Analysis of synthetic flames

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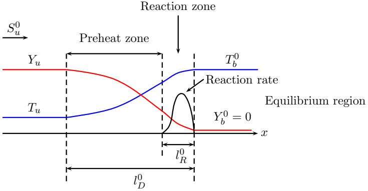
Outline

Definition

The normal propagation velocity of fresh gas relative to a fixed, planar flame front



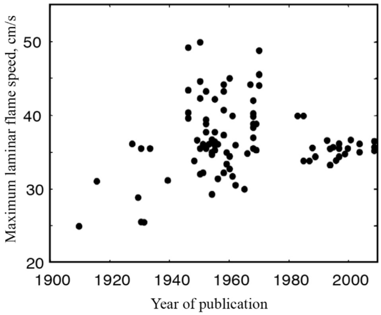
A measure of the mixture reactivity and diffusivity

An important fundamental parameter

- Turbulent combustion models
- Multi-zone internal combustion engine model
- Reaction model development
- Reaction model validation

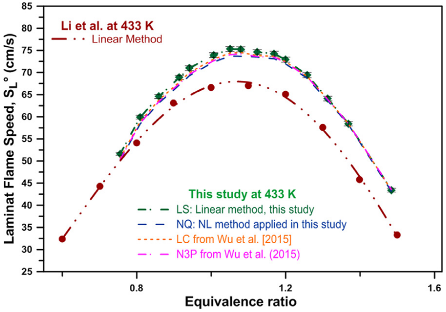
Typical results

CH_4-air



Egolfopoulos et al.

1-pentanol-air



Nativel et al.

Significant improvement since ∼2000

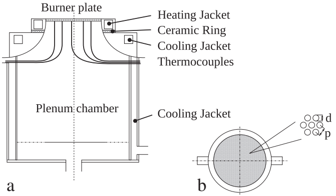
Discrepancies remain

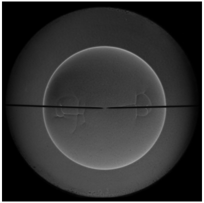
Measurement Techniques

Counter flow

Heat flux burner

Expanding flame



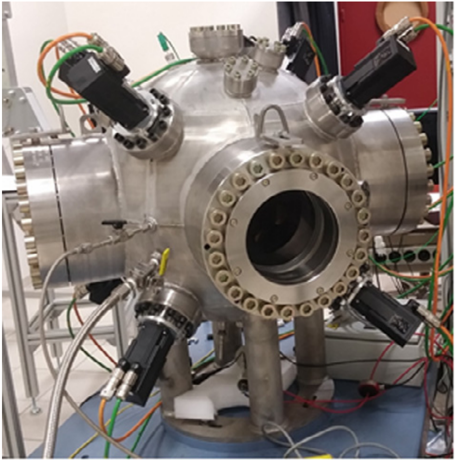


Spherically expanding flame (SEF) is widely used

Enables access to high pressure conditions

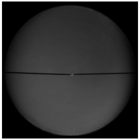
SEF Experiments (1/5)

Typical experimental set-up at ICARE-Orleans

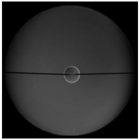


SEF Experiments (2/5)

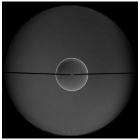
H_2-air mixture. $\Phi = 2$; $P = 82.4$ **kPa;** $T = 296$ **K**



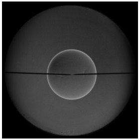
a) $t = 0$ ms



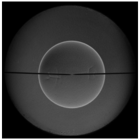
b) $t = 0.72$ ms



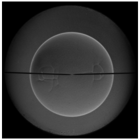
c) $t = 1.52$ ms



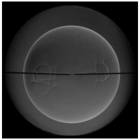
d) $t = 2.32$ ms



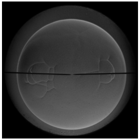
e) $t = 3.12$ ms



f) $t = 3.92$ ms

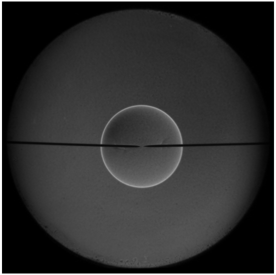


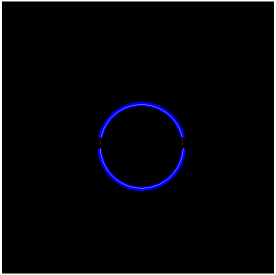
g) $t = 4.52$ ms

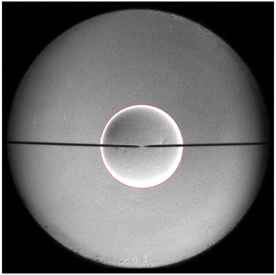


h) $t = 5.12$ ms

Flame radius measurement (in-house code from ICARE-Orleans)

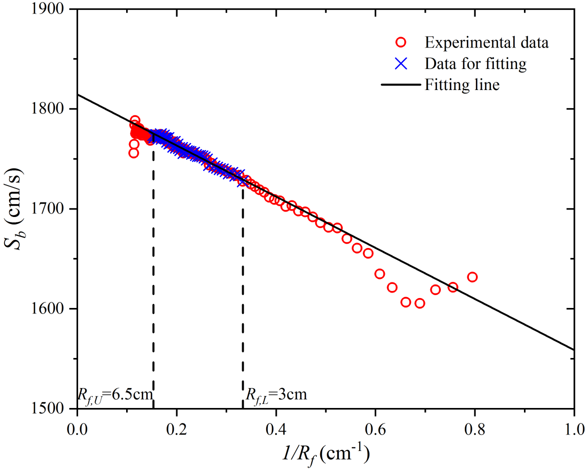






SEF experiments (4/5)

Extrapolation to zero-stretch rate



SEF experiments (5/5)

Perturbations for SEF experiments (Lipatnikov et al.)

i. Spark ignition energy (small radii)
ii. Confinement effects (large radii)
iii. Heat losses through radiation (large radii)
iv. Product density non-uniformity (small radii)
v. Compression effects (large radii)
vi. Flame instabilities (large radii)
vii. Stretch effects (all radii)

Focus on the effect of extrapolation method

Extrapolation Models

- Linear stretch (LS): $S_b = S_b^0 - L_B \kappa$
- Linear curvature (LC): $S_b = S_b^0 - 2S_b^0 L_B / R_f$
- Nonlinear quasi-steady (NQ): $\ln(S_b) = \ln(S_b^0) - 2S_b^0 L_B / (R_f S_b)$
- Finite thickness expression (FTE):

$$\left(S_b/S_b^0 + 2\delta^0/R_f\right) \ln\left(S_b/S_b^0 + 2\delta^0/R_f\right) = -2\left(L_B - \delta^0\right)/R_f$$

- Taylor expansion of nonlinear model (NE) about L_B/R_f:

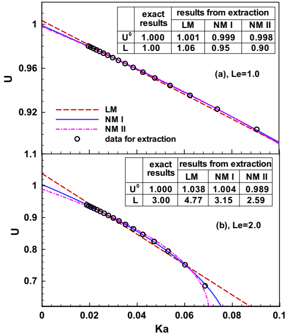
$$S_b/S_b^0 \left(1 + 2L_B/R_f + 4L_B^2/R_f^2 + 16L_B^3/3R_f^3 + ...\right) = 1$$

- Nonlinear model with 3 fitting parameters (N3P):

$$S_b/S_b^0 = 1 - L_B/R_f + C/R_f^2$$

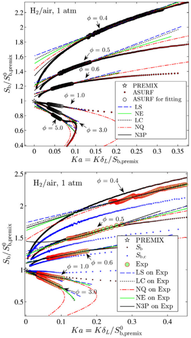
Extrapolation Behavior

Chen



CH_4-air

Wu et al. (2014)



H_2-air

Liang et al. (2016)

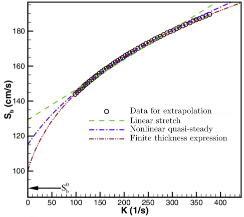


*Figure font modified from original article by Coronel

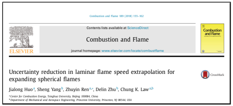
H_2-air

Evaluation of Models (1/2)

How are extrapolation results affected by data set characteristics?

- Range of flame radii, radius upper and lower bounds, number of points in data set, noise in data, etc.

Huo et al. 2018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Uncertainty reduction in laminar flame speed extrapolation for expanding spherical flames

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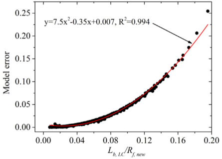


- Error = $7.5x^2 - 0.35x + 0.007$

$$x = L_{B,LC}/R_{f,\text{new}}$$

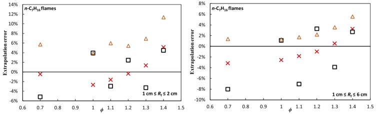
$$R_{f,\text{new}} = \frac{R_{f,L} R_{f,U} \sqrt{s^2+1}}{-sR_{f,L} + R_{f,U}}$$

$$s = -1.72$$

- Error less than 2% when $L_B/R_{f,\text{new}} < 0.06$
- At least 30 points recommended for extrapolation

Evaluation of Models (2/2)

Jayachandra et al. 2015



Error values represented by symbols: (×) linear method for S_b; (□) non-linear method for S_b; and (△) non-linear method for U_n.

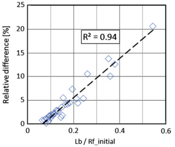
- Relative error decreased when increasing flame radius range: $10 \leq R_f \leq 20$ mm to $10 \leq R_f \leq 60$ mm

Halter et al. 2010


Combustion and Flame

Nonlinear effects of stretch on the flame front propagation

F. Halter, T. Tahtouh, C. Mounaïm-Rousselle



- Comparison of linear and nonlinear methodologies
- CH_4/air, iso-octane/ air ($P = 100$ kPa, $T = 300$ and 400 K)
- For $\Phi = 0.8$, the relative difference between the two model results is reduced to 1% from 10% when increasing the initial radius from 8 mm to 20 mm

Conclusions/Summary of Previous Work

- Extrapolation results are affected by the flame radius range and data set size
- A systematic study on effect of data set size has not been performed (experimentally or numerically)
- Nonlinear model is accurate for mixtures with small Lewis number
- Linear curvature model is accurate for mixtures with large Lewis number
- Models can lead to large errors away from stoichiometric conditions

Objective of Present Study

Objective

- Systematically evaluate nonlinear model by varying data range and size, and noise levels
- Evaluate relative differences between linear and nonlinear models

Approach

- Generate synthetic data through integration of nonlinear expression
  - Experimental data generation is expensive and time consuming
  - Numerical simulations can be computational expensive
- Introduce noise to simulate experimental environment
- Assess recovery of flame parameters by quantifying uncertainty and standard deviation

Outline

Methodology

Extrapolation models (recall)

- Linear stretch:

$$S_b = S_b^0 - L_B \kappa$$

- Nonlinear quasi-steady:

$$\ln\left(S_b\right) = \ln\left(S_b^0\right) - 2S_b^0 \frac{L_B}{R_f S_b}$$

Definitions

- R_f : flame radius; $\kappa = 2S_b/R_f$: stretch rate; S_b : $\mathrm{d}R_f/\mathrm{d}t$

Parametric Study

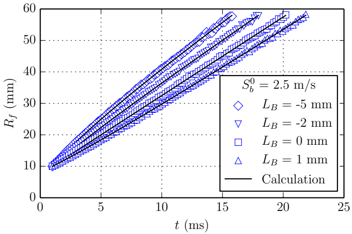
	Synthetic	Experimental
Range	$R_f = [R_{f,L}, R_{f,U}]$ 1% noise; $R_{f,L} = 10$ mm $R_{f,U} = \{25, 38, 58, 70\}$ mm	$R_{f,N}$: combustion vessel windows and flame instabilities; $R_{f,L}$: initial energy deposition
Size	$\lvert R_f \rvert = \{10, 20, 50, 100\}$ $R_{f,L} = 10$ mm; $R_{f,U} = 58$ mm; 1% noise	Camera framing rate; mixture composition; initial energy deposition
Noise	Gaussian: $1, 3, 5, 10\%$ $R_{f,L} = 10$ mm; $R_{f,U} = 58$ mm; $\lvert R_f \rvert = 100$	Camera resolution; flame sphericity; flame detection algorithm; flame instabilities

Data Generation

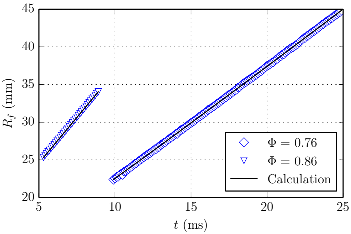
- Numerically integrate (`ode15i`) equation below to obtain $R_f(t)$ for values of S_b^0 and L_B

$$\frac{1}{S_b^0}\frac{\mathrm{d}R_f}{\mathrm{d}t}\ln\left(\frac{1}{S_b^0}\frac{\mathrm{d}R_f}{\mathrm{d}t}\right) = -2\frac{L_B}{R_f}$$

- Add different levels of Gaussian noise to synthetic $R_f(t)$
- R_f will have size $|R_f|$, lower bound $R_{f,L}$, and upper bound $R_{f,U}$



$|R_f| = 100$, $[R_{f,L}, R_{f,U}] = [10, 58]$ mm, 1% noise



Experimental flame radius: *n*-hexane/air

Steps to Solve for S_b^0 and L_B (1/2)

1. Use synthetic $R_f(t)$ in analytic solution of linear model to find S_b^0 and L_B

$$S_b = S_b^0 - L_B \kappa \rightarrow \frac{\mathrm{d}R_f}{\mathrm{d}t} = S_b^0 - 2\frac{L_B}{R_f}\frac{\mathrm{d}R_f}{\mathrm{d}t}$$

$$\boldsymbol{S_b^0}(t - t_U) = R_f - R_{f,U} + 2\boldsymbol{L_B} \ln\left(\frac{R_f}{R_{f,U}}\right) + C$$

2. Solutions of linear model, $S^0_{b,\mathrm{guess}}$ and $L_{B,\mathrm{guess}}$, used as initial guesses in nonlinear model

$$\frac{1}{S^0_{b,\mathrm{guess}}}\frac{\mathrm{d}R_f}{\mathrm{d}t} \ln\left(\frac{1}{S^0_{b,\mathrm{guess}}}\frac{\mathrm{d}R_f}{\mathrm{d}t}\right) = -2\frac{L_{B,\mathrm{guess}}}{R_f}$$

3. Integration of nonlinear differential equation yields new values of $R_f(t) : R_f^{\mathrm{trial}}$

Steps to Solve for S_b^0 and L_B (2/2)

4. Objective function calculated

$$z = \sum_{i=0}^{N} \left[R_f - R_f^{\text{trial}} \right]^2$$

   where i corresponds to the i^{th} data point and N is the size of R_f

5. L_B and S_b^0 are iteratively refined by minimizing the objective function using the Levenberg-Maarquardt minimization algorithm

Uncertainty

- Jacobian

$$J_{ik}^2 = \frac{\partial^2 r_i}{\partial a_k^2} \text{ where } r_i = R_{f,i} - R_{f,i}^{\text{trial}} \text{ and } a_k = \{L_B, S_b^0\}$$

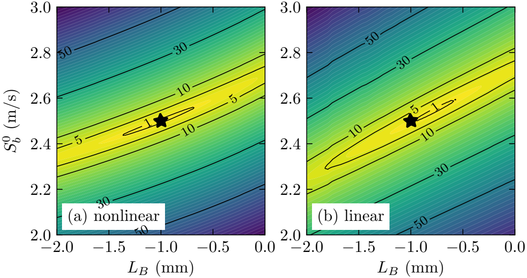
$$\Delta a_k = \left[3 \sum_i^N \Delta R_{f,i}^2 / \sum_i J_{ik}^2 \right]^{1/2}$$

- $\Delta R_{f,i}$: uncertainty in the i^{th} point; $\Delta a_k = \{\Delta L_B, \Delta S_b^0\}$

Outline

Performance of Levenberg-Maarquardt minimization algorithm

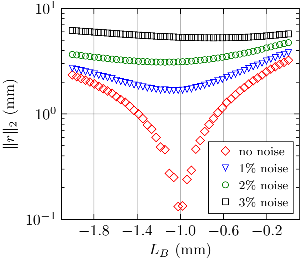
- Synthetic data generated for $S_b^0 = 2.5$ m/s and $L_B = -1$ mm (no added noise) using nonlinear model



- Elongated contours characteristic of linear and nonlinear expressions

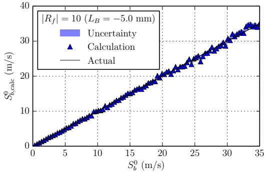
How much is L_B affected by noise?

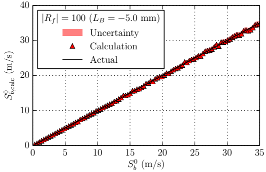
- Global minimum at the correct solution; shallower minimum as noise increases
- Shifted to more negative Markstein lengths as noise increases (not the case for 3%)
- Minimum error behavior is consistent across different types of noise (e.g. uniform noise and noise that decreases with increasing flame radius)



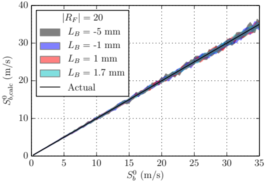
Effect of Size on S_b^0: $S_b^0 \in [0.3, 35]$ m/s; $L_B = \{-5.0, -1.0, 1.0, 1.7\}$ mm

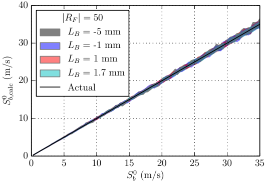
$R_{f,L} = 10$ mm, $R_{f,U} = 58$ mm, $|R_f| = \{10, 20, 50, 100\}$; 1% Gaussian noise





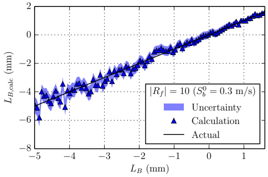
- 10 points: incorrect S_b^0 calculation in the range $S_b^0 \in [18, 35]$ m/s
- 100 points: correct S_b^0 calculation (within the uncertainty) over entire S_b^0 range
- ~50 points: correct S_b^0 calculation for $L_b = \{-5.0, -1.0, 1.0, 1.7\}$ mm



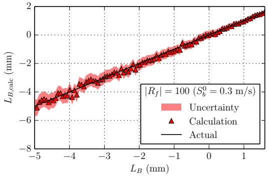


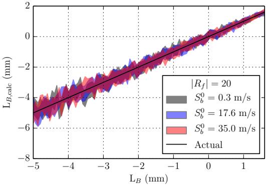
Effect of Size on L_B: $S_b^0 = \{0.3, 17.6, 35.0\}$ m/s; $L_B \in [-5.0, 1.7]$ mm

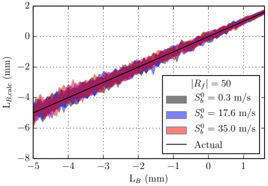
$R_{f,L} = 10$ mm, $R_{f,U} = 58$ mm, $|R_f| = \{10, 20, 50, 100\}$; 1% Gaussian noise



- 10 points: incorrect L_B calculation in the range $L_B \in [-5, -1]$ mm
- 100 points: correct L_B calculation (within the uncertainty) over entire L_B range
- ~50 points: correct L_B calculation for $S_b^0 = \{0.3, 17.6, 35.0\}$ m/s

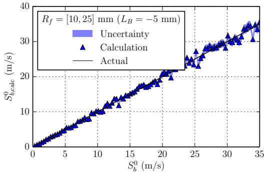


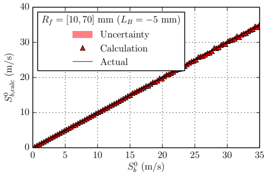




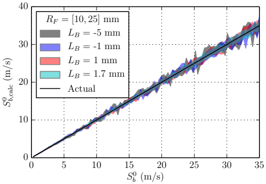
Effect of Range on S_b^0: $S_b^0 \in [0.3, 35]$ m/s; $L_B = \{-5.0, -1.0, 1.0, 1.7\}$ mm

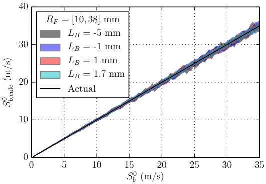
$R_{f,L} = 10$ mm, $R_{f,U} = \{25, 38, 58, 70\}$ mm, $|R_f| = 100$; 1% Gaussian noise





- $R_{f,U} = 25$ mm: incorrect S_b^0 calculation in the range $S_b^0 \in [8, 35]$ m/s
- $R_{f,U} = 70$ mm: correct S_b^0 calculation (within the uncertainty) over entire S_b^0 range
- $\sim R_{f,U} = 38$ mm: correct S_b^0 calculation for $L_b = \{-5.0, -1.0, 1.0, 1.7\}$ mm

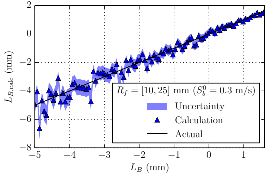


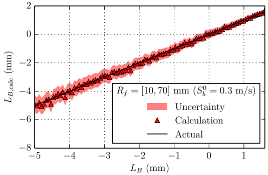


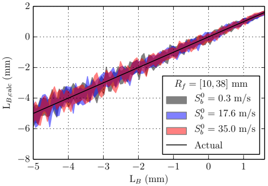
Effect of Range on L_B: $S_b^0 = \{0.3, 17.6, 35.0\}$ m/s; $L_B \in [-5.0, 1.7]$ mm

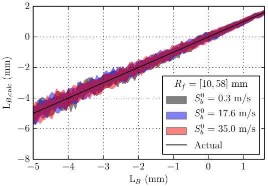
$R_{f,L} = 10$ **mm,** $R_{f,U} = \{25, 38, 58, 70\}$ **mm,** $|R_f| = 100$**;** 1% **Gaussian noise**

- $R_{f,U} = 25$ mm: incorrect L_B calculation in the range $L_B \in [-5, 0]$ mm
- $R_{f,U} = 70$ mm: correct L_B calculation (within the uncertainty) over entire L_B range
- $\sim R_{f,U} = 58$ mm: correct L_B calculation for $S_b^0 = \{0.3, 17.6, 35.0\}$ m/s



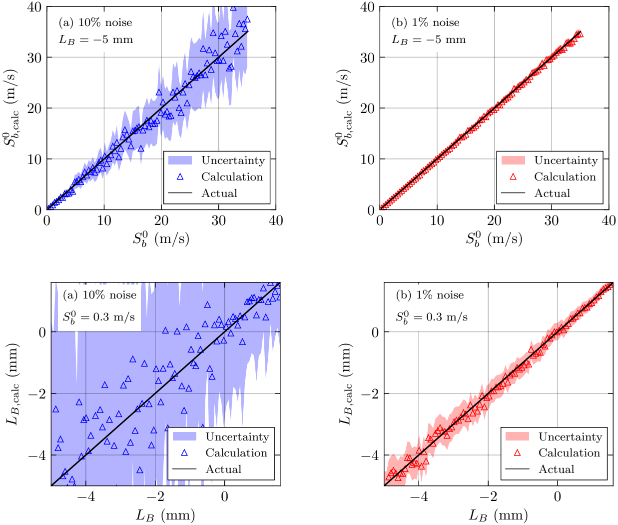






Effect of Noise

$R_{f,L} = 10$ mm, $R_{f,U} = 58$ mm, $|R_f| = 100$; $1, 3, 5, 10\%$ Gaussian noise



Outline

Conclusions

- The objective function exhibits a shallow minimum that depends only weakly on the Markstein length
- When noise is added to the synthetic data, the local minimum in the objective function becomes shallower
- To determine the flame speed and Markstein length with accuracy and minimize the uncertainty, the present results indicate that the experiments should result in data with a large number of points (> 50), a large flame radius range (> 58 mm), and low noise

Acknowledgment

Thank you