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Back to Basics – NO concentration measurements in atmospheric lean-to-rich, low-temperature, premixed hydrogen-air flames diluted with argon

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Supplemental material A: Experimentally-measured boundary conditions

Table 1 reports the experimental conditions required to perform simulations of quasi-1D flames. Uncertainties in the measured conditions are shown in parentheses. Measurements are performed at atmospheric conditions with an ambient pressure of $p_\infty = 1.000\ (0.005)$ atm. Reported below are: the equivalence ratio ϕ; the mole fraction of argon diluted in air $X_{\mathrm{Ar,\,in\,air}}$; the computational domain length l; the inlet velocity u_{in}, velocity gradient $\mathrm{d}u/\mathrm{d}z|_{in}$, and temperature T_{in}; and the stagnation surface temperature T_{wall}. Thermal mass flow controllers, calibrated with a dry-piston calibrator (±0.45%), monitor the fuel (Bronkhorst F-201-CV-10K-ABD-22-V), air (Bronkhorst F-211-CV-20K-ABD-22-V), argon (Bronkhorst F-211-CV-5K0-ABD-22-V), and nitrogen (Bronkhorst F-211-CV-50K-ABD-22-V) flows for the current set of experiments.

Table 1: Experimentally-measured boundary conditions.

ϕ [−]	$X_{\mathrm{Ar,\,in\,air}}$ [−]	l [mm]	u_{in} [m/s]	$(\mathrm{d}u/\mathrm{d}z\|_{in})/2$ [1/s]	T_{in} $[K]$	T_{wall} $[K]$
0.7 (0.005)	0.2497 (0.0017)	6.32 (0.05)	1.605 (0.003)	204.3 (4.4)	293 (2)	416 (5)
0.8 (0.006)	0.3778 (0.0027)	6.93 (0.05)	1.359 (0.002)	160.9 (4.1)	291 (2)	414 (5)
0.9 (0.006)	0.4686 (0.0033)	7.69 (0.05)	1.112 (0.005)	146.1 (12.0)	292 (2)	415 (5)
1.0 (0.007)	0.5349 (0.0038)	7.78 (0.05)	1.012 (0.003)	137.2 (7.3)	292 (2)	412 (5)
1.1 (0.008)	0.5239 (0.0037)	7.63 (0.05)	1.166 (0.004)	205.4 (19.7)	292 (2)	416 (5)
1.2 (0.008)	0.5094 (0.0035)	7.59 (0.05)	1.445 (0.004)	214.9 (17.7)	291 (2)	412 (5)
1.3 (0.009)	0.4939 (0.0033)	7.63 (0.05)	1.570 (0.007)	247.5 (25.9)	291 (2)	412 (5)
1.4 (0.010)	0.4774 (0.0031)	7.50 (0.05)	1.634 (0.008)	277.9 (41.7)	292 (2)	414 (5)
1.5 (0.010)	0.4598 (0.0029)	7.25 (0.05)	1.944 (0.009)	273.1 (26.3)	291 (2)	423 (5)

Supplemental material B: Calibration of optical constant C_{opt}

Calibration of the optical constant, C_{opt}, is necessary to quantify "raw" LIF signals and allow for direct comparison with model predictions across different operating conditions. The methodology used to quantify signals has been used extensively in [1–4]. It should be minimally affected by the choice of nitrogen chemistry, provided that the base chemistry adequately captures reactivity and thermochemistry, even if the model used for calibration is shown to be inaccurate for the calibration case. Figure 1 shows an example of the calibration process performed with a) the NUIG and b) the GRI mechanisms for a lean hydrogen-air flame with a known seeding of 10 ppm of NO molecules in the reactants stream. These two mechanisms are selected to demonstrate that models with inherent differences and discrepancies in their predictions still yield the same optical constant value within uncertainty.

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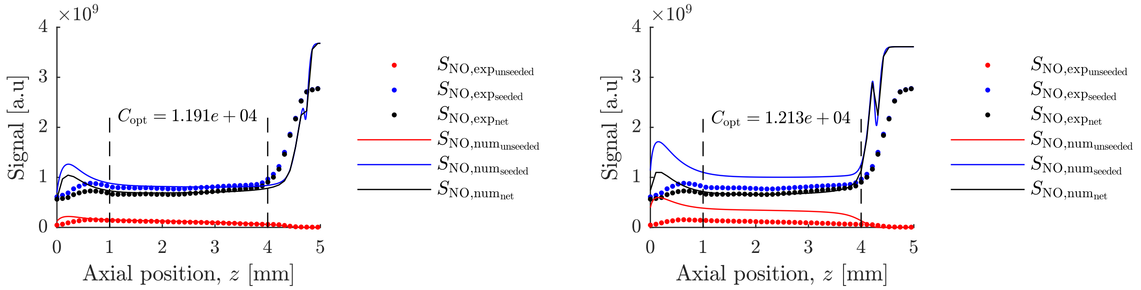
Experimental measurements are performed for the unseeded calibration flame, $\phi = 0.7$, and for different known seeding amount of NO in the flow (5, 10, and 15 ppm). The measured signal intensity for the seeded case, $S_{\mathrm{NO,exp_{seeded}}}$, then includes the fluorescence signal from the known seeded amount, n ppm, plus the NO produced in the flame (Eq. 1). The unseeded signal measurement, $S_{\mathrm{NO,exp_{unseeded}}}$, only captures the fluorescence of the NO that is produced in the flame (Eq 2). Under the assumptions that at lean conditions and low-temperatures there is no reburn or recombination of NO species [5], the subtraction of the unseeded signal from the seeded signal results in an experimental signal intensity of the known seeded amount of NO molecules only, $S_{\mathrm{NO,exp_{net}}}$ (Eq. 3). These experimental signals are shown in Fig. 1 with red, blue, and black symbols for the unseeded, seeded, and net signals, respectively.

$$S_{\mathrm{NO_{seeded}}} = S_{\mathrm{NO}_{n\,\mathrm{ppm}}} + S_{\mathrm{NO_{produced}}} \tag{1}$$

$$S_{\mathrm{NO_{unseeded}}} = S_{\mathrm{NO_{produced}}} \tag{2}$$

$$S_{\mathrm{NO_{net}}} = S_{\mathrm{NO_{seeded}}} - S_{\mathrm{NO_{unseeded}}} = S_{\mathrm{NO}_{n\,\mathrm{ppm}}} \tag{3}$$

With known experimentally-measured boundary conditions, the calibration cases can be simulated with any mechanisms using the quasi-1D axisymmetric model. Numerical fluorescence signals can be obtained by processing the simulation results with a LIF model to produce numerical unseeded, seeded, and net signals, $S_{\mathrm{NO,num_{unseeded}}}$, $S_{\mathrm{NO,num_{seeded}}}$, and $S_{\mathrm{NO,num_{net}}}$, respectively, shown by solid curves in Fig. 1 with colors consistent with experimental measurements. The net numerical signal obtained is then minimally affected by the nitrogen chemistry of the model used to perform the calibration since it describes only the seeded and non-reacting NO molecules. As can be seen in Supplemental Fig. 1, the net signals that arise from use of either kinetic model are in good agreement, even if they predict very different rates of NO formation under these conditions (see Fig. 3g). C_{opt} is calculated by minimizing the least square difference between the net numerical and experimental signals in the post-flame region unaffected by the thermal boundary layer near the water-cooled stagnation surface. This procedure is repeated for the three NO seedings used and the average optical constant value is used to quantify the signals. After calibration, C_{opt} values obtained with the NUIG and GRI mechanisms differ by ~1%, well within the uncertainty on the optical constant of ~20%.



(a) Calibration with NUIG

(b) Calibration with GRI

Figure 1: Calibration procedure for the lean $\phi = 0.7$ H_2 flame with 10 ppm NO seeded performed with a) NUIG and b) GRI.

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