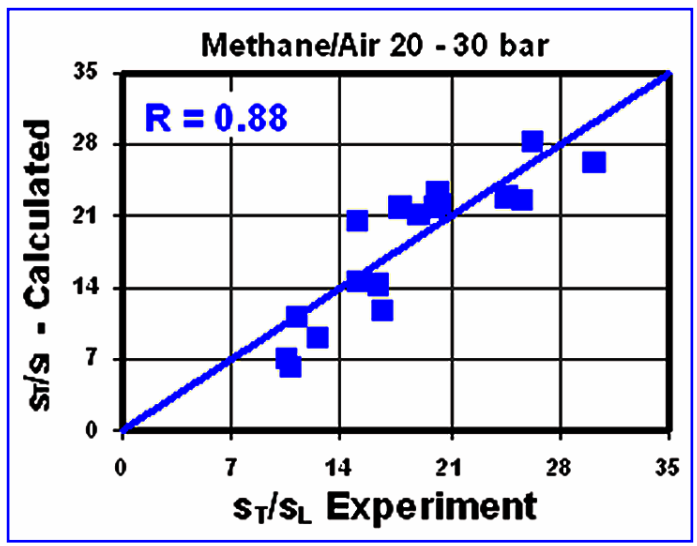


Le = 1.2



Le = 1.62

Extrapolation zu 20 und 30 bar (Vorhersage)



Muppala et al., Comb. Flame 140, 257 (2005)

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Berechnung turbulenter Vormischflammen

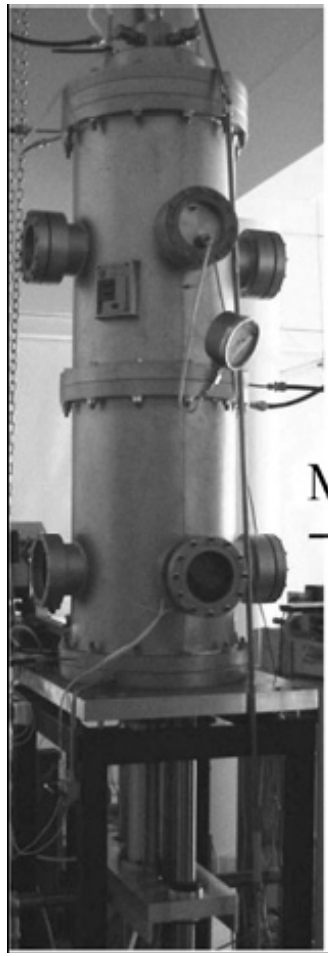
- Reaktionsfortschritts-Modell mit Druck- und Brennstoffeinfluss
- Exkurs Lewis Number
- Methane/Hydrogen Flames
- Effective Lewis Number
- Zusammenfassung

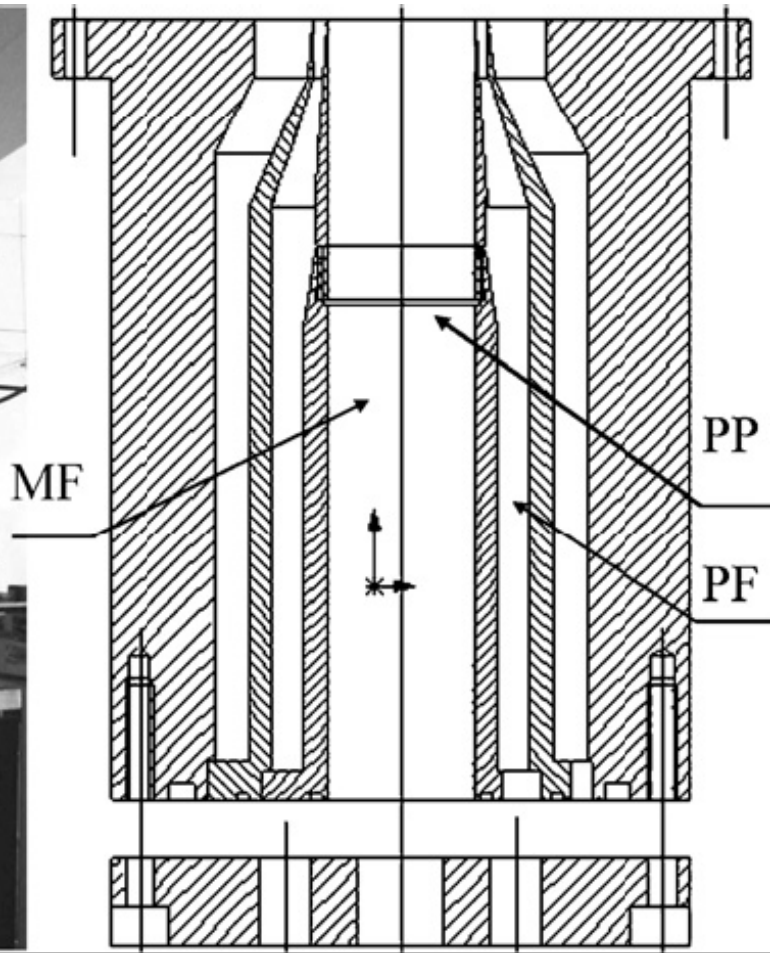
Hochdruck-Bunsenflammen Orleans

F. Halter, C. Chauveau, I. Gökalp (Univ. Orléans)

Bunsenflamme D = 25 mm
H_2-Pilotierung
Turbulenzgitter
Brennkammer 600 mm hoch, D = 300
Druck 1, 5, 9 bar

Methane/Hydrogen - Luft
Mager vorgemischt $\Phi = 0{,}6$
U = 2.1 m/s
u' = 0,15 m/s





Hochdruck-Bunsenflammen Orleans

D = 25 mm, Mager vorgemischt Φ = 0,6
U = 2.1 m/s, u' = 0,15 m/s

0.1MPa 0.5MPa 0.9MPa

Pressure Variation

$\alpha = 0$ $\alpha = 0.1$ $\alpha = 0.2$

Hydrogen Addition

C. Cohé, F. Halter, C. Chauveau, I. Gökalp (31. Symp.)

Hochdruck-Bunsenflammen Orleans

Table 1: Experimental inflow conditions (U = 2.1 m/s, Φ = 0.6)

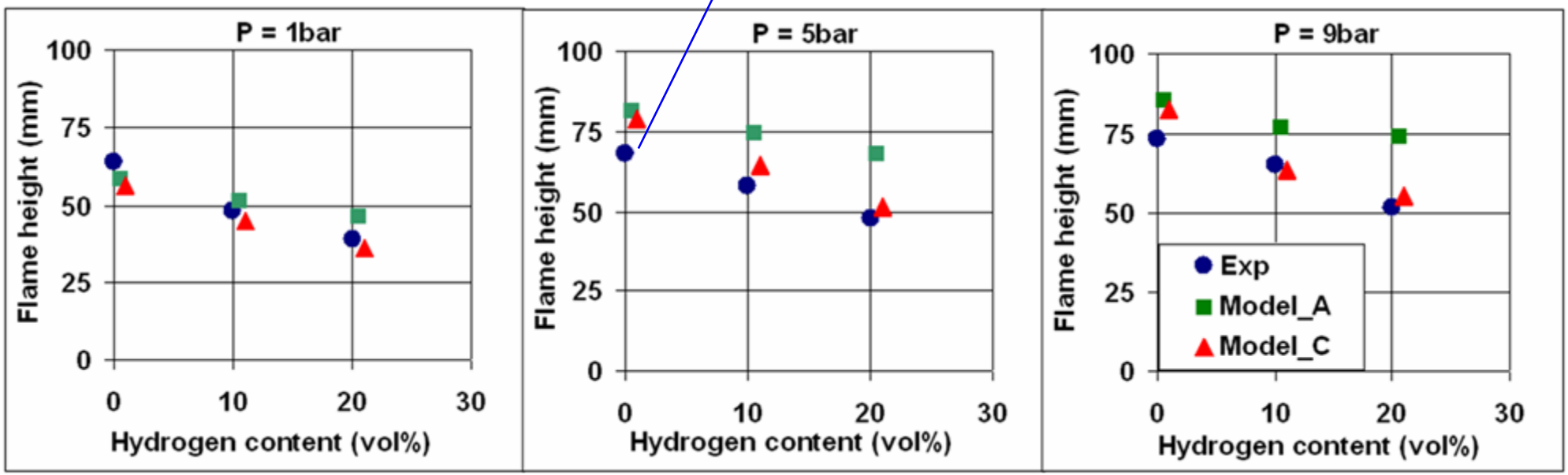
% H_2	p (MPa)	u' (m/s)	v' (m/s)	l_x (mm)	s_L (m/s)	u'/s_L
0	0.1	0.15	0.12	6.69	0.112	1.36
10	0.1	0.15	0.14	4.30	0.121	1.26
20	0.1	0.16	0.14	3.51	0.132	1.20
0	0.5	0.18	0.14	7.37	0.041	4.36
10	0.5	0.18	0.14	6.97	0.044	4.07
20	0.5	0.19	0.17	6.84	0.048	3.92
0	0.9	0.16	0.11	5.77	0.029	5.32
10	0.9	0.15	0.12	5.45	0.031	4.92
20	0.9	0.16	0.14	5.66	0.033	4.85

Hochdruck-Bunsenflammen Orleans

$\alpha = 0$ $\alpha = 0.1$ $\alpha = 0.2$

Einfluss Wasserstoff-Zufügung

Blau: Experiment (Orléans)



Modell-Ansatz

Modell-Ansatz valied also for Methane/Hydrogen Flames ???

$$\frac{A_T}{A_L} = 1 + \frac{0.46}{Le} \cdot \mathrm{Re}_t^{\,0.25} \cdot \left(\frac{u'}{s_L}\right)^{0.3} \cdot \left(\frac{p}{p_0}\right)^{0.2}$$

But: Which Lewis Number for Methane/Hydrogen-Air Flames ???

Effective Lewis Number following Law

Model A: **Effective Lewis Number following Law et al. (2005): (with q-weighted average)**

$$q\,(Le^* - 1) = q_1\,(Le_1 - 1) + q_2\,(Le_2 - 1)$$ (with q = heat release)

Lewis Number

Le_{H2} = 0.29

Le_{CH4} = 0.955

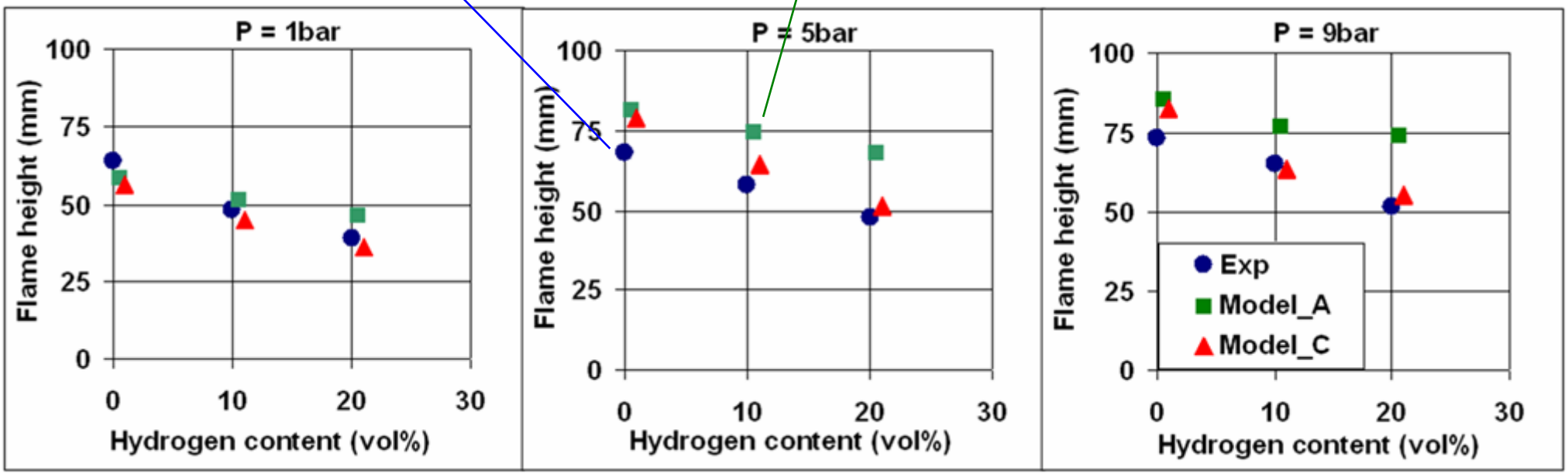
gives

Le^*	= 0.955	at 0 % H2
Le^*	= 0.935	at 10 % H2
Le^*	= 0.918	at 20 % H2

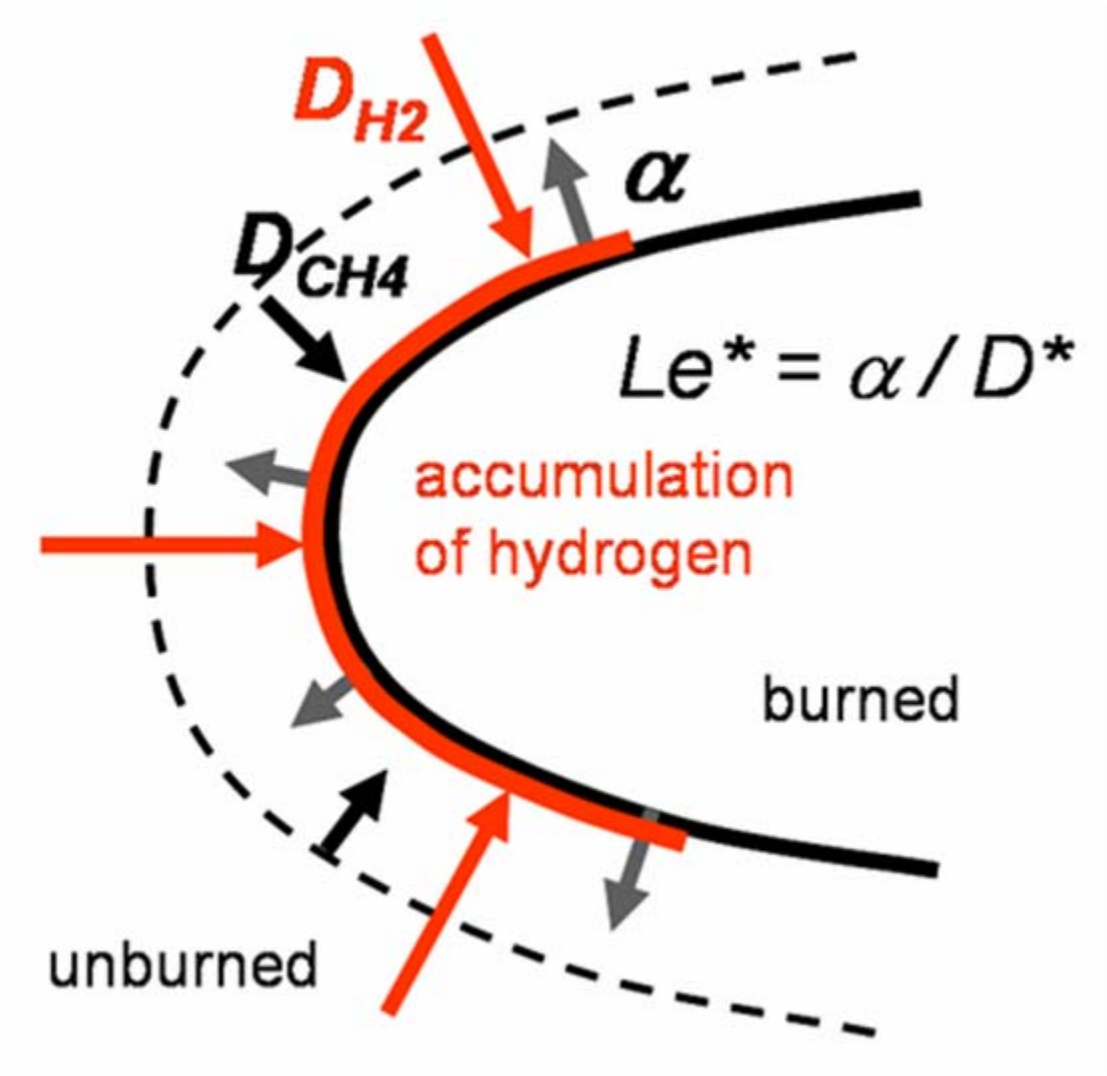
Hochdruck-Bunsenflammen Orleans

Blue:
Experiment

Green: Model A:
Effective Lewis Number foll. Law et al.



Methane/Hydrogen Flame



Effective Lewis Number *Le
following Dinkelacker:**

$$Le^* = \alpha / D^*$$

$$D^* = x_{H2} D_{H2} + x_{CH4} D_{CH4}$$

Dinkelacker et al., Dt. Flammentag (2007)

Effective Lewis Number following Dinkelacker

Model C: **Effective Lewis Number from effective diffusivity D* (Dinkelacker 2007):**

$$Le^* = \alpha / D^*$$

mit α = thermal diffusivity
x = mole fraction

$$D^* = x_{H2} D_{H2} + x_{CH4} D_{CH4}$$

$$\rightarrow \quad \frac{1}{Le^*} = \frac{D^*}{a} = \frac{x_{CH4} D_{CH4}}{a} + \frac{x_{H2} D_{H2}}{a} = \frac{x_{CH4}}{Le_{CH4}} + \frac{x_{H2}}{Le_{H2}}$$

Lewis Number

Le_{H2} = 0.29
Le_{CH4} = 0.95

gives

Le^*	= 0.95	at 0 % H2
Le^*	= 0.77	at 10 % H2
Le^*	= 0.65	at 20 % H2

Hochdruck-Bunsenflammen Orleans

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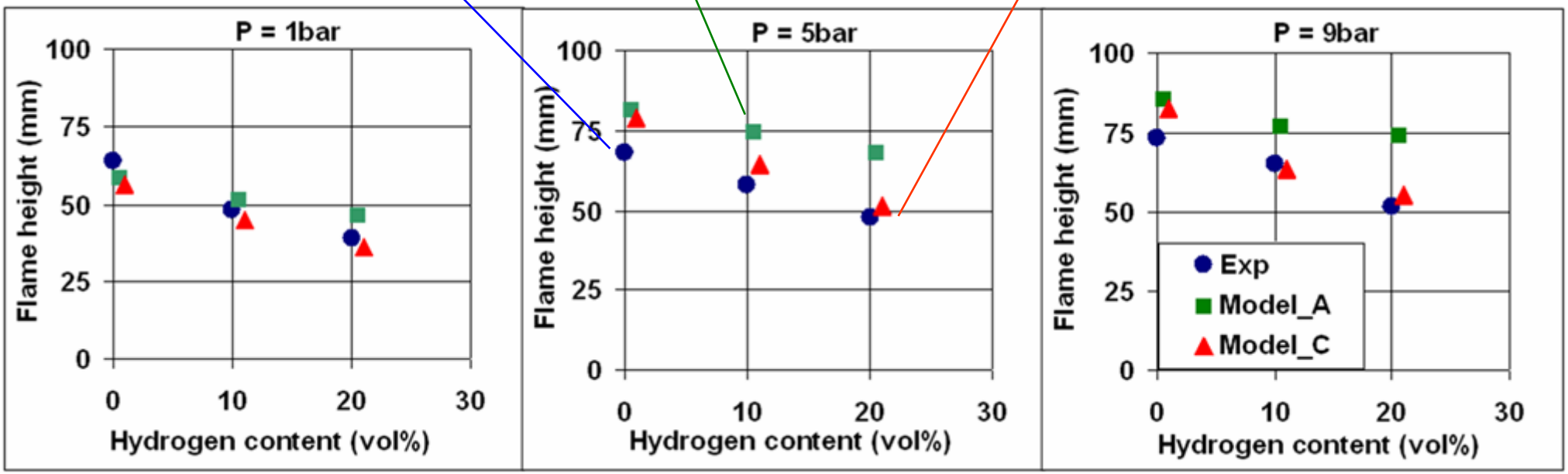
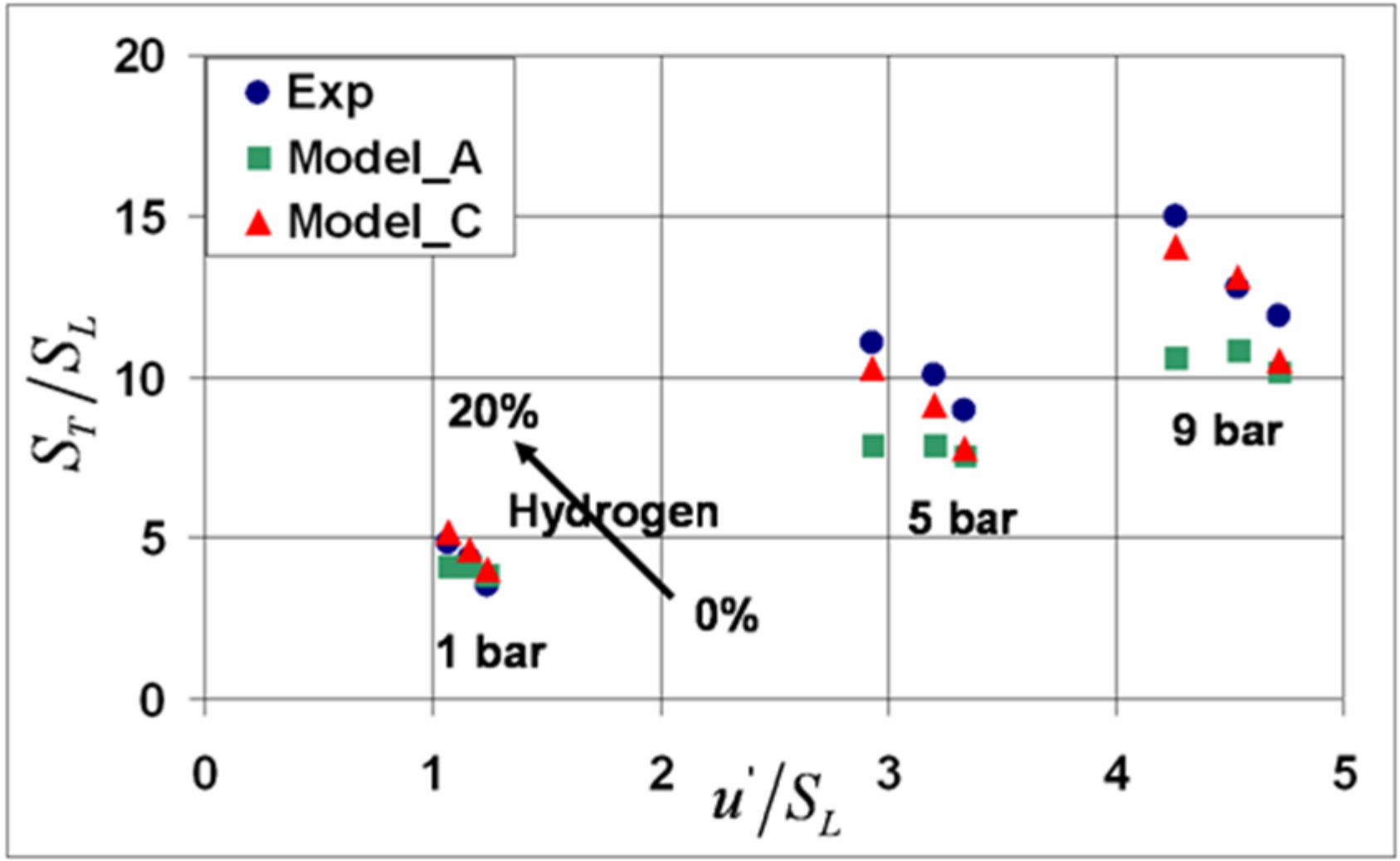
Modell A:
Effective Lewis Number nach Law et al.

Experiment

Modell C:
Effective Lewis Number mittels Effectiver Diffusivität D*



Methane/Hydrogen Flame



Summary

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Numerical calculation of turbulent premixed flames

- **Modelling of mean reaction term**
  (TFC Model, good for 1 bar)

- **Calculation of Pressure- + Fuel Influence**
  (Muppala-Dinkelacker Model)

$$\frac{A_T}{A_L} = 1 + \frac{0.46}{Le} \cdot \mathrm{Re}_t^{\,0.25} \cdot \left(\frac{u'}{s_L}\right)^{0.3} \cdot \left(\frac{p}{p_0}\right)^{0.2}$$

for lean Methane, Ethylene, Propane-Flames 1 - 10 bar (30 bar)

- **Le-Influence may be explained with Leading Edge Concept**

- **Calculation of H_2-CH_4 / air flames (1 - 9 bar)**

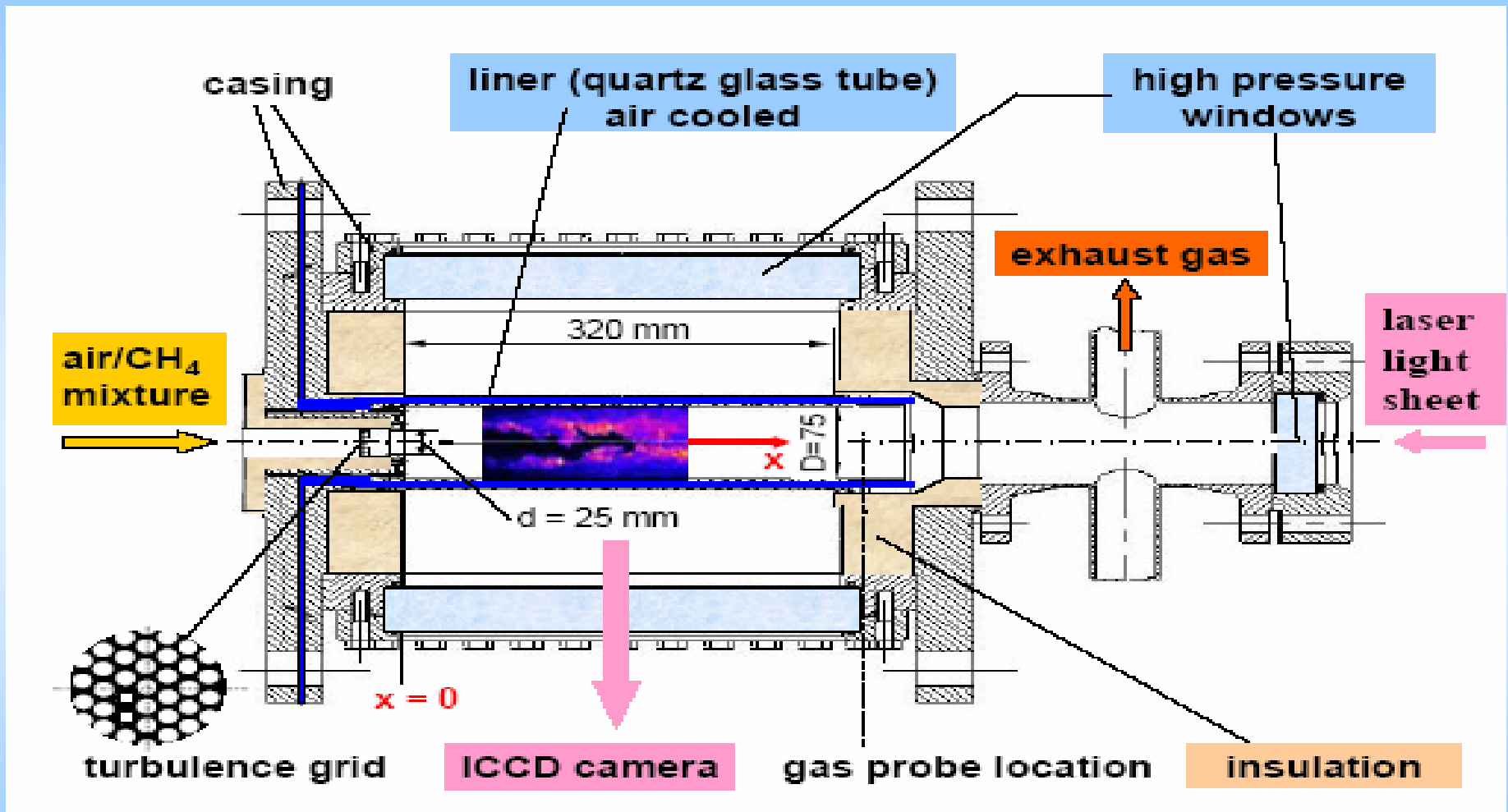
not for more than 20% hydrogen

- **Effective Lewis Number based on Effective Diffusivity of Fuel Mixture**

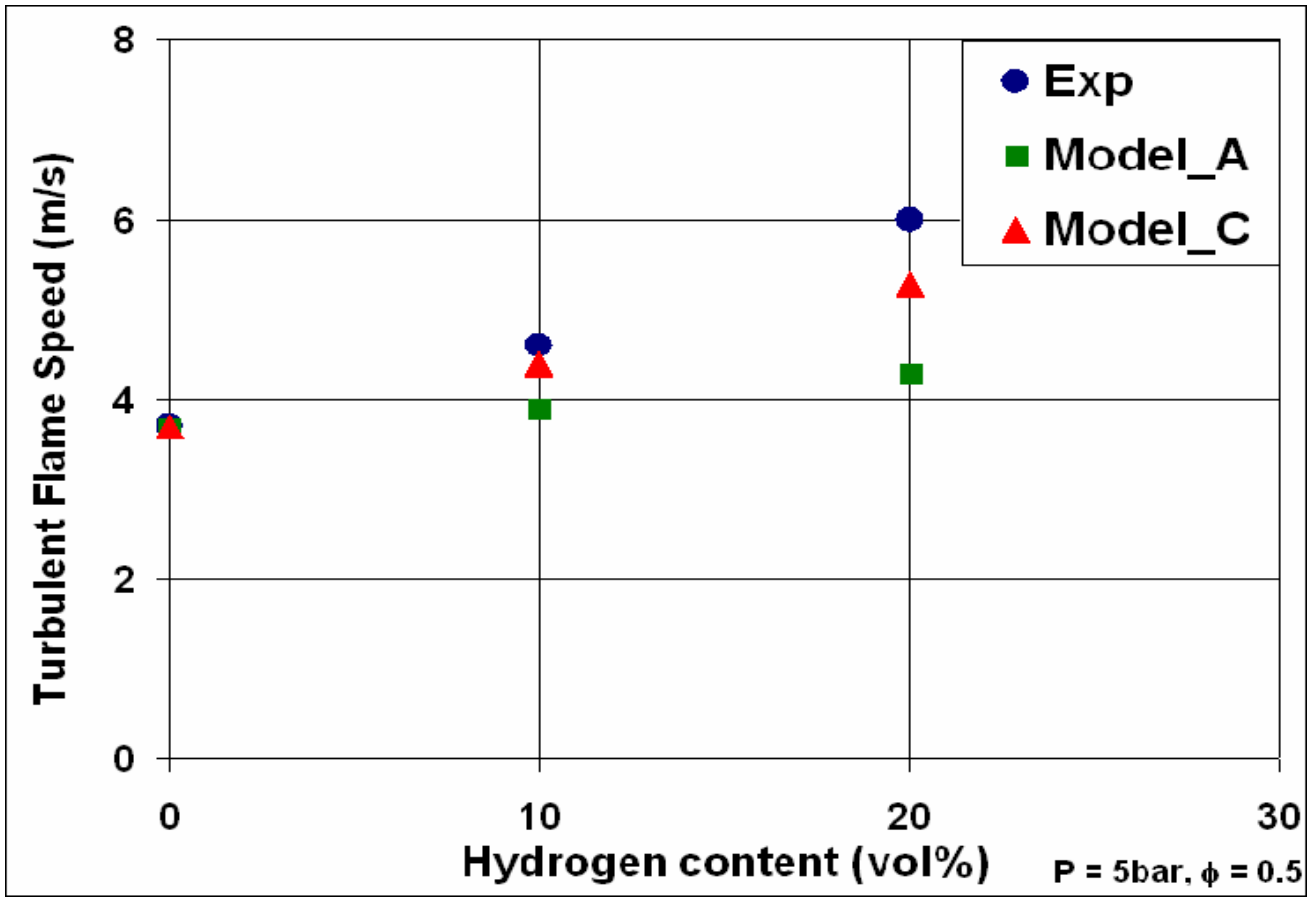
$$Le^* = a / D^*$$
$$D^* = x_{H2} D_{H2} + x_{CH4} D_{CH4}$$

PSI Burner (Griebel, et al.)

5 bar, $\Phi = 0.5$, Methane/Hydrogen - Air



High-pressure combustor (PSI)

PSI Burner (Griebel, et al.)

Methane/Hydrogen - Air, 5 bar, $\Phi = 0.5$