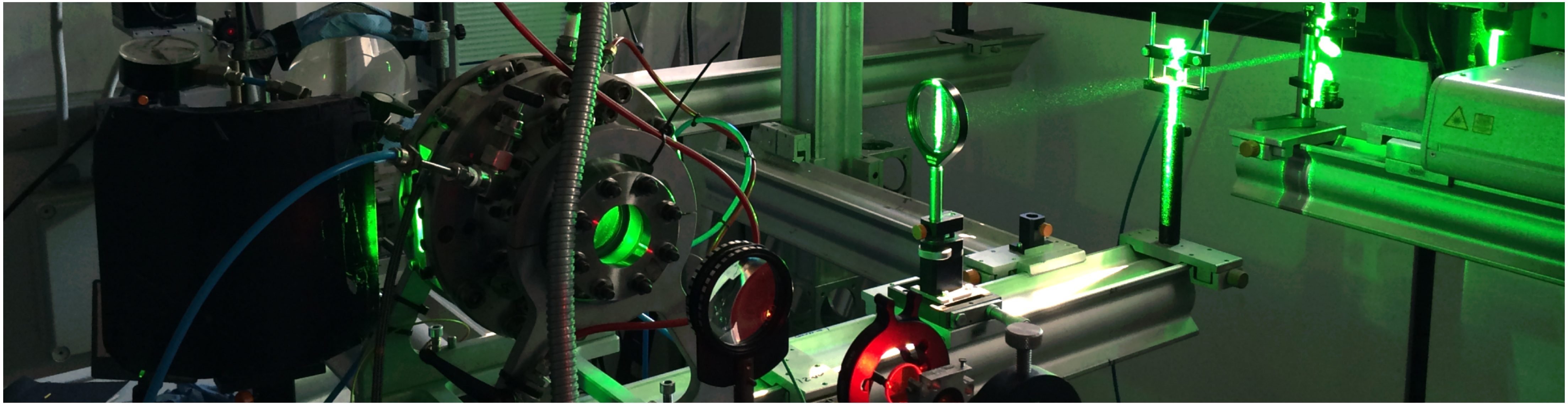

Laminar burning velocities of refrigerants under the impact of buoyancy and radiation

J. Beeckmann[a], R. Hesse[a], L. Berger[a], H. Pitsch[a], R. Burrell[b], and G. Linteris[b]

[a]Institute for Combustion Technology RWTH Aachen University, Germany

[b]Energy and Environment Division, National Institute of Standards and Technology (NIST), USA

LBV workshop 2019 –
New Perspectives, Methods, and Applications for Laminar Burning Velocity
Lisbon, Portugal - April 14th 2019

NIST National Institute of Standards and Technology U.S. Department of Commerce

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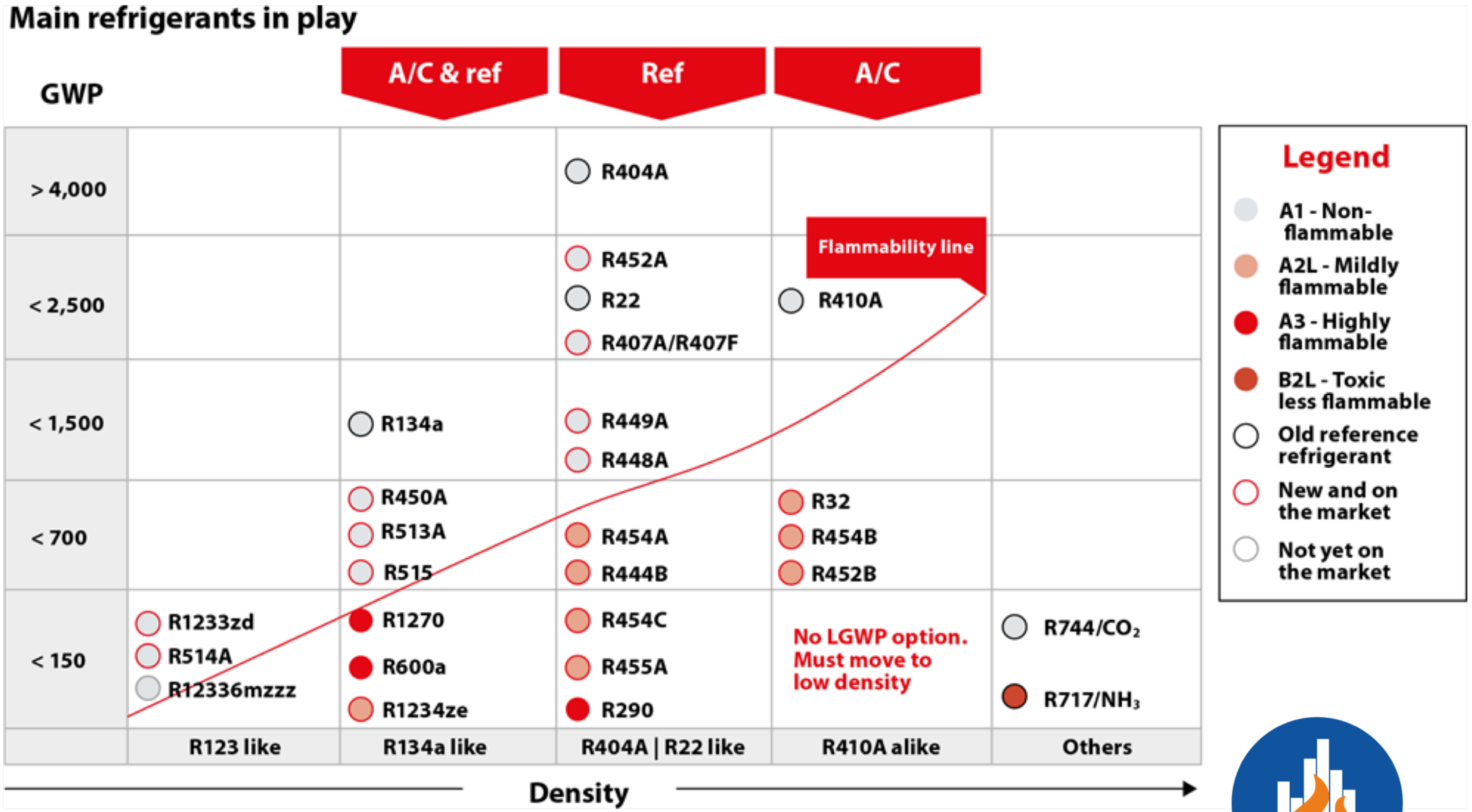
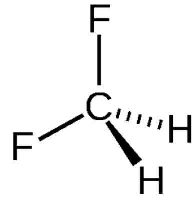
Phase Out of HFC Refrigerants with a High Global Warming Potential (GWP)

What are the alternatives?...



Source: www.danfoss.com

$$CH_2F_2 + O_2 = CO_2 + 2HF$$



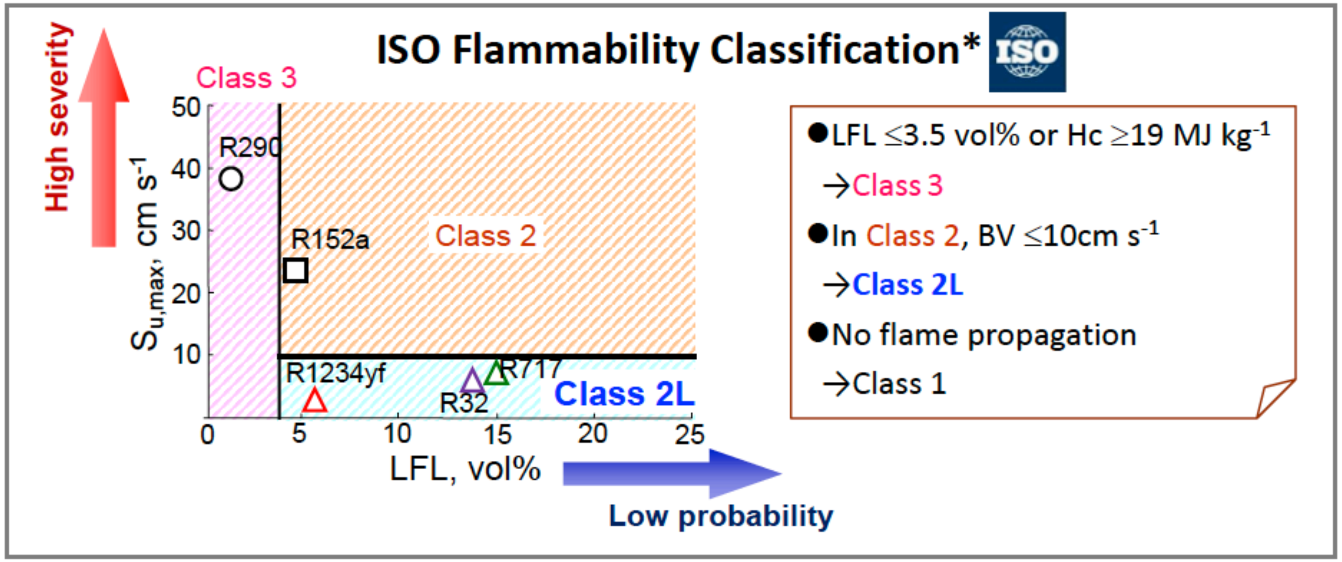
Suitable metric?

... Low-GWP refrigerants are mildly flammable

Challenges to describe S_L?...

… Flammable, but only mildly flammable

Very low burning velocities!!!



Takizawa, ICR2015 Workshop on Risk Assessment of Mildly Flammable Refrigerants (1963)
**ISO817, Refrigerants—Designation and safety classification (2014)*

Challenges to describe S_L?...

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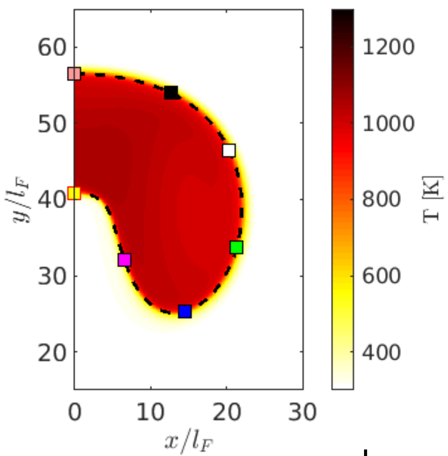
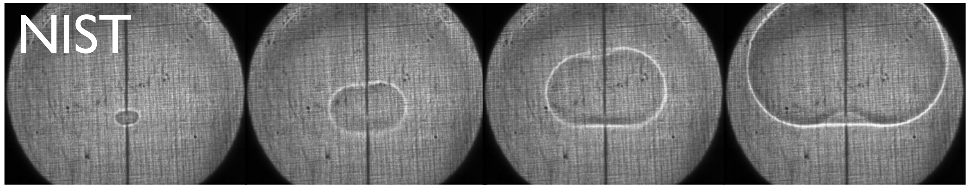
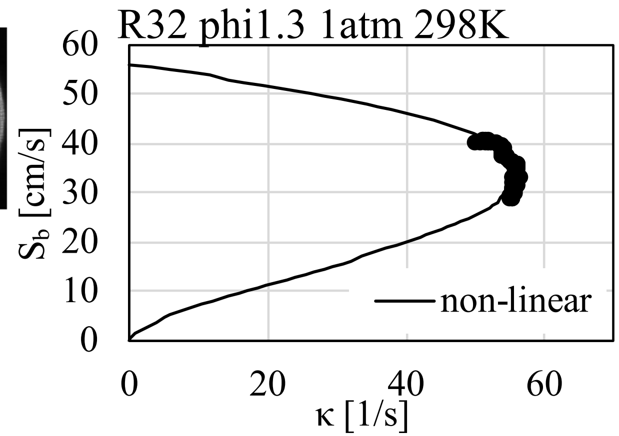
Very low burning velocities!!!







$$s_L = s_L^0 - s_L^0 \mathcal{L}\kappa - \mathcal{L}S$$

$g\downarrow$

Effect of buoyancy?

Effect of radiation?

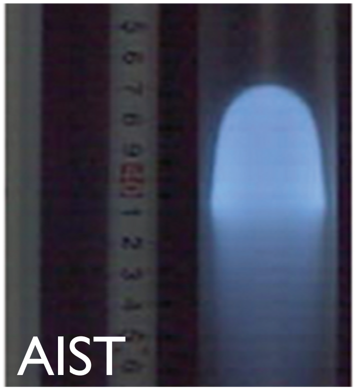
NIST = National Institute of Standards and Technology, USA

Outline

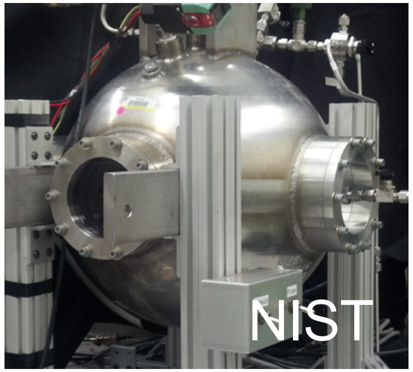
- Experiments and Methodologies
- Results
- Summary/Suggestions

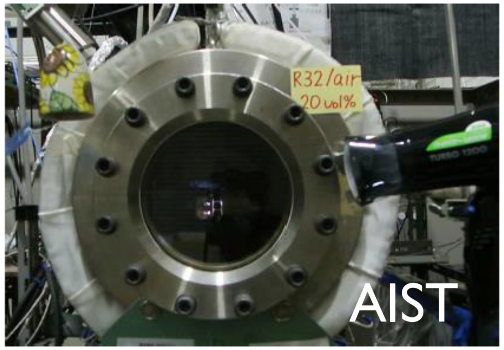
Experiments -
Sparse data, only about 6 groups worldwide measure refrigerents

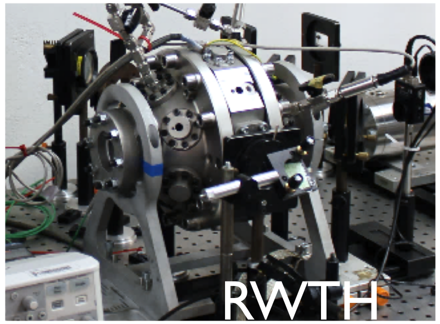
Tube

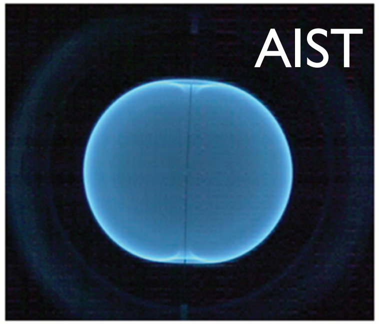


Vessels



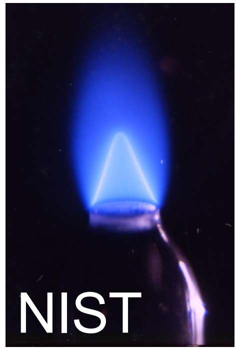






Burner

Mache-Hebra

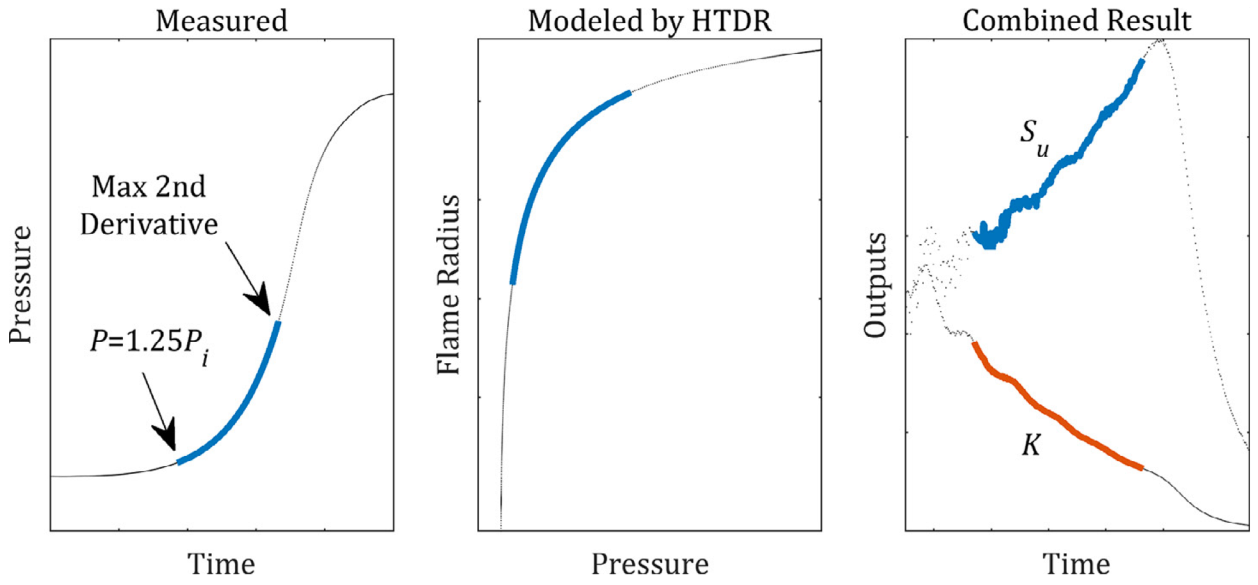


AIST = National Institute of Advanced Industrial Science and Technology, Japan
NIST = National Institute of Standards and Technology, USA
RWTH = RWTH Aachen University, Germany
UTRC = United Technologies Research Center
MINES = Mines Paris Tech, France
KR = R&D Center, Korean Register of Shipping, Korea

Methodologies – pressure based
Data reduction process (S_u)

Fiock and Marvin:

$$S_u = \frac{\mathrm{d}R_f}{\mathrm{d}t} - \frac{R_w^3 - R_f^3}{tR_f^2\gamma_u P}\frac{\mathrm{d}P}{\mathrm{d}t}$$

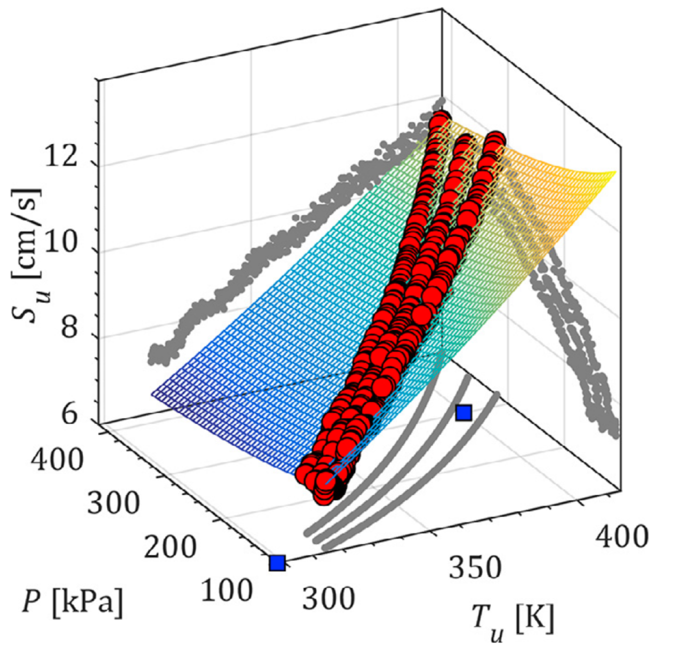


Fiock and Marvin, Chem. Rev. (1937)
Takizawa et al., ASHRAETransactions (2013)
R. Burell et al., Proc. Combust. Inst. (2019)

HTDR = Hybrid ThermoDynamic-Radiation
RADCAL = Radiation Calculations

Power law surface, e.g. [2]:

$$\widehat{S_u}(T_u, P) = S_{u,ref}\left(\frac{T_u}{T_{ref}}\right)^{\gamma}\left(\frac{P_u}{P_{ref}}\right)^{\beta}$$



Methodologies – optical based
Extrapolation to zero stretch (S_{b0})

Propagation speed :

$$s_b = \frac{\mathrm{d}r_f}{\mathrm{d}t}$$

Stretch:

$$\kappa = \frac{1}{A}\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{2}{r_f}\frac{\mathrm{d}r_f}{\mathrm{d}t}$$

Linear model:

$$s_b^0 - s_b = \mathcal{L}_b\kappa$$

Non-linear models:

$$\left(\frac{s_b}{s_b^0}\right)^2 \ln\left(\frac{s_b}{s_b^0}\right)^2 = -\frac{2\mathcal{L}_b\kappa}{s_b^0} \quad [1, 2]$$

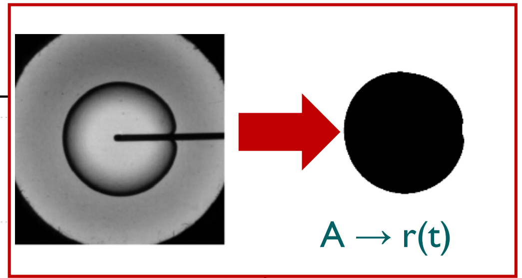
$$\frac{s_b}{s_b^0} = 1 - \mathcal{L}_b\frac{2}{r_f} \quad [3]$$

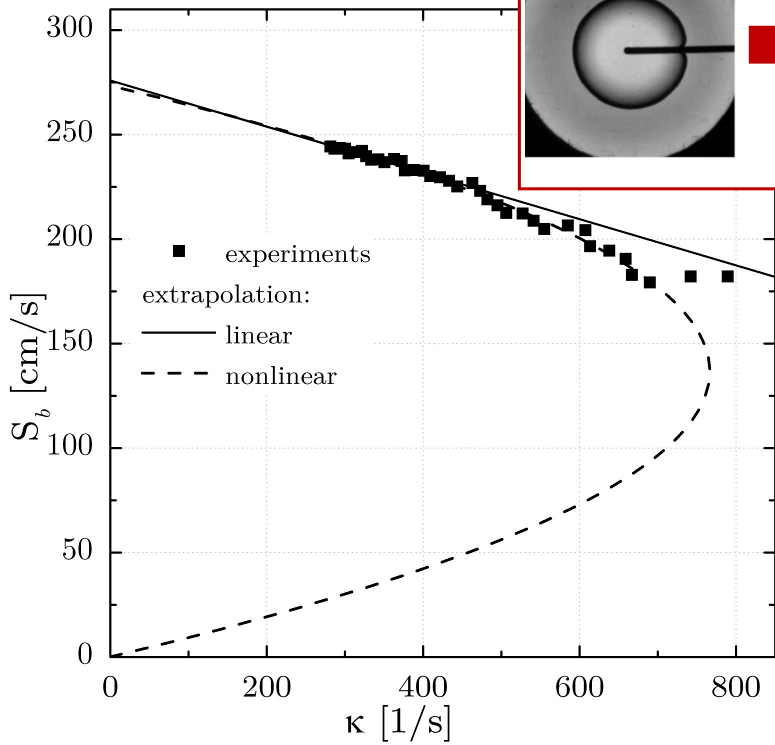
$$\frac{s_b}{s_b^0}\left[1 + \frac{2\mathcal{L}_b}{r_f} + \frac{4\mathcal{L}_b^2}{r_f^2} + \frac{16\mathcal{L}_b^3}{3r_f^3} + o^4\left(\frac{\mathcal{L}_b}{r_f}\right)\right] = 1 \quad [4]$$

$$\left(\frac{s_b}{s_b^0} + \frac{2\delta^0}{r_f}\right)\ln\left(\frac{s_b}{s_b^0} + \frac{2\delta^0}{r_f}\right) = -\frac{2(\mathcal{L}_b - \delta^0)}{r_f} \quad [5]$$

$$\frac{s_b}{s_b^0} = 1 - \frac{2\mathcal{L}_b}{r_f} + \frac{C}{r_f^2} \quad [6]$$

[1] *Halter et al., Combust. Flame (2010)*
[2] *Kelly and Law, Combust. Flame (2009)*
[3] *Frankel and Sivashinsky. Combust. Sci. Technol. (1983)*
[4] *Kelly et al, J. Fluid Mech. (2012)*
[5] *Liang et al., Proc. Combust. Inst.(2017)*
[6] *Wu et al., Proc. Combust. Inst.(2015)*





High speed Schlieren arrangement: J. Beeckmann et al., Fuel (2014)

Outline

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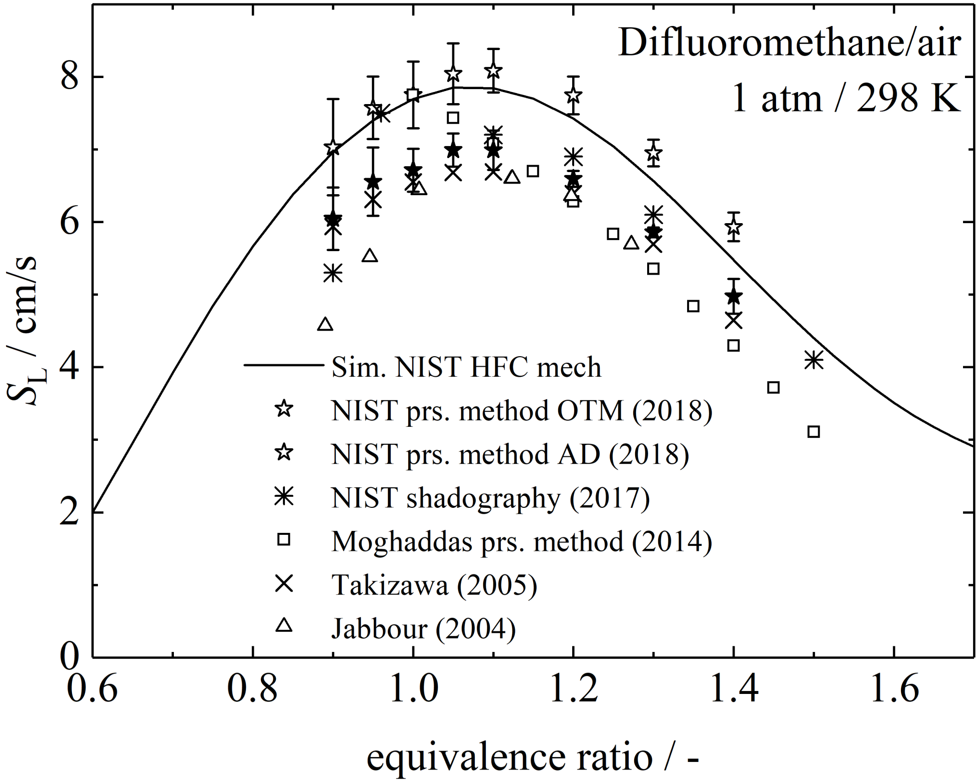
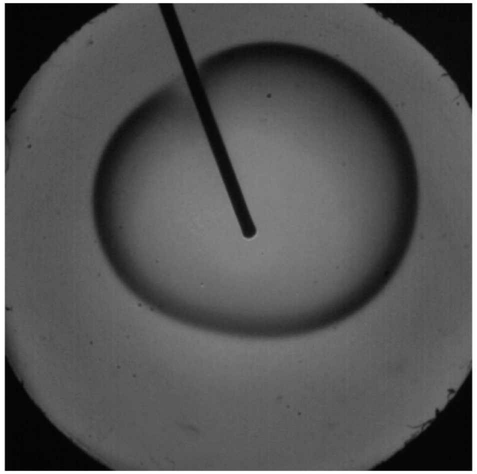
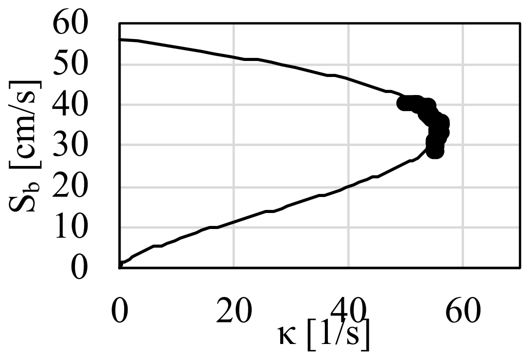
Results comparison - R32 case
Literature

R32 phi1.3 1atm 298K







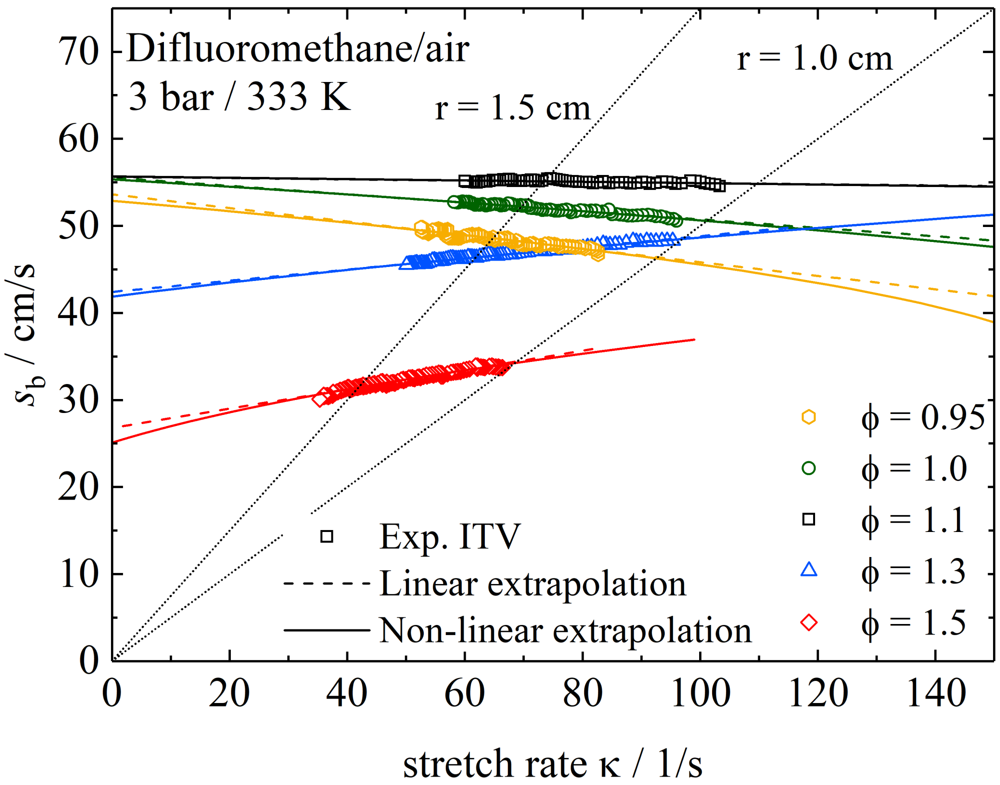
atmospheric conditions difficult to measure (high sens. to stretch & small density gradient)

Beeckmann et al., Proc. Combust. Inst. (2019)

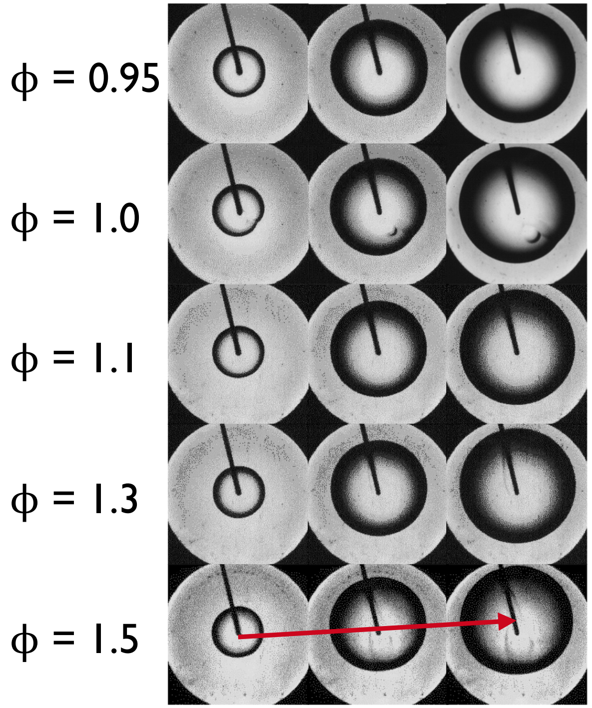
In order to reduce exp. uncetainty → increase p and T

Simulation performed with detailed mechanism provided by NIST: R. Burgess, Jr et al., submitted to Combust. Flame (2019)

Results comparison - R32 case
Higher pressure and temperature



Elevated pressure reduces sensitivity to stretch



Marginal influence of gravitation visible

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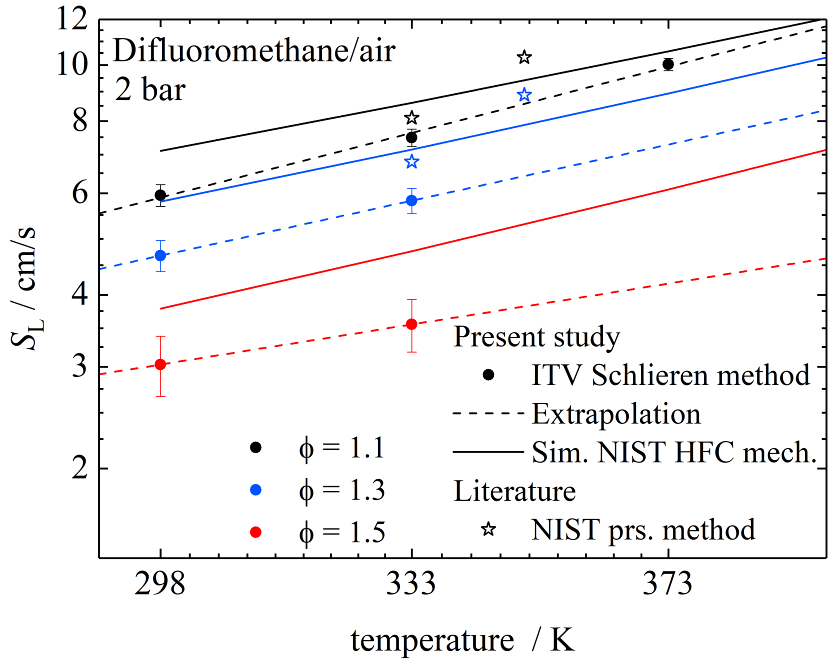
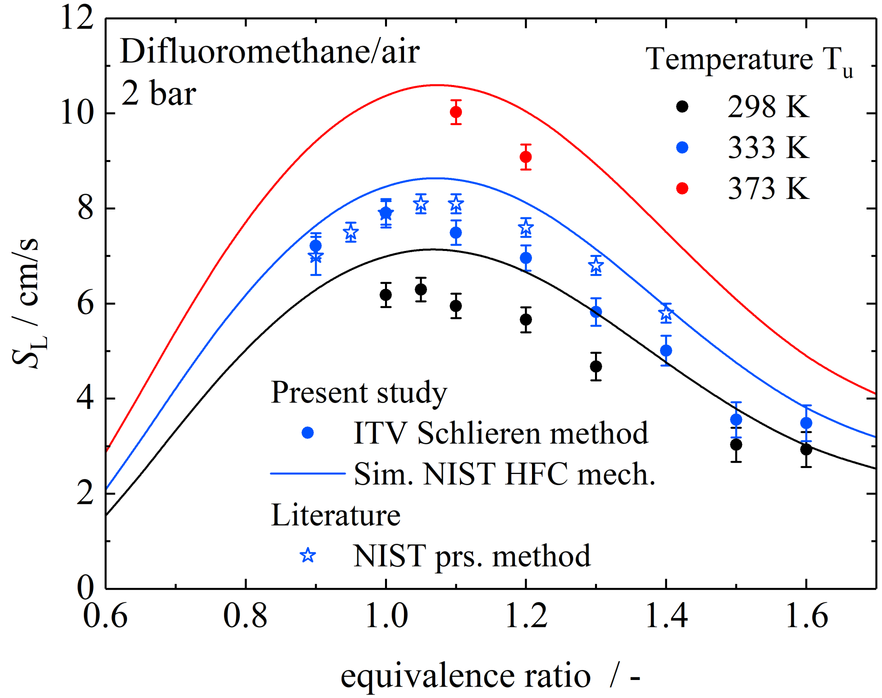
Results comparison - R32 case
Pressure and temperature sensitivity

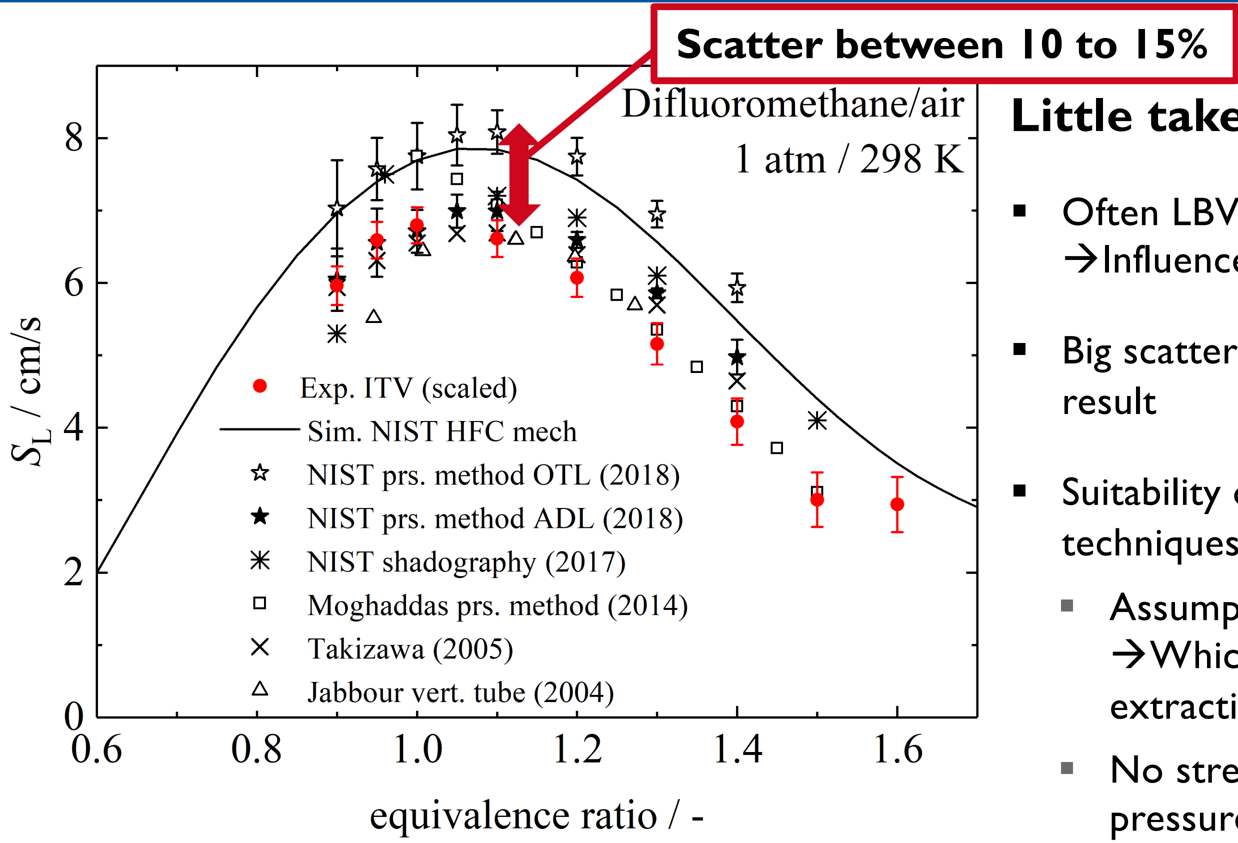




Agreement seems within the limits of comparison >>> OTM vs adiabatic

Simulation performed with detailed mechanism provided by NIST: R. Burgess, Jr et al., submitted to Combust. Flame (2019)

Results comparison - R32 case
ITV data scaled to ambient conditions



Little take away:

- Often LBV obtained with adiabatic model
  →Influence of radiation unknown
- Big scatter between adiabatic and radiation result
- Suitability of the different measurement techniques has to be further assessed:
  - Assumption of perfect spheres
    →Which flame radius for flame speed extraction in buoyant flames?
  - No stretch effects taken into account in pressure model (+/- 12 %[1])

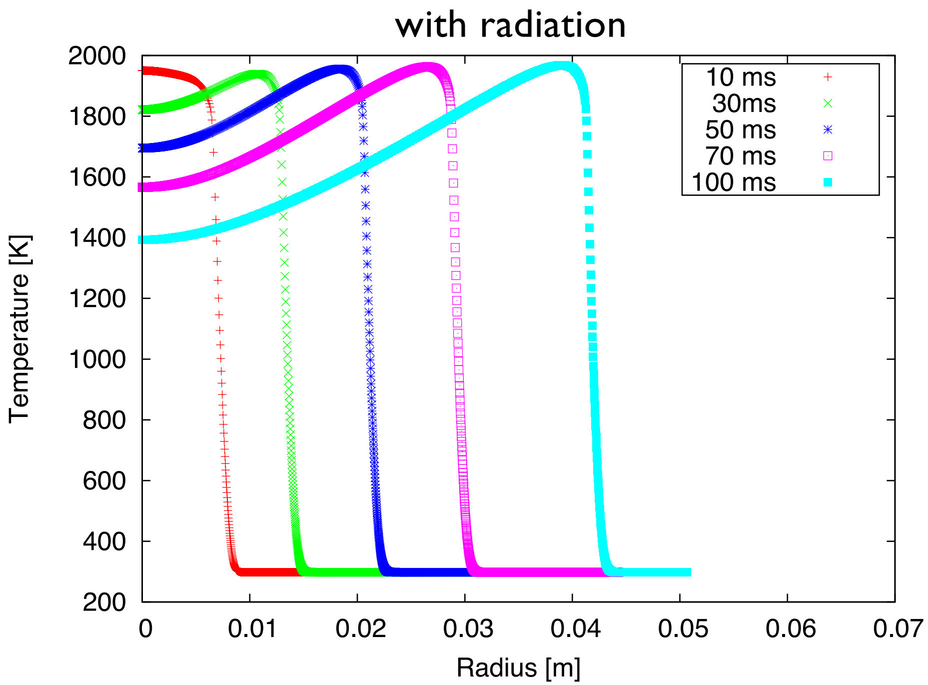
Assess buoyancy and radiation effects by DNS simulations

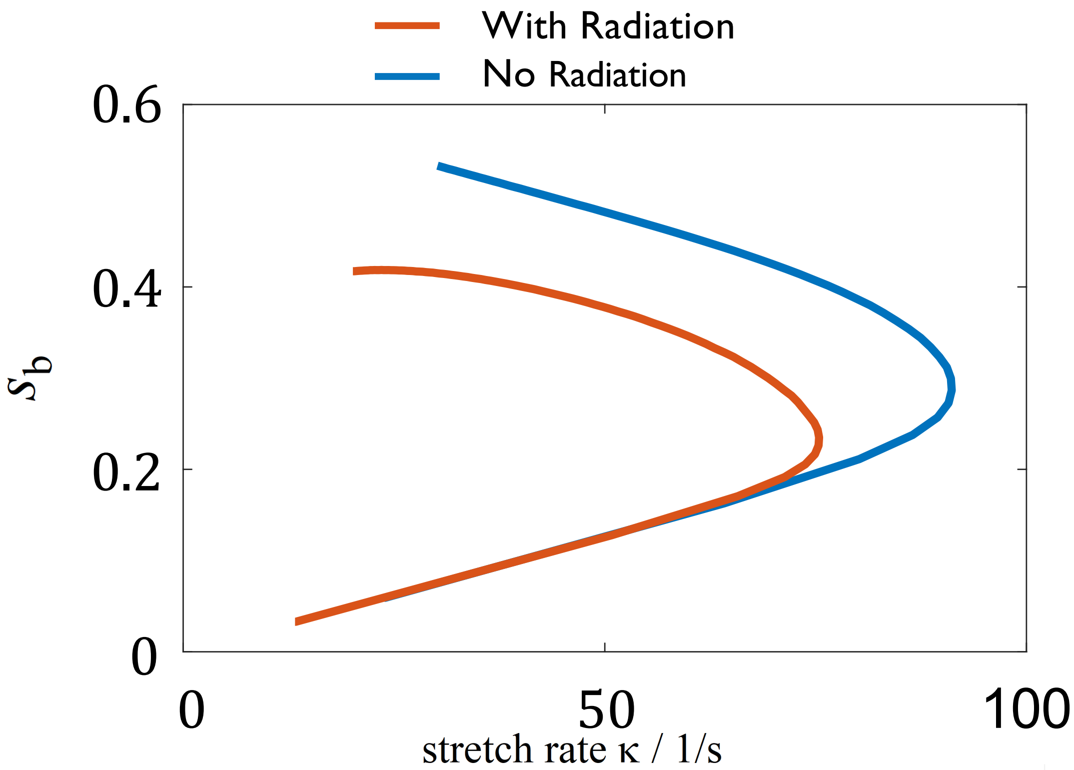
[1] *Burrel et al., Proc. Combust. Inst. (2019)*

Results comparison - R32 case
Radiation

$$\dot{Q} = 4\sigma(T^4 - T_b{}^4)\sum_i (p_i a_{p_i}) \left\{ \begin{array}{l} \text{Species:} \\ CO_2, CO, H_2O, CH_4, \text{HF} \end{array} \right.$$

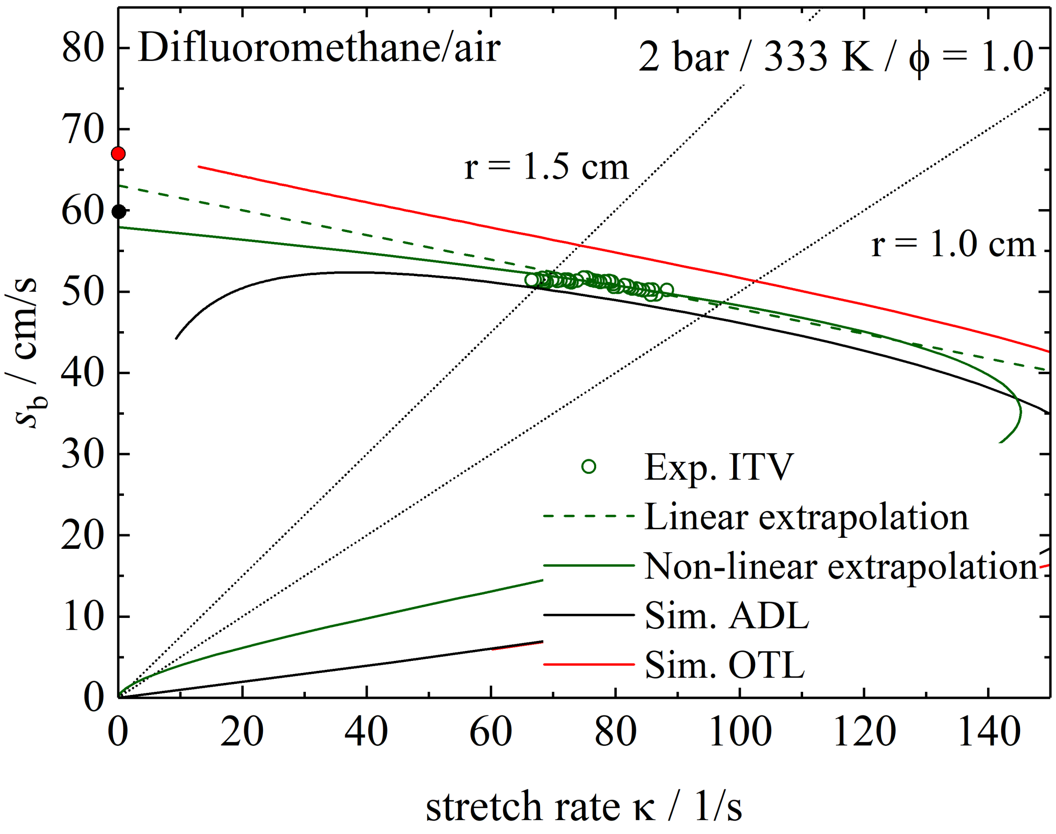
R-32 spherical flame
(ϕ = 1.0, 1bar, T_u=298K)





Simulation with FlameMaster code, 1D spherical flame module

Results comparison - R32 case
Radiation

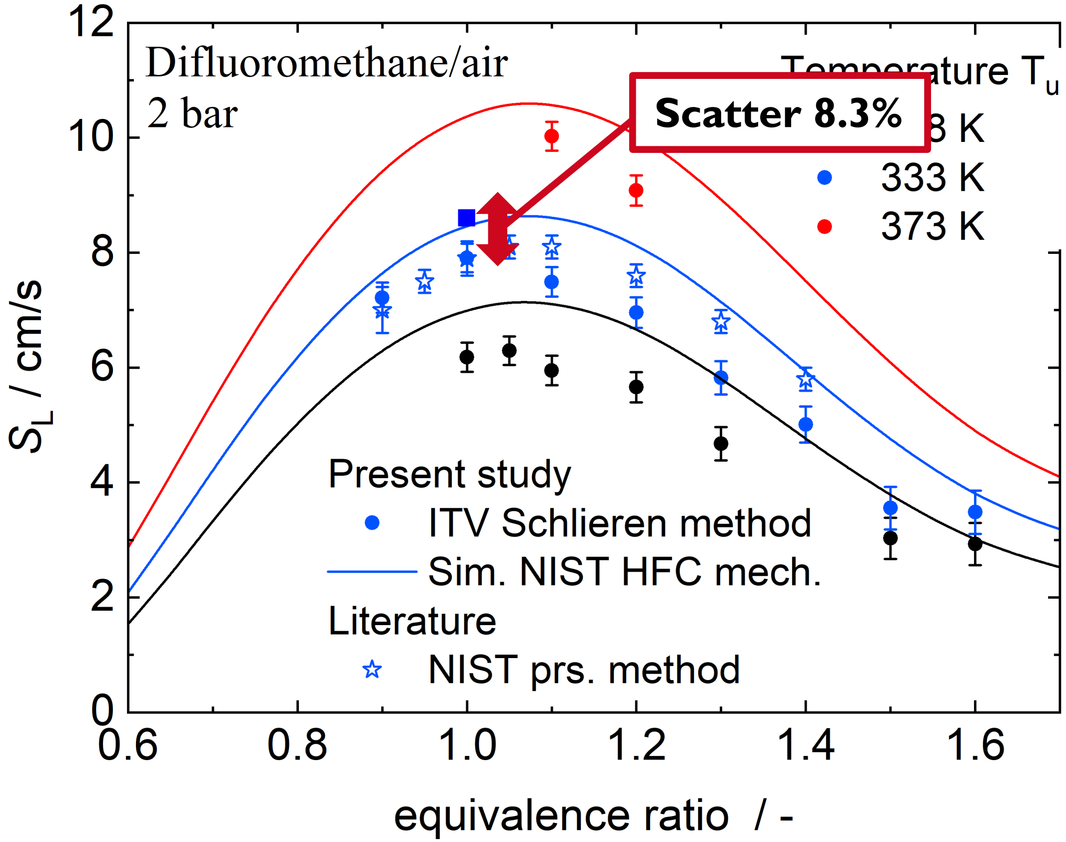


Little more take away:

- Exp. raw data can be used together:
  - Upper limit (adiabatic, red circle)
  - Lower limit (OTM, black circle)
- Exp. data do not need to be between simulation before mechanism modification

Simulation with FlameMaster code, 1D spherical flame module

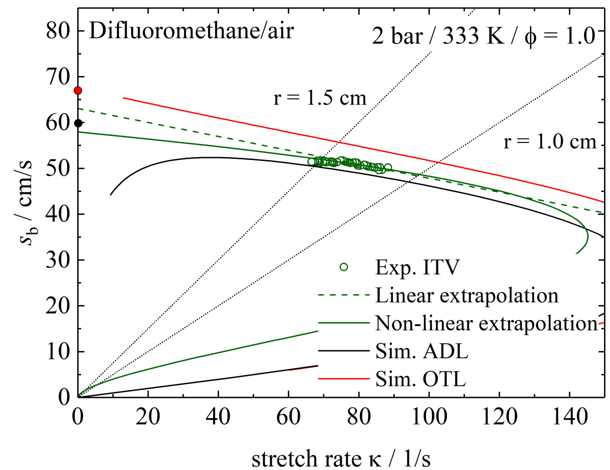
Results comparison - R32 case
Radiation



Little more take away:

- SL, EXP (ADIABATIC) = 7.90 cm/s
- SL,EXP (OTM) = 8.614 cm/s

→ 8.3% difference

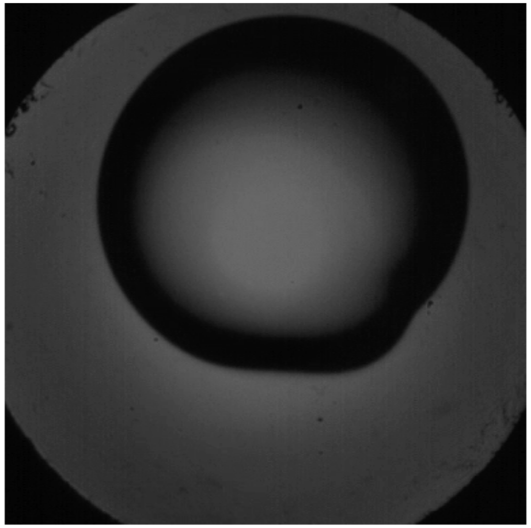


Simulation with FlameMaster code, 1D spherical flame module

Results – DNS simulation
Buoyancy

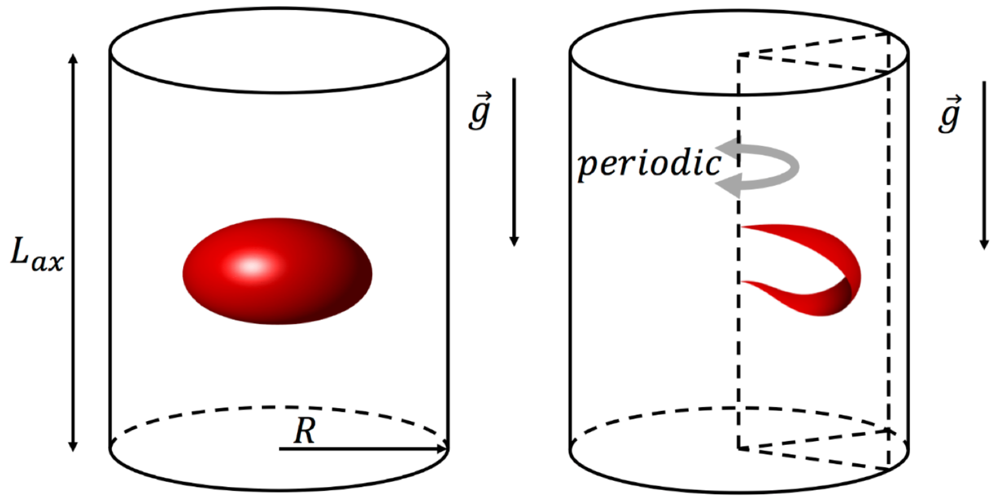
Berger et al.; ECM 2019 Poster

CH_4 / ϕ = 0.6 / 2.5 bar / 298 K



Laser ignition

DNS:



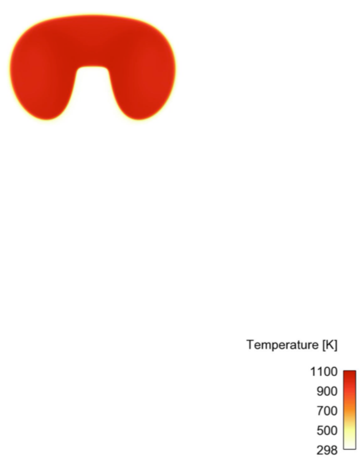
Variation of flame speed by dilution

- Diluted H_2 ($\phi = 1.8, T_u = 298K, p = 1bar$)
- CH_4

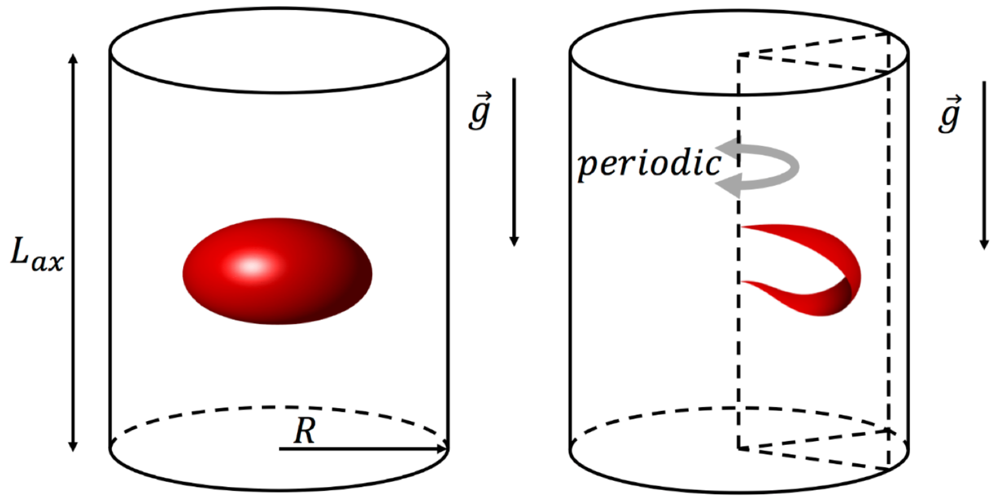
Results – DNS simulation
Buoyancy

Berger et al.; ECM 2019 Poster

Diluted H_2 ($\phi = 1.8, T_u = 298K, p = 1bar$)



DNS[1]:



Variation of flame speed by dilution

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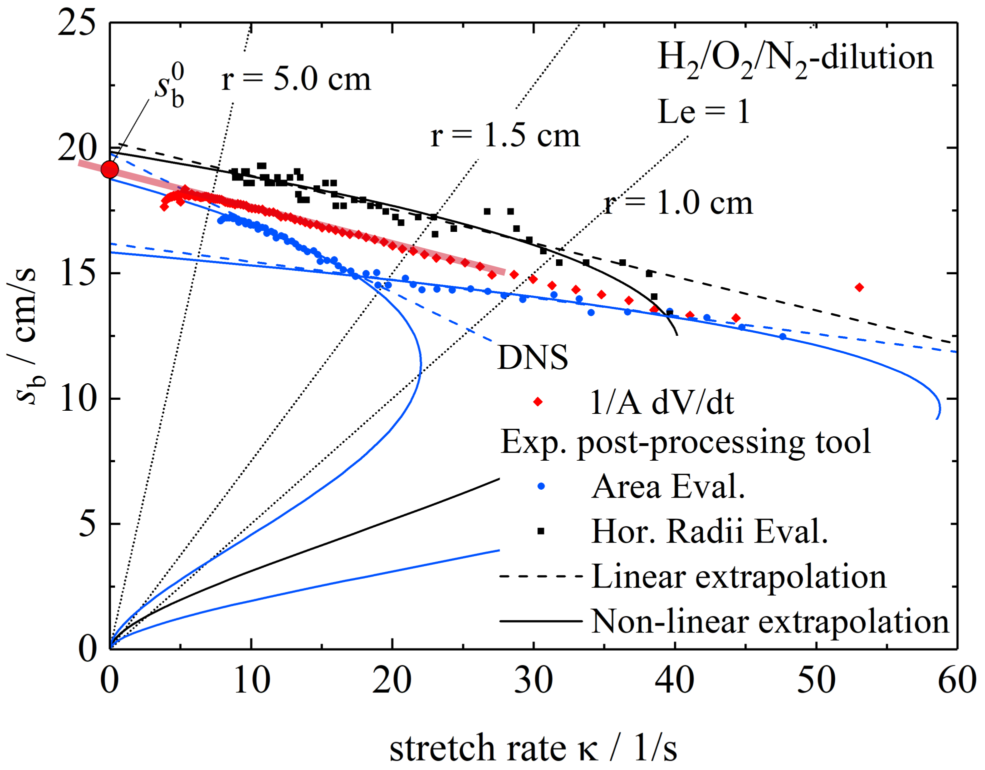
Results – DNS simulation
Buoyancy



Method 1/A dV/dt seems promising

Take away:

- Exp. post processing tools either:
  - Underpredict (Area Eval.)
  - Overpredict (Hor. Radii Eval.)
- Proposed DNS extrapolation agrees well with unstretched value

Outline

- Experiments and Methodologies
- Results
- Summary/Outlook

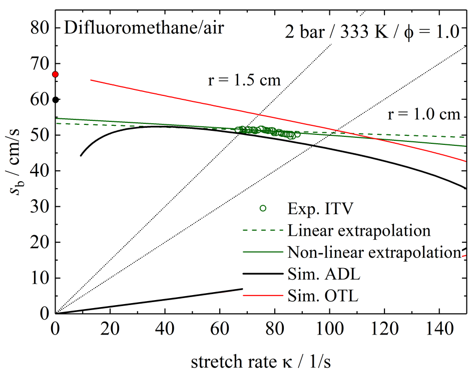
Summary/Outlook

Summary:

- Non-linearities in extrapolation very pronounce at ambient conditions
  → Increase pressure and temperature to use linear extrapolation
- Effect of radiation is very pronounce and cannot be described satisfactory
- Buoyancy for R32 in acceptable range

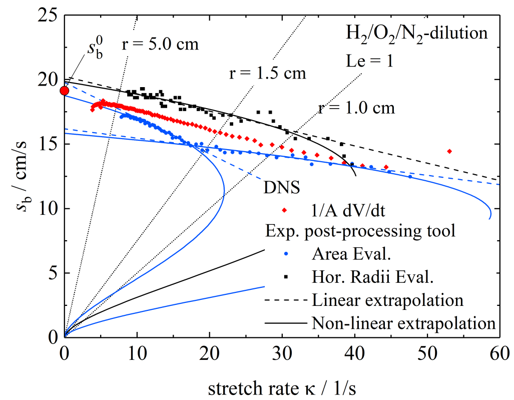
Outlook (I):

- Uncertainty description due to radiation (model)
- Investigate stretch/strain
- Quantify effect of radiation in experiments



Outlook (II):

- PIV measurements
- New methodology for buoyant flames based on: experiments/DNS



Institute for Combustion Technology | Joachim Beeckmann | 3rd LBV workshop

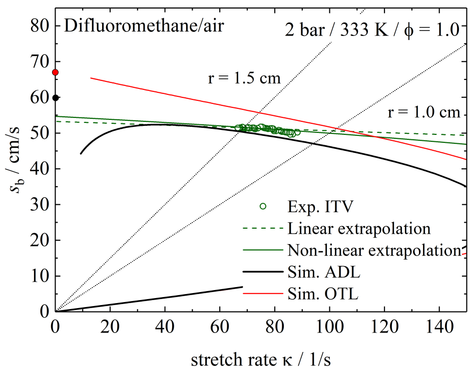
Driving questions:

Summary:

- What uncertainty do we need for flammability metrics?
- Is 15% enough?
- Hybrid method:
  - How to use optical and pressure based method best? (also couple together with simulations?)
- What is limit for buoyant flames?

Outlook (I):

- Uncertainty description due to radiation (model)
- Investigate stretch/strain
- Quantify effect of radiation in experiments



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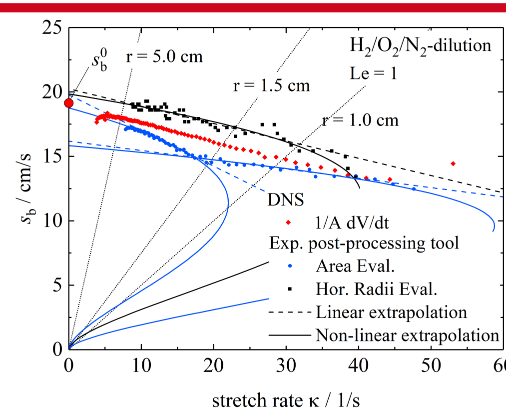

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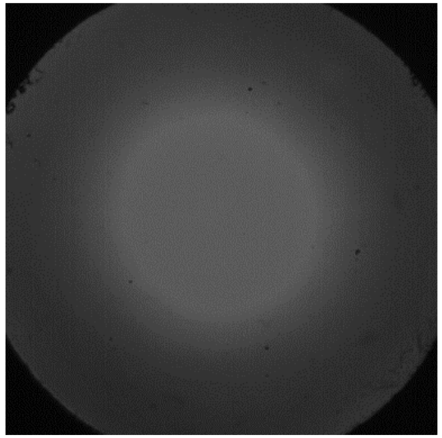
This work was performed as part of the Cluster of Excellence ”Fuel Science Center", which is funded by the Excellence Initiative of the German federal state. The support is gratefully acknowledged.



Thank you for your attention

Joachim Beeckmann

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