Appendix B: Uncertainty Analysis

The proper estimation of errors in dependent or independent variables is critical to the interpretation of any experimental data. Recognizing that insufficient or inappropriate consideration of errors and error propagation can lead to serious misinterpretations of data, the following sections describe the methodology for estimating the errors associated with parameters of interest reported in this work.

B.1 Systematic versus Random Errors

From the outset, it is important to note that two types of error are important in the interpretation of the present data set. Systematic (or bias) errors result from defects in a parameter model (e.g. Nusselt number) or measuring equipment (e.g. pressure gauges) which cause deviations from the true behavior in a given system. Such errors result in reproducible inaccuracies that tend to impact the entire data set in a largely equivalent manner. Random errors, on the other hand, are fluctuations in measured data based upon the precision of the measurement device. Such errors are statistical in nature, and can be minimized through averaging multiple observations. These definitions are important to the present analysis because, while the total uncertainty (including both systematic and random errors) is relevant for the comparison of the present data set to other experimental data or numerical predictions, only the random error is applicable when comparing data points within the current data set since all data should be affected essentially equally by systematic errors (if any). Moreover, this random error is particularly relevant to the measured ignition temperatures, where it represents the variability associated with repeated measurements at the same operating conditions. The random error can be estimated by finding the standard error of the mean ($SE_{\bar{x}}$):

$$SE_{\bar{x}} = \frac{\sigma}{\sqrt{n}}, \hspace{4cm} \text{B.1.1}$$

where σ is the standard deviation of the set of measurements and n is the number of measurements at a given condition. Using this estimate, the maximum random error observed for any ignition temperature measurement is 5 K. Therefore, when comparing any two ignition temperatures within the current experimental dataset, the relevant uncertainty should be considered as ±5 K.

The total uncertainty in each of the four system variables/responses – i.e., pressure, fuel loading, strain rate, and air boundary temperature – is estimated in terms of the uncertainty in the variable's constituent components, added in quadrature. This simple approach is demonstrated in Ref. [1]. The general form for this relation is:

$$\delta q = \sqrt{\left(\frac{\partial q}{\partial x_1}\delta x_1\right)^2 + \left(\frac{\partial q}{\partial x_2}\delta x_2\right)^2 + \cdots \left(\frac{\partial q}{\partial x_n}\delta x_n\right)^2},$$
B.1.2

where δq is the uncertainty in a system variable, $\frac{\partial q}{\partial x_n}$ is the partial derivative of the relation for q with respect to the nth independent variable x_n, and δx_n is the estimated uncertainty in the independent variable x_n. Thus, as long as a closed-form, differentiable relationship can be defined between q and x_n, the uncertainty in q can be readily obtained. Representative total estimated uncertainties are plotted with experimental ignition temperatures in the main text.

B.2 Estimated Error in Pressure Measurements

Since chamber pressure is a directly-measured quantity by way of the chamber pressure gauge, the estimated error in pressure is quite simple, and is only a function of the instrument uncertainty and readout resolution. As provided by the manufacturer (Cecomp), the uncertainty in the pressure measurement is ±0.25% of full-scale range, in this case resulting in an uncertainty of ±0.75 psi. Added in quadrature with a readout resolution of 1 psi, the resulting estimated uncertainty in pressure is ±1.25 psi, and is included where applicable in the following analyses.

B.3 Estimated Error in Fuel Loading

The experimental fuel loading is calculated based upon Eqn. B.3.1:

$$X_F = \frac{M_F}{M_F + M_N},$$

B.3.1

where X_F is the fuel loading, M_F is the molar flow rate of fuel, and M_N is the molar flow rate of nitrogen. The uncertainty in fuel loading based upon Eqn. B.3.1 is:

$$\delta X_F = \sqrt{\left(\frac{\partial X_F}{\partial M_F} \delta M_F\right)^2 + \left(\frac{\partial X_F}{\partial M_N} \delta M_N\right)^2},$$

B.3.2

where δX_F, δM_F, and δM_N are the uncertainties in fuel loading, fuel molar flow rate, and nitrogen molar flow rate, respectively. The individual uncertainties δM_F and δM_N thus need to be defined. The uncertainty in fuel flow rate is related to the accuracy of the syringe pump, and over the flow rates of interest for the present study, the pump has been found to have a maximum deviation of 2% from the expected value based upon average measurements of total fluid flow over extended time periods at various flow rates, measured by a precision digital mass balance. As a result, δM_F is estimated as $0.02 M_F$. The uncertainty in the molar flow rate of nitrogen is related to the uncertainty in the fit line created from experimentally obtained flow rate data during the calibration of the sonic nozzles used to meter the flow rates of gaseous components, as well as the uncertainty associated with readout resolution. The fit line takes the form of Eqn. B.3.3, with the overall uncertainty given as Eqn. B.3.4:

$$M_N = mx + b$$

B.3.3

$$\delta M_N = \sqrt{\left(\frac{\partial M_N}{\partial m} \delta m\right)^2 + \left(\frac{\partial M_N}{\partial b} \delta b\right)^2 + \left(\frac{\partial M_N}{\partial x} \delta x\right)^2}.$$

B.3.4

The uncertainties in the slope (δm) and intercept (δb) of the fit line are taken as the standard error in the fit coefficients as calculated by the Excel function LINEST, while δx is the readout error of ± 1 psi. Strictly speaking, both δm and δb are dependent on the readout error (δx), however the inclusion of such a dependence would require an alternative error treatment and is

not expected to significantly alter the estimated uncertainty in fuel loading. It should also be noted that since the sonic nozzles are calibrated with the same pressure gauges used for experiments, unlike the pressure measurements in Section B.2 only the readout error is relevant to δx. The resulting uncertainties in fuel loading (δX_F) range from ± 0.0025 at the lowest fuel loading to ± 0.01 at the highest.

B.4 Error in Strain Rate

The strain rate is calculated from the estimated densities and bulk velocities issuing from both the fuel and oxidizer sides, as shown in Eqn. B.4.1:

$$k = \frac{2V_O}{L}\left(1 + \frac{V_F\sqrt{\rho_F}}{V_O\sqrt{\rho_O}}\right),$$

B.4.1

where V and ρ are the bulk velocity and density, respectively, the subscripts O and F refer to the flows issuing from the oxidizer and fuel ducts, respectively, and L is the separation distance between the two duct exits. The uncertainty in this strain rate is thus:

$$\delta k = \sqrt{\left(\frac{\partial k}{\partial V_O}\delta V_O\right)^2 + \left(\frac{\partial k}{\partial V_F}\delta V_F\right)^2 + \left(\frac{\partial k}{\partial \rho_F}\delta \rho_F\right)^2 + \left(\frac{\partial k}{\partial \rho_O}\delta \rho_O\right)^2 + \left(\frac{\partial k}{\partial L}\delta L\right)^2},$$

B.4.2

with nomenclature definitions similar to that previously described in Section B.3. Since each of these quantities – with the exception of L – is itself a calculated value based upon a number of uncertain values, each uncertainty is likewise determined through an identical procedure. For the sake of brevity in the following discussion, the subscripts N and O refer to the properties associated with nitrogen and oxygen gases, respectively, and when used in conjunction with the linear fit parameters for sonic nozzles, refer to the values specific to the nitrogen or oxygen nozzle used in the relevant – i.e., fuel or oxidizer side – flow.

The bulk velocity issuing from the fuel side is described by Eqn. B.4.3:

$$V_F = \frac{(m_N x_N + b_N)\rho_{\text{ref},N}\frac{T_{\text{ref}}}{T} + \dot{m}_F\frac{R_{sp}T}{P}}{\frac{\pi}{4}D^2},$$

B.4.3

where m_N and b_N are the nitrogen nozzle linear fit parameters as described previously, x_N is the pressure gauge readout for the nitrogen nozzle, $\rho_{\text{ref},N}$ is a reference density of nitrogen at a given chamber operating pressure and 300 K, T_{ref} is 300 K, T is the temperature of the stream in question, $\dot{m}_F$ is the mass flow rate of the fuel issuing from the fuel pump, R_{sp} is the specific gas constant for vaporized fuel, P is the chamber pressure, and D is 19 mm, the inner diameter of the fuel and oxidizer ducts. The resulting estimated uncertainty in fuel-side bulk velocity is therefore:

$$(\delta V_F)^2 = \left(\frac{\partial V_F}{\partial m_N}\delta m_N\right)^2 + \left(\frac{\partial V_F}{\partial x_N}\delta x_N\right)^2 + \left(\frac{\partial V_F}{\partial b_N}\delta b_N\right)^2 + \left(\frac{\partial V_F}{\partial \rho_{\text{ref},N}}\delta \rho_{\text{ref},N}\right)^2 + \cdots$$

$$\cdots + \left(\frac{\partial V_F}{\partial T}\delta T\right)^2 + \left(\frac{\partial V_F}{\partial \dot{m}_F}\delta \dot{m}_F\right)^2 + \left(\frac{\partial V_F}{\partial P}\delta P\right)^2 + \left(\frac{\partial V_F}{\partial D}\delta D\right)^2. \qquad \text{B.4.4}$$

Equation B.4.4 shows the squares of the uncertainties for the purposes of visual clarity given the overall length of the equations. It should be noted that both R_{sp} and T_{ref} are constants and therefore have no uncertainty. While the nitrogen reference density is also a constant, the uncertainty in pressure results in an uncertainty in the accuracy of the reference density. Based upon the uncertainty in pressure the uncertainty in reference density for all ρ_{ref} terms is estimated as ±0.08 kg/m^3. The uncertainty in temperature is variable and calculated based upon the results of Section B.5; however, this uncertainty does not play a significant part in the overall uncertainty in strain rate. In a similar fashion, the bulk velocity of the oxidizer stream, consisting of purely gaseous components, may be described by:

$$V_O = \frac{(m_N x_N + b_n)\rho_{\text{ref},N}\frac{T_{\text{ref}}}{T} + (m_O x_O + b_O)\rho_{\text{ref},O}\frac{T_{\text{ref}}}{T}}{\frac{\pi}{4}D^2}, \qquad \text{B.4.5}$$

Thus, the resulting estimated uncertainty in oxidizer-side bulk velocity is:

$$(\delta V_O)^2 = \left(\frac{\partial V_O}{\partial m_N}\delta m_N\right)^2 + \left(\frac{\partial V_O}{\partial x_N}\delta x_N\right)^2 + \left(\frac{\partial V_O}{\partial b_N}\delta b_N\right)^2 + \left(\frac{\partial V_O}{\partial \rho_{\text{ref},N}}\delta \rho_{\text{ref},N}\right)^2 + \cdots$$

$$\cdots + \left(\frac{\partial V_O}{\partial m_O} \delta m_O\right)^2 + \left(\frac{\partial V_O}{\partial x_O} \delta x_O\right)^2 + \left(\frac{\partial V_O}{\partial b_O} \delta b_O\right)^2 + \left(\frac{\partial V_O}{\partial \rho_{ref,O}} \delta \rho_{ref,O}\right)^2 + \cdots$$

$$\cdots + \left(\frac{\partial V_O}{\partial T} \delta T\right)^2 + \left(\frac{\partial V_F}{\partial D} \delta D\right)^2, \qquad \text{B.4.6}$$

with the sole difference being the presence of an additional set of sonic nozzle fit parameters for the oxygen sonic nozzle.

The remaining uncertainties needed are the uncertainties in fuel- and oxidizer-stream densities:

$$\rho_F = X_F \frac{R_{sp}T}{P} + (1 - X_F)\rho_{ref,N} \frac{T_{ref}}{T} \qquad \text{B.4.7}$$

$$\delta \rho_F = \sqrt{\left(\frac{\partial \rho_F}{\partial X_F} \delta X_F\right)^2 + \left(\frac{\partial \rho_F}{\partial P} \delta P\right)^2 + \left(\frac{\partial \rho_F}{\partial T} \delta T\right)^2 + \left(\frac{\partial \rho_F}{\partial \rho_{ref,N}} \delta \rho_{ref,N}\right)^2} \qquad \text{B.4.8}$$

$$\rho_O = X_O \rho_{ref,O} \frac{T_{ref}}{T} + (1 - X_O)\rho_{ref,N} \frac{T_{ref}}{T} \qquad \text{B.4.9}$$

$$\delta \rho_O = \sqrt{\left(\frac{\partial \rho_O}{\partial X_O} \delta X_O\right)^2 + \left(\frac{\partial \rho_F}{\partial T} \delta T\right)^2 + \left(\frac{\partial \rho_F}{\partial \rho_{ref,O}} \delta \rho_{ref,O}\right)^2 + \left(\frac{\partial \rho_F}{\partial \rho_{ref,N}} \delta \rho_{ref,N}\right)^2} \qquad \text{B.4.10}$$

In Eqns. B.4.9 and B.4.10, the term X_O refers to the mole fraction of oxygen in the oxidizer stream, set as 0.21 for all experiments. It should be noted that the dominant term driving uncertainty in strain rate (k) is $\delta \rho_{ref,N}$ as a direct result of the prevalence of nitrogen in both streams. The resulting uncertainty in k ranges from ± 7–12 s^{-1} for the range of strain rates used in the present study.

B.5 Error in Boundary Temperatures

Two temperatures are important in the above discussion: the fuel and oxidizer boundary temperatures. The former, being a relatively low temperature measurement, is not subject to appreciable radiative heating, and therefore the error in said measurement may be described simply as a function of the stated accuracy of the thermocouple, or 0.75%. For both measurements, the precision error associated with the readout resolution is sufficiently small to be neglected.

As described in Appendix A, the gas temperature of the air stream is described by:

$$T_g = T_b + \frac{\varepsilon_b \sigma d_b}{k_g \, \text{Nu}} (T_b^4 - \varepsilon_\infty F_{b-\infty} T_\infty^4), \qquad\qquad \text{B.5.1}$$

where T_g is the estimated gas temperature, T_b is the measured thermocouple temperature, ε_b is the emissivity of the thermocouple bead, d_b is the thermocouple bead diameter, k_g is the thermal conductivity of the gas, Nu is the Nusselt number as described in Appendix A, ε_∞ is the estimated emissivity of the chamber wall, $F_{b-\infty}$ is the configuration factor from the bead to the chamber wall, and T_∞ is the estimated surroundings temperature, taken here as the fuel boundary temperature. The estimated error in the gas temperature is then given by:

$$\left(\delta T_g\right)^2 = \left(\frac{\partial T_g}{\partial T_b} \delta T_b\right)^2 + \left(\frac{\partial T_g}{\partial \varepsilon_b} \delta \varepsilon_b\right)^2 + \left(\frac{\partial T_g}{\partial d} \delta d\right)^2 + \left(\frac{\partial T_g}{\partial \varepsilon_\infty} \delta \varepsilon_\infty\right)^2 + \cdots$$

$$\cdots + \left(\frac{\partial T_g}{\partial T_\infty} \delta T_\infty\right)^2 + \left(\frac{\partial T_g}{\partial \text{Nu}} \delta \text{Nu}\right)^2 + \left(\frac{\partial T_g}{\partial k_g} \delta k_g\right)^2 \qquad \text{B.5.2}$$

The error in T_b and T_∞ is taken as 0.75% of the measured value per manufacturer's specifications and the error in bead diameter d_b is taken as 0.01 mm. Since the value of the gas conductivity k_g is a calculated value based upon an experimental fit [2], it is difficult to ascertain an appropriate estimate of the error. Thus a highly conservative estimate of 20% of k_g is used. It should be noted that this choice does not appreciably impact the estimated error in T_g.

As mentioned in Appendix A, emissivity values for any practical surface are exceedingly difficult to define, and even more so in high-temperature oxidizing environments. The uncertainty in ε_∞ can be neglected *a priori* as its effect on the magnitude of the radiation correction is negligible. However, varying the value of ε_b will significantly alter the magnitude of the radiation correction. Unfortunately, as described in Appendix A, there is no accessible methodology for defining either a precise value or bounds on the uncertainty of the bead emissivity. As a result, any estimation of uncertainty would be purely conjecture; this uncertainty is therefore neglected, and it is merely stated that significant changes in emissivity will result in appreciable, but largely uniform, changes in the magnitude of the radiation correction as demonstrated in Appendix A.

The remaining uncertainty, that of the Nusselt number Nu, is ultimately the most significant factor in the estimation of error in the gas temperature measurement, and is simultaneously the most difficult to define. The Nusselt number is a surrogate for the convective heat transfer coefficient needed to define the energy balance around the thermocouple bead. Since this coefficient cannot be defined directly, the Nusselt number is used instead. However, numerous correlations exist to estimate Nusselt number, and each depends upon the specific geometry of the object in question. For the case of a thermocouple bead, Shaddix [3] reviewed several correlation options, and compared the results for spherical and cylindrical treatments, concluding that a cylindrical treatment was more appropriate for the thermocouple geometry at issue in the present study. However, even within the domain of cylindrical correlations, the relations shown by Shaddix [3] differ by as much as 20% in the low Reynolds number regime. To fully account for this disparity, the estimated error δNu is taken as double the largest deviation in observed by

Shaddix [3], or 40% Nu. The resulting error estimate for the gas temperature based upon the above assumptions is 20–35 K for typical ignition conditions.

References:

[1] J.R. Taylor, An introduction to error analysis: The study of uncertainties in physical measurements, 1st ed., University Science Books, Mill Valley, CA, 1982.

[2] M.D. Scadron, I. Warshawsky, Experimental determination of time constants and Nusselt numbers for bare-wire thermocouples in high-velocity air streams and analytic approximation of conduction and radiation errors, NACA Technical Note 2599, 1952.

[3] C.R. Shaddix, Correcting thermocouple measurements for radiation loss: a critical review, Proc. 33rd Natl. Heat Transf. Conf., Albuquerque, NM, 1999, pp. 1–10.