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# Logistic-Regression-Based Meta-Analysis of Factors Affecting Flame Stability in a Shock Tube

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## ABSTRACT

This work describes a meta-analysis performed in an effort to better understand the parameters controlling flame stability in shock-tube flame experiments. The data set used in the analysis was aggregated from multiple prior studies employing the shock-tube flame speed method, as well as previously unreported results. Flames are first qualitatively classified as being smooth, distorted, or wrinkled based on end-wall images. A subset of trials capturing the stability transition from stable to unstable flames are then selected from each set of experiments. Across all data sets, the transition between stable and unstable flames is analyzed as a binary classification problem using logistic regression. The resulting classification model, cast in terms of a multivariate power-law expression for the critical temperature ( $T_{crit}$ ) at which flames become unstable, is found to be highly predictive of the stability transition. Consideration of the trained model coefficients allows the effects of different experimental parameters on  $T_{crit}$  to be identified. Model parameters provide significant new insight into the selection of diluents in experiments; the use of a test gas with a high heat capacity ratio is found to have the most beneficial effect toward increasing  $T_{crit}$ , while the effects of Lewis number and molecular weight are determined to be negligible. Ignition-location and pressure effects are less well quantified due to limited available data and are identified as key areas of further study.

## ARTICLE HISTORY

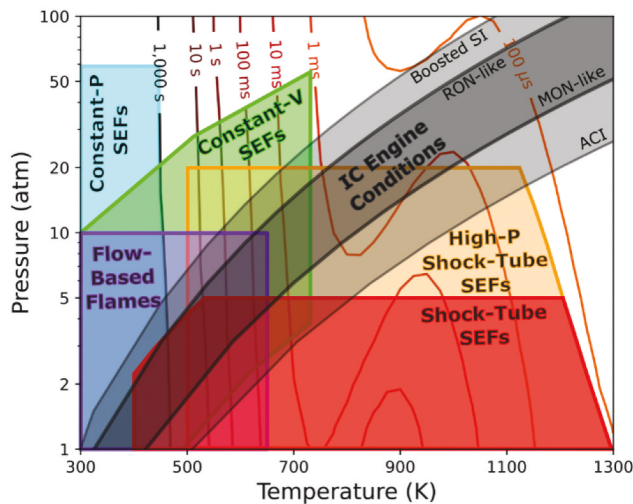
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## KEYWORDS

Shock tube; laminar flame speed; instability

## Introduction

At the extreme conditions reached within modern combustion engines, flame propagation and spontaneous ignition chemistry can occur simultaneously, coupling with one another to jointly govern engine operability and performance (Puduppakkam et al. 2020). Efforts to predict the behavior of laminar flames at high unburned-gas temperatures at which the fuel – air mixture becomes spontaneously reactive have employed numerous simulation-based methods (e.g., Sankaran 2015; Pan et al. 2016; Krisman, Hawkes, and Chen 2018; Ansari, Jayachandran, and Egolfopoulos 2019; Faghih et al. 2019; Zhang et al. 2020). However, while significant advancements have extended the range of pressures accessible to experimental laminar flame speed ( $S_L$ ) measurement (e.g., Tse, Zhu, and Law 2000; Xiouris et al. 2016), practical limitations have consistently hindered efforts to extend  $S_L$  measurements to higher temperatures.



**Figure 1.** Temperature–pressure regime diagram comparing the approximate domains accessible to different  $S_L$  measurement approaches compared to an isentropic approximation of IC-engine-relevant conditions and IDT contours for  $n$ -heptane at  $\phi = 1$ .

The approximate unburned-gas temperature ( $T_u$ ) and pressure ( $P_u$ ) regimes accessible to different experimental approaches for the measurement of  $S_L$  are presented in Figure 1. Contours represent ignition delay times (IDTs) simulated for a stoichiometric (unity equivalence ratio,  $\phi = 1$ ) mixture of  $n$ -heptane at constant pressure using a skeletal reaction mechanism from University of California at San Diego (2016). Conditions traditionally relevant to IC engines (dark gray) are shown bounded by air-standard isentropic trajectories from the research and motor octane number (RON and MON) intake conditions (ASTM D 2699: 2017–11 2017; ASTM D 2700: 2017–11 2017). An extended regime (light-gray) relevant to state-of-the-art engine technologies is shown bounded by isentropes originating from boosted spark ignition (SI) and advanced compression ignition (ACI) intake conditions (Szybist and Splitter 2020).

Flame speed measurements performed using constant-pressure (–P) spherically expanding flames (SEFs) can reach pressures as high as 60 atm (Tse, Zhu, and Law 2004), but are limited to low-  $T_u$  conditions by the long mixture residence time (on the order of 10 minutes) and are subject to fuel-loading constraints (Egolfopoulos et al. 2014). Constant-volume (–V), confined SEFs use dynamic heating of the unburned-gas mixture ahead of the flame to reach elevated temperatures.  $S_L$  measurements have been demonstrated up to 720 K using contemporary constant-V methods (Wang et al. 2020), with spontaneous autoignition of the preheated unburned gas limiting the ability of the method to reach higher  $T_u$  (Lawson et al. 2020). Flow-based flame speed measurements employing counterflow, Bunsen, or diverging-channel configurations use inline heating of the unburned gas to reach elevated temperatures. To the authors’ knowledge, the 873-K data reported by Kurata, Takahashi, and Uchiyama (1994) using a Bunsen-flame configuration represent the highest- $T_u$   $S_L$  measurements reported in the literature prior to the introduction of the shock-tube flame speed method, though Bunsen flame data are often viewed as being subject to elevated uncertainty (Egolfopoulos et al. 2014). Heated, diverging channels have been employed in

$S_L$  measurements up to about 650 K (e.g., 2012). Rapid compression machines (RCMs) have been employed to measure burning velocities at  $T_u$  up to 1,000 K (e.g., Assanis, Wagnon, and Wooldridge 2015); while flame wrinkling and pressure rise typically precludes the determination of  $S_L$  values from RCM experiments, recent progress realizing stable flames in RCMs has been reported at more moderate  $T_u$  conditions (Goyal and Samimi-Abianeh 2022).

The shock-tube flame speed method, first introduced by Ferris et al. (2019b), provides significant potential to enable  $S_L$  measurements at previously inaccessible  $T_u$  conditions (Figure 1). By pairing the ability of the shock-tube to nearly instantaneously heat an unburned-gas mixture with non-intrusive laser-induced ignition of a SEF and high-speed imaging diagnostics, the spontaneous-reactivity limits facing other  $S_L$  measurement methods can be overcome. The theoretical regime boundaries shown for shock-tube SEFs are described in (Susa 2022, 45–47). Despite this significant potential, early applications of the method (e.g., Susa et al. 2019a, 2019b) were, in practice, limited by the occurrence of wrinkling, instability, and distortion of flames with increasing temperature. The schlieren-based propane measurements reported in Susa, Zheng, and Hanson (2021), performed using an oxidizer mixture of  $O_2$  and Ar and with flames ignited much nearer the end wall than in previous studies, broke through these limits and demonstrated  $S_L$  measurements in excess of 1,000 K for the first time. Those results significantly expanded the demonstrated capability of the shock-tube flame speed method and motivate the present analysis of the factors that allowed that study to succeed.

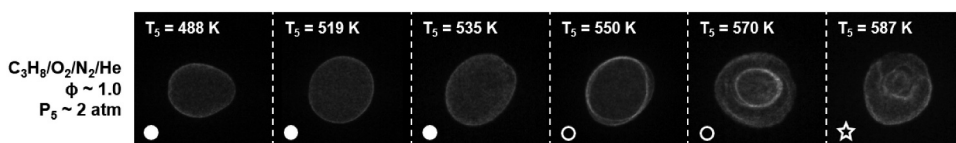
This work describes a meta-analysis performed in an effort to better understand the parameters controlling flame stability in shock-tube flame experiments. The dataset used in the analysis was aggregated from multiple prior flame speed studies (Ferris et al. 2019a, 2019b; Ferris 2020a; Susa et al. 2019a; 2019b; Susa, Zheng, and Hanson 2021) as well as previously unreported results. The flame in each experiment is first classified by its stability, and a subset of trials capturing the transition from stable to unstable flames with increasing  $T_u$  is selected. The binary classification between stable and unstable is then analyzed using logistic regression. The resulting model, cast in terms of a multivariate power-law expression for the critical temperature ( $T_{crit}$ ) at which flames become unstable, is found to be highly predictive of the stability transition. Consideration of the trained model coefficients allows the effects of different experimental parameters on the predicted stable  $T_u$  limit to be identified and informs the optimal design of future experiments.

## Flame stability classifications

Flame stability is classified in this study by the subjective appearance of the flame at a characteristic diameter of approximately 3 cm. Flames are classified by three categories – stable ●, distorted ○, and wrinkled ☆ — selected to be analogous to those used in Susa et al. (2019a) and associated with a corresponding symbol used throughout this chapter. While the distorted and wrinkled categories are later lumped together to form the “unstable” binary class, they are distinguished in the classification phase to reflect the distinct appearances, illustrated by elevated-pressure propane– $O_2/N_2/He$  flame images in Figure 2. The “distorted” name used to describe flames exhibiting concentric rings of emission is adopted from the side-wall imaging results of Susa and Hanson (2022) that found the rings seen in

Table 1. Experimental parameters.

Label	Fuel	Oxidizer			$\phi$ (-)	$P_5$ (atm)	$\gamma_1$ (-)	$\bar{M}$ (g/mol)	$\bar{Le}$ (-)	$z_s$ (cm)	$T_5$ (K)	Ref.
		O <sub>2</sub>	N <sub>2</sub>	He								
CH <sub>4</sub> -Air	CH <sub>4</sub>	0.21	0.79	-	1.0	1.0	1.39	27.6	1.02	10.25	491–573	(Ferris et al. 2019b)
C <sub>2</sub> H <sub>6</sub> -Air	C <sub>2</sub> H <sub>6</sub>	0.21	0.79	-	1.0	1.0	1.38	28.9	1.20	10.25	582–607	(Ferris 2020b)
C <sub>3</sub> H <sub>8</sub> -Air	C <sub>3</sub> H <sub>8</sub>	0.21	0.79	-	1.0	1.0	1.37	29.5	1.35	10.25	459–534	(Ferris et al. 2019a)
C <sub>3</sub> H <sub>8</sub> -He-2 atm	C <sub>3</sub> H <sub>8</sub>	0.21	0.32	0.47	1.0	2.0	1.44	18.6	2.48	10.25	537–551	-
C <sub>3</sub> H <sub>8</sub> -Ar	C <sub>3</sub> H <sub>8</sub>	0.21	-	-	1.0	1.0	1.51	38.5	1.26	10.25	496–556	(Ferris et al. 2019b)
C <sub>3</sub> H <sub>8</sub> -Ar-2 cm	C <sub>3</sub> H <sub>8</sub>	0.21	-	-	1.0	1.0	1.51	38.5	1.20	2.0	572–606	-
n-C <sub>7</sub> H <sub>16</sub> -Air	n-C <sub>7</sub> H <sub>16</sub>	0.21	0.79	-	0.9	1.0	1.36	30.1	2.27	10.25	488–587	-
i-C <sub>8</sub> H <sub>18</sub> -Air	i-C <sub>8</sub> H <sub>18</sub>	0.21	0.79	-	0.9	1.0	1.36	30.1	2.33	10.25	547–826	(Susa, Zheng, and Hanson 2021)
n-C <sub>7</sub> H <sub>16</sub> -He	n-C <sub>7</sub> H <sub>16</sub>	0.18	0.41	0.41	0.9	1.0	1.43	20.1	3.83	10.25	806–1,190	(Susa et al. 2019b)
i-C <sub>8</sub> H <sub>18</sub> -He	i-C <sub>8</sub> H <sub>18</sub>	0.18	0.41	0.41	0.9	1.0	1.43	20.1	4.00	10.25	401–595	(Susa et al. 2019b)
											502–594	(Susa et al. 2019b)
											512–689	(Susa et al. 2019b)
											505–641	(Susa et al. 2019a)



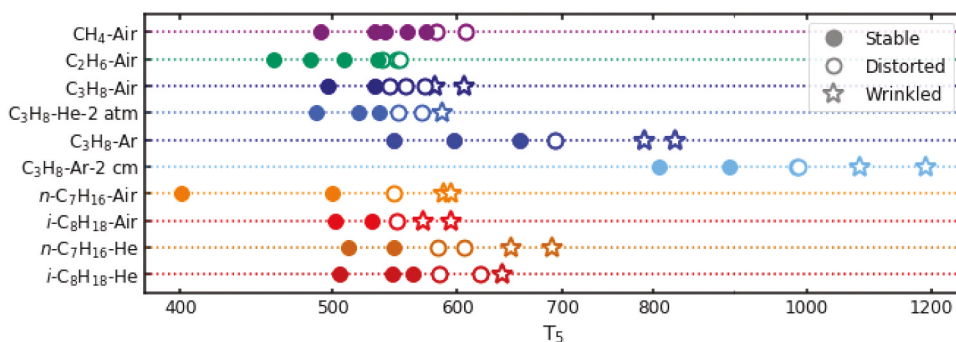
**Figure 2.** Propane–O<sub>2</sub>/N<sub>2</sub>/He flames ( $\phi = 1.0$ ) at elevated pressure ( $P_5 \approx 2$  atm). Symbols indicate the stability classification. Experiments represented in this figure are previously unpublished.

end-wall images to be associated with axial flame distortion. The nominal conditions of the 10 groupings of experiments included in the aggregate data set are detailed in Table 1; corresponding stability classifications vs. post-reflected-shock unburned-gas temperature ( $T_5$ ) are presented in Figure 3.

It is noted that the radius used here to characterize flame stability is somewhat larger than the maximum radius required to perform a  $S_L$  measurement. As a result, flames at conditions classified as “unstable” in this chapter may, in fact, have been suitably stable for a reliable  $S_L$  measurement to be performed at smaller radii, as was the case for the methane, ethane, and propane experiments from Ferris et al. (2019a, 2019b) and Susa, Zheng, and Hanson (2021). In the cases of the *n*-heptane and *iso*-octane results (Susa et al. 2019a, 2019b), the presence of a fully stable radius range was less assured, such that axial flame distortion (Susa and Hanson 2022) is believed to have been a contributing factor to the observed negative temperature dependence reported in those experiments. Experiments from Ferris (2020b) were reported specifically for the purpose of illustrating the presence of non-ideal structure and thus not used in performing flame-speed measurements.

## Analytical method

Logistic regression analysis is applied to estimate the extent to which different experimental parameters make a flame more or less prone to propagating in a stable manner. Logistic regression (Berkson 1944; Walker and Duncan 1967) is a method for estimating the value of



**Figure 3.** Stability of flames at different temperatures,  $T_5$ , grouped by experiment set. Each symbol represents a single shock-tube experiment, with the symbol shape corresponding to the stability classification. Y-axis labels correspond to those used in Table 1.

a binary dependent variable,  $y$ , from a set of  $n$  scalar independent variables,  $\mathbf{x} = [1, x_1, x_2, \dots, x_n]$ ; the  $x_0 = 1$  feature is included to allow for a non-zero intercept. In the logistic model, the probability,  $P$ , of a given binary outcome,  $y = 1$ , given  $\mathbf{x}$  is defined as:

$$P(y = 1|\mathbf{x}) = \sigma(t) = \frac{1}{1 + e^{-t}}, \quad (1)$$

$$t = \mathbf{B}\mathbf{x}^T = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n = \sum_{i=0}^n \beta_i x_i, \quad (2)$$

where  $\sigma$  is the logistic function,  $t$  is a scalar value known as the “logit,” and  $\mathbf{B} = [\beta_0, \beta_1, \beta_2, \dots, \beta_n]$  are a set of weights. Values of  $t > 0$  are associated with the expected result that  $y = 1$ ;  $t < 0$  corresponds with an expectation of  $y = 0$ . In this work, the weights  $\mathbf{B}$  are trained using a stochastic gradient descent (SGD) method (*i.e.*, SGDClassifier) implemented in the open-source Scikit-learn package (Pedregosa et al. 2011).

A typical shock-tube flame speed study consists of experiments performed over a range of  $T_5$ 's while maintaining constant the other experimental parameters (pressure, mixture, *etc.*). Therefore, in order to predict the critical temperature ( $T_{\text{crit}}$ ) at which a stable flame will no longer be realized in a given study, a power-law expression of the following form is sought:

$$T_{\text{crit}} = c T_0 \prod_{i=2}^n \left( \frac{a_i}{a_{i,0}} \right)^{\theta_i} \begin{cases} > T_5, \text{ stable} \\ < T_5, \text{ unstable} \end{cases}, \quad (3)$$

where  $c$  is a constant and each independent parameter,  $a_i$ , non-dimensionalized by some characteristic value  $a_{i,0}$ , is taken to a power,  $\theta_i$ , that defines the sensitivity of  $T_{\text{crit}}$  to that parameter. Letting  $a_1 = T_5$ ,  $a_{1,0} = T_0$ , and  $\theta_1 = -1$ , Eqn. 3 can be rewritten as:

$$c \prod_{i=1}^n \left( \frac{a_i}{a_{i,0}} \right)^{\theta_i} \begin{cases} > 1, \text{ stable} \\ < 1, \text{ unstable} \end{cases}. \quad (4)$$

Taking the natural logarithm converts Eqn. 4 into the form of a logit,  $t$  (Eqn. 2):

$$\ln(c) + \sum_{i=1}^n \theta_i \ln \left( \frac{a_i}{a_{i,0}} \right) = \ln(c) + \sum_{i=1}^n \theta_i (\alpha_i - \alpha_{i,0}) \begin{cases} > 0, & \text{stable} \\ < 0, & \text{unstable} \end{cases} = t, \quad (5)$$

where  $\alpha_i \equiv \ln a_i$ . SGD performs most reliably when the independent variables comprising  $\mathbf{x}$  are standardized to zero mean and unit variance (scikit-learn developers n.d). Zero mean is realized for the  $(\alpha_i - \alpha_{i,0})$  terms in Eqn. 5 if  $\alpha_{i,0} = \mu_{\alpha,i}$ , where  $\mu_{\alpha,i}$  is the mean-log value of all values  $a_i$  in the training set. Division by the standard deviation,  $s_{\alpha,i}$ , of the  $\alpha_i$  values enforces unit variance and is balanced by multiplying  $\theta_i$  by  $s_{\alpha,i}$ :

$$t = \ln(c) + \sum_{i=1}^n (\theta_i s_{\alpha,i}) \left( \frac{\alpha_i - \mu_{\alpha,i}}{s_{\alpha,i}} \right). \quad (6)$$

Equation 6 is now exactly in the form of Eqn. 2, with:

$$\beta_0 = \ln(c), \quad (7)$$

$$\beta_{i \in \{1 \dots n\}} = \theta_i s_{\alpha, i}, \quad (8)$$

$$x_{i \in \{1 \dots n\}} = \frac{\alpha_i - \mu_{\alpha, i}}{s_{\alpha, i}}, \quad (9)$$

such that the parameters  $\mathbf{B}$  trained on standardized features  $\mathbf{x}$  can be interpreted as coefficients  $\theta$  in the power-law form of Equation (3) and thus can provide physical insight into the factors affecting flame stability.

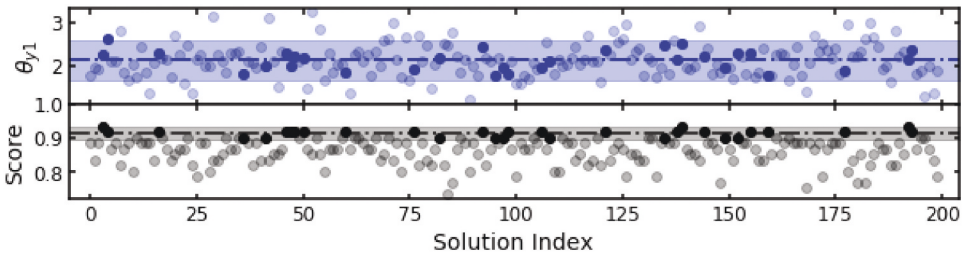
## Results and discussion

Logistic regression was performed on the aggregate data set with the binary classifications of  $y = 0$  assigned to stable flames and  $y = 1$  assigned to both distorted and unstable flames. The resulting data set was closely balanced, containing 28 stable flames out of 61 total experiments. Six independent variables were selected to describe the experimental conditions:  $T_5$  and  $P_5$  characterize the thermodynamic state of the unburned gas; the room-temperature ratio of specific heats ( $\gamma_1$ ), mixture-averaged molecular weight ( $\bar{M}$ ), and Lewis number (Le) characterize the unburned-gas mixture; and the axial distance ( $z_5$ ) from the end wall at which the flame is ignited characterizes the experimental configuration. Equivalence ratio is not independently considered in the present analysis as all available experiments were performed with  $\phi$  near unity ( $0.9 \leq \phi \leq 1.0$ ).

As SGD exhibits both sample-ordering and random-seed dependencies, a total of 200 training runs were performed using different seeds and ordering of the data. The mean and 95% confidence interval of each  $\theta_i$  was calculated considering the 30 solutions producing the highest-scoring sets of weights, a process illustrated for  $\theta_{\gamma_1}$  in Figure 4. Training results are tabulated for all  $\theta_i$  coefficients in Table 2. Terms in the table correspond to an equation for  $T_{\text{crit}}$  of the following form, where  $T_{\text{ref}} = cT_0$  and the units of dimensional quantities are specified:

$$T_{\text{crit}} = T_{\text{ref}} \left( \frac{P_5}{1.07 \text{ atm}} \right)^{\theta_{P_5}} \left( \frac{\gamma_1}{1.41} \right)^{\theta_{\gamma_1}} \left( \frac{\bar{M}}{27.4 \text{ g/mol}} \right)^{\theta_{\bar{M}}} \left( \frac{\text{Le}}{1.69} \right)^{\theta_{\text{Le}}} \left( \frac{z_5}{8.77 \text{ cm}} \right)^{\theta_{z_5}}. \quad (10)$$

The first row in Table 2 represents the results of the full, six-variable model, which scores 93% at predicting stability in the current data set using the average  $\theta_i$  values. Outputs of the



**Figure 4.** Coefficient  $\theta_{\gamma_1}$  (top) and model score (bottom) resulting corresponding to 200 trained solutions. Mean values (dot-dash lines) and 95% confidence intervals (shaded regions) are calculated considering only the highest-scoring solutions (opaque symbols).



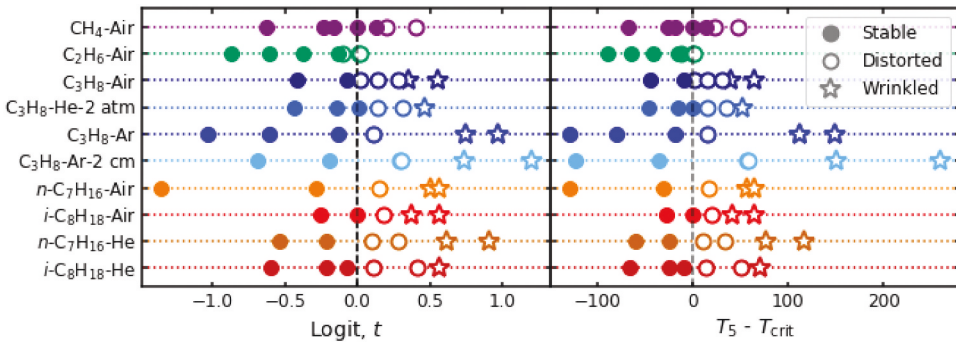
**Table 2.** Trained parameter values and confidence intervals.

Model	$T_{\text{ref}}$ (K)	$\theta_{\rho_5}$	$\theta_{\gamma_1}$	$\theta_{\bar{M}}$	$\theta_{\text{Le}}$	$\theta_{z_5}$
Full	590 $\pm$ 9	-0.13 $\pm$ 0.10	2.14 $\pm$ 0.45	0.05 $\pm$ 0.05	-0.02 $\pm$ 0.03	-0.19 $\pm$ 0.04
Drop Le	588 $\pm$ 7	-0.12 $\pm$ 0.10	2.10 $\pm$ 0.39	0.05 $\pm$ 0.04	$\emptyset$	-0.19 $\pm$ 0.05
Drop $\bar{M}$	586 $\pm$ 10	-0.15 $\pm$ 0.09	2.27 $\pm$ 0.49	$\emptyset$	-0.04 $\pm$ -0.03	-0.18 $\pm$ 0.05

full model are displayed in Figure 5 in terms of both the logit,  $t$ , and the difference between the experimental and predicted critical temperatures,  $T_5 - T_{\text{crit}}$ . As neither  $\theta_{\text{Le}}$  nor  $\theta_{\bar{M}}$  are found to be statistically non-zero in the full model, two five-variable models are additionally considered, each dropping one of Le or  $\bar{M}$  as independent variables. The “drop” model parameters are shown in the bottom two rows of the table; both matched the 93% score of the full model. It is found that when one of Le or  $\bar{M}$  is dropped from the model,  $\theta$  of the other becomes slightly statistically non-zero, such that one, but not both, of these parameters seems necessary in characterizing experimental conditions with respect to stability.

These empirical models provide insights into the experimental parameters affecting the stability limits in shock-tube flame experiments. The ratio of specific heats,  $\gamma_1$ , is found to be the parameter with the strongest effect, with larger values of  $\gamma_1$  being beneficial to increasing  $T_{\text{crit}}$ . This strongly motivates the use of monatomic diluents (Ar and He,  $\gamma = 5/3$ ) over diatomic nitrogen ( $\text{N}_2$ ,  $\gamma \approx 7/5$ ) for use in high-temperature flame experiments. It is further noted that the value  $\theta_{\gamma_1}$  in these models reflects a weaker scaling than that applied to the closely related post-incident-shock ratio of specific heats ( $\gamma_2^{-2.66}$ ) in an empirical expression describing the height of a reflected-shock bifurcation reported by Petersen and Hanson (2006). As such, at least one physical mechanism that could reasonably be expected to influence flame stability is known to exist that would explain a relationship of at least this magnitude.

While the strong correlation between  $\gamma_1$  and stability motivates the use of Ar or He, it does not differentiate between the two. Furthermore, the nearly statistically nonexistent relationships between Le or  $\bar{M}$  and stability do not provide a strong case for one over the other. Therefore, a different metric is required to identify the preferred diluent of Ar or He for experiments performed using the shock-tube flame speed method. The effect of the

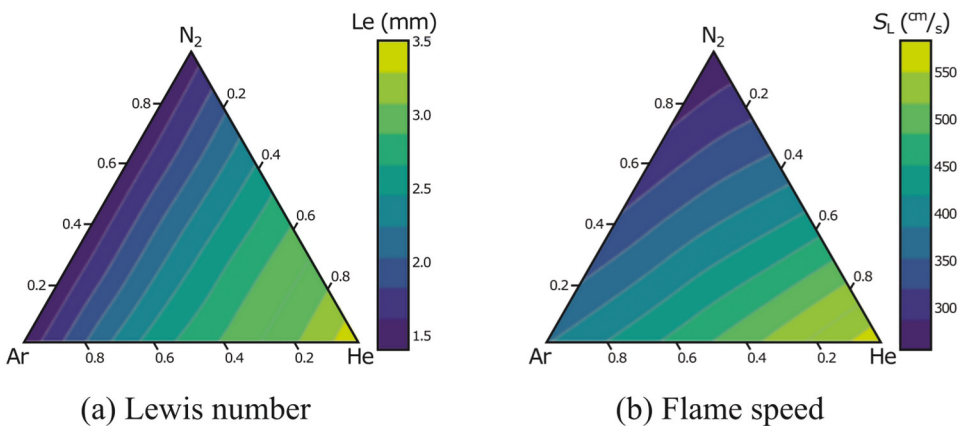


**Figure 5.** Results of the six-variable model applied to all data sets in term of the logit,  $t$  (left) and as the difference between  $T_5$  and  $T_{\text{crit}}$  (right). Y-axis labels correspond to the labels in Table 1 and Figure 3. The vertical dashed lines represent the model predicted stability criteria. The modeled  $T_{\text{crit}}$  captures the stability transition (from filled to open symbols) across all experiment sets within about 20 K.

diluent selection on  $Le$  and the simulated  $S_L$  for a stoichiometric mixture of propane is shown in Figure 6. Viewing first the relationship between diluent selection and  $Le$ , it is seen that  $Le$  for mixtures diluted with Ar nearly exactly match those diluted with  $N_2$ , suggesting flames ignited in those mixtures would exhibit similar stretch responses. As  $N_2$  is the air-relevant diluent for which data would generally be preferred by combustion practitioners, the use of Ar over He would be expected to provide more relevant data than early studies using He dilution with the shock-tube flame speed method (Ferris et al. 2019b; Susa et al. 2019a, 2019b) as well as many state-of-the-art  $S_L$  methods that use He dilution to suppress hydrodynamic instabilities (e.g. Rozenchan et al. 2002; Tse, Zhu, and Law 2004; Xiouris et al. 2016; Wang et al. 2020). Looking next to  $S_L$ , it can be seen that both monotonic diluents lead to an increase compared to  $N_2$  on account of higher equilibrium temperatures. However, the increase seen using Ar is only about half that induced by He, once again making Ar-diluted mixtures more relevant to air than those containing He.

The axial position of the flame ( $z_5$ ) exhibits the next strongest effect on the critical temperature. While the magnitude of  $\theta_{z_5}$  is not particularly large, the wide range over which  $z_5$  may be varied can nonetheless lead to a significant effect on  $T_{crit}$  predicted by the present model. This is observable in Figure 3 by comparing the baseline “C<sub>3</sub>H<sub>8</sub>-Ar” data set with the “C<sub>3</sub>H<sub>8</sub>-Ar-2 cm” data; reducing  $z_5$  from 10.25 cm to 2 cm resulted in a significant increase in  $T_{crit}$ , from below 700 K to over 900 K. Based on the measurements reported in Susa and Hanson (2021) of axial velocity within the region-5 environment that is expected to increase in magnitude with distance from the end wall, this positional effect may be associated with igniting the flame in a more quiescent environment.

While  $z_5$  clearly has some significant effect on flame stability, the magnitude and nature of the effect are made uncertain by the availability of only a single data set using a value  $z_5$  other than 10.25 cm. For this reason, the identification and characterization of the specific mechanism underlying the positioning effect and are identified as a high-priority topic for further study. One preliminary study of positional effects was reported in Susa et al. (2022b), which revealed a more complex relationship between the position and stability than the simple, monotonic scaling



**Figure 6.** Ternary diagrams illustrating the effect of the diluent on (a) mixture Lewis number ( $Le$ ), and (b) laminar flame speed ( $S_L$ ) for propane ( $\phi = 1$ ) in an oxidizer containing 21% O<sub>2</sub> and 79% diluent (N<sub>2</sub>, Ar, He) at  $T_u = 800$  K and  $P_u = 1$  atm.

contained in the present analysis. For this reason, while the positional term in the present model might offer some general guidance, the authors urge caution in the model being assumed quantitatively predictive with respect to the positioning term.

The effect of unburned-gas pressure,  $P_5$ , is found to be small and uncertain. The uncertainty is attributed to only the single “C<sub>3</sub>H<sub>8</sub>-He-2 atm” data set being available at a pressure other than one atmosphere. Within the limits of the present model, it is expected that flames studied at higher pressure will experience a modest decrease in  $T_{\text{crit}}$ ; for example, a 10-fold increase in pressure is predicted to result in a 22% decrease in  $T_{\text{crit}}$ . The magnitude of  $\theta_{P_5}$  is strikingly similar to the pressure exponent of  $-0.14$  associated with the analytical form of shock attenuation (Petersen and Hanson 2001), which could reflect a physical mechanism giving rise to the effect. However, further investigation is warranted to increase confidence in  $\theta_{P_5}$  before conclusions regarding pressure effects can be drawn.

## Conclusion

A regression-based meta-analysis of flame stability in a shock-tube environment was reported. A binary classifier was trained on an aggregate set of flame-stability data using SGD. The resulting model was cast as a power-law expression for predicting the critical temperature at which flames will become unstable in a shock tube, providing physical insight into the experimental parameters controlling flame stability. The strongest effect was found to be associated with  $\gamma_1$ , where increasing the value through the use of monatomic diluents promotes stability. Mixture Le and  $\bar{M}$  were found to have negligible effect on  $T_{\text{crit}}$  in the limit of the  $\text{Le} > 1$  conditions evaluated in the present study; an evaluation of diluent effects on  $S_L$  and Le demonstrated that the use of Ar should be favored over He for maximizing the relevance to flames in air, as was used to good effect in a pair of recent studies (Susa et al. 2022a; Susa, Zheng, and Hanson 2022). The effect of  $z_5$  is predicted by the model to be important but is uncertain on account of the limited availability of data and is identified as a topic of particular importance for further study. The effect of  $P_u$  is found to be relatively small but similarly uncertain; future applications of the shock-tube flame speed method at higher pressures will provide additional insight into the magnitude of the effect on flame stability.

Using this analytical framework and these preliminary results as guides, shock-tube flame speed experiments can now be designed to maximize the temperature range for stable flames, particularly through the informed selection of Ar as the diluent in the oxidizer. Future experiments designed using the present model as a guide will naturally interrogate the accuracy of the model parameters, and the incorporation of future results into an expanded aggregate data set will enable the predictive model to be iteratively refined over time. As additional experimental results become available to bolster and broaden the aggregate data set, further value could be realized by incorporating additional independent variables into the model, such as equivalence ratio. While the present model considers only a single flame radius, future analysis could treat the radius as an independent variable in order to predict  $T_{\text{crit}}$  at a specific radius of interest. Facility-specific parameters, including the radius of the shock tube, incident-shock attenuation rate, and  $T_1$  (for heated shock tubes), may additionally be expected to affect  $T_{\text{crit}}$  and could become candidates for inclusion in future studies following this analysis methodology once results from other shock-tube facilities become available.

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