Experimental *n*-Hexane-Air Expanding Spherical Flames

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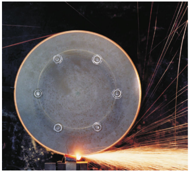
Outline

Thermal Ignition Hazards

Motivation: understand thermal ignition hazards present in the aviation, nuclear, mining, and manufacturing sectors.

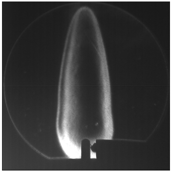


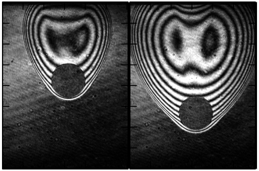
Frictional sparks and hot spots[†]

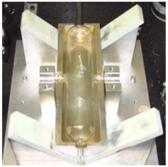
China Air flight 120, 2007

TWA flight 800, 1996

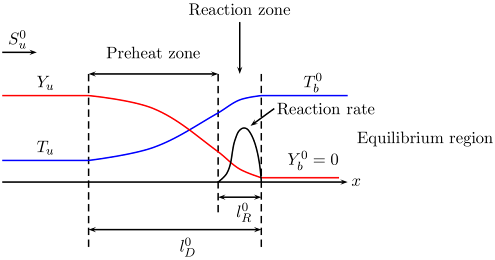
Previous work: extensive work has been performed at Caltech in the context of aviation safety using ***n*-hexane** as a surrogate for kerosene.







Laminar Flame Properties



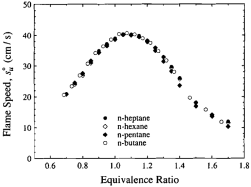
Why study flame properties?

- Development of clean combustion technologies
- Development of cleaner alternative fuels
- Goals motivate the development and validation of **chemical reaction mechanisms**
    - Turbulent combustion models
    - Multi-zone internal combustion engine model

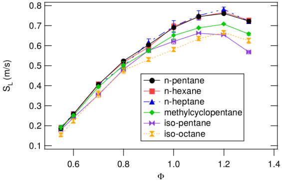
Why study *n*-hexane?

- Ease of use in laboratory environment (high vapor pressure)
- "Simple" single component surrogate for kerosene based fuels
- Limited number of studies

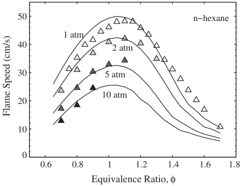
Davis and Law (1998)



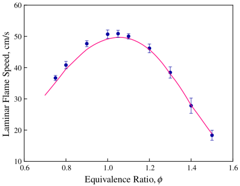
Farrell et al. (2004)



Kelley et al. (2010)



Ji et al. (2010)

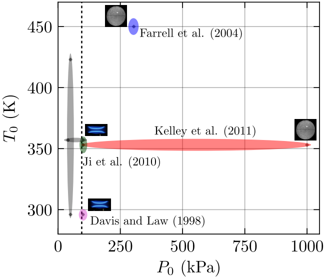


n-Hexane Previous Studies

Pressure conditions ≥ 100 kPa

Ref.	P_0 (kPa)	T_0 (K)	Φ	N
[1]	100	300	0.85 – 1.70	16
[2]	304	450	0.55 – 1.30	9
[3]	100	353	0.75 – 1.70	19
[3]	100 – 1000	353	0.9	4
[4]	100	353	0.75 – 1.50	10

- Experiments at pressure conditions of ≤ 100 kPa, relevant to conditions in aircraft fuel tanks, have not been performed



Objective of Present Study

Objective

- Obtain laminar flame properties at sub-atmospheric conditions ($P_0 \leq 100$ kPa)

Effect	P_0 (kPa)	T_0 (K)	Φ	N
Pressure	$40 - 100$	357	0.9	4
Temperature	50	$296 - 423$	$0.9, 1.1, 1.4$	15
Composition	100	296	$0.76 - 1.42$	7
	50	296	$0.86 - 1.90$	12

Approach

- Perform spherically expanding flame experiments
- Use nonlinear extrapolation methodology to extract flame properties
- Compare experimental results with several chemical kinetic mechanisms

Outline

Introduction

Methodology

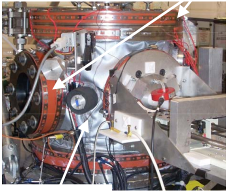
Results & Discussion

Summary & Conclusions

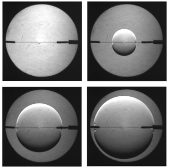
Experimental Setup

Spherically expanding flame experimental setups

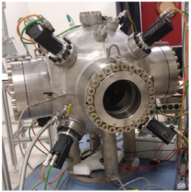
GALCIT



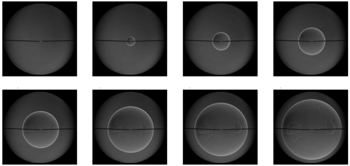
22 L cylindrical
$10,000$ fps (Phantom v711)
512×512 px^2



ICARE



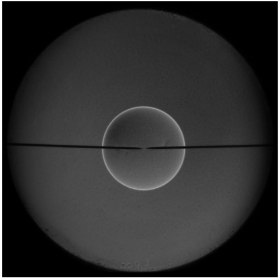
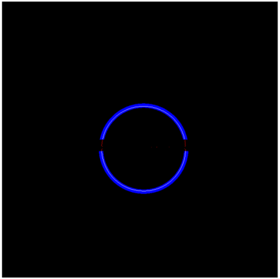
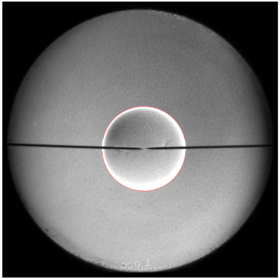
56 L spherical
$25,000$ fps (Phantom v1610)
768×768 px^2



Extracting Flame Radii

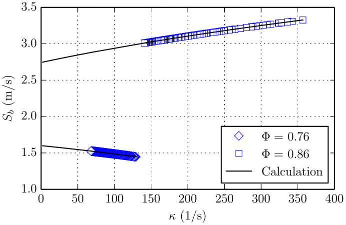
Flame radius extraction software developed at ICARE

- Apply mask: removes background (electrodes)
- Edge detection operator: Canny
- Fit detected edge: ellipse
- Ellipse: obtain equivalent flame radius R_f

Extracting Flame Parameters

- LS: $S_b = S_b^0 - L_B \kappa$
- LC: $S_b = S_b^0 - 2S_b^0 L_B / R_f$
- **NQ:** $\ln\left(S_b\right) = \ln\left(S_b^0\right) - 2S_b^0 L_B / \left(R_f S_b\right)$
- FTE:
  $\left(S_b/S_b^0 + 2\delta^0/R_f\right)\ln\left(S_b/S_b^0 + 2\delta^0/R_f\right) = -2\left(L_B - \delta^0\right)/R_f$
- NE: $S_b/S_b^0\left(1 + 2L_B/R_f + 4L_B^2/R_f^2 + 16L_B^3/3R_f^3 + \ldots\right) = 1$
- N3P: $S_b/S_b^0 = 1 - L_B/R_f + C/R_f^2$



$\kappa = 2S_b/R_f$: stretch rate

$S_b = \mathrm{d}R_f/\mathrm{d}t$: unstretched flame speed

δ^0 : flame thickness

L_b : Markstein length

Implementation of Nonlinear Methodology (1/2)

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

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

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

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

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

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

Implementation of Nonlinear Methodology (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
6. Calculate S_u^0 through expansion ratio: $S_u^0 = S_b^0/\sigma$ where $\sigma = \rho_u/\rho_b$

1-D freely propagating flame calculations using FlameMaster

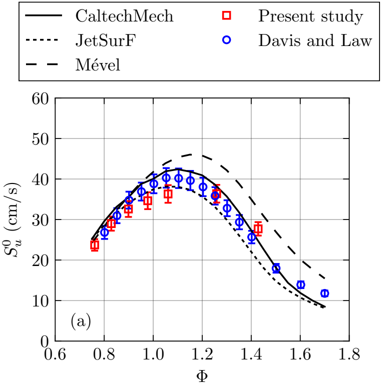
- Neglect Soret and Dufour effect
  - Xin et al. (2012): $1-2\%$ increase in S_u^0 when accounting for Soret effect in *n*-heptane-air
  - Bongers and Goey (2003): Dufour effect negligible in C_3 laminar premixed flames
- Mixture-averaged formulation for the transport properties
  - Ji et al. (2010): 1 cm/s increase in S_u^0 of C_5-C_{12} flames

Chemical kinetic mechanisms

- CaltechMech: 172 species and $1,119$ reactions; importance on modeling of formation of soot precursors for fuel surrogates
- JetSurF: 348 species and $2,163$ reactions
- Mével: 531 species and $2,628$ reactions; validated for ignition delay time

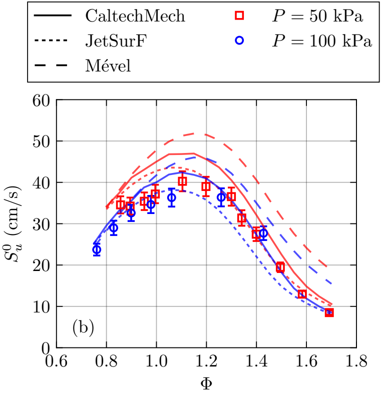
Outline

Comparison with previous work



- A Mann-Whitney-Wilcoxon (MWW) RankSum test indicates that differences are not statistically significant

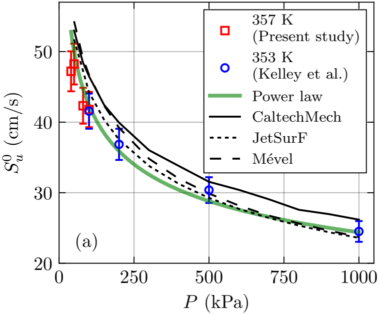
Comparison of flame parameters at 50 kPa and 100 kPa



- The MWW RankSum test indicates that the differences in S_u^0 at 100 kPa and 50 kPa are not statistically significant

Pressure Effect on S_u^0

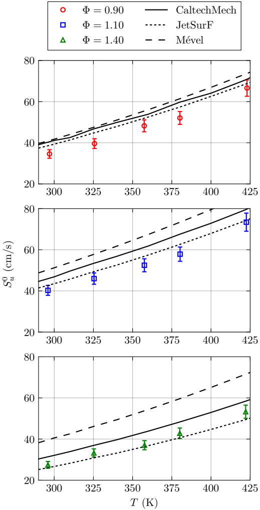
Flame parameters at $40 - 1000$ kPa and 353 and 357 K



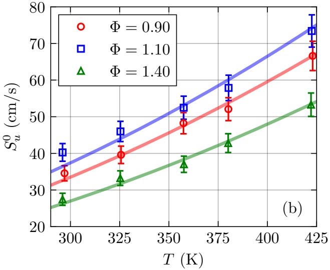
- S_u^0 decreases 20% between 50 and 100 kPa
- S_u^0 decreases 53% between 50 and 1000 kPa
- Power law: $S_u^0(P) = 128 \times P^{-0.24}$ (P has units of kPa) standard deviations for the pre-exponential and exponent are 12 and 0.02, respectively

Temperature Effect on S_u^0

Flame parameters at 50 kPa and $296 - 422$ K

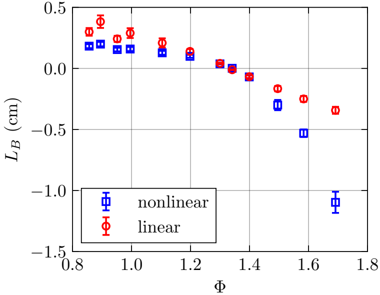


- From 296 K to 422 K, S_u^0 increases by approximately 93%, 82%, and 94% for $\Phi = 0.90, 1.10,$ and,1.40, respectively
- Profiles can be fit to power law, $S_u^0 \sim T^2$, shown below



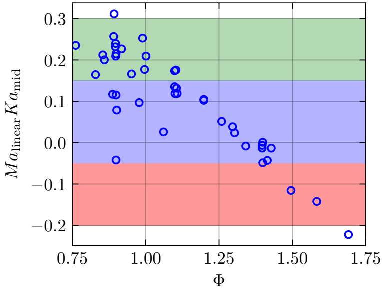
Markstein Length (1/2)

Flame parameters at 50 kPa and $\Phi = 0.86 - 1.90$



- Lean and rich mixtures exhibit positive and negative Markstein lengths
- The transition from positive to negative L_B occurs at $\Phi = 1.3$
- Deviations of the nonlinear and linear L_B occur for both rich and lean conditions

Flame parameters at 50 kPa and $\Phi = 0.86 - 1.90$

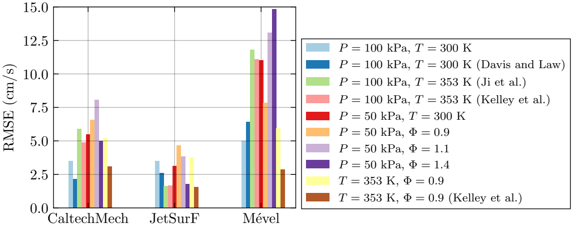


- Ma_{linear} : Markstein number (linear method); Ka_{mid} : Karlovitz number (evaluated at mid-point of flame radii profiles)
- $Ma_{\mathrm{linear}}Ka_{\mathrm{mid}}$ suggested by Wu et al. (2015) to evaluate extrapolation errors
- Blue, green, and red: $\leq 5\%$, $5 - 12\%$, and $5 - 40\%$
- Points in red region: rich conditions (strong flame instabilities)

Root-mean-squared error (RMSE)

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(S_{\mathrm{calc}}^{(i)} - S_{\mathrm{exp}}^{(i)}\right)^2}$$

where N is the number of tests and i is the i^{th} test



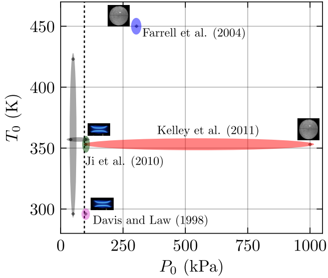
- Mean RMSE: 5.0 cm/s (CaltechMech), 2.8 cm/s (JetSurF), and 9.0 cm/s (Mével)

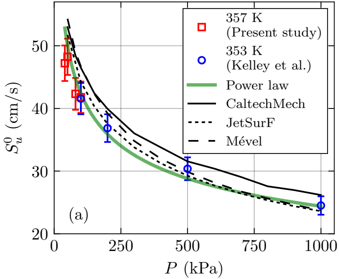
Outline

Summary & Conclusions

- *n*-Hexane-air mixtures characterized through experimental measurements and calculations of the laminar burning speed
- The laminar burning speed was obtained by using a nonlinear methodology
- The laminar burning speed was observed to increase as pressure decreases ($T_0 = 357$ K) and as temperature increases
- Laminar burning speed increases at comparable rates as temperature increases for mixtures $\Phi = 0.90, 1.10, 1.40$
- The predictive capabilities of three chemical kinetic mechanisms was quantified using RMSE
- JetSurF yielded the lowest mean RMSE across a wide range of experimental conditions

Thank you


Farrell et al. (2004)
Kelley et al. (2011)
Ji et al. (2010)
Davis and Law (1998)
450
400
350
300
0
250
500
750
1000
T_0 (K)
P_0 (kPa)


357 K
(Present study)
353 K
(Kelley et al.)
Power law
CaltechMech
JetSurF
Mével
(a)
50
40
30
20
0
250
500
750
1000
S_u^0 (cm/s)
P (kPa)