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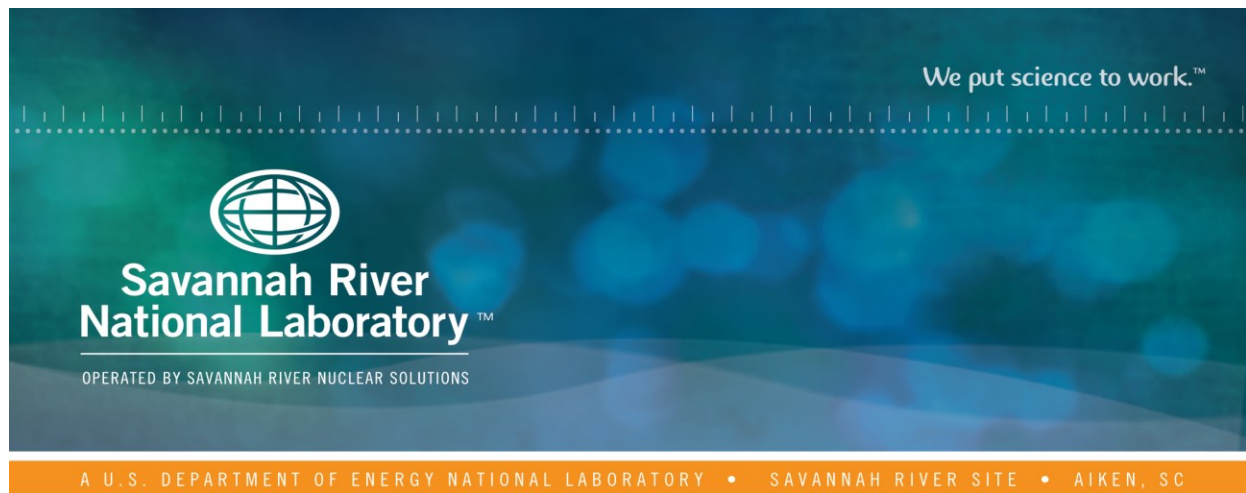
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Dissolution of Material and Test reactor Fuel in an H-Canyon Dissolver

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January 2017

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EXECUTIVE SUMMARY

In an amended record of decision for the management of spent nuclear fuel (SNF) at the Savannah River Site, the US Department of Energy has authorized the dissolution and recovery of U from 1000 bundles of Al-clad SNF. The SNF is fuel from domestic and foreign research reactors and is typically referred to as Material Test Reactor (MTR) fuel. Bundles of MTR fuel containing assemblies fabricated from U-Al alloys (or other U compounds) are currently dissolved using a Hg-catalyzed HNO_3 flowsheet. Since the development of the existing flowsheet, improved experimental methods have been developed to more accurately characterize the offgas composition and generation rate during laboratory dissolutions. Recently, these new techniques were successfully used to develop a flowsheet for the dissolution of High Flux Isotope Reactor (HFIR) fuel. Using the data from the HFIR dissolution flowsheet development and necessary laboratory experiments, the Savannah River National Laboratory (SRNL) was requested to define flowsheet conditions for the dissolution of MTR fuels. With improved offgas characterization techniques, SRNL will be able to define the number of bundles of fuel which can be charged to an H-Canyon dissolver with much less conservatism.

Laboratory-scale experiments were performed to evaluate the dissolution of MTR fuels using both Al 1100 and 30 wt % U-Al alloys. The Al 1100 alloy was considered a representative surrogate since it provided an upper bound on the generation of flammable (i.e., H_2) gas during the dissolution process. The dissolution of the 30 wt % U-Al alloy proceeded at a slower rate than the Al 1100 alloy and was used to verify that the target Al concentration in solution could be achieved for the selected Hg concentrations. Raman spectroscopy was used to provide continuous monitoring of the concentration of H_2 and other permanent gases in the dissolution offgas allowing the development of H_2 generation rate profiles. The H_2 generation rates were subsequently used to evaluate how many L-Bundles could be dissolved in an H-Canyon dissolver without exceeding 60% of the calculated lower flammability limit (LFL) for H_2 at a given Hg concentration.

Complete dissolution of the Al 1100 and 30 wt % U-Al alloys up to a final Al concentration of 2 M was obtained using a HNO_3 solution containing a 0.002 M Hg catalyst. However, following the dissolutions, solids were observed in the solutions. Analysis of the solids generally showed amorphous material or Si and SiO_2 which likely originated from the Si present in the alloys. No crystalline materials, such as $\text{UO}_2(\text{NO}_3)_2$ or $\text{Al}(\text{NO}_3)_3$ were observed. Amorphous and silicon-containing solids from the dissolution of MTR fuels should be easily removed by the Head End centrifuge using the standard gelatin strike process. In experiments performed to develop the HFIR fuel dissolution flowsheet, the H_2 generation data showed that delaying the addition of Hg once the HNO_3 solution reached the boiling point can reduce the total offgas and H_2 generation rates. The delay in starting the Hg addition is not necessary for MTR fuel dissolution, but could allow more L-Bundles to be processed during the initial charge.

The potential to generate flammable concentrations of H_2 in the offgas during a MTR fuel dissolution was evaluated using the experimental data. The predicted H_2 concentration in the dissolver offgas stream was compared with 60% of the calculated H_2 LFL at 200 °C using several prototypical experiments. The calculations showed that four L-Bundles can be initially dissolved using nominally 0.002 M Hg to catalyze the dissolution when the dissolving solution is allowed to boil for 45 minutes prior to starting the Hg addition. The number of allowable bundles which can be charged to a dissolver in subsequent charges was defined as a function of the Al concentration. When the Hg concentration is increased to 0.003 or 0.004 M and the Hg is added when the solution reaches the boiling point, two and one L-Bundles, respectively, can be initially dissolved.

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LIST OF ABBREVIATIONS

CVAA	cold vapor atomic absorption
DOE	Department of Energy
HFIR	High Flux Isotope Reactor
ICPES	inductively-coupled plasma emission spectroscopy
LFL	lower flammability limit
MTHM	metric tons of heavy metal
MTR	Material Test Reactor
MURR	Missouri University Research Reactor
NIST	National Institute of Standards and Technology
ROD	record of decision
SNF	Spent Nuclear Fuel
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
XRD	x-ray diffraction

1.0 Introduction

In 2013, the US Department of Energy (DOE) issued an amended record of decision (ROD) for the management of spent nuclear fuel (SNF) at the Savannah River Site (SRS). The amended ROD stated that DOE will manage approximately 3.3 metric tons of heavy metal (MTHM) from the projected inventory of 22 MTHM at SRS by conventional processing at the H-Canyon facility. The 3.3 MTHM includes up to 200 High Flux Isotope Reactor (HFIR) cores, approximately 1000 bundles of Al-clad SNF currently stored at SRS, as well as target residue material containing enriched U.¹ The SNF is fuel from domestic and foreign research reactors and is typically referred to as Material Test Reactor (MTR) fuel. Bundles of MTR fuel containing assemblies fabricated from U-Al alloys (or other U compounds) are currently dissolved using a Hg-catalyzed, HNO₃ flowsheet.^{2,3} The Hg catalyst is added gradually after the dissolver has reached boiling to achieve a maximum catalyst concentration of 0.012 – 0.015 M. The existing flowsheet also requires the addition of 0.17 M Al (as Al(NO₃)₃) to the dissolving solution and severely limits the number of fuel bundles charged in the first several dissolutions until higher Al concentrations are obtained (Table 1-1) to control the estimated H₂ concentration in the offgas from an H-Canyon dissolver below 60% of the lower flammability limit (LFL).

Table 1-1. Maximum Bundles of SNF Containing 16-68.8 wt % U-Al Alloy in an H-Canyon Dissolver Charge³

Dissolved [Al] (M)	Maximum Bundles
[Al] ≤ 0.17	0
0.17 < [Al] ≤ 0.30	1
0.30 < [Al] ≤ 0.34	2
0.34 < [Al] ≤ 0.39	3
0.39 < [Al] ≤ 0.44	4
0.44 < [Al] ≤ 0.66	7
0.66 < [Al] ≤ 0.84	8
0.84 < [Al] ≤ 0.88	9
0.88 < [Al] ≤ 2.00	10

Since the development of the existing MTR fuel dissolution flowsheet,^{2,3} improved experimental methods have been developed to more accurately characterize the offgas composition and generation rate during laboratory dissolutions. Recently, these new techniques were successfully used to develop a flowsheet for the dissolution of HFIR fuel.⁴ Using the data from the HFIR dissolution flowsheet development and any necessary laboratory experiments, SRNL will define flowsheet conditions for the dissolution of MTR fuels using a Hg concentration between 0.002 and 0.004 M.^{5,6} With improved offgas characterization techniques, SRNL will be able to define the number of bundles of fuel which can be charged to an H-Canyon dissolver with much less conservatism.

Following dissolution of the MTR fuels, the U-containing solution will be processed through Head End and centrifuged to remove particulate matter. After Head End treatment, the U will be recovered and purified by solvent extraction (1st and 2nd U Cycles), and the waste processed for transfer to the H-Area Tank Farm. The enriched U from the MTR fuels will be down-blended into low-enriched U for subsequent use as commercial reactor fuel. The relatively high Al content in the dissolved fuel limits the downstream processing due to issues associated with Al solubility.⁷ The number of bundles dissolved in a batch will be dependent on the final Al concentration in the solution. Typically, H-Canyon does not exceed approximately 1.7 M Al(NO₃)₃ in the dissolver (at 2 M HNO₃), but higher Al(NO₃)₃

concentrations (≤ 2 M) will be evaluated as part of this study. The initial HNO_3 concentration used during dissolution is dependent on the amount of Al and U to be dissolved, targeting a final HNO_3 concentration of 0.5–1.0 M after completion of the dissolution of the last charge. Boric acid or $\text{Gd}(\text{NO}_3)_3$ may be used as a nuclear safety poison. Concentrations up to 2 g/L B or 2 g/L Gd in surrogate dissolver solutions have been observed to be stable from precipitation.⁷

1.1 Objectives

The objective of this work was to identify flowsheet conditions through literature review and laboratory experimentation to safely and efficiently dissolve U-Al alloy MTR fuels (or fuels fabricated from other U compounds) in H-Canyon. During this task, we evaluated the generation of H_2 from the dissolution of the fuels to determine the number of bundles which can be charged to an H-Canyon dissolver without exceeding 60% of the H_2 LFL during the initial and subsequent charges. In addition, the downstream processing of the dissolver solution (including Head End and solvent extraction operations) were evaluated to ensure any processing issues were identified and resolved.

2.0 Experimental Procedure

2.1 Surrogate Materials

During the development of the dissolution flowsheet for HFIR fuel, scouting experiments were performed using both Al 1100 and Al 6061 T6 alloys to establish which Al alloy provides a bounding estimate for the generation of H_2 . Generally Al 1100 is used to manufacture the fissionable component of MTR fuels and Al 6061 alloy is used for the cladding and structural components. The L-Bundle used to store and transfer MTR fuels is also generally fabricated from Al 6061 alloy. In dissolution experiments designed to characterize the offgas from the two alloys, Daniel et al. demonstrated that the Al 1100 alloy was bounding in terms of the H_2 generation rate when compared to the dissolution of the Al 6061 T6 alloy.⁴ Based on these results, data from the dissolution of Al 1100 were used to evaluate the H_2 generation rate from the dissolution of MTR fuels.

2.2 Alloy Dissolution

Two prior experiments (97, 98) performed to define a dissolution flowsheet for HFIR fuel⁴ and four additional experiments (105-108) were used to define the dissolution conditions using Al 1100 and 30 wt % U-Al alloys. A summary of the objective and dissolution conditions for each experiment are provided in Table 2-1. All experiments were performed at the boiling point of the solution.

Table 2-1. Al Alloy Dissolution Experiments

Exp. No. ⁽¹⁾	Objective (Evaluate ...)	Al Alloy	Hg Conc. (M)	Target Al Conc. (M)
97	offgas generation rate at 0.002 M Hg with hold on Hg addition	Al 1100	0.002	2.0
98	offgas generation rate at 0.004 M Hg with hold on Hg addition	Al 1100	0.004	2.0
105	offgas generation rate at 0.004 M Hg without pausing Hg addition	Al 1100	0.004	2.0
106	offgas generation rate at 0.002 M Hg without pausing Hg addition	Al 1100	0.002	2.0
107	offgas generation rate at 0.003 M Hg without pausing Hg addition	Al 1100	0.003	2.0
108	offgas generation rate at 0.002 M Hg without pausing Hg addition	30 wt % U-Al	0.002	2.0

(1) Experimental numbering sequence corresponds to data recording practices

2.2.1 Preparation of Coupons

The Al 1100 alloys used in the dissolution experiments were prepared by cutting corrosion coupons to the desired length. The coupons were lightly sanded, washed with soap and water, and then weighed and measured. The coupons were sanded to maximize reactivity as well as to generate consistent results. The coupons used for the majority of the experiments had a mass of approximately 6 g each with a surface area of approximately 5 cm².

The 30 wt % U-Al alloy coupon was previously cut to model the dissolution of Denmark Reactor (DR-3) fuels during the development of a modified dissolution flowsheet for Sodium Reactor Experiment (SRE) and DR-3 fuels.² The coupon was lightly sanded, washed with soap and water, and then weighed and measured prior to the dissolution.

The masses, dimensions, and surface areas of the coupons used in the experiments are provided in Table 2-2. The surface areas are based on a 10 mm immersion depth along the length of each coupon in the HNO₃ solution. The calculations are illustrated by equation 2,

$$SA \text{ (cm}^2\text{)} = 2(1 \text{ cm})(t \text{ (cm)}) + 2(1 \text{ cm})(w \text{ (cm)}) + (t \text{ (cm)})(w \text{ (cm)}) \quad (2)$$

where SA is the surface area of the immersed coupon, t is the thickness of the coupon, and w is the width of the coupon.

Table 2-2. Alloy Coupon Characteristics

Exp. No.⁽¹⁾	Mass	Length	Width	Thickness	Surface Area⁽²⁾
	(g)	(cm)	(cm)	(cm)	(cm²)
97	6.0599	4.090	1.905	0.290	4.942
98	6.2206	4.210	1.910	0.291	4.958
105	6.0797	4.150	1.921	0.291	4.983
106	5.9958	4.238	1.913	0.277	4.910
107	5.9227	4.177	1.918	0.275	4.914
108	9.7914	2.659	1.396	0.913	5.893

(1) Experiments 97, 98 and 105-107 used Al 1100 alloy; Experiment 108 used 30 wt % U-Al alloy

(2) Surface areas were calculated for a 10 mm coupon immersion

2.2.2 Dissolving System

The vessel and offgas condenser used to perform the Al alloy dissolution experiments were fabricated from borosilicate glass by the SRNL Glass Shop. The dissolving vessel was made from a 300-mL round-bottom flask. Penetrations were added for a condenser, Hg addition (using a syringe pump), thermocouple, and gas purge. The bottom of the flask was flattened slightly to facilitate heating and agitation using a hot plate/stirrer with a magnetic stir bar. During dissolution, a coupon was charged to the dissolver in a glass basket suspended by a glass rod which was held in place by a compression fitting. The compression fitting allows adjustment of the basket height during dissolution. The solution temperature was controlled using an external thermocouple monitored by the hot plate. Offgas exiting the dissolving vessel can be sampled for analysis by mass spectrometry using a sample line connected to a port just above the condenser; although, this capability was not used. A manometer, also connected to the offgas sample port, acts as a pressure relief device and provides a measurement of the pressure in the system. The offgas leaving the condenser subsequently passes through a cell containing a Raman probe and terminates in a bubbler (i.e., beaker containing 700 mL or 3.5 in of deionized water). The bubbler prevents air in-leakage from the vent side of the system. The Raman spectrometer was used to measure non-condensable gases such as H₂, N₂, O₂, Ar, NO, N₂O and NO₂ in real time during the experiment. A photograph of the equipment is shown in Figure 2-1.

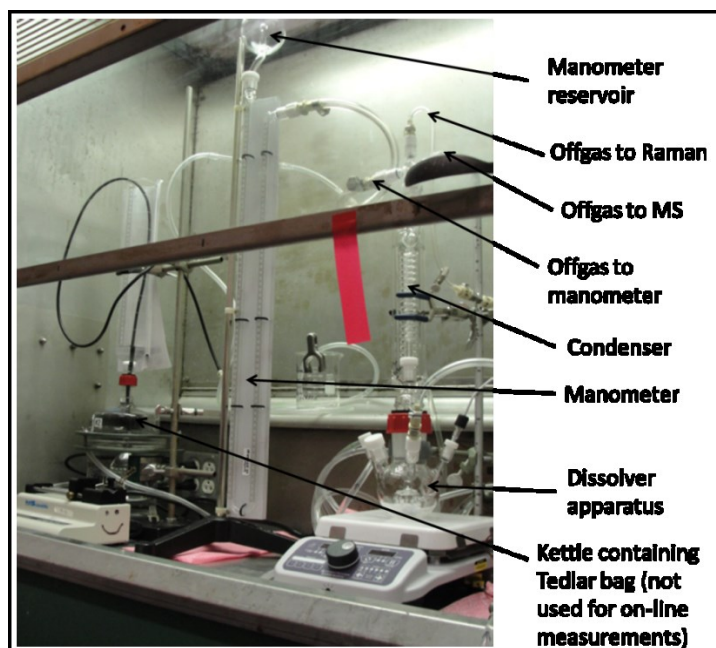


Figure 2-1. Dissolver Setup with Online MS and Raman Offgas Analyzers

2.2.2.1 Raman Spectrometer

The Raman spectrometer non-intrusively analyzes the offgas through a quartz window using the excitation of a laser passing through a fixed portion of the offgas stream. The Raman scattering technique identifies and measures the concentration of gases in the offgas stream. The Raman spectrometer was calibrated using the standard gases shown in Table 2-3. The Raman spectrometer measures the concentrations of the offgas species approximately every 12-13 seconds. Since the Raman spectrometer directly measures the concentrations in the offgas stream, there is zero dead time between the offgas concentration measurement and the reading other than the analysis time of 12-13 seconds. The Raman spectrometer was controlled by and data was logged using a computer running EZRamanReader v8.3.9 software and an Excel spreadsheet.

Table 2-3. Calibration Gases for Raman Analyzer

Supplier	Gas	Ar	N ₂	N ₂ O	NO ₂	NO	O ₂	H ₂
		(%)	(%)	(%)	(%)	(%)	(%)	(%)
Air Liquide	20% N ₂ O-80% Ar	80.00	—	20.00	—	—	—	—
Liquid Technology	5% NO ₂ -20% O ₂ -75% Ar	74.89	—	—	4.98	—	20.13	—
Air Liquide	20% NO-80% Ar	80.00	—	—	—	20.00	—	—
Air Liquide	5% N ₂ -10% H ₂ -85% Ar	85.00	5.00	—	—	—	—	10.00
SRNL	Ar ⁽¹⁾	99.9	—	—	—	—	—	—
SRNL	N ₂ ⁽¹⁾	—	99.9	—	—	—	—	—
SRNL	Air ⁽¹⁾	0.94	78.03	—	—	—	20.99	—

(1) purity not measured; supplied from SRNL facility gases

To calculate offgas generation rates, a CO₂ tracer gas was metered into the system through a flow controller at a set rate (20, 30, or 50 cm³/min @ 70 °F, 1 atm). The total offgas rate was then calculated by dividing the set input rate by the measured CO₂ concentration in the offgas.

Calibration of the Raman spectrometer and treatment of the data is discussed in Appendix A.

2.2.3 Dissolution Experiments

Prior to performing a dissolution experiment, the dissolving system was checked for leaks by connecting a Tedlar[®] bag inside a glass kettle filled with water (Figure 2-1.) to the dissolver and adding sufficient Ar, N₂, or CO₂ to the bag to generate a column of water 18-28 cm tall. The Tedlar[®] bag system was then closed and monitored for any observable decrease in the water column height over approximately 3 min. After the system integrity was confirmed, the experiment was started.

To perform a dissolution, the Al or U-Al alloy coupon was initially placed in a perforated glass basket. The basket was lowered until the coupon was immersed 10 mm lengthwise into a 7 M HNO₃ dissolving solution at room temperature. The solution was then heated to boiling. Chilled water (at 3 °C) was circulated through the condenser during the dissolution to remove water vapor from the offgas stream before the gas flowed through the Raman cell. Once the solution reached boiling, either the Hg solution was added right away or there was a hold time before starting the Hg addition to reduce the initial offgas surge. The initial volume of HNO₃ and the volume of the Hg solution added (Table 2-4) were based on the mass of the Al coupon and the target Al and Hg concentrations.

During the dissolution of Al 1100 alloy in Experiments 97 and 98, it was found that holding the coupon in the boiling HNO₃ solution for 45 min significantly reduced the initial surge of offgas for the lower Hg concentration (i.e., 0.002 M). The reduced reactivity of the Al coupons was likely due to the passivation of the surface by the HNO₃ solution during the hold time.

Table 2-4. Dissolving Solution Volume and Composition

Exp. No.	Initial Volume	Hg Solution Volume	Target Hg Concentration	Target Al Concentration
	(mL)	(mL)	(M)	(M)
97	124	1.48	0.002	1.8
98	114	2.75	0.004	2.0
105	110	2.67	0.004	2.0
106	110	1.32	0.002	2.0
107	108	1.95	0.003	2.0
108	126	1.50	0.002	2.0

To simulate the Hg addition performed in the 6.4D dissolver,⁸ the time of the Hg addition relative to total fuel dissolution time was scaled in an effort to match the Hg addition to the increasing concentration of Al in solution. It was assumed that the 6.4 D dissolver takes about 36 h to dissolve a charge of fuel and 6 h of that time was used to add 0.012 M Hg. Therefore, one-sixth of the total dissolution time was used for adding Hg. For the lab scale experiments, approximately 76 min were needed to dissolve the Al-1100 alloy coupons starting with 7 M HNO₃ (with the Al concentration increasing to approximately 1.6 M). Therefore, on the lab scale, the Hg was added over 76/6 or 12.67 min. The Hg solution for the dissolution of the Al alloys was obtained from H-Canyon Tank 201 and contained 4.31 wt % Hg(NO₃)₂ (0.169 M Hg) and 37.79 wt % (7.64 M) HNO₃. Therefore, on the lab scale, 10 mL of the Hg solution would be added to 130 ml of HNO₃ solution giving an effective Hg addition rate of 10 mL/12.67 minutes or 0.79 mL/min (47.4 mL/h).

During the experiments, samples of the final dissolving solutions were collected for analysis. Samples were submitted to SRNL Analytical Development to measure the HNO_3 (free acid), Hg, and metals concentrations in reagents and in final dissolving solutions. The free acid, Hg, and metals concentrations were determined by titration, cold vapor atomic absorption (CVAA) spectroscopy, and inductively-coupled plasma emission spectroscopy (ICPES), respectively. Some final dissolution solutions (Experiments 97 and 106) were filtered and the filtered solids were examined by x-ray diffraction (XRD) analysis. Samples of the initial 7 M HNO_3 dissolving solution were also submitted for free acid analysis. Samples of the H-Canyon Hg solution were submitted for free acid and Hg analysis. The analyses were used as checks on the concentrations since the initial and final volumes of the dissolver solutions were measured as well as the mass of Al added to each solution.

2.3 Quality Assurance

Requirements for performing reviews of technical reports and the extent of review are established in manual E7, 2.60. SRNL documents the extent and type of review using the SRNL Technical Report Design Checklist contained in WSRC-IM-2002-00011, Rev. 2.

3.0 Results and Discussion

3.1 Effect of Hg Addition on Offgas Generation

During the dissolution of the Al-1100 alloy, it was observed that holding the coupon in the boiling HNO_3 solution for 45 min prior to starting the Hg addition significantly reduced the initial surge of offgas and the H_2 generation rate. In Experiment 106, Al 1100 was dissolved in 7 M HNO_3 and the addition of 0.002 M Hg was initiated immediately after reaching the solution boiling point. In Experiment 97, Al 1100 was dissolved in 7 M HNO_3 and the addition of 0.002 M Hg was initiated 45 min after the solution reached the boiling point. The H_2 generation rates for the two experiments are shown in Figure 3-1 and demonstrate that holding the solution at the boiling point for 45 min and then starting the Hg addition reduces the H_2 generation rate especially during the peak H_2 generation at the beginning of the dissolution.

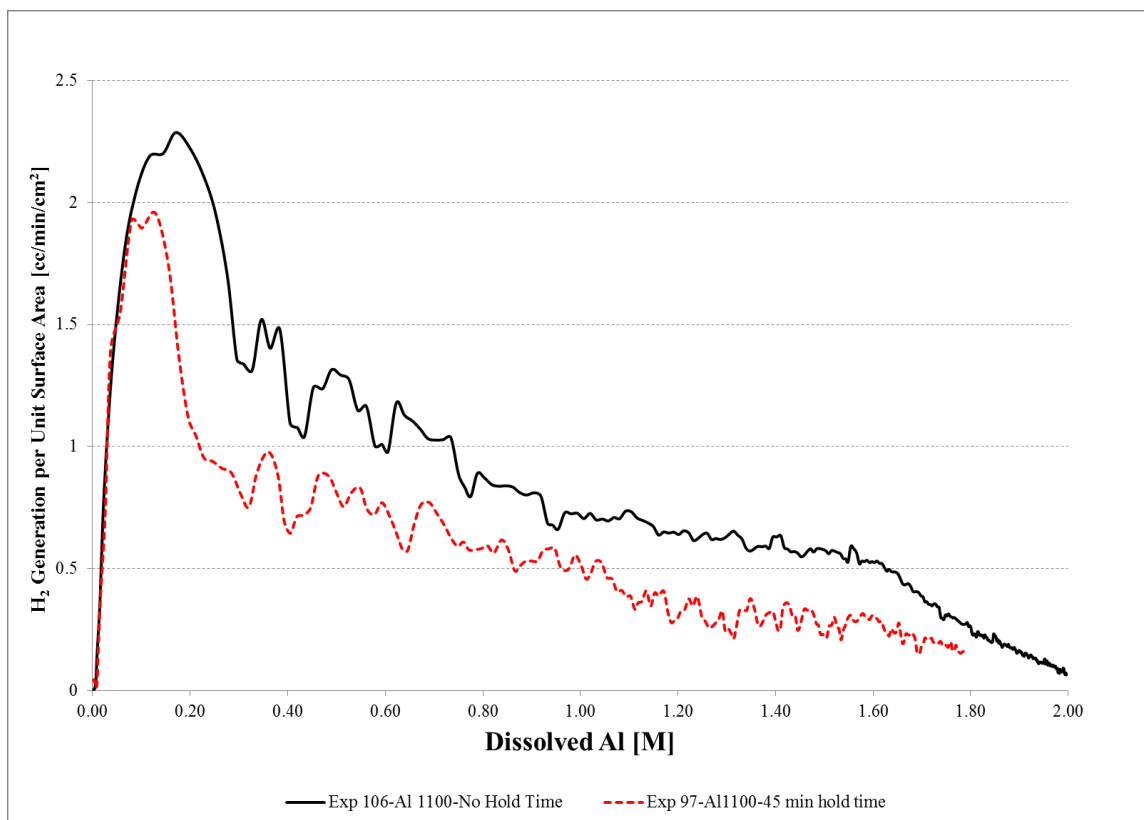


Figure 3-1. Effect of Hold Time on H₂ Generation Rate

3.2 Flowsheet Development

3.2.1 Maximum Dissolved Al Concentration

Experiments were performed using the Al-1100 alloy with high targeted Al end points (e.g., 1.8-2.0 M) to evaluate the rate of dissolution and to determine if there were any solubility issues following dissolution. Experiment 108 was performed to illustrate that a 30 wt % U-Al alloy is not a concern with respect to Al concentrations approaching 2 M. Experiments 97, 98, 105, 106, and 107 performed with the Al 1100 alloy, targeted final Al concentrations of 1.8, 2.0, 2.0, 2.0, and 2.0 M, respectively. The H₂ generation curves (which illustrate the extent of dissolution) for the experiments are plotted as a function of time in Figure 3-2. Time zero for each curve represents the start of the Hg addition. The figure shows that the Al 1100 alloy dissolves much faster than the 30 wt % U-Al alloy. In fact, an Al concentration of 1.9 M was only reached after 21,902 seconds (6.08 hours) when the 30 wt % U-Al alloy was dissolved. Complete dissolution of the U-Al alloy required 173,170 seconds (48.1 hours) (see Figure 3-3); however, the unusually long dissolution time was exacerbated due to complete consumption of the 7 M HNO₃. Additional acid was required to complete the dissolution.

Complete dissolution of the Al coupons was achieved in each experiment. However, following the dissolution experiments, solids were observed in the solution. Analysis of the solids by XRD generally showed amorphous material or Si and SiO₂ as shown in Figure 3-4. No crystalline materials, such as UO₂(NO₃)₂ or Al(NO₃)₃ were observed. This result is consistent with several previous Al 1100 dissolution experiments in which unidentifiable amorphous solids were recovered from the dissolving solution by filtration. In other experiments, undissolved solids were identified by XRD as elemental Si.² Amorphous and silicon-containing solids from the dissolution of MTR fuel (including U₃Si₂ fuels) in an H-Canyon dissolver should be easily removed by the Head End centrifuge using the standard gelatin strike process.⁹

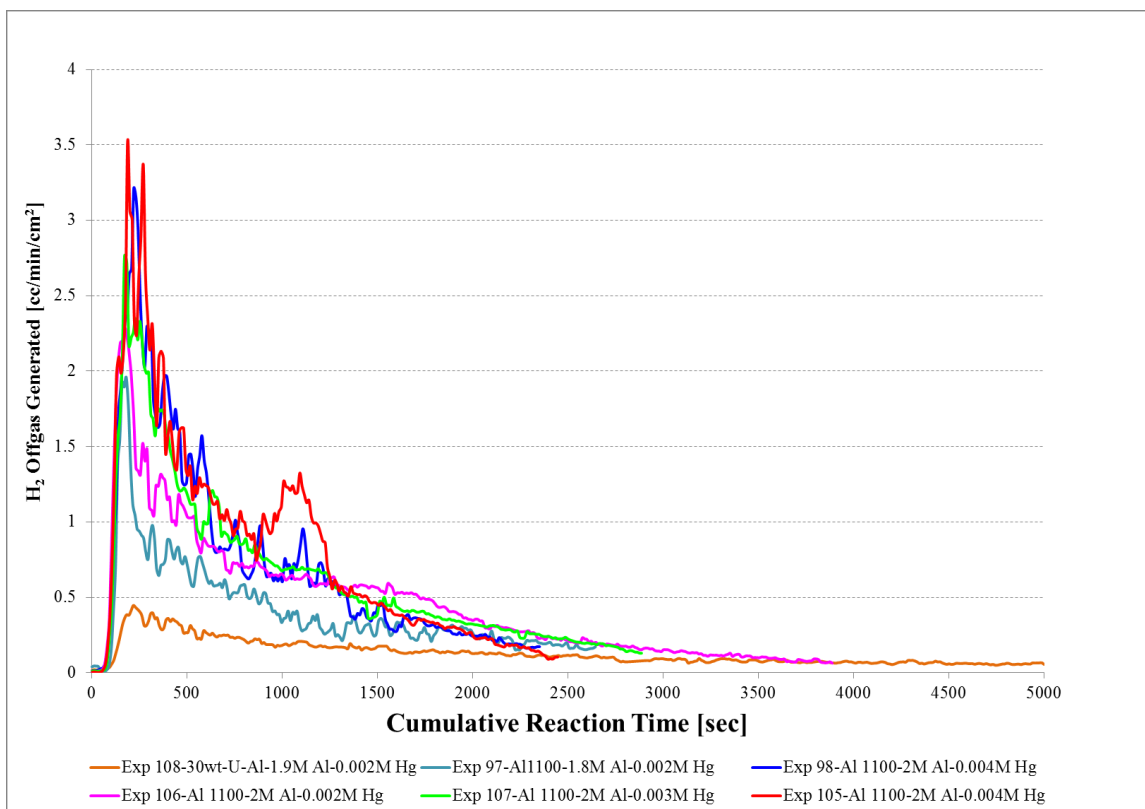


Figure 3-2. H₂ Generation Rate for Experiments Targeting High Concentrations of Al

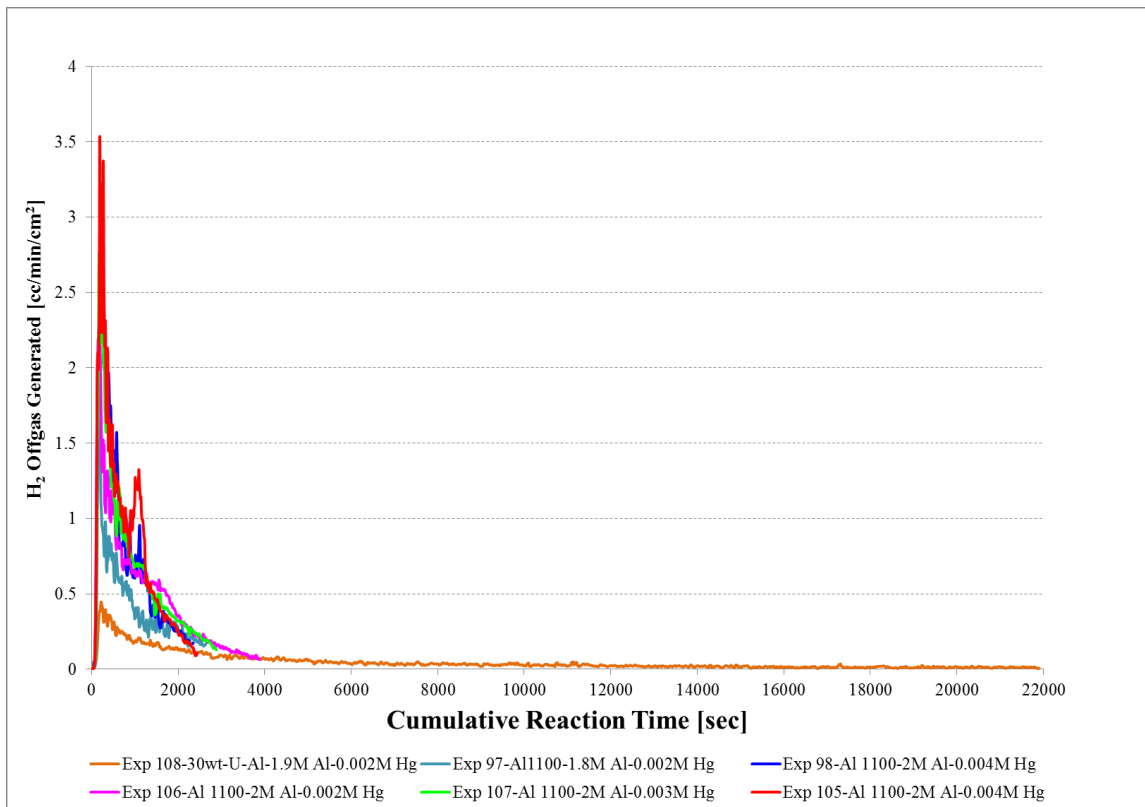


Figure 3-3. H₂ Generation Rate for Experiment 108 up to 1.9 M Al

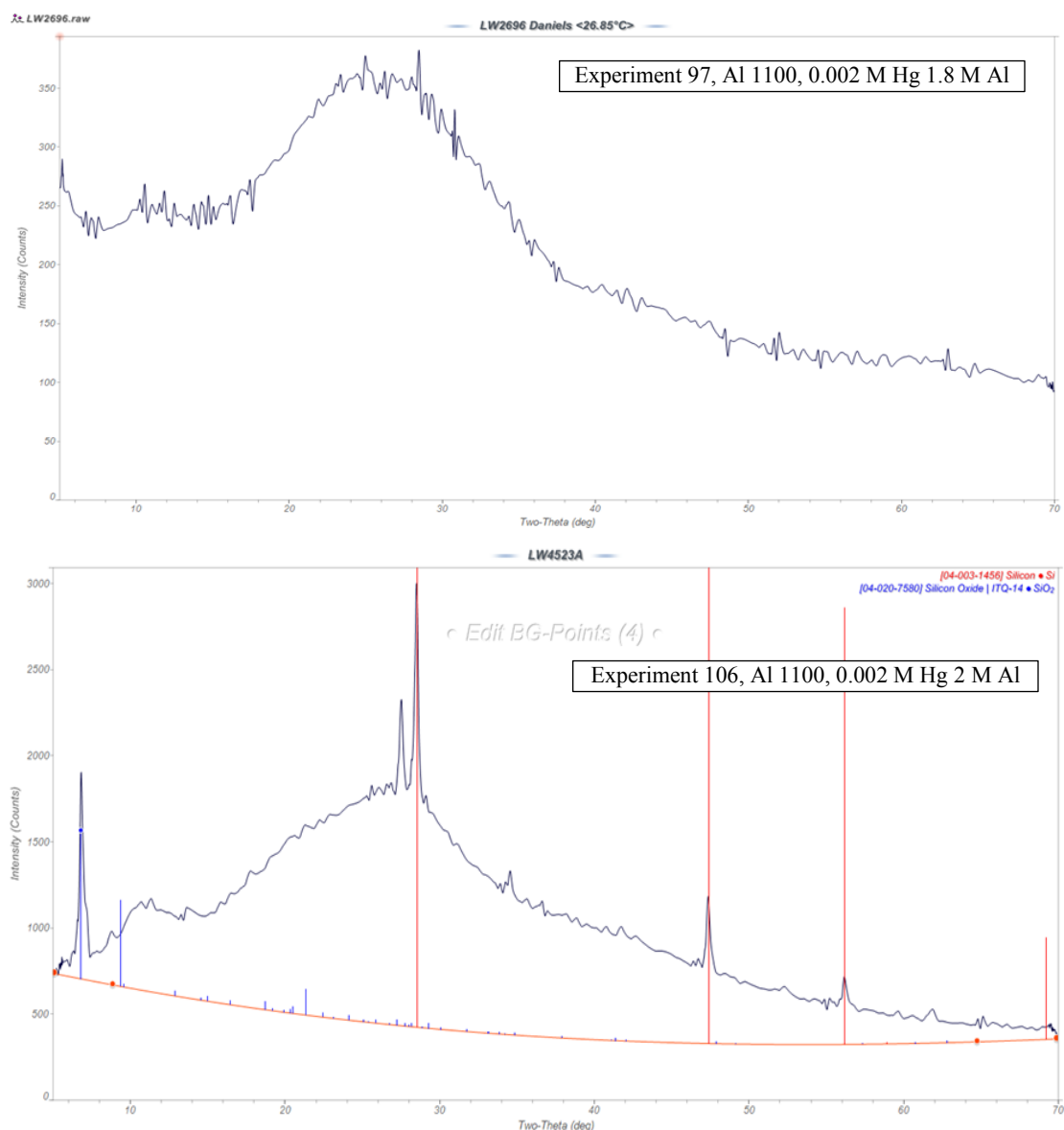


Figure 3-4. XRD Results for Solids Generated During Al Alloy Dissolutions

3.2.2 Flammable Gas Generation

The rate of flammable gas generation from MTR fuel is proportional to the surface area exposed to the dissolving solution. The MTR fuel will be packaged in L-Bundles which dissolve first. The L-Bundles have the largest surface area and off-gas generation compared to fuels similar to Missouri University Research Reactor (MURR) fuel.¹⁰ Although, most research reactor fuel assemblies are fabricated from multiple plates, the spacing between plates is sufficiently close that fresh dissolving solution cannot continuously fill the small void between adjacent surfaces and dissolve Al. The offgas generation from the dissolution of Al would also hinder the flow of fresh solution to the close surfaces. During the development of a dissolution flowsheet for SRS U-Al alloy tubular fuel, Caracciolo¹¹ demonstrated that the dissolution rate for two concentric fuel tubes containing a 16 wt % U-Al alloy was essentially the same as for a single tube of the same alloy. This result indicated that the outside surface area of the outer tube controlled the dissolution rate. For previous dissolution flowsheets, the peak offgas generation rate during the dissolution of fuel assemblies was based on the outer surface area of the L-Bundle.^{2,7,10,12} For

the MTR fuel dissolution flowsheet, the peak offgas rate will also be based on the outer surface area of the L-Bundle.

To estimate the concentration of H_2 in the offgas during the dissolution of MTR fuel, experiments were performed using Al 1100 alloy. A dissolution experiment using a 30 wt % U-Al alloy (Experiment 108) demonstrated that the dissolution of the Al 1100 alloy was bounding in terms of the H_2 generation rate when compared to the dissolution of the 30 wt % U-Al alloy. Experiments 97, 98, 105, 106, and 107 were performed to measure the H_2 generation rate for Al 1100 at nominally 0.002 M, 0.003 M, and 0.004 M Hg. In experiments 97-98, the Hg addition was started after the solution had boiled for about 45 minutes. In Experiments 105-107, the Hg addition was started as soon as the solution reached boiling. In each case, 7 M HNO_3 was used as the dissolving solution.

The H_2 generation rates for Experiments 97, 98, 105, 106, and 107 are plotted as a function of the dissolved Al concentration in Figure 3-5. The H_2 generation rates were calculated from the measured offgas generation rates, measured H_2 concentrations, and the measured surface area of the Al 1100 coupons. The concentration of Al in the dissolving solution as a function of time was estimated using the method described by Almond et al.² The figure shows that the H_2 generation rates surge after the start of the Hg addition and the rates for Experiment 98 (0.004 M Hg) are approximately twice the values for Experiment 97 (0.002 M Hg). The figure also shows that when the Hg level is low (0.002 M), holding for 45 minutes at boiling before starting the Hg addition does reduce the H_2 generation rate after the initial surge. However, at higher Hg levels (0.004 M), holding for 45 minutes at boiling before starting the Hg addition does not reduce the H_2 generation rate significantly.

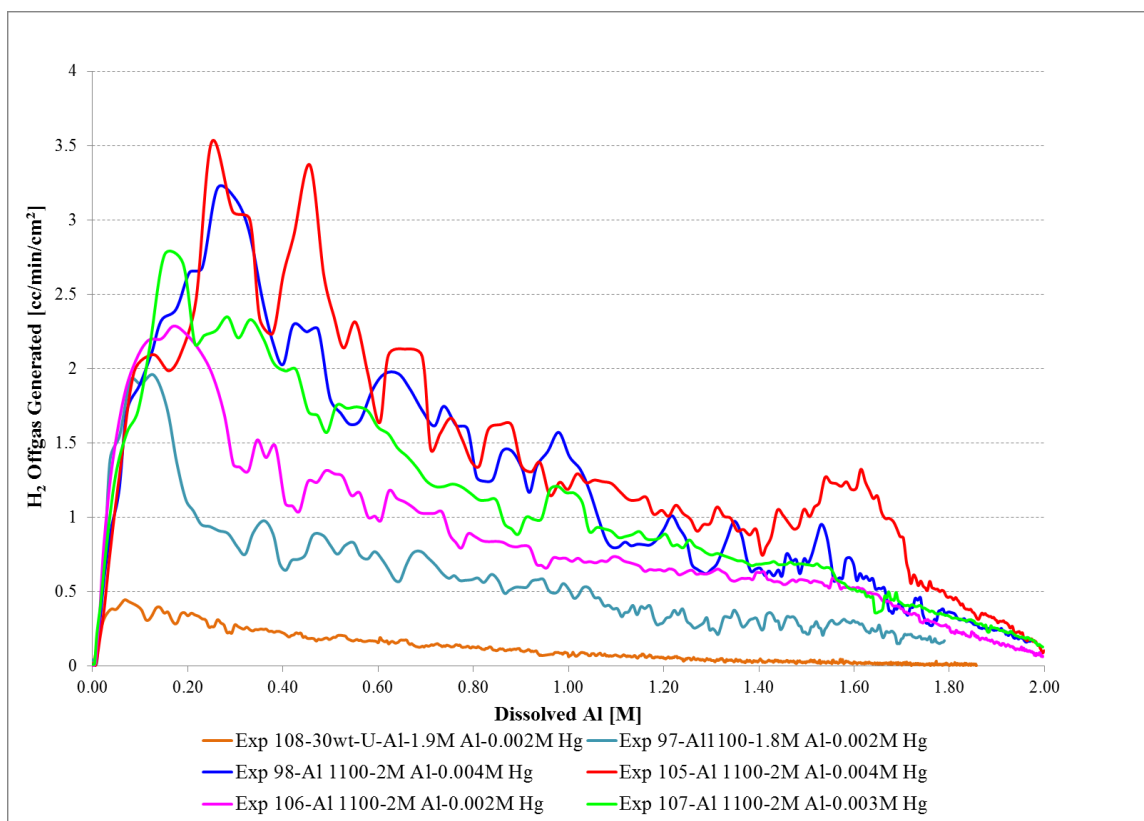


Figure 3-5. H_2 Generation Rate from the Dissolution of Al 1100 and 30-wt % U/Al Alloy

The criterion of not exceeding 60% of the H_2 LFL in the dissolver offgas (at 200 °C) was used for the flammable gas calculations in this report and is consistent with the criterion used for other fuel dissolution

flowsheets.^{2,4,7,10,12} When automatic instrumentation with safety interlocks is provided, the combustible concentration is permitted to be maintained at or below 60% of the LFL.¹³ The H₂ LFL at 200 °C is required due to the iodine reactor in the offgas stream of the H-Canyon dissolvers which operates at this temperature. Lower flammability limit data reported by Scott et al.¹⁴ for air, H₂, NO, and N₂O mixtures were used to calculate the LFL for comparison to the H₂ concentrations calculated for an H-Canyon dissolver. Three data sets for NO:N₂O ratios of 2.57, 1.00, and 0.33 are shown in Appendix B. The H₂ LFL data in Appendix B were correlated using a second order polynomial to allow interpolation at varying concentrations of air (Table 3-1).

Table 3-1. Correlations for H₂ LFL Data

NO:N ₂ O Ratio ⁽¹⁾ (vol %/vol %)	Correlation
$x \geq 2.57$	$H_2 \text{ LFL (vol \%)} = 6.038 + 3.174 * 10^{-2} (\text{Air vol \%}) - 5.401 * 10^{-4} (\text{Air vol \%})^2$
$1 \leq x < 2.57$	$H_2 \text{ LFL (vol \%)} = 3.425 + 1.207 * 10^{-1} (\text{Air vol \%}) - 1.186 * 10^{-3} (\text{Air vol \%})^2$
$x < 1$	$H_2 \text{ LFL (vol \%)} = 5.479 - 1.067 * 10^{-3} (\text{Air vol \%}) - 1.400 * 10^{-4} (\text{Air vol \%})^2$

(1) x is defined as the NO:N₂O ratio

The NO:N₂O volume ratios for dissolution experiments 97, 98, 105, 106, and 107, which were used to estimate the H₂ LFL in the offgas during dissolution of MTR fuel, are shown in Figure 3-6. The LFL data for H₂ provided in Appendix B show that normally higher NO:N₂O ratios result in higher values for the H₂ LFL; likewise, lower NO:N₂O ratios normally will result in lower values of the H₂ LFL.

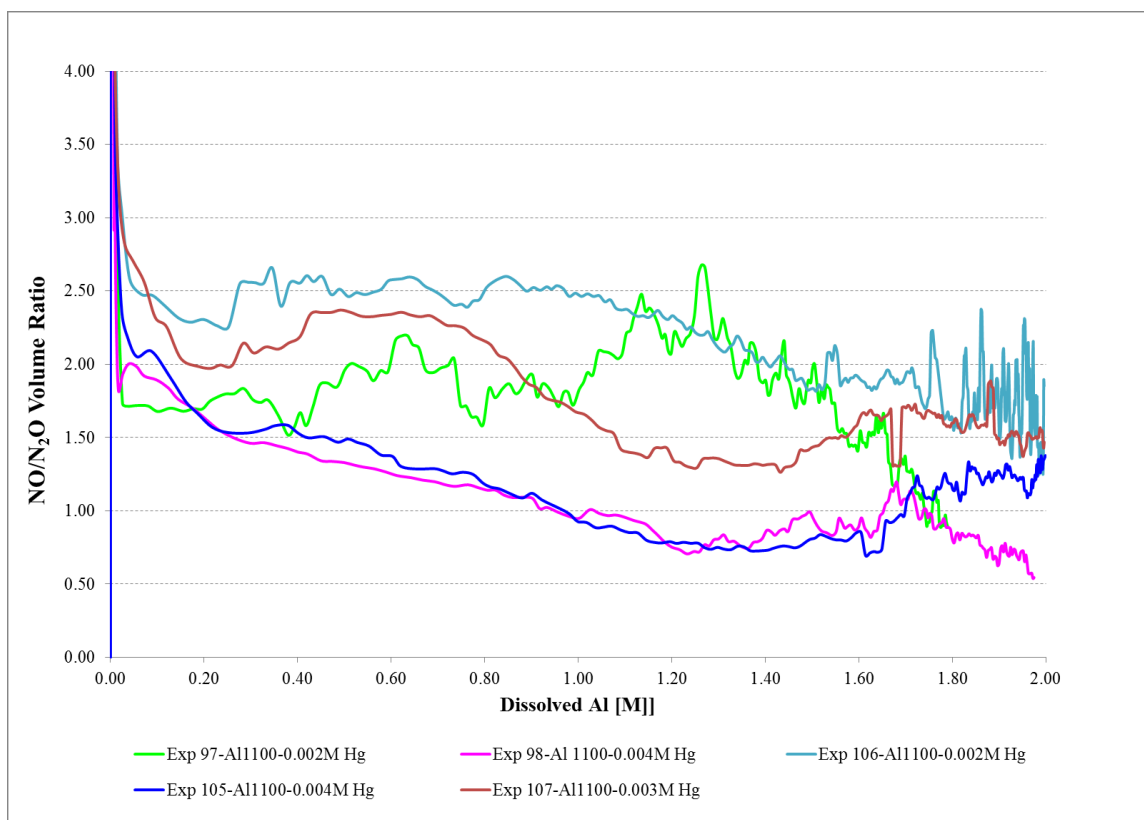


Figure 3-6. NO:N₂O Volume Ratio from the Dissolution of Al 1100 Alloy

The maximum concentration of H₂ calculated during the dissolution of MTR fuel must be compared to the appropriate percentage of the LFL for H₂ at the maximum temperature of the offgas. Since the offgas from the H-Canyon dissolvers flow through the iodine reactor, which operates at 200 °C, the LFL for H₂ must be corrected for the increase in temperature. The LFL is corrected using equation 3:¹⁵

$$LFL_T = LFL_{ref} (1 - A(T - T_{ref})) \quad (3)$$

where LFL_T is the LFL at temperature T (°C), LFL_{ref} is the LFL at the reference temperature, A is an empirical coefficient (Zabetakis attenuation factor) equal to 0.0011, and T (°C) is the temperature at which the LFL is evaluated. For the H₂ LFL data provided in Appendix B, which were measured at 28 °C, equation 3 can be simplified to equation 4 for use at 200 °C.

$$LFL_{200\text{ }^{\circ}\text{C}} = LFL_{28\text{ }^{\circ}\text{C}} (0.811) \quad (4)$$

The H₂ generation rates calculated for Experiments 97, 98, 105, 106, and 107 (Figure 3-5) were used to predict the H₂ concentration in the offgas stream from an H-Canyon dissolver. The experiments were performed using 0.002 to 0.004 M Hg and targeted a final Al concentration of 1.8 to 2 M. The offgas generation rate for an L-Bundle was based on the outer surface area of the L-Bundle since the L-Bundle surface area is bounding for MURR-like fuel.⁷ For the normal 54 in. immersion of the L-Bundle in the H-Canyon dissolver, the exposed outer surface area per L-Bundle is 6.4546 ft².¹⁰

To estimate the H₂ concentration in the dissolver offgas stream, the total offgas generation rate was initially predicted for a single L-Bundle (equation 5).

$$\text{Predicted Offgas Rate (SCFM)} = \text{Measured Offgas Rate} \left(\frac{\text{SCFM}}{\text{ft}^2} \right) (6.4546 \text{ ft}^2) \quad (5)$$

The predicted H₂ generation rate for the L-Bundle was calculated in a similar manner (equation 6) by scaling-up the H₂ generation rate calculated from the experimental data (Figure 3-5).

$$\text{Predicted H}_2 \text{ Offgas Rate (SCFM)} = \text{Measured H}_2 \text{ Offgas Rate} \left(\frac{\text{SCFM}}{\text{ft}^2} \right) (6.4546 \text{ ft}^2) \quad (6)$$

The predicted H₂ concentration in the dissolver offgas stream was subsequently calculated from the predicted H₂ offgas rate, the predicted (total) offgas rate, and the volumetric flow rate of air used to sparge (i.e., mix) the solution and purge the dissolver (equation 7). A dissolver sparge/purge rate of 40 SCFM was used for all calculations.

$$\text{Predicted H}_2 \text{ Conc (vol \%)} = \frac{\text{Predicted H}_2 \text{ Offgas Rate (SCFM)}}{\text{Predicted Offgas Rate (SCFM)} + 40 \text{ SCFM}} \left(\frac{100 \text{ vol \%}}{1} \right) \quad (7)$$

The predicted H₂ concentration (with air dilution) in the dissolver offgas stream is compared with 60% of the calculated H₂ LFL at 200 °C in Figure 3-7 through Figure 3-11 for Experiments 97, 98, 105, 106, and 107, respectively, to determine how many L-Bundles could be charged to the dissolver without exceeding the calculated LFL over the Al concentration range from 0 to 2 M. The number of L-Bundles that can be charged while staying below the calculated LFL varied depending on the concentration of Hg being used and whether the Hg was added when boiling was reached or delayed for 45 minutes after boiling was reached. Figure 3-10 shows that when the Hg addition is started at boiling for a final Hg concentration of

0.002 M, 3 L-Bundles could be charged to begin the dissolution since the predicted H_2 concentration is below 60% of the LFL. It should be noted that the margin between the predicted H_2 concentration and the calculated LFL is greater for 0.002 M Hg when the dissolving solution was allowed to boil for 45 min prior to initiating the Hg addition (Figure 3-7). The comparison of the predicted H_2 concentration to 60% of the LFL with 0.004 M Hg (normal Hg addition for Experiment 105 in Figure 3-9 and Hg addition after 45 minute pause for Experiment 98 in Figure 3-8), shows that 2 L-Bundles could be charged initially. If the Hg addition is paused at boiling for 0.004 M Hg then more L-Bundles are allowed once the dissolved Al concentration increases.

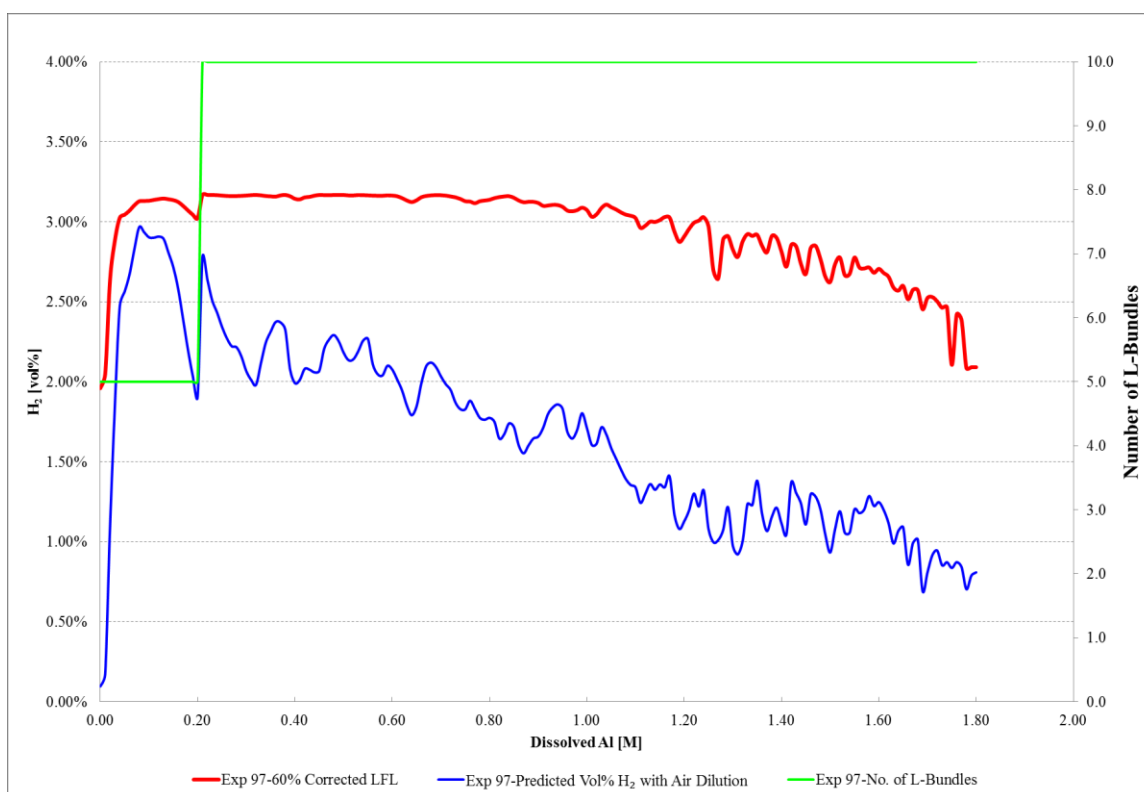


Figure 3-7. H_2 LFL for Exp. 97 – 7 M HNO_3 , 0.002 M Hg, and 45 min Hold Time

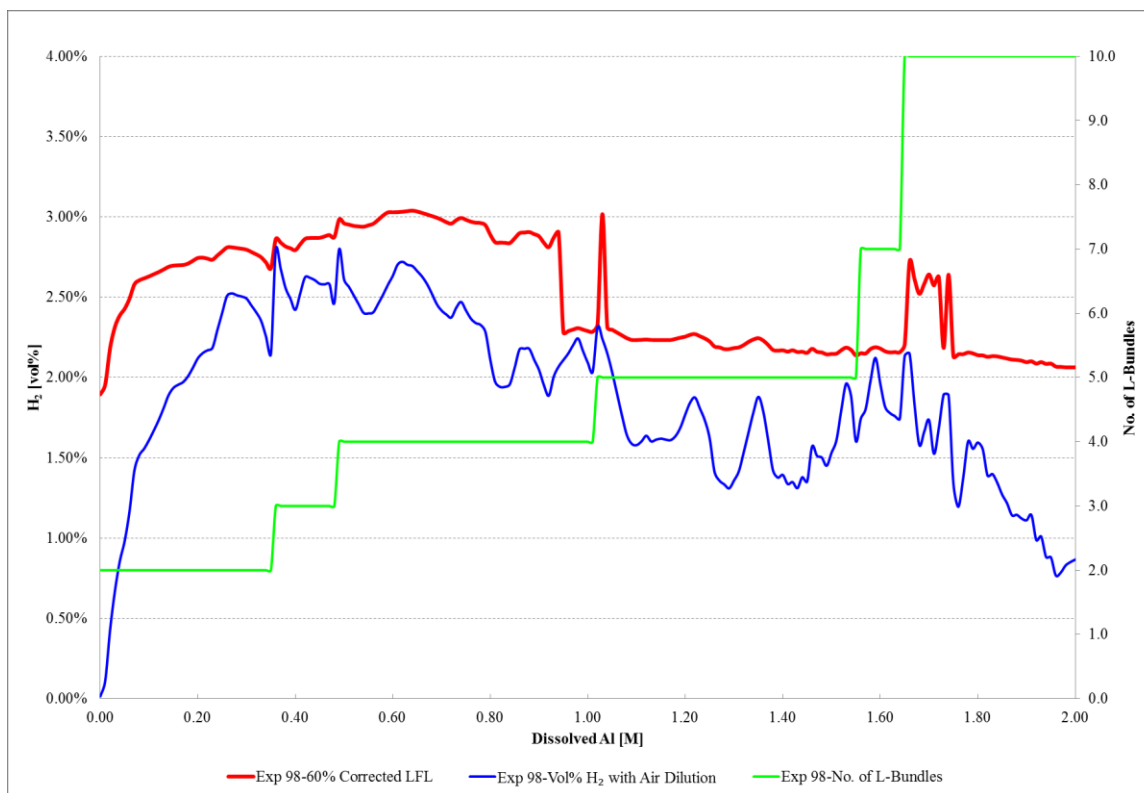


Figure 3-8. H₂ LFL for Exp. 98 – 7 M HNO₃, 0.004 M Hg, and 45 min Hold Time

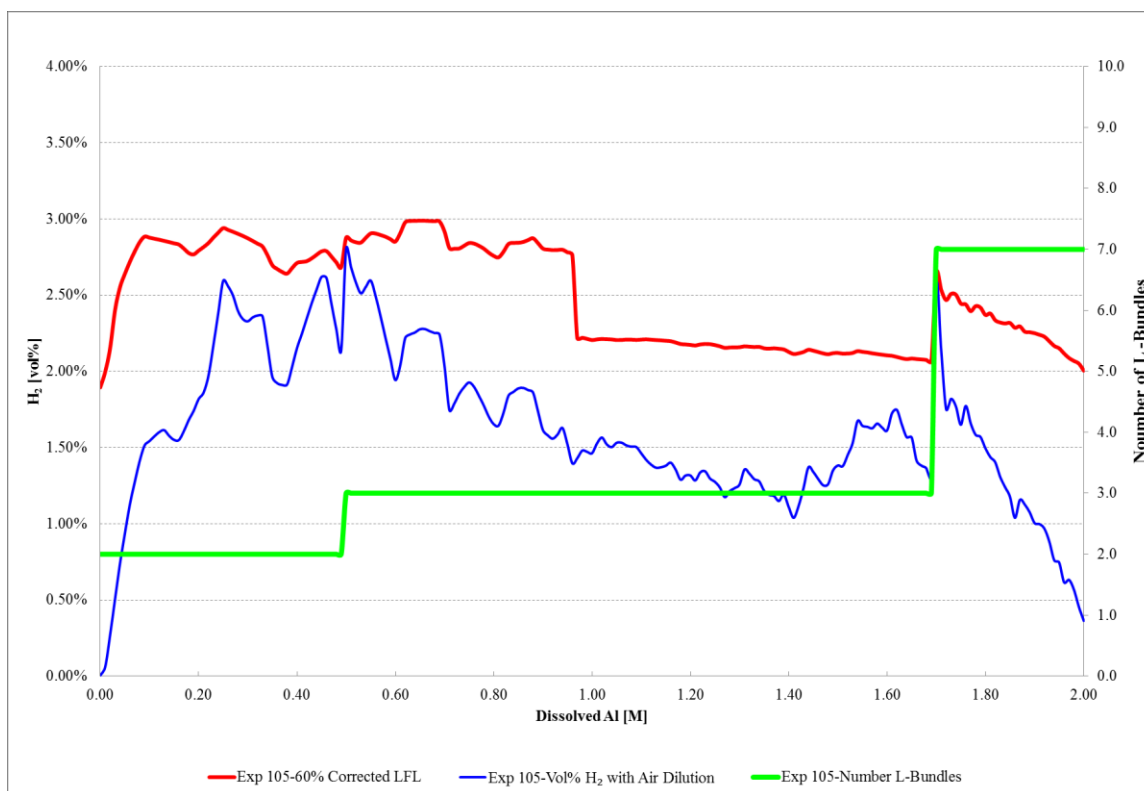


Figure 3-9. H₂ LFL for Exp. 105 – 7 M HNO₃, 0.004 M Hg, and No Hold Time

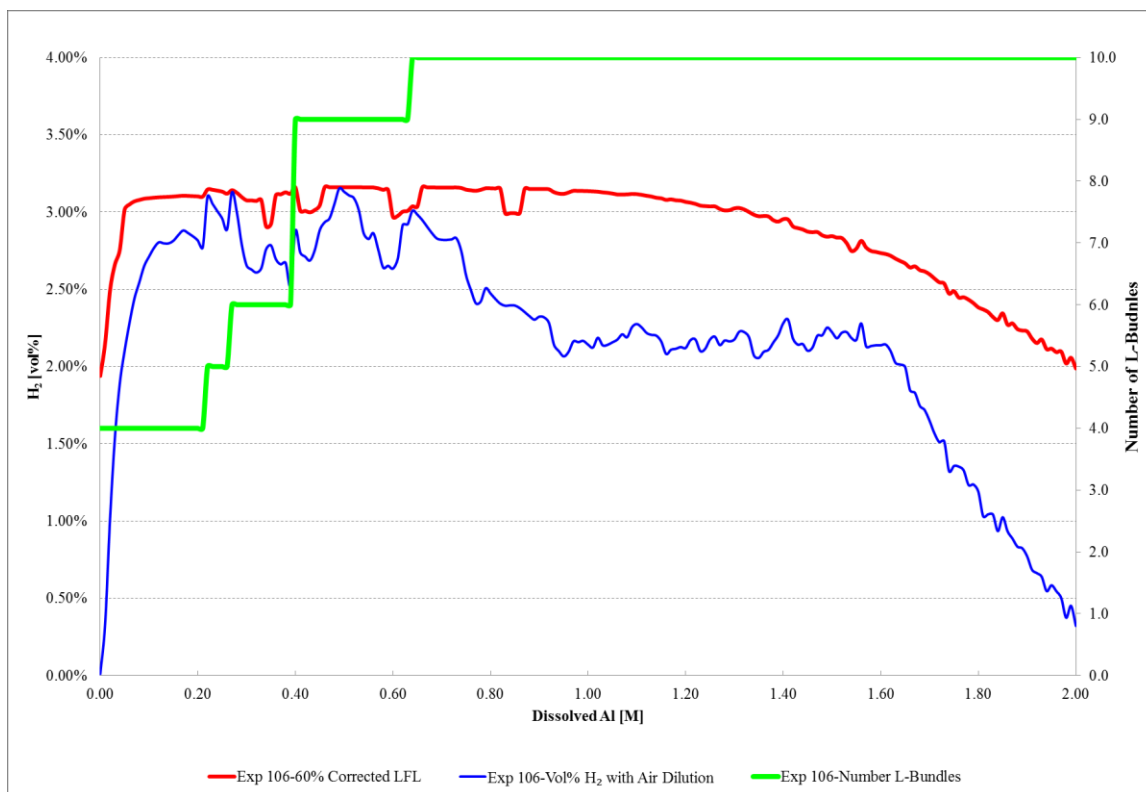


Figure 3-10. H₂ LFL for Exp. 106 – 7 M HNO₃, 0.002 M Hg, and No Hold Time

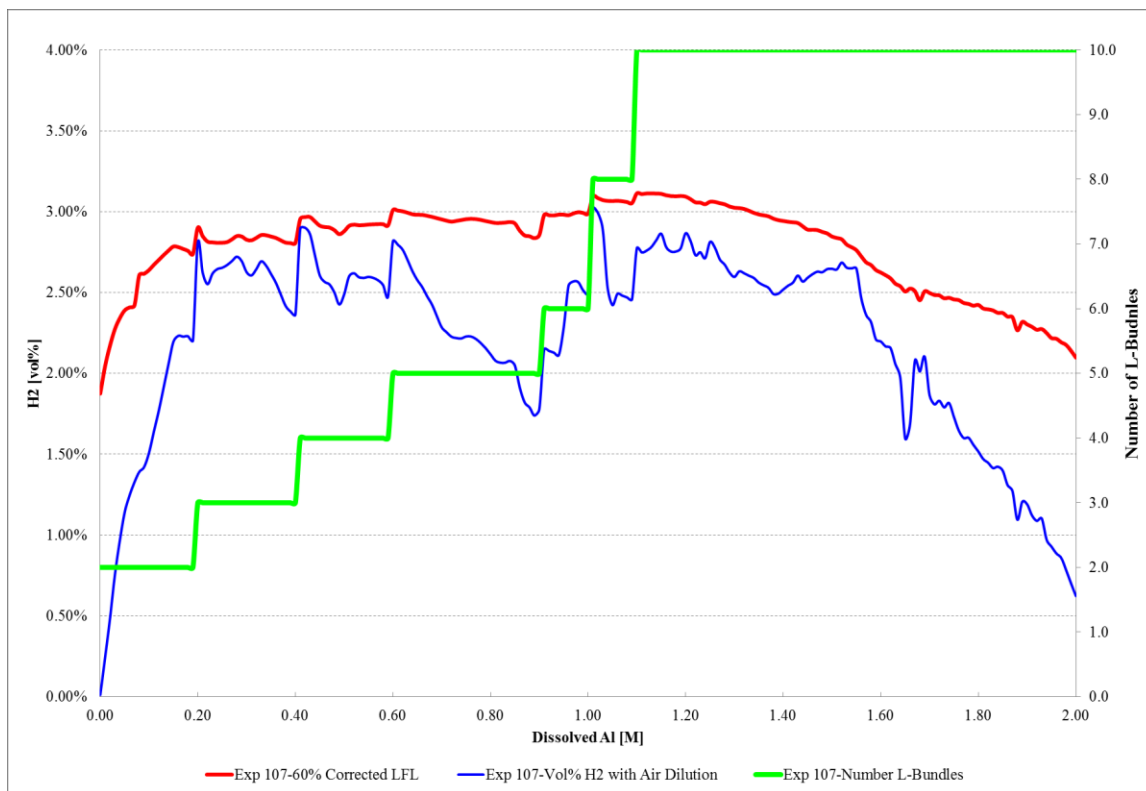


Figure 3-11. H₂ LFL for Exp. 107 – 7 M HNO₃, 0.003 M Hg, and No Hold Time

The uncertainties associated with the calculations performed to determine the number of L-Bundles that can be charged to an H-Canyon dissolver (at a given Hg concentration) were not evaluated; however, the uncertainties associated with the offgas analyses were examined. The Raman spectrometer was calibrated using NIST-traceable standards and calibration gases checked before each experiment. The 2σ value or twice the standard deviation for the Raman spectrometer H_2 analysis is <2 vol % (see Appendix A). A summary of the 2σ uncertainties for all calibrated gases is provided in Table 3-2.

Table 3-2. Two Sigma Uncertainties for Gas Concentrations Measured by Raman Spectroscopy

Gas	2σ Uncertainty (vol %)
CO ₂	4.10
N ₂	2.36
O ₂	0.80
H ₂	1.14

To understand how small uncertainties in the offgas concentration measurements performed by Raman spectroscopy affected the calculations performed to determine how many L-Bundles could be charged to a dissolver, the measured H_2 concentrations in Experiments 97 and 106 were increased by 1.14 vol % (2σ uncertainty). The maximum number of L-Bundles that could be charged with the increased H_2 concentrations at 0-2 M Al decreased for the normal (Figure 3-12 and Figure 3-13) and the paused additions of 0.002 M Hg (Figure 3-14 and Figure 3-15) as expected. Combining the results from Experiments 97 and 106, Table 3-3 provides the maximum number of L-Bundles for 0-2 M Al when the H_2 concentration was increased by 1.14 vol %. The initial charge of L-Bundles is based on the addition of 0.002 M Hg 45 minutes after reaching the boiling point of the solution (Experiment 97). The allowable number of L-Bundles for higher concentrations of Al is based on the more conservative results from Experiment 106 in which 0.002 M Hg was added when the solution began to boil. The decrease in the number of allowable L-Bundles (from 4 to 3) between 0.15 and 0.23 M Al is a reflection of the transition in the data from the paused to the normal addition of Hg used in the two experiments. A reduction in the number of allowable L-Bundles in this concentration range guards against the surge in the offgas and H_2 generation rates if bundles of fuel (which were not passivated by 45 minutes at the solution boiling point) are charged to a dissolver at relatively low Al concentrations to a solution already containing 0.002 M Hg. However, if the first charge of fuel results in an Al concentration which is between 0.23 and 0.35 M, then a second charge of 4 L-Bundles is permitted.

Table 3-3. Maximum Number of L-Bundles based on Al Concentration and H_2 vol% + 1.14 vol % with Paused Addition of 0.002 M Hg

Dissolved Al [M]	No. L-Bundles
$0.00 < Al[M] \leq 0.15$	4
$0.15 < Al[M] \leq 0.23$	3
$0.23 < Al[M] \leq 0.35$	4
$0.35 < Al[M] \leq 0.38$	5
$0.38 < Al[M] \leq 0.65$	6
$0.65 < Al[M] \leq 0.74$	8
$0.74 < Al[M] \leq 2.00$	10

Other aspects of the calculations have built-in conservatism which further address the uncertainty in the calculations. The calculated H_2 concentration in the offgas stream is compared to 60% of the LFL which provides a layer of conservatism. The saturated water vapor in the offgas stream is ignored and would further dilute the H_2 concentration. Given the conservative nature of the experimental design and the calculations performed, the maximum number of L-Bundles that can be charged to an H-Canyon dissolver using nominally 0.002 M Hg to catalyze the dissolution adequately incorporates the many uncertainties associated with the experimental and modeling work.

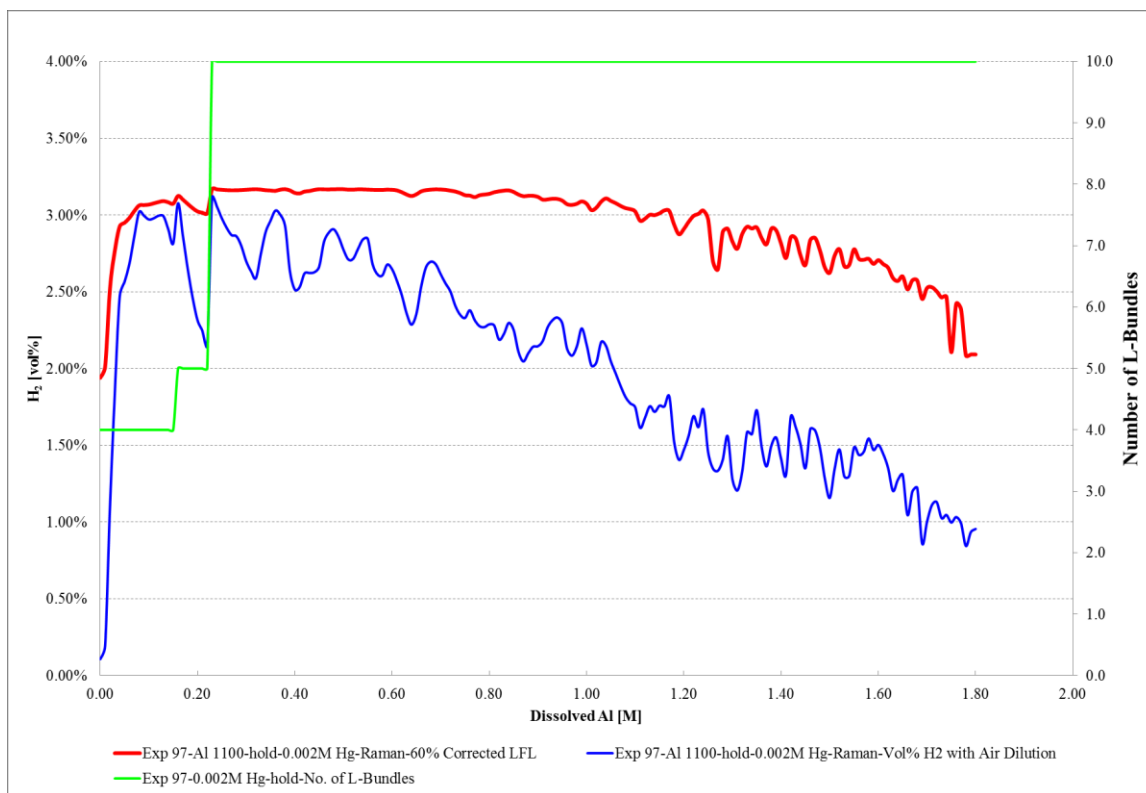


Figure 3-12. H₂ LFL Comparison for Exp. 97 with Predicted H₂ Increased by 1.14 vol %

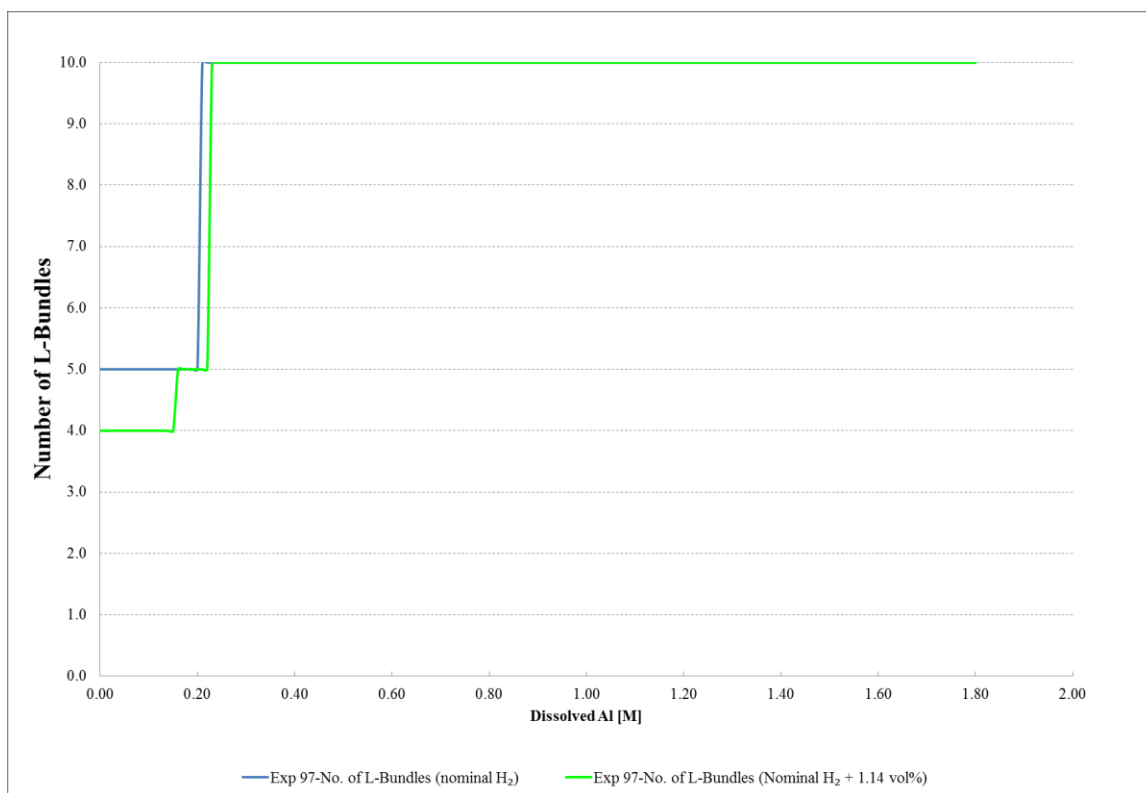


Figure 3-13. H₂ LFL Comparison for Exp. 97 with unadjusted H₂ and H₂ increased by 1.14 vol %

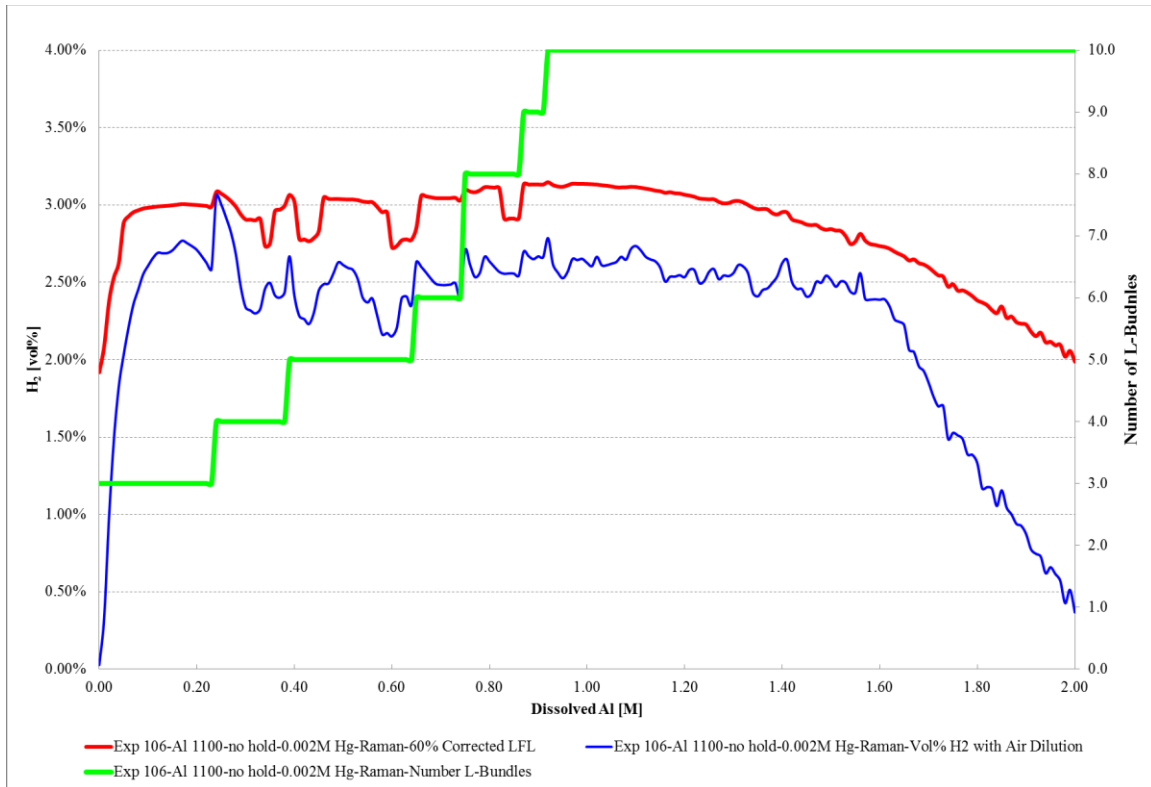


Figure 3-14. H₂ LFL Comparison for Exp. 106 with Predicted H₂ Increased by 1.14 vol %

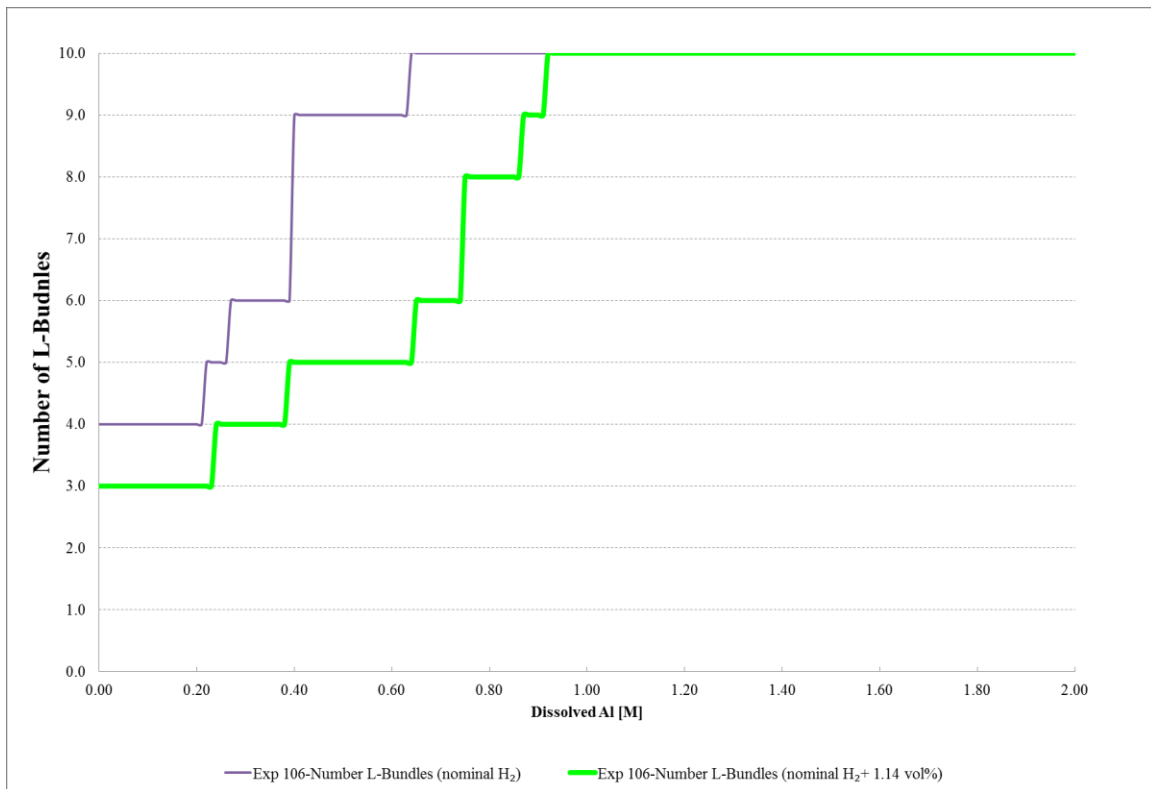


Figure 3-15. H₂ LFL Comparison for Exp. 106 with unadjusted H₂ and H₂ increased by 1.14 vol %

3.3 Downstream Processing of MTR Fuel

Following dissolution of the MTR fuels, the solution will be processed through Head End and the 1st and 2nd Cycles of solvent extraction to recover the enriched U for subsequent down-blending for use as commercial reactor fuel. No issues associated with the processing of the enriched U solutions through Head End and solvent extraction are anticipated. The dissolution of the MTR fuels will generate undissolved solids such as transition metal fission products (e.g., Zr, Mo, Ru, Tc, Pd, and Ag) and Si (as SiO₂) which is present in the Al alloys and produced from the transmutation of Al during fuel irradiation. These solids should be easily removed by the Head End centrifuge using the standard gelatin strike process. Once the solution is clarified, purification by solvent extraction should proceed in the same manner as in previous campaigns. High and low activity waste generated from the processing will be neutralized and prepared for disposal using existing SRS facilities. No issues are anticipated in this process.

4.0 Conclusions

To achieve complete dissolution of L-Bundles containing MTR fuels, a Hg-catalyzed HNO₃ dissolution flowsheet was demonstrated. In laboratory experiments, Al 1100 and 30 wt % U-Al alloys were dissolved starting with a 7 M HNO₃ solution. A Hg catalyst concentration of 0.002 M was sufficient to dissolve Al alloy coupons up to a final Al concentration of ≤ 2 M. Complete dissolution of the Al coupons was achieved; however, following the dissolutions, solids were observed in the solution. Analysis of the solids generally showed amorphous material or Si and SiO₂ which likely originated from the Si present in the alloys. No crystalline materials, such as UO₂(NO₃)₂ or Al(NO₃)₃ were observed. During the course of the experiments, it was determined that delaying the addition of Hg once the HNO₃ solution reaches boiling can reduce the total offgas and H₂ generation rates. The delay in starting the Hg addition is not necessary, but increases the number of L-Bundles that can be initially charged based on the Al concentration.

The potential to generate flammable concentrations of H₂ in the offgas during MTR fuel dissolution was evaluated using the experimental data. The predicted H₂ concentration (with air dilution) in the dissolver offgas stream was compared with 60% of the calculated H₂ LFL at 200 °C using several prototypical experiments. The calculations showed that four L-Bundles can be dissolved initially when the dissolving solution is allowed to boil for 45 min prior to starting the addition of 0.002 M Hg. The number of allowable bundles which can be charged to a dissolver in subsequent charges was defined as a function of the Al concentration. When the Hg concentration is increased to 0.003 or 0.004 M and the Hg is added when the solution reaches the boiling point, two and one L-Bundles, respectively, can be initially dissolved.

5.0 Flowsheet Recommendations

Flowsheet recommendations were developed for the dissolution of MTR fuels using either the 6.4D or 6.1D dissolver. The process conditions required to ensure that the predicted H₂ concentration in the offgas from dissolution is less than 60% of the H₂ LFL at 200 °C are summarized below.

- The flowsheet analysis assumes 54 inch immersion of the L-Bundle in the dissolver solution.
- A dissolver air sparge/purge flow rate of at least 40 SCFM is required.
- The initial HNO₃ concentration shall be based on the mass of Al and U charged to the dissolver. The concentration is typically 5 to 7.5 M.
- A Hg concentration of nominally 0.002 M shall be used to catalyze the dissolution of the MTR fuel. The Hg shall be added to the 6.4D dissolver as described in Procedure 221-H-4101 after waiting 45 minutes after the solution reaches boiling.⁸ A similar Hg addition method shall be used for the 6.1D dissolver.
- The HNO₃ concentration in the dissolver solution at the completion of the dissolution of a batch of MTR fuel shall be greater than 0.5 M.

The maximum L-Bundles containing MTR fuel that may be processed varies based on the Hg concentration, how the Hg is added, and the dissolved Al concentration. The maximum L-Bundles that can be charged assuming a H₂ concentration with measurement uncertainty using 0.002 M Hg is shown in Table 3-3. Variations in the Hg concentration added to the dissolver shall not exceed $\pm 25\%$ of the required concentration (0.0020 ± 0.0005). Based on past MTR fuel dissolution history, the recommended flowsheet should result in an estimated dissolution time of 24 to 48 h for a dissolver charge. The dissolution times would be expected to increase as the Al concentration in the dissolver also increases.

6.0 References

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Appendix A. Raman Calibration and Sampling Method

The Raman spectrometer was calibrated using a set of calibration gases as shown in Table 2-3. Due to the nature of the Raman technique, the instrument only needs to be calibrated once for the intensities (or quantities) of the calibration gases. The wavelengths for the various calibration gases are known and also remain fixed. As an additional check before and after each experiment, air, 99.9 vol % CO₂, and/or a 2.67 vol % H₂ gas (balance Ar) were analyzed using the Raman cell to ensure the calibration was still good. If the calibration checks were off for these gases, the Raman calibration model was adjusted for those gases after the run. For the Al dissolutions performed in Experiments 97 and 98, the calibration checks are shown in Table A-1. The calibration check indicates if the calibration was successful and provides an indication of the variance of the measurements since the calibration gas is analyzed for several samples.

The Raman readings should be positive and sum to 100% except for the 2.67 vol % H₂ gas which is 97.33 vol % Ar (which is not detected by the Raman spectrometer). Due to the noise in the Raman signal, any raw readings that are less than zero are fixed to zero and then all the gas readings for H₂, NO₂, N₂, O₂, N₂O, NO, CO₂, CO, H₂O and NH₃ are normalized to 100% except for the 2.67 vol % H₂ gas. These fixed and normalized Raman readings are the values reported in Table A-1 except for the 2.67 vol % H₂ gas where the raw readings are provided. Due to rounding to the nearest hundredth, the numbers in the table may not sum exactly to 100 vol % but all the decimal places were carried in the calculations performed for this report.

The total offgas flow is calculated from the fixed normalized sum of the CO₂ and CO concentrations divided into the CO₂ tracer flow rate coming into the system as shown in Table A-2. The noise in the concentrations measured by the Raman spectrometer propagates into the total offgas flow rate so moving averages of the total offgas flow rates were performed using equation A-1:

$$\text{Offgas flow rate}_{t_i} (\text{cm}^3/\text{min}) = \frac{\sum_{k=t_i-1}^{t_i+1} \text{Offgas flow rate}_k}{3} \quad (\text{A-1})$$

where Offgas flow rate = offgas generated by the dissolution in cm³/min
 t_i = time at integer time step i
 k = integer time step t_{i-1} , t_i , and t_{i+1} .

The moving average offgas flow rates and fixed normalized moving average Raman offgas concentrations for Experiment 97, 98, 105, 106 and 107 are shown in Appendix C, D, E, F, and G, respectively.

Table A-1. Pre-run Check of Calibration Gases for Al Dissolution Experiments 97-107

Gas Description	Exp.	H ₂ (%)	NO ₂ (%)	N ₂ (%)	O ₂ (%)	N ₂ O (%)	NO (%)	CO ₂ (%)	CO (%)	H ₂ O (%)	NH ₃ (%)
99.9% CO ₂	97	0.00	0.24	0.00	0.40	0.00	0.00	98.62	0.26	0.49	0.00
	97	0.00	0.29	0.28	0.70	0.00	0.04	98.05	0.00	0.58	0.07
	97	0.21	0.28	0.04	0.78	0.00	0.00	98.45	0.00	0.19	0.06
	97	0.00	0.25	0.22	0.00	0.00	0.15	98.01	0.55	0.64	0.18
	97	0.23	0.24	0.00	0.65	0.00	0.00	98.64	0.00	0.24	0.00
	97	0.07	0.21	0.05	0.48	0.00	0.00	98.60	0.06	0.53	0.00
	97	0.17	0.29	0.37	0.39	0.00	0.04	98.42	0.00	0.32	0.00
	97	0.00	0.23	0.00	0.66	0.00	0.01	98.46	0.29	0.35	0.00
	Avg.	0.09	0.25	0.12	0.51	0.00	0.03	98.41	0.15	0.42	0.04
	98	0.02	0.30	0.61	0.96	0.00	0.26	97.58	0.00	0.16	0.12
	98	0.00	0.21	0.51	0.29	0.00	0.00	98.72	0.00	0.21	0.06
	98	0.31	0.26	0.80	0.96	0.00	0.31	96.54	0.13	0.42	0.26
	98	0.00	0.26	0.17	0.90	0.00	0.00	97.89	0.00	0.65	0.13
	98	0.00	0.25	0.71	0.67	0.00	0.00	98.01	0.24	0.12	0.00
	98	0.11	0.25	0.53	0.42	0.00	0.11	98.19	0.28	0.11	0.00
	98	0.08	0.23	0.17	1.35	0.00	0.00	97.73	0.00	0.44	0.00
	98	0.02	0.23	0.54	0.58	0.00	0.00	98.60	0.00	0.00	0.03
	Avg.	0.07	0.25	0.51	0.77	0.00	0.09	97.91	0.08	0.26	0.08
	105	0.34	0.29	0.00	0.93	0.11	0.51	97.35	0.00	0.47	0.00
	105	0.00	0.30	0.00	0.60	0.38	0.00	97.38	0.11	1.14	0.09
	105	0.00	0.29	0.06	0.79	0.23	0.00	97.32	0.15	0.67	0.49
	105	0.00	0.25	0.00	0.41	0.07	1.27	97.43	0.00	0.55	0.02
	105	0.00	0.31	0.00	1.10	0.46	0.00	97.46	0.00	0.66	0.00
	105	0.00	0.27	0.02	0.00	0.00	0.21	97.80	0.09	1.07	0.53
	105	0.00	0.29	0.00	0.13	0.13	0.96	97.16	0.00	0.79	0.53
	105	0.16	0.36	0.00	1.48	0.56	0.00	96.36	0.00	0.83	0.25
	Avg.	0.06	0.30	0.01	0.68	0.24	0.37	97.28	0.04	0.77	0.24
	106	0.00	0.21	0.64	0.00	0.00	0.23	98.00	0.00	0.91	0.00
	106	0.14	0.33	0.57	0.29	0.00	0.00	97.19	0.42	0.84	0.22
	106	0.00	0.30	0.63	0.23	0.00	0.00	97.72	0.00	1.03	0.09
	106	0.22	0.28	0.65	0.21	0.00	0.36	97.72	0.00	0.26	0.31
	106	0.01	0.28	0.40	0.03	0.00	1.05	97.16	0.00	1.06	0.00
	106	0.11	0.26	0.58	1.27	0.00	0.00	97.44	0.00	0.34	0.00
	106	0.09	0.28	0.08	0.00	0.00	0.29	98.68	0.00	0.59	0.00
	106	0.00	0.28	0.55	0.23	0.00	0.31	98.06	0.00	0.57	0.00
	Avg.	0.07	0.28	0.51	0.28	0.00	0.28	97.75	0.05	0.70	0.08
	107	0.15	0.27	0.00	0.07	0.00	0.14	98.60	0.00	0.51	0.27
	107	0.00	0.22	0.01	0.51	0.00	0.00	99.00	0.21	0.04	0.00
	107	0.00	0.25	1.07	0.40	0.00	0.00	98.03	0.22	0.00	0.02
	107	0.07	0.22	0.00	0.57	0.00	0.00	98.12	0.40	0.48	0.14
	107	0.00	0.19	0.81	0.26	0.00	0.52	98.21	0.00	0.00	0.00
	107	0.00	0.24	0.81	0.50	0.00	1.05	96.90	0.15	0.16	0.19
	107	0.00	0.23	0.00	0.24	0.00	0.00	99.39	0.00	0.00	0.14
	107	0.48	0.30	0.33	0.85	0.20	0.00	97.56	0.00	0.29	0.00
	Avg.	0.09	0.24	0.38	0.43	0.03	0.21	98.23	0.12	0.19	0.10
Air (78.0% N ₂ -21.0% O ₂ -0.9% Ar)	97	0.21	0.35	77.04	20.59	0.22	0.00	0.63	0.00	0.76	0.20
	97	0.00	0.35	77.09	20.63	0.00	0.00	1.15	0.07	0.67	0.04
	97	0.05	0.36	77.52	20.66	0.00	0.00	0.89	0.00	0.51	0.00
	97	0.37	0.34	76.83	20.00	0.01	0.00	0.54	0.00	1.06	0.85

Gas Description	Exp.	H ₂ (%)	NO ₂ (%)	N ₂ (%)	O ₂ (%)	N ₂ O (%)	NO (%)	CO ₂ (%)	CO (%)	H ₂ O (%)	NH ₃ (%)
	97	0.00	0.37	77.20	20.38	0.01	0.13	0.89	0.00	0.75	0.28
	97	0.00	0.36	76.20	20.41	0.08	0.93	1.23	0.00	0.72	0.07
	97	0.14	0.31	77.12	19.46	0.00	0.19	1.29	0.85	0.48	0.15
	97	0.51	0.37	77.03	20.34	0.03	0.09	0.85	0.53	0.08	0.16
	Avg.	0.16	0.35	77.00	20.31	0.04	0.17	0.93	0.18	0.63	0.22
	98	0.23	0.08	77.90	20.88	0.00	0.00	0.00	0.17	0.73	0.00
	98	0.00	0.12	77.81	20.68	0.17	0.64	0.25	0.00	0.33	0.00
	98	0.12	0.12	77.07	20.35	0.00	0.78	0.84	0.16	0.38	0.19
	98	0.05	0.09	78.31	20.40	0.00	0.00	0.00	0.80	0.36	0.00
	98	0.00	0.09	78.47	20.44	0.00	0.00	0.57	0.00	0.42	0.00
	98	0.01	0.10	78.08	20.25	0.16	0.67	0.00	0.00	0.40	0.33
	98	0.04	0.12	77.60	20.56	0.07	0.35	0.00	0.30	0.65	0.31
	98	0.00	0.06	77.21	20.95	0.12	0.59	0.00	0.00	0.79	0.27
	Avg.	0.06	0.10	77.81	20.56	0.07	0.38	0.21	0.18	0.51	0.14
	105	0.13	0.01	76.90	20.94	0.31	0.00	0.90	0.00	0.74	0.08
	105	0.19	0.03	76.17	20.84	0.00	0.72	1.16	0.00	0.63	0.26
	105	0.37	0.05	75.76	21.22	0.00	0.56	1.55	0.06	0.44	0.00
	105	0.12	0.02	75.18	21.99	0.54	0.00	1.11	0.49	0.55	0.00
	105	0.16	0.04	77.05	20.63	0.33	0.26	0.96	0.00	0.49	0.09
	105	0.00	0.07	76.18	20.75	0.94	0.00	1.19	0.00	0.51	0.35
	105	0.24	0.00	76.66	21.31	0.20	0.00	1.03	0.00	0.56	0.00
	105	0.02	0.00	77.97	20.64	0.00	0.09	0.87	0.00	0.40	0.00
	Avg.	0.15	0.03	76.48	21.04	0.29	0.20	1.10	0.07	0.54	0.10
	106	0.00	0.03	77.06	20.53	0.00	0.14	0.81	0.75	0.68	0.00
	106	0.07	0.06	76.66	20.40	0.00	0.84	1.06	0.00	0.52	0.40
	106	0.11	0.02	77.63	20.78	0.26	0.00	0.00	0.60	0.61	0.00
	106	0.00	0.00	77.94	21.16	0.00	0.03	0.00	0.00	0.87	0.00
	106	0.00	0.03	77.12	20.80	0.01	0.00	1.20	0.08	0.50	0.25
	106	0.00	0.01	77.08	21.60	0.00	0.00	0.81	0.00	0.51	0.00
	106	0.00	0.07	76.67	21.00	0.00	0.56	0.83	0.00	0.88	0.00
	106	0.26	0.00	76.38	21.10	0.00	0.73	0.91	0.00	0.61	0.00
	Avg.	0.06	0.03	77.07	20.92	0.03	0.29	0.70	0.18	0.65	0.08
	107	0.00	0.00	76.87	21.12	0.13	0.36	1.51	0.00	0.00	0.01
	107	0.06	0.01	76.54	20.51	0.31	0.61	1.55	0.03	0.31	0.07
	107	0.00	0.00	74.24	22.88	0.00	0.00	2.32	0.00	0.56	0.00
	107	0.29	0.05	77.66	20.10	0.08	0.00	1.77	0.00	0.05	0.00
	107	0.00	0.02	77.12	20.40	0.00	0.00	1.96	0.00	0.50	0.00
	107	0.38	0.00	76.53	20.05	0.10	0.36	1.61	0.72	0.17	0.09
	107	0.00	0.00	77.29	20.69	0.20	0.31	1.07	0.23	0.20	0.00
	107	0.09	0.03	78.39	20.22	0.02	0.00	0.87	0.03	0.35	0.02
	Avg.	0.10	0.01	76.83	20.75	0.11	0.21	1.58	0.13	0.27	0.02
2.67% H ₂ - 97.33% Ar	97	3.54	0	0	0	0	0	0	0	0	0
	97	3.22	0	0	0	0	0	0	0	0	0
	97	3.02	0	0	0	0	0	0	0	0	0
	97	3.34	0	0	0	0	0	0	0	0	0
	97	3.58	0	0	0	0	0	0	0	0	0
	97	3.39	0	0	0	0	0	0	0	0	0
	97	3.30	0	0	0	0	0	0	0	0	0
	97	3.25	0	0	0	0	0	0	0	0	0
	Avg.	3.33	0	0	0	0	0	0	0	0	0

Gas Description	Exp.	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO	CO ₂	CO	H ₂ O	NH ₃
		(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)
	98	3.04	0	0	0	0	0	0	0	0	0
	98	3.53	0	0	0	0	0	0	0	0	0
	98	3.46	0	0	0	0	0	0	0	0	0
	98	3.20	0	0	0	0	0	0	0	0	0
	98	3.51	0	0	0	0	0	0	0	0	0
	98	3.00	0	0	0	0	0	0	0	0	0
	98	3.37	0	0	0	0	0	0	0	0	0
	98	3.11	0	0	0	0	0	0	0	0	0
	Avg.	3.28	0	0	0	0	0	0	0	0	0
	105	3.34	0	0	0	0	0	0	0	0	0
	105	2.11	0	0	0	0	0	0	0	0	0
	105	3.00	0	0	0	0	0	0	0	0	0
	105	3.07	0	0	0	0	0	0	0	0	0
	105	2.57	0	0	0	0	0	0	0	0	0
	105	2.87	0	0	0	0	0	0	0	0	0
	105	2.80	0	0	0	0	0	0	0	0	0
	105	2.97	0	0	0	0	0	0	0	0	0
	Avg.	2.84	0	0	0	0	0	0	0	0	0
	106	3.34	0	0	0	0	0	0	0	0	0
	106	3.27	0	0	0	0	0	0	0	0	0
	106	3.14	0	0	0	0	0	0	0	0	0
	106	3.31	0	0	0	0	0	0	0	0	0
	106	3.12	0	0	0	0	0	0	0	0	0
	106	3.19	0	0	0	0	0	0	0	0	0
	106	3.39	0	0	0	0	0	0	0	0	0
	106	3.07	0	0	0	0	0	0	0	0	0
	Avg.	3.23	0	0	0	0	0	0	0	0	0
	107	3.32	0	0	0	0	0	0	0	0	0
	107	2.76	0	0	0	0	0	0	0	0	0
	107	3.90	0	0	0	0	0	0	0	0	0
	107	3.44	0	0	0	0	0	0	0	0	0
	107	2.96	0	0	0	0	0	0	0	0	0
	107	3.30	0	0	0	0	0	0	0	0	0
	107	3.59	0	0	0	0	0	0	0	0	0
	107	3.44	0	0	0	0	0	0	0	0	0
	Avg.	3.34	0	0	0	0	0	0	0	0	0

The values in Table A-1 should be constant since the Raman is reading constant sources (calibration gases) without being connected to the dissolution equipment. The variance seen in these values represent the instrument noise and should not be counted as part of the process noise or variance. For this reason, the values in Table A-1 are averaged per experiment and these averages are then compared to the calibration values to determine measurement uncertainty. To estimate the measurement uncertainty of the Raman spectroscopy, the average of the pre-run check values of Table A-1 were compared to the standard values across Experiments 97, 98, 105, 106 and 107. Sample standard deviations of the measured average concentrations with respect to the calibrated concentrations for the data were calculated. These sample standard deviations were then doubled to get an idea of the variability in the Raman spectroscopy concentration measurements. Table A-3 shows the sample standard deviation of the measured concentrations with respect to their calibrated values. For the H₂ and O₂ gases, the 2 σ values or twice the standard deviation is < 2 vol%. The 2 σ value for N₂ is < 3 vol % and the 2 σ value for CO₂ is < 4.5 vol %.

Table A-2. Raman Tracer Gas Flow Rates

Experiment	CO₂ Flow (cm³/min)
97	20
98	20
105	20
106	20
107	20

Table A-3. Standard Deviation of Raman Concentrations with Respect to Calibrated Values

Gas	Standard Deviation (σ) (vol %)	2*Standard Deviation (2σ) (vol %)
CO ₂	2.05	4.10
N ₂	1.18	2.36
O ₂	0.40	0.80
H ₂	0.57	1.14

Appendix B. Lower Flammability of H₂

Lower flammability data reported by Scott et al.¹⁴ for air, H₂, NO, and N₂O mixtures were used to calculate the LFL for comparison to the H₂ concentrations calculated for an H-Canyon dissolver. Three data sets for NO:N₂O ratios of 2.57, 1.00, and 0.33 are shown in Table B-1. The H₂ LFL data in Table B-1 marked with an asterisk did not propagate a flame.

Table B-1. Lower Flammability Limits for H₂ (1 atm and 28 °C)

	NO:N ₂ O = 2.57	NO:N ₂ O = 1.00	NO:N ₂ O = 0.33
Air	H ₂ LFL	H ₂ LFL	H ₂ LFL
(vol %)	(vol %)	(vol %)	(vol %)
1.5	6.2	-	-
4.6	6.4	-	-
6.2	5.9*	-	-
21.7	6.4	-	-
34.5	6.1*	-	-
52.6	7.2	-	-
60.8	5.5*	-	-
66.8	6.6	-	-
74.1	4.3*	-	-
28.7	-	6.3	-
40.6	-	5.1	-
54.2	-	7.0	-
57.1	-	6.9*	-
61.3	-	6.9	-
68.9	-	6.3	-
81.2	-	4.2*	-
33.5	-	-	5.3
45.7	-	-	4.5*
50.3	-	-	6.3
52.0	-	-	4.5*
59.4	-	-	5.6
62.5	-	-	4.1*

* Did not propagate flame

The H₂ LFL data in Table B-1 were correlated using a second order polynomial to allow interpolation at varying concentrations of air. The correlations including parameters for the polynomials are shown in Figures B-1 to B-3 for NO:N₂O ratios of 2.57, 1.00, and 0.33, respectively.

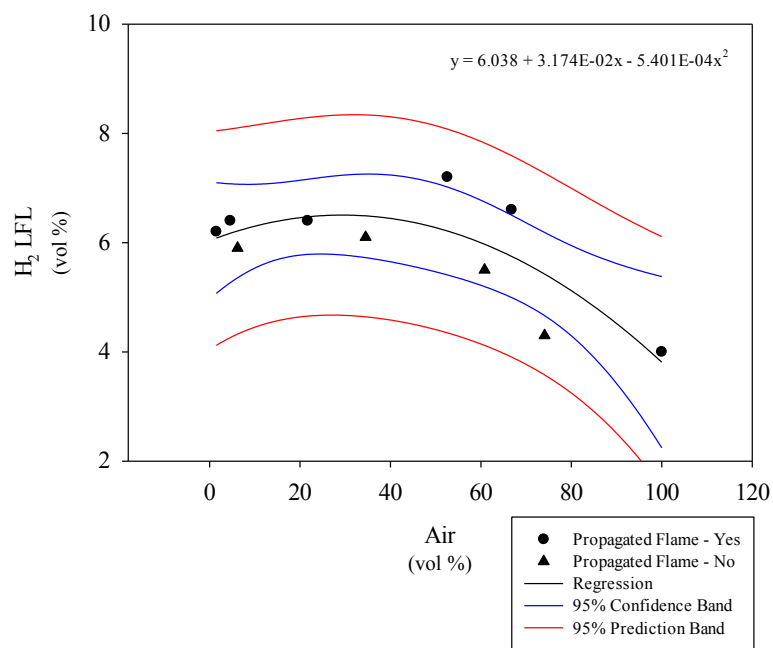


Figure B-1. Lower Flammability of H₂ (NO:N₂O = 2.57).

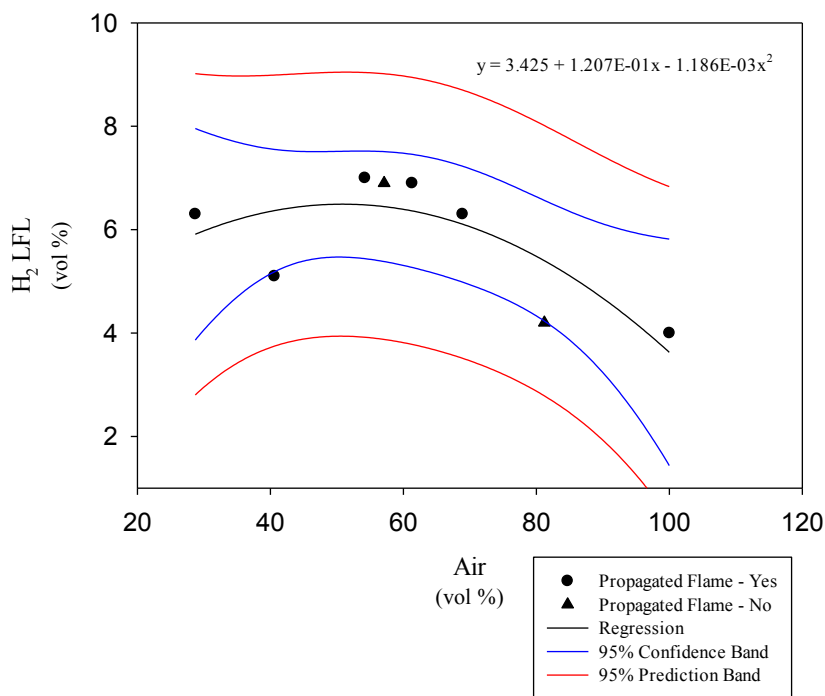


Figure B-2. Lower Flammability of H₂ (NO:N₂O = 1.00).

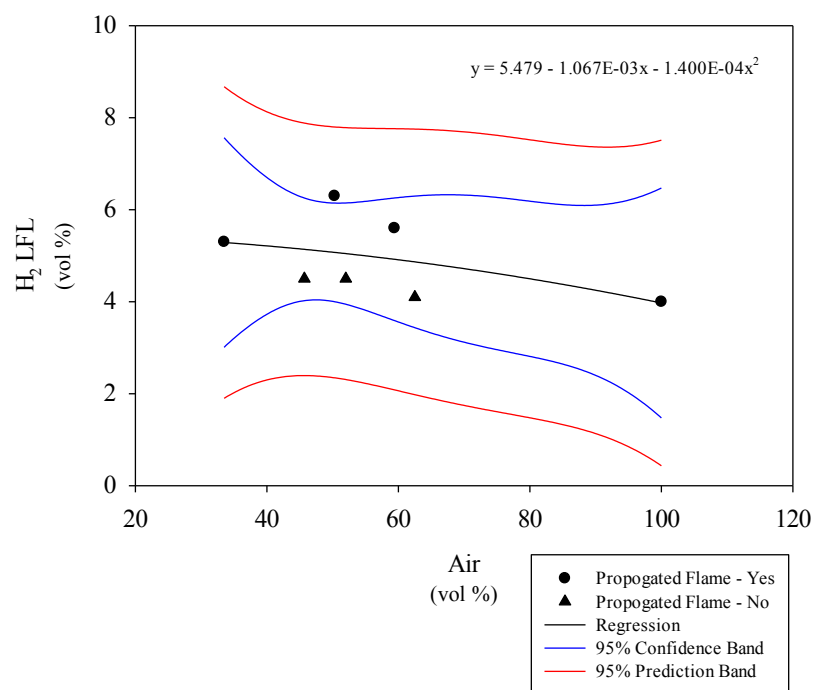


Figure B-3. Lower Flammability of H₂ (NO:N₂O = 0.33)

Appendix C. Raman Offgas Data for Experiment 97

As discussed in Appendix A, the Raman readings should be positive and sum to 100% except in cases where there is significant Ar present. Due to the noise in the Raman signal, any raw readings that are less than zero are fixed to zero and then all the gas readings for H₂, NO₂, N₂, O₂, N₂O, and NO are normalized to 100 vol %. Even with these corrections, the Raman readings have noise in them. To reduce this noise, moving averages of the fixed and normalized readings were performed using equation C-1:

$$\text{Gas } t_i (\text{vol}\%) = \frac{\sum_{k=t_i-2}^{t_i+2} \text{Gas } k}{5} \quad (\text{C-1})$$

where Gas = H₂, NO₂, N₂, O₂, N₂O, NO concentrations (vol %)

t_i = time at integer time step i

k = integer time step t_{i-2}, t_{i-1}, t_i, t_{i+1}, and t_{i+2}.

These moving averages do not eliminate all the noise but smooth the values so comparisons and calculations can be performed. The fixed, normalized, and moving average Raman gas concentrations are reported in Table C-1. Due to rounding to the nearest hundredth, the numbers in the table may not sum to exactly 100 vol % but all the decimal places were carried in the calculations performed for this report.

Table C-1. Fixed Normalized Moving Average Raman Data for Experiment 97

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
2	0.001	77.62	5.785	3.40	13.51	1.53	4.46	0.43	76.67
13	0.002	77.44	5.846	3.80	13.54	1.61	5.26	0.43	75.35
24	0.003	77.92	5.677	3.79	13.54	1.61	5.27	0.47	75.31
35	0.004	77.17	5.919	3.43	13.88	1.49	5.26	0.41	75.53
47	0.005	77.27	5.883	1.45	13.39	2.54	4.38	0.26	77.99
58	0.006	77.39	5.845	1.30	13.14	2.09	4.22	0.26	78.99
69	0.008	77.56	5.787	0.91	12.90	1.60	4.11	0.32	80.16
80	0.009	77.45	5.824	1.64	12.68	1.82	3.80	5.80	74.26
92	0.010	70.98	8.765	2.91	12.06	2.29	3.22	11.45	68.08
103	0.011	55.99	20.288	3.81	11.47	2.10	3.67	16.94	62.01
114	0.016	39.03	36.850	5.27	11.06	2.64	3.12	22.36	55.56
126	0.026	27.53	54.390	6.54	11.01	2.75	3.14	28.04	48.52
137	0.037	20.22	93.209	7.36	10.95	3.18	3.11	27.79	47.61
148	0.057	17.79	102.797	7.44	11.42	2.74	3.25	27.64	47.50
160	0.080	14.07	130.602	7.29	12.20	2.22	3.40	27.58	47.31
171	0.101	13.94	132.625	7.06	13.19	2.25	3.43	27.67	46.40
182	0.129	12.52	142.597	6.78	14.02	2.77	3.32	27.07	46.03
194	0.156	13.31	132.931	6.47	15.22	2.90	3.62	26.80	45.00

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
		(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
205	0.177	15.56	109.729	6.17	16.32	2.96	3.68	26.29	44.58
216	0.196	17.99	95.048	5.82	17.26	3.20	4.00	25.88	43.84
228	0.212	18.30	92.080	5.60	17.93	3.35	4.49	24.99	43.64
239	0.228	18.39	91.547	5.15	18.67	3.24	4.36	24.71	43.87
250	0.246	16.73	100.205	4.63	19.05	2.95	4.33	24.68	44.36
262	0.265	16.18	105.707	4.26	19.21	3.37	4.77	24.43	43.95
273	0.285	16.29	105.017	4.20	19.55	3.58	4.23	24.14	44.29
284	0.304	17.20	99.721	3.98	19.89	3.77	4.45	24.62	43.30
296	0.321	17.95	92.604	4.02	19.84	3.93	5.26	24.44	42.51
307	0.337	16.48	104.164	4.26	19.90	4.03	5.40	24.11	42.29
319	0.360	15.70	108.608	4.45	20.77	3.74	5.65	24.75	40.65
330	0.379	18.91	92.293	4.75	21.48	3.48	6.35	25.41	38.54
341	0.393	21.55	74.873	4.56	21.93	3.37	5.09	25.30	39.75
353	0.406	23.16	66.693	4.78	22.49	3.42	4.13	24.41	40.77
364	0.418	21.36	73.875	4.76	22.91	3.87	4.65	24.72	39.08
376	0.433	20.76	76.674	4.63	22.29	3.67	4.56	23.93	40.92
387	0.447	18.89	86.529	4.28	21.69	3.65	4.26	23.14	42.98
398	0.463	17.10	98.972	4.40	21.43	3.43	5.98	22.54	42.21
410	0.484	18.23	94.124	4.62	21.65	2.84	7.24	22.37	41.28
421	0.501	19.22	88.215	4.53	21.23	1.94	8.28	21.63	42.39
433	0.515	20.07	81.297	4.58	21.30	1.85	8.72	21.15	42.40
444	0.531	18.66	87.606	4.58	21.53	2.10	9.00	21.03	41.76
456	0.548	19.36	84.413	4.86	21.89	1.85	7.96	21.48	41.96
467	0.562	19.79	81.655	4.50	21.61	1.71	7.95	22.25	41.98
479	0.578	20.00	80.518	4.43	21.71	1.78	6.93	22.03	43.13
490	0.593	19.09	84.846	4.49	22.07	1.60	6.79	22.08	42.99
502	0.609	20.19	79.336	4.45	22.31	1.21	7.10	20.53	44.40
513	0.623	22.56	70.396	4.52	22.19	1.27	8.01	20.04	43.96
525	0.635	23.99	64.063	4.47	22.32	1.34	7.63	20.11	44.13
536	0.646	24.02	63.916	4.44	22.53	1.23	8.15	20.31	43.34
548	0.659	21.32	74.625	4.52	22.33	1.13	8.20	20.51	43.31
559	0.673	19.73	81.868	4.60	21.99	0.87	7.55	21.94	43.04
571	0.690	18.70	86.964	4.38	22.02	0.63	7.58	22.22	43.17
582	0.706	19.31	83.789	4.28	21.96	0.72	7.76	21.95	43.33
594	0.722	20.75	77.099	4.33	21.84	1.03	7.24	21.91	43.65
605	0.735	21.57	72.916	4.24	21.86	1.13	6.87	21.69	44.20
617	0.748	23.60	65.558	4.46	23.00	2.26	7.79	23.00	39.48

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
		(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
628	0.760	23.82	64.759	4.65	23.02	2.60	7.50	22.91	39.32
640	0.772	24.55	61.765	4.61	23.19	3.05	7.29	23.41	38.45
651	0.783	23.06	66.774	4.28	23.28	2.64	7.82	23.49	38.49
663	0.796	23.08	66.705	4.31	23.19	2.69	7.92	23.93	37.96
675	0.809	21.87	71.985	4.07	22.02	1.88	6.80	23.00	42.23
686	0.822	21.01	75.917	3.67	22.00	1.98	7.50	23.40	41.45
698	0.838	20.03	79.928	3.82	21.76	1.52	7.93	22.93	42.04
709	0.852	22.12	71.738	3.97	21.63	2.28	7.60	22.51	42.02
721	0.865	24.34	63.148	3.84	21.87	2.78	7.84	22.73	40.93
732	0.875	24.10	64.300	3.92	21.86	2.60	8.54	22.39	40.69
744	0.889	23.99	64.637	4.06	21.84	2.65	8.03	21.93	41.48
756	0.902	24.92	62.205	4.21	22.38	2.42	7.95	21.52	41.52
768	0.912	26.01	57.548	4.57	22.78	2.36	7.92	22.47	39.91
780	0.923	25.37	59.656	4.75	22.85	1.76	7.64	21.98	41.01
792	0.936	25.22	60.021	4.79	22.82	2.03	7.87	21.99	40.49
804	0.947	25.58	58.755	4.91	22.98	1.83	7.81	22.49	39.98
816	0.958	27.36	53.573	4.71	22.63	2.51	7.65	23.06	39.44
828	0.969	27.74	52.681	4.61	22.29	2.59	7.54	22.42	40.56
840	0.978	27.56	53.311	4.67	21.92	3.21	7.58	22.29	40.33
852	0.989	26.31	56.699	4.84	22.85	2.98	7.02	22.90	39.40
865	1.002	27.97	53.508	4.71	22.51	3.26	6.87	22.16	40.48
877	1.011	30.25	47.268	4.78	22.07	3.15	6.44	22.10	41.47
890	1.020	29.41	50.156	4.67	21.95	3.10	5.70	21.93	42.65
902	1.031	26.44	56.770	4.61	21.95	2.92	5.70	22.16	42.66
914	1.043	24.63	61.457	4.22	20.92	3.52	5.97	21.16	44.21
926	1.054	27.18	54.091	4.23	20.78	3.39	5.75	21.34	44.51
938	1.065	26.92	54.904	4.12	21.20	3.14	6.16	21.23	44.16
950	1.075	29.41	48.872	4.11	21.42	3.22	6.18	21.26	43.80
962	1.085	28.60	50.754	4.00	21.66	3.76	5.96	21.28	43.35
974	1.094	29.70	47.656	3.99	21.82	3.66	5.63	21.15	43.74
985	1.103	30.09	46.966	4.07	22.91	4.18	5.97	19.58	43.28
997	1.112	34.16	39.759	4.14	22.75	4.14	5.25	19.73	43.99
1009	1.118	33.26	42.232	4.21	22.59	3.92	5.12	19.37	44.80
1020	1.126	33.36	42.058	4.29	22.52	3.04	4.74	19.31	46.11
1032	1.135	29.64	48.400	4.18	22.38	2.73	4.62	19.00	47.08
1044	1.144	32.87	41.289	4.15	21.16	2.26	3.86	20.40	48.18
1056	1.152	30.17	47.352	4.18	20.82	2.78	4.03	20.15	48.04

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
		(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
1067	1.160	29.91	47.984	4.00	21.00	2.69	4.42	20.26	47.63
1079	1.171	30.22	47.508	4.23	21.33	3.48	4.89	20.20	45.87
1091	1.179	34.09	39.613	4.02	21.69	3.85	4.67	20.70	45.08
1103	1.186	37.43	33.463	4.12	21.49	4.12	6.06	20.04	44.17
1115	1.192	36.76	34.546	4.07	22.22	3.81	5.94	20.68	43.29
1126	1.198	36.22	35.335	4.10	21.96	3.81	5.38	21.08	43.67
1138	1.206	32.98	41.234	3.89	21.45	3.06	5.29	20.58	45.73
1150	1.214	34.00	39.640	4.15	20.96	2.81	5.67	20.92	45.50
1162	1.222	31.13	45.437	4.09	21.31	1.97	4.26	21.91	46.47
1174	1.230	31.14	45.405	3.77	20.93	2.16	4.41	21.64	47.08
1185	1.240	29.51	48.118	3.96	20.78	2.50	4.82	21.17	46.77
1197	1.248	32.39	42.297	3.56	19.94	2.69	5.00	20.67	48.15
1209	1.256	33.45	39.978	3.51	20.26	3.17	5.08	18.90	49.08
1221	1.264	36.14	35.865	3.54	20.28	3.70	5.39	18.25	48.85
1233	1.271	37.78	33.649	3.87	19.76	3.67	5.53	18.33	48.84
1244	1.276	36.78	35.846	3.78	20.33	3.06	5.40	18.97	48.46
1256	1.283	37.77	34.715	4.15	20.93	3.23	4.93	19.90	46.86
1268	1.291	36.09	36.999	4.36	20.42	3.12	4.53	21.24	46.33
1280	1.297	39.51	30.928	3.90	20.29	3.36	4.54	21.44	46.47
1292	1.303	39.18	31.285	3.99	20.57	3.55	4.19	20.93	46.77
1304	1.309	41.13	28.687	4.05	19.90	3.97	4.23	20.48	47.37
1316	1.314	41.75	27.918	3.77	19.72	3.75	5.18	20.74	46.85
1327	1.319	37.85	33.869	3.73	19.84	3.09	5.04	21.48	46.81
1339	1.326	35.08	37.832	4.30	19.95	2.78	5.25	21.70	46.02
1351	1.335	35.29	37.584	4.35	19.87	3.13	5.33	22.75	44.57
1363	1.341	35.74	36.680	4.43	19.71	3.33	5.14	23.22	44.17
1375	1.348	35.12	37.844	4.93	20.23	3.77	3.97	22.92	44.17
1387	1.356	37.00	35.928	4.66	20.01	4.67	4.79	21.76	44.11
1399	1.363	41.10	30.188	4.57	19.52	5.15	4.13	22.19	44.45
1411	1.367	41.73	29.008	4.48	19.24	4.96	4.34	21.32	45.66
1423	1.374	39.30	31.584	4.39	19.08	4.61	4.27	21.52	46.13
1435	1.380	35.35	37.036	4.14	18.67	3.98	4.58	22.29	46.33
1447	1.387	36.16	35.688	4.42	18.84	3.85	3.87	23.79	45.24
1459	1.395	35.66	36.347	4.39	19.53	3.49	4.15	23.82	44.61
1470	1.401	41.15	29.478	4.64	19.76	2.92	3.92	23.79	44.97
1482	1.406	45.36	24.659	4.88	19.96	3.21	4.92	24.03	43.00
1494	1.410	44.82	25.423	4.95	19.59	3.93	4.74	23.89	42.90

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
		(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
1506	1.415	39.37	32.212	5.26	19.47	2.82	5.35	23.18	43.91
1518	1.423	38.16	33.320	5.35	18.57	2.81	5.42	23.08	44.77
1530	1.429	38.20	33.257	5.11	18.30	3.35	5.23	23.45	44.56
1542	1.435	41.99	28.006	5.36	18.45	3.05	4.48	22.41	46.24
1554	1.441	44.23	26.079	5.75	18.75	2.62	4.68	21.60	46.60
1566	1.445	48.17	21.701	5.65	19.20	3.65	3.75	23.13	44.61
1578	1.449	47.60	22.311	5.65	19.30	3.71	3.58	23.35	44.41
1590	1.453	43.63	26.167	5.51	19.05	3.41	3.47	23.99	44.58
1602	1.459	39.04	31.557	5.23	18.71	3.48	3.21	25.06	44.32
1614	1.466	38.03	32.777	4.96	18.37	3.76	3.19	25.81	43.91
1626	1.472	38.23	32.524	5.06	17.58	3.52	3.38	24.87	45.60
1638	1.478	40.24	29.715	5.19	18.64	3.68	3.33	25.08	44.07
1650	1.484	46.10	24.479	5.53	18.78	3.80	3.88	24.90	43.12
1662	1.488	46.28	24.258	5.45	18.81	4.17	4.24	23.85	43.48
1674	1.492	49.81	20.925	5.42	19.10	4.17	3.98	23.28	44.05
1687	1.497	48.65	21.688	5.25	19.13	4.01	4.28	23.43	43.90
1699	1.501	49.11	21.156	5.06	18.08	4.22	4.12	23.08	45.43
1711	1.505	47.94	22.101	4.88	17.82	4.54	4.51	22.73	45.53
1723	1.510	43.56	26.169	4.99	17.41	4.67	4.68	23.65	44.60
1735	1.515	43.09	26.712	4.94	17.20	4.89	5.04	24.80	43.12
1747	1.520	41.27	28.483	5.21	17.10	5.29	4.90	23.84	43.66
1759	1.526	46.21	24.039	5.36	16.90	5.14	5.64	24.22	42.74
1771	1.530	47.09	23.044	5.41	17.16	4.70	5.43	23.55	43.75
1783	1.534	51.43	19.387	5.29	17.32	4.45	5.25	23.80	43.89
1795	1.538	47.75	22.421	5.40	17.16	3.78	5.12	24.25	44.30
1808	1.543	45.75	24.854	5.27	17.02	3.60	5.10	25.25	43.75
1820	1.548	41.58	28.340	5.20	17.08	3.44	4.98	25.35	43.96
1832	1.554	41.58	28.336	5.39	16.94	3.87	4.74	26.96	42.10
1844	1.559	44.13	25.341	5.61	16.97	3.61	4.58	27.29	41.93
1857	1.564	44.88	24.567	5.67	16.93	3.96	4.84	26.78	41.82
1869	1.569	44.60	24.867	5.75	16.91	3.74	5.41	26.98	41.21
1881	1.574	44.24	25.228	5.98	16.71	3.67	5.60	26.94	41.11
1893	1.579	43.89	25.575	6.11	17.06	3.71	6.01	27.51	39.60
1905	1.584	45.60	23.940	6.23	16.93	3.96	6.25	27.19	39.44
1917	1.588	45.75	23.779	6.16	16.76	4.25	6.73	27.09	39.01
1929	1.593	45.91	23.625	6.09	16.66	4.51	6.96	26.87	38.92
1942	1.598	44.45	24.999	6.07	16.73	4.33	6.84	27.41	38.63

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
		(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
1954	1.603	44.94	24.525	5.96	16.17	3.52	6.56	26.63	41.16
1966	1.608	45.28	24.185	6.03	16.38	3.39	7.13	27.17	39.91
1978	1.612	46.39	23.118	6.02	16.51	3.43	7.01	27.21	39.81
1990	1.617	46.56	22.960	6.12	16.66	3.44	6.38	27.67	39.73
2002	1.621	47.06	22.503	5.71	16.26	3.96	9.34	25.54	39.19
2015	1.626	50.20	20.155	5.78	16.12	4.54	9.47	25.50	38.58
2027	1.630	50.37	20.003	5.71	15.92	4.55	9.07	25.52	39.22
2039	1.633	51.06	19.416	5.71	15.99	4.54	8.43	25.93	39.41
2051	1.637	48.67	21.112	5.93	16.01	4.86	9.28	24.15	39.76
2064	1.642	53.18	17.958	6.58	16.16	5.12	5.72	26.22	40.19
2076	1.645	52.80	18.278	6.36	15.78	5.37	4.49	25.98	42.01
2088	1.648	51.43	19.490	6.14	15.87	5.69	4.26	26.54	41.49
2100	1.653	48.09	21.672	6.32	15.90	5.77	4.61	25.28	42.13
2112	1.657	52.51	18.688	5.99	15.80	5.16	3.97	27.29	41.79
2125	1.660	54.33	17.114	5.55	15.85	5.32	3.85	27.55	41.88
2137	1.663	54.04	17.347	5.75	16.50	5.75	4.37	28.97	38.65
2149	1.667	50.65	19.495	5.90	16.56	5.80	4.20	29.19	38.35
2162	1.671	50.87	19.330	5.84	16.42	5.73	4.10	31.14	36.77
2174	1.675	50.80	19.384	5.82	16.32	6.30	3.88	31.19	36.49
2186	1.679	50.96	19.260	6.07	16.18	6.14	4.39	30.98	36.24
2198	1.683	50.75	19.420	5.80	16.11	6.15	4.88	30.73	36.33
2211	1.687	52.57	18.085	5.64	16.29	6.47	5.08	28.60	37.92
2223	1.690	57.71	15.136	5.00	16.21	6.68	4.80	28.56	38.75
2235	1.693	58.26	14.725	5.17	16.18	7.13	4.24	28.73	38.56
2248	1.696	57.37	15.341	4.92	16.41	6.96	3.78	29.32	38.61
2260	1.699	53.41	17.467	5.15	16.06	6.79	3.68	28.79	39.54
2272	1.702	52.91	17.845	5.24	15.40	6.40	3.93	30.37	38.66
2285	1.706	53.26	17.592	6.05	15.28	6.08	4.06	30.21	38.32
2297	1.710	52.95	17.801	5.81	15.19	6.00	5.24	29.96	37.81
2309	1.713	53.73	17.224	6.12	14.85	6.04	5.84	29.40	37.74
2322	1.717	53.90	17.107	6.13	15.10	6.03	6.05	29.86	36.83
2334	1.720	54.32	16.828	6.29	15.43	6.56	6.17	30.53	35.03
2346	1.723	55.64	15.967	6.16	15.51	6.87	6.24	30.80	34.41
2359	1.726	56.44	15.443	6.27	15.57	6.37	5.66	31.14	35.00
2371	1.729	56.44	15.442	6.11	15.69	6.51	5.21	31.63	34.85
2383	1.732	55.89	15.786	6.00	15.46	6.62	5.31	32.05	34.55
2396	1.736	55.50	16.036	6.10	15.24	5.73	5.58	31.77	35.58

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
		(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
2408	1.739	55.79	15.854	6.27	15.52	6.45	5.99	32.33	33.44
2421	1.742	56.76	15.261	5.91	15.71	7.02	6.44	32.84	32.08
2433	1.745	57.93	14.532	6.29	15.95	7.18	7.13	33.49	29.95
2445	1.748	58.55	14.158	6.46	15.99	7.07	6.75	33.18	30.54
2458	1.751	58.29	14.315	6.37	15.97	7.29	6.48	33.24	30.64
2470	1.754	58.18	14.377	6.08	15.63	6.61	6.10	33.10	32.47
2483	1.757	58.05	14.455	6.46	15.37	6.18	6.11	33.02	32.86
2495	1.759	57.73	14.647	6.72	15.69	5.98	6.10	30.73	34.78
2507	1.762	62.70	12.317	6.57	15.55	5.56	6.95	30.63	34.74
2520	1.765	62.83	12.240	6.58	15.51	5.87	7.04	30.78	34.23
2532	1.767	63.80	11.673	6.98	15.83	5.81	6.90	31.35	33.13
2545	1.770	60.28	13.208	6.97	15.77	5.75	6.53	31.39	33.59
2557	1.772	60.87	12.870	6.43	15.54	5.90	6.99	34.15	31.00
2570	1.775	62.06	12.244	6.44	15.58	6.02	6.82	34.54	30.60
2582	1.777	61.69	12.433	6.16	15.57	5.84	6.78	34.64	31.00
2595	1.780	62.00	12.264	6.15	15.35	5.54	7.46	34.30	31.22
2607	1.782	61.77	12.384	6.26	15.35	6.21	7.57	34.02	30.59
2620	1.785	61.56	12.495	6.36	15.04	6.10	6.52	33.47	32.52
2632	1.787	61.83	12.353	6.50	15.15	5.92	6.02	34.54	31.87
2645	1.790	60.98	12.803	6.63	15.17	5.82	6.19	34.99	31.20

Appendix D. Raman Offgas Data for Experiment 98

As discussed in Appendix A, the Raman readings should be positive and sum to 100% except in cases where there is significant Ar present. Due to the noise in the Raman signal, any raw readings that are less than zero are fixed to zero and then all the gas readings for H₂, NO₂, N₂, O₂, N₂O, and NO are normalized to 100 vol %. Even with these corrections, the Raman readings have noise in them. To reduce this noise, moving averages of the fixed and normalized readings were performed using equation C-1.

These moving averages do not eliminate all the noise but smooth the values so comparisons and calculations can be performed. The fixed, normalized, and moving average Raman gas concentrations are reported in Table D-1. Due to rounding to the nearest hundredth, the numbers in the table may not sum to exactly 100 vol % but all the decimal places were carried in the calculations performed for this report.

Table D-1. Fixed Normalized Moving Average Raman Data for Experiment 98

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
4	0.001	78.40	5.546	1.24	13.66	1.92	6.48	8.11	68.60
15	0.002	78.22	5.600	1.19	12.76	1.61	6.20	14.90	63.34
27	0.004	78.02	5.672	1.28	12.51	1.32	4.54	15.66	64.69
38	0.005	78.20	5.618	1.70	13.01	1.86	4.79	8.94	69.71
50	0.006	78.23	5.609	2.40	12.41	1.68	4.04	14.66	64.81
61	0.007	76.34	6.360	2.76	11.62	1.37	3.96	20.40	59.89
73	0.009	67.42	10.461	3.42	11.36	2.01	3.71	19.03	60.47
84	0.012	53.97	18.868	4.55	10.29	2.11	3.69	23.38	55.99
95	0.017	40.87	32.233	5.27	9.32	1.90	3.08	28.48	51.96
107	0.026	29.86	51.773	6.06	8.76	2.55	2.50	27.35	52.77
118	0.039	23.87	65.473	6.97	8.35	2.97	2.03	26.54	53.15
130	0.056	20.87	75.981	7.73	8.20	3.23	1.81	26.49	52.54
141	0.072	17.81	101.001	8.40	8.20	3.40	1.57	26.86	51.57
153	0.098	16.54	107.388	8.71	8.10	3.91	2.07	26.69	50.52
164	0.124	15.37	114.632	9.09	7.96	4.24	2.11	26.99	49.61
175	0.144	14.92	122.086	9.43	7.88	4.09	2.22	27.65	48.73
187	0.176	14.72	123.372	9.65	7.81	4.14	2.55	28.09	47.76
198	0.204	13.50	135.208	9.71	7.79	4.07	2.59	28.90	46.94
210	0.230	13.75	130.870	10.15	7.81	3.87	2.19	29.74	46.23
221	0.262	11.64	152.469	10.44	7.87	3.50	2.54	30.27	45.39
233	0.298	12.04	147.849	10.56	7.93	3.54	2.35	30.73	44.90
244	0.328	12.94	136.113	10.68	7.96	3.62	2.05	30.71	44.98
256	0.357	15.26	113.227	10.80	8.03	3.77	2.27	30.76	44.38
267	0.379	16.64	102.107	10.54	8.11	3.74	2.56	30.95	44.10
279	0.400	17.12	97.603	10.31	8.21	3.76	2.65	31.27	43.81

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
		(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
290	0.422	15.35	112.805	10.08	8.27	4.10	2.93	31.26	43.36
302	0.450	15.30	113.152	9.85	8.43	3.96	3.27	31.82	42.67
313	0.474	14.81	117.849	9.52	8.56	4.15	3.25	31.89	42.63
325	0.499	16.62	102.324	8.73	8.79	4.33	3.50	32.05	42.61
336	0.521	17.30	98.491	8.56	8.99	4.25	3.48	32.33	42.39
348	0.541	17.39	97.560	8.26	9.16	4.10	3.72	32.54	42.23
359	0.562	16.72	102.125	8.03	9.31	3.94	4.21	32.57	41.94
371	0.588	14.44	119.599	7.70	9.39	3.68	5.52	32.54	41.17
382	0.613	14.39	120.165	8.11	9.51	3.57	5.55	32.71	40.55
394	0.643	14.00	123.319	7.91	9.69	3.43	5.59	32.97	40.41
405	0.667	14.67	116.593	7.91	9.98	3.31	5.44	33.21	40.15
417	0.693	15.43	109.735	7.75	10.24	3.66	4.99	33.37	39.99
429	0.718	16.70	100.828	7.94	10.56	3.82	4.03	33.85	39.80
440	0.738	15.79	110.617	7.83	10.82	3.89	3.88	33.95	39.61
452	0.764	16.94	103.377	7.76	11.04	3.74	3.87	33.80	39.80
463	0.788	17.16	102.164	7.74	11.27	4.01	3.73	33.98	39.28
475	0.807	19.92	80.468	7.85	11.46	3.78	3.61	34.25	39.05
486	0.823	20.01	80.002	7.71	11.66	3.80	3.49	34.26	39.10
498	0.841	20.08	79.644	7.83	11.85	3.89	3.12	34.80	38.50
510	0.860	18.42	89.973	7.95	11.86	4.29	3.38	34.70	37.83
521	0.880	18.19	91.172	7.88	12.09	4.25	3.14	34.72	37.92
533	0.902	19.38	86.002	7.69	12.26	4.38	3.44	34.65	37.58
544	0.918	21.46	73.819	7.85	12.54	4.70	3.47	35.47	35.97
556	0.934	19.59	88.167	7.57	12.52	4.97	3.82	35.15	35.96
568	0.956	17.72	97.202	7.36	12.88	4.90	3.77	35.71	35.38
579	0.979	15.80	108.156	7.21	12.83	5.17	4.14	36.00	34.65
591	1.002	16.96	98.106	7.12	12.86	6.28	3.79	35.90	34.05
603	1.025	17.39	95.539	6.85	12.73	6.21	3.66	35.13	35.41
614	1.044	18.98	86.078	6.78	13.06	6.14	3.79	35.43	34.81
626	1.063	21.55	73.909	6.66	13.17	6.61	3.56	35.58	34.41
638	1.078	23.87	64.543	6.54	13.31	6.09	4.10	35.49	34.47
649	1.091	24.99	60.117	6.61	13.57	4.80	4.46	35.92	34.64
661	1.105	24.94	60.261	6.59	13.79	4.43	4.72	36.14	34.33
673	1.119	24.58	61.391	6.74	13.97	4.21	4.63	36.44	34.02
684	1.132	24.90	60.339	6.65	14.06	4.11	4.72	36.64	33.82
696	1.145	24.95	60.155	6.76	14.04	4.50	4.85	36.63	33.23
708	1.159	24.97	60.092	6.74	14.07	4.86	4.97	37.16	32.20

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
		(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
719	1.172	24.86	60.438	6.69	14.11	5.17	5.04	37.74	31.25
731	1.186	23.90	63.960	6.60	14.17	5.34	5.45	38.37	30.05
743	1.201	23.02	67.148	6.82	14.18	4.97	6.09	38.81	29.13
755	1.217	21.40	73.678	6.81	14.47	4.74	5.76	39.33	28.88
766	1.233	23.61	66.624	6.91	14.73	4.59	6.15	39.64	27.97
778	1.248	25.74	59.971	7.00	14.83	3.95	6.29	39.45	28.48
790	1.259	29.06	48.864	6.95	15.18	3.74	6.04	39.60	28.50
802	1.270	29.66	47.480	6.82	15.35	3.63	5.55	38.83	29.83
813	1.280	30.96	44.683	7.03	15.45	3.33	5.66	38.94	29.59
825	1.290	30.97	44.670	6.90	15.30	3.34	5.52	38.25	30.68
837	1.300	30.23	46.393	6.95	15.32	3.55	5.45	38.03	30.71
849	1.311	29.63	47.587	7.14	14.95	3.61	5.54	37.45	31.31
860	1.321	28.01	51.906	7.25	14.89	4.11	5.65	38.05	30.05
872	1.333	25.83	59.057	7.22	14.77	4.23	5.52	38.10	30.17
884	1.348	23.75	64.569	7.48	15.10	4.16	5.32	38.67	29.26
896	1.364	26.72	57.590	7.56	15.22	4.04	5.69	38.72	28.77
907	1.374	30.45	47.084	7.60	15.10	3.98	6.03	37.72	29.56
919	1.383	32.81	41.011	7.70	15.16	4.16	6.39	37.22	29.36
931	1.393	31.81	42.916	7.54	15.22	4.03	6.71	36.77	29.73
943	1.403	31.85	42.827	7.62	14.89	3.79	7.21	35.62	30.87
955	1.413	33.50	39.977	7.55	14.80	4.17	6.86	35.91	30.71
966	1.421	32.14	43.248	7.34	15.11	4.49	6.69	36.21	30.16
978	1.431	34.32	39.906	7.55	15.09	3.95	6.52	35.86	31.02
990	1.441	33.82	40.683	7.89	15.07	4.16	6.20	35.54	31.14
1002	1.449	34.97	37.851	7.94	15.00	4.42	5.83	35.95	30.87
1014	1.458	30.66	46.071	8.13	15.10	4.89	6.05	33.95	31.88
1026	1.470	35.28	40.684	8.60	14.95	4.53	5.70	34.07	32.15
1038	1.478	35.22	40.809	8.70	15.03	4.40	5.30	33.93	32.64
1050	1.486	38.07	34.704	8.89	15.01	4.65	5.41	33.48	32.56
1061	1.495	33.80	39.540	9.06	15.11	4.61	5.73	32.86	32.63
1073	1.503	35.56	36.254	9.49	14.98	4.02	5.57	33.95	31.99
1085	1.511	34.43	38.271	9.75	15.06	4.37	5.76	34.33	30.74
1097	1.521	31.86	43.284	9.79	14.89	5.06	6.16	34.44	29.67
1109	1.531	29.66	47.596	9.94	15.04	5.46	6.66	34.00	28.90
1121	1.543	33.40	42.111	10.23	15.35	5.67	6.31	34.10	28.34
1133	1.551	38.41	33.978	10.26	15.42	5.87	6.29	33.47	28.68
1145	1.557	41.83	27.926	10.19	15.57	5.63	6.36	31.96	30.30

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
		(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
1156	1.563	42.77	26.964	10.68	16.01	5.83	6.34	31.79	29.36
1168	1.570	42.53	27.219	10.84	16.21	5.45	6.08	32.65	28.77
1180	1.576	42.13	27.764	10.54	15.99	5.50	6.04	32.73	29.19
1192	1.582	37.35	34.401	10.34	16.03	5.63	6.06	32.54	29.40
1204	1.591	37.67	34.061	10.62	16.01	5.79	5.62	33.17	28.80
1216	1.599	38.33	33.180	10.21	16.07	5.33	5.32	33.40	29.66
1228	1.606	41.19	28.639	9.96	15.83	5.59	4.95	32.61	31.05
1240	1.612	40.09	29.887	10.34	16.33	6.10	4.98	33.04	29.21
1252	1.619	41.60	28.181	10.35	16.41	6.13	4.90	33.55	28.65
1264	1.626	40.57	29.582	10.14	16.58	6.80	5.38	33.61	27.51
1276	1.632	41.75	28.249	10.11	16.37	7.00	5.45	32.84	28.23
1288	1.639	41.08	28.960	10.09	16.53	6.98	5.31	32.74	28.36
1300	1.645	43.50	25.988	9.89	16.15	6.57	5.17	31.68	30.54
1312	1.651	43.37	26.131	9.95	16.21	6.21	5.30	31.40	30.93
1324	1.657	43.74	25.723	10.04	16.00	5.94	4.87	30.87	32.29
1336	1.663	44.05	25.418	10.31	16.26	6.31	5.64	29.73	31.76
1348	1.669	48.43	21.864	10.25	16.29	6.63	6.22	28.26	32.35
1360	1.673	52.72	18.370	10.11	16.35	6.49	6.22	28.54	32.29
1372	1.677	53.28	17.840	10.29	16.66	6.84	6.18	27.67	32.36
1384	1.681	54.06	17.371	10.14	16.61	7.01	6.43	27.24	32.57
1396	1.685	50.73	19.916	9.78	16.54	6.95	5.67	28.94	32.12
1408	1.690	51.12	19.566	9.72	16.66	6.32	4.48	30.77	32.06
1420	1.695	47.49	22.124	9.53	16.49	6.43	4.52	30.37	32.65
1432	1.700	47.46	22.156	9.24	16.41	6.73	4.89	30.15	32.58
1444	1.705	50.86	19.720	9.24	16.51	6.42	4.56	30.45	32.83
1456	1.709	51.12	19.496	9.04	16.32	6.32	4.58	29.88	33.86
1468	1.713	51.87	18.829	9.06	16.05	6.65	5.33	29.53	33.38
1481	1.719	48.28	21.433	9.18	16.33	6.59	5.13	30.08	32.70
1493	1.724	48.66	21.122	9.30	15.87	6.83	4.56	31.56	31.89
1505	1.728	46.28	23.488	9.63	16.01	7.06	5.42	31.82	30.06
1517	1.734	47.35	22.598	9.75	15.87	7.40	5.20	31.64	30.14
1529	1.739	47.19	22.726	10.06	16.15	7.64	5.15	30.32	30.68
1541	1.744	54.01	17.404	10.19	16.02	8.31	5.26	30.00	30.21
1553	1.748	53.88	17.502	9.10	16.61	8.26	5.54	30.99	29.51
1565	1.751	55.19	16.517	8.71	16.47	8.02	4.84	31.26	30.70
1577	1.756	51.45	18.901	7.55	16.71	7.87	4.77	32.02	31.07
1589	1.760	51.97	18.506	7.36	16.58	7.87	4.92	33.66	29.61

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
		(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
1602	1.765	51.23	19.040	7.19	16.62	7.68	5.10	33.80	29.62
1614	1.769	51.87	18.561	8.43	16.26	8.13	5.19	32.68	29.31
1626	1.773	51.89	18.550	8.19	15.84	8.61	6.26	31.97	29.13
1638	1.777	50.92	19.329	9.44	15.47	8.68	6.46	31.24	28.72
1650	1.782	49.92	20.097	9.28	15.31	9.07	5.87	31.07	29.40
1662	1.787	49.98	20.048	9.54	15.40	9.59	6.02	31.50	27.96
1674	1.791	51.62	18.780	9.30	15.45	9.33	5.68	31.93	28.31
1687	1.796	53.03	17.720	10.11	15.59	9.37	5.06	31.93	27.93
1699	1.800	52.84	17.867	10.12	15.79	9.99	5.37	32.48	26.25
1711	1.804	53.21	17.608	10.17	15.66	9.98	6.29	32.52	25.39
1723	1.808	52.87	17.849	9.94	15.42	9.80	5.77	32.20	26.87
1735	1.812	53.27	17.553	9.91	15.30	10.33	5.51	31.88	27.06
1747	1.816	53.71	17.262	9.45	15.67	10.19	5.34	32.95	26.39
1760	1.820	54.58	16.668	9.32	15.36	9.95	5.67	32.33	27.36
1772	1.824	54.31	16.866	9.13	15.49	10.31	5.29	32.60	27.18
1784	1.828	54.17	16.958	9.22	15.38	10.47	5.48	32.63	26.81
1796	1.832	53.58	17.356	9.12	15.21	10.63	5.87	32.38	26.80
1808	1.836	54.27	16.863	8.84	14.90	11.39	5.85	32.03	26.99
1821	1.840	54.06	16.997	8.89	15.09	11.33	5.05	32.60	27.04
1833	1.844	54.65	16.602	9.04	14.97	11.14	4.74	32.76	27.35
1845	1.848	54.92	16.421	8.90	15.05	11.17	5.05	32.80	27.04
1857	1.851	55.23	16.217	8.63	15.15	11.21	5.33	32.88	26.80
1870	1.855	55.61	15.969	8.65	15.25	10.84	5.17	32.81	27.29
1882	1.859	56.00	15.718	8.75	15.41	11.29	6.01	33.12	25.42
1894	1.863	56.75	15.251	8.45	15.37	11.66	6.61	32.91	25.01
1906	1.866	56.76	15.244	8.36	15.33	11.76	6.88	33.07	24.61
1919	1.870	57.37	14.866	8.44	15.22	12.05	6.67	33.27	24.35
1931	1.873	56.99	15.097	8.77	15.28	12.59	6.84	33.63	22.90
1943	1.877	57.68	14.682	8.48	15.15	12.37	6.05	33.52	24.43
1956	1.880	57.68	14.682	8.59	15.18	12.41	5.74	33.46	24.63
1968	1.884	57.69	14.676	8.58	15.21	12.56	5.00	33.55	25.10
1980	1.887	57.52	14.775	8.72	15.73	12.94	4.67	34.69	23.24
1992	1.890	58.69	14.112	8.67	15.77	12.19	4.22	35.00	24.16
2005	1.894	59.69	13.519	8.84	15.77	12.75	4.18	34.76	23.70
2017	1.897	60.14	13.262	9.11	16.01	13.17	3.89	35.58	22.24
2029	1.900	60.14	13.259	9.10	15.84	13.16	4.14	35.27	22.50
2042	1.903	59.88	13.406	9.26	15.30	12.02	4.19	34.03	25.20

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
		(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
2054	1.906	59.71	13.504	8.85	15.01	12.90	4.57	33.32	25.37
2066	1.909	59.08	13.855	9.12	15.03	12.60	4.95	33.92	24.38
2079	1.913	59.43	13.655	8.54	14.82	12.05	5.56	33.19	25.84
2091	1.916	59.88	13.404	8.77	15.50	12.70	4.62	33.92	24.49
2103	1.919	61.79	12.412	8.58	15.48	13.39	4.55	34.22	23.78
2116	1.922	61.99	12.300	8.69	15.29	13.13	4.78	34.36	23.75
2128	1.925	61.43	12.619	8.12	15.09	13.07	4.86	33.61	25.25
2140	1.928	59.58	13.574	8.50	15.35	12.92	4.59	34.48	24.16
2153	1.931	60.40	13.150	8.12	14.79	12.09	5.68	34.16	25.16
2165	1.934	61.37	12.612	7.75	14.78	12.11	6.00	34.23	25.13
2178	1.937	62.11	12.206	7.61	15.15	12.48	5.48	34.94	24.33
2190	1.940	62.12	12.199	7.78	15.19	12.53	5.09	35.39	24.02
2202	1.943	62.19	12.162	7.75	15.03	13.17	5.48	35.16	23.41
2215	1.946	62.61	11.949	7.60	14.63	13.18	5.41	34.55	24.63
2227	1.948	61.61	12.475	7.69	14.65	13.08	5.01	34.54	25.05
2240	1.952	61.98	12.282	7.63	14.56	13.06	5.64	34.27	24.85
2252	1.954	62.18	12.181	7.66	14.94	13.53	5.87	35.11	22.89
2264	1.957	63.96	11.277	7.71	14.97	12.72	5.00	35.09	24.52
2277	1.960	65.26	10.659	7.65	15.61	12.37	4.45	36.44	23.48
2289	1.962	66.00	10.306	7.79	15.78	12.87	4.98	37.17	21.42
2302	1.965	66.03	10.291	8.01	15.84	13.00	4.48	37.40	21.27
2314	1.967	65.63	10.473	8.01	15.70	12.95	4.35	37.51	21.47
2327	1.970	65.68	10.452	7.93	15.56	12.54	5.28	37.30	21.39
2339	1.972	65.69	10.446	8.20	15.39	13.13	6.12	37.16	20.00
2352	1.975	65.77	10.212	8.40	15.67	11.54	6.26	37.63	20.49

Appendix E. Raman Offgas Data for Experiment 105

As discussed in Appendix A, the Raman readings should be positive and sum to 100% except in cases where there is significant Ar present. Due to the noise in the Raman signal, any raw readings that are less than zero are fixed to zero and then all the gas readings for H₂, NO₂, N₂, O₂, N₂O, and NO are normalized to 100 vol %. Even with these corrections, the Raman readings have noise in them. To reduce this noise, moving averages of the fixed and normalized readings were performed using equation C-1.

These moving averages do not eliminate all the noise but smooth the values so comparisons and calculations can be performed. The fixed, normalized, and moving average Raman gas concentrations are reported in Table D-1. Due to rounding to the nearest hundredth, the numbers in the table may not sum to exactly 100 vol % but all the decimal places were carried in the calculations performed for this report.

Table E-1. Fixed Normalized Moving Average Raman Data for Experiment 105

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
4	0.001	78.68	5.467	0.39	2.58	7.96	1.11	6.81	81.14
15	0.002	76.01	6.368	0.39	2.39	6.85	1.11	7.98	81.27
27	0.004	74.52	6.848	0.20	2.14	7.78	0.82	9.55	79.52
38	0.005	75.85	6.387	0.16	1.96	6.83	0.82	10.27	79.96
50	0.006	76.75	6.062	0.52	1.92	7.43	1.22	12.38	76.53
61	0.007	69.59	9.462	1.07	1.84	6.59	1.32	14.73	74.45
73	0.010	55.45	19.700	1.46	1.75	6.63	1.32	19.31	69.53
84	0.015	39.14	35.680	2.41	1.67	6.56	1.23	22.21	65.92
96	0.024	28.65	51.849	3.64	1.33	7.30	1.23	25.80	60.71
108	0.037	20.94	87.049	4.35	1.19	6.45	0.82	27.40	59.79
119	0.056	15.74	121.214	5.26	1.20	5.80	0.94	28.45	58.35
131	0.087	10.56	176.004	5.61	1.18	5.83	1.33	27.86	58.19
143	0.128	11.42	166.668	6.26	1.22	6.44	2.04	28.88	55.15
154	0.161	12.05	158.260	6.25	1.29	6.62	2.70	30.27	52.86
166	0.186	12.93	137.616	7.63	1.43	5.60	2.70	31.02	51.62
178	0.217	11.36	158.339	7.74	1.53	5.74	2.22	32.20	50.56
189	0.250	9.46	196.748	8.92	1.63	5.09	2.47	32.31	49.57
201	0.294	11.36	175.020	8.71	1.62	5.00	2.03	32.65	49.98
213	0.331	12.94	154.223	9.70	1.70	4.68	1.41	32.28	50.24
224	0.351	14.44	120.856	9.63	1.68	5.20	1.42	31.81	50.26
236	0.378	16.56	109.488	10.18	1.58	4.66	1.50	31.76	50.31
248	0.401	15.17	126.731	10.34	1.57	4.68	0.85	32.62	49.92
259	0.423	14.99	129.382	11.17	1.67	4.11	1.47	32.67	48.93
271	0.456	11.92	149.355	11.24	1.62	4.57	1.48	32.36	48.72
283	0.486	14.83	121.670	10.77	1.67	4.41	1.64	33.03	48.49
295	0.508	15.60	111.882	10.44	1.70	4.68	1.10	32.96	49.11

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
306	0.528	16.13	106.735	9.99	1.70	4.96	1.21	33.30	48.84
318	0.552	13.97	123.627	9.32	1.72	5.89	0.65	33.75	48.66
330	0.578	14.64	117.464	8.37	1.74	6.57	0.93	34.61	47.79
342	0.603	15.91	108.601	7.51	1.72	6.52	1.43	34.93	47.89
353	0.621	14.10	144.940	7.19	1.82	6.31	2.02	35.91	46.75
365	0.656	13.97	145.982	7.28	1.84	6.58	2.15	35.95	46.19
377	0.692	14.35	143.958	7.21	1.82	4.86	1.83	36.85	47.43
388	0.710	16.94	99.880	7.28	1.85	4.43	1.54	37.35	47.55
400	0.730	16.86	100.560	7.75	1.87	4.58	0.87	37.71	47.22
412	0.753	15.52	108.905	7.63	1.85	4.53	0.40	37.82	47.77
424	0.776	16.44	102.324	7.44	1.87	4.39	0.20	38.32	47.78
436	0.796	17.92	92.385	7.40	1.85	5.62	0.63	38.61	45.89
447	0.813	18.29	89.657	7.49	1.83	5.08	1.26	39.02	45.32
459	0.831	16.30	107.682	7.36	1.82	4.80	1.26	39.43	45.33
471	0.857	16.20	108.210	7.48	1.76	5.23	1.14	39.92	44.47
483	0.880	15.39	114.627	7.05	1.71	5.17	1.16	40.68	44.23
495	0.901	16.91	99.723	6.74	1.68	4.89	0.80	40.52	45.36
506	0.922	17.15	98.466	6.61	1.65	5.78	0.96	40.96	44.05
518	0.940	17.10	98.987	6.89	1.63	5.68	1.11	41.41	43.28
530	0.961	18.21	92.361	6.20	1.66	5.05	1.26	42.61	43.23
542	0.982	17.78	94.650	6.51	1.67	4.74	1.61	43.20	42.25
554	0.999	18.73	87.115	6.80	1.70	5.03	2.60	43.54	40.33
566	1.018	18.06	90.839	7.10	1.72	4.24	1.78	44.36	40.81
578	1.037	18.27	89.689	6.85	1.75	4.86	1.72	45.00	39.80
589	1.054	18.75	86.731	7.19	1.73	5.13	1.58	44.69	39.68
601	1.071	18.40	89.021	6.95	1.69	5.83	1.16	44.52	39.85
613	1.091	18.66	87.710	6.98	1.65	5.63	0.10	45.82	39.83
625	1.109	18.33	89.640	6.50	1.64	6.06	0.23	46.24	39.34
637	1.127	18.63	87.671	6.36	1.60	5.86	0.13	46.53	39.52
649	1.146	19.03	85.824	6.49	1.39	6.31	0.22	47.59	38.01
661	1.163	19.43	83.492	6.78	1.37	5.75	0.66	47.90	37.54
672	1.179	20.93	75.979	6.70	1.35	5.69	0.66	48.08	37.52
685	1.196	21.40	74.038	7.05	1.33	5.36	0.66	47.84	37.75
697	1.210	21.83	71.834	7.00	1.29	5.04	1.36	48.00	37.32
709	1.225	20.84	76.357	7.06	1.47	5.19	1.53	47.48	37.27
720	1.241	21.09	75.437	6.78	1.46	5.37	1.09	47.98	37.32
732	1.256	22.10	71.199	6.91	1.48	5.55	1.25	47.67	37.14
744	1.270	23.38	65.559	6.90	1.48	5.65	1.39	48.37	36.20

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
756	1.284	23.01	66.954	7.09	1.49	6.19	0.69	48.67	35.87
768	1.298	23.07	66.726	7.17	1.49	5.70	0.76	48.49	36.39
780	1.312	22.29	69.964	7.62	1.50	5.13	1.28	48.59	35.87
792	1.326	22.92	67.626	7.43	1.52	5.23	1.12	48.83	35.87
804	1.341	22.76	68.220	7.26	1.49	5.78	1.03	48.02	36.40
816	1.354	24.23	62.658	7.24	1.49	5.82	1.34	47.95	36.15
828	1.367	23.66	64.752	7.07	1.53	6.33	1.02	48.65	35.40
840	1.381	24.12	63.118	6.97	1.52	6.99	1.03	48.40	35.09
852	1.394	24.92	60.832	7.53	1.47	7.41	1.26	47.64	34.69
864	1.406	29.41	49.773	7.51	1.50	6.73	1.25	47.94	35.07
876	1.415	28.86	51.740	7.74	1.51	6.73	1.03	47.64	35.34
888	1.426	28.49	52.739	8.23	1.48	6.88	1.03	47.01	35.37
900	1.439	24.79	60.984	8.57	1.49	7.22	0.80	46.54	35.38
912	1.451	25.57	58.294	8.67	1.55	6.69	1.11	46.71	35.28
924	1.463	27.29	54.231	8.82	1.58	7.03	0.93	46.73	34.90
936	1.474	28.51	50.802	9.04	1.57	7.09	0.83	46.34	35.12
948	1.484	28.88	49.667	9.44	1.55	6.79	0.85	45.71	35.65
960	1.495	26.86	54.597	9.63	1.52	6.59	0.90	45.10	36.25
972	1.507	28.47	51.221	9.78	1.51	7.15	0.57	44.65	36.35
984	1.517	28.32	51.682	10.32	1.45	7.25	0.71	43.69	36.57
996	1.527	28.36	51.543	10.64	1.44	7.28	1.05	43.51	36.08
1008	1.539	25.78	57.572	10.98	1.44	7.73	1.32	43.33	35.20
1020	1.551	26.54	55.496	11.09	1.42	8.26	1.68	43.04	34.51
1032	1.562	27.02	54.138	11.30	1.33	8.24	1.48	43.12	34.52
1044	1.573	28.05	51.326	11.74	1.28	8.34	2.01	42.72	33.91
1056	1.584	28.56	50.111	12.33	1.31	8.72	1.66	41.82	34.15
1068	1.594	29.26	48.360	12.26	1.28	8.76	1.46	41.25	35.00
1081	1.605	29.96	46.780	12.75	1.28	9.10	1.31	40.78	34.78
1093	1.614	30.14	46.379	14.23	1.40	10.01	1.83	42.82	29.71
1105	1.624	32.34	42.229	14.59	1.41	10.27	1.16	42.37	30.21
1117	1.632	33.07	40.796	14.40	1.38	10.39	1.87	41.80	30.16
1129	1.640	33.78	39.337	14.28	1.42	10.91	1.83	41.68	29.88
1141	1.649	32.93	40.749	13.99	1.43	10.63	1.44	41.80	30.71
1153	1.657	33.41	39.907	12.94	1.34	10.26	1.17	38.48	35.81
1165	1.666	33.96	38.908	12.72	1.35	10.89	1.68	38.22	35.14
1177	1.674	34.11	38.633	12.82	1.37	10.68	1.17	38.41	35.54
1190	1.682	34.95	37.312	12.99	1.33	11.15	1.53	37.39	35.61
1202	1.690	36.90	34.420	13.36	1.37	11.23	1.36	36.80	35.89

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
1214	1.697	38.15	32.473	13.37	1.35	11.55	1.56	36.78	35.40
1226	1.703	38.92	31.419	13.69	1.39	12.15	1.65	34.10	37.01
1238	1.710	45.49	25.851	13.49	1.36	13.26	1.81	33.02	37.05
1250	1.715	46.87	24.106	13.23	1.36	13.35	1.76	32.58	37.72
1263	1.719	48.48	22.248	12.44	1.38	13.71	2.20	32.45	37.81
1275	1.725	44.70	24.889	12.28	1.39	13.85	2.10	31.43	38.95
1287	1.730	45.04	24.513	12.03	1.36	13.17	2.08	32.82	38.55
1299	1.735	45.71	23.853	11.32	1.41	13.42	1.77	33.30	38.79
1311	1.740	45.29	24.229	11.78	1.46	14.27	1.54	33.76	37.19
1324	1.745	47.90	21.823	12.29	1.43	15.19	1.33	33.48	36.28
1336	1.750	48.21	21.534	12.18	1.43	15.71	1.10	33.25	36.33
1348	1.754	48.44	21.333	11.91	1.48	16.52	1.26	33.06	35.77
1361	1.759	48.11	21.596	13.16	1.48	16.29	1.21	32.70	35.15
1373	1.763	49.81	20.209	13.08	1.51	15.72	1.22	32.36	36.12
1385	1.767	50.56	19.576	13.31	1.50	15.63	0.99	31.71	36.85
1397	1.771	51.03	19.205	13.42	1.54	15.98	1.13	31.64	36.30
1409	1.776	49.83	20.152	12.80	1.53	16.64	0.97	31.49	36.58
1422	1.780	49.09	20.777	12.03	1.44	17.38	1.46	30.45	37.25
1434	1.785	48.36	21.359	11.92	1.38	18.07	1.33	29.84	37.46
1446	1.789	49.27	20.633	12.13	1.39	18.88	1.67	29.94	35.99
1458	1.793	50.81	19.391	12.14	1.43	18.76	1.91	30.09	35.67
1471	1.797	52.18	18.336	12.57	1.41	19.23	1.32	30.00	35.47
1483	1.801	52.22	18.307	12.70	1.49	19.62	1.61	30.14	34.44
1495	1.805	51.70	18.702	12.31	1.49	20.40	2.02	29.82	33.97
1507	1.809	51.70	18.700	11.90	1.49	20.14	2.46	29.16	34.86
1520	1.813	51.71	18.695	12.32	1.50	21.59	2.10	29.61	32.89
1532	1.817	53.62	17.350	12.82	1.54	21.45	2.10	30.06	32.04
1544	1.821	54.40	16.824	12.76	1.56	21.33	1.32	29.65	33.38
1557	1.824	55.41	16.104	12.72	1.57	21.51	0.95	29.94	33.32
1569	1.828	54.91	16.424	12.73	1.58	21.45	0.17	30.25	33.82
1582	1.831	55.11	16.293	12.03	1.56	20.69	0.04	29.17	36.51
1594	1.835	55.18	16.246	11.79	1.59	20.60	0.92	27.89	37.22
1606	1.838	55.60	15.978	11.95	1.56	20.60	2.11	28.08	35.70
1619	1.842	55.26	16.198	11.68	1.52	20.66	2.60	27.63	35.92
1631	1.845	55.12	16.291	11.71	1.54	21.15	2.96	27.41	35.24
1643	1.848	55.22	16.230	11.23	1.53	21.81	3.06	27.22	35.15
1656	1.852	55.25	16.205	10.99	1.51	22.28	2.18	27.98	35.06
1668	1.855	56.20	15.593	10.81	1.59	23.27	1.25	27.95	35.13

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
		(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
1680	1.859	56.96	15.136	10.49	1.67	22.78	1.48	28.59	34.99
1693	1.862	57.40	14.855	10.60	1.70	22.78	1.49	28.87	34.57
1705	1.865	56.77	15.250	11.08	1.64	22.55	1.85	28.89	33.99
1718	1.869	56.23	15.572	11.44	1.60	22.80	2.01	28.21	33.94
1730	1.872	57.04	15.087	11.45	1.60	22.63	1.79	28.02	34.51
1743	1.875	58.24	14.350	12.30	1.58	23.29	1.18	27.70	33.95
1755	1.878	58.63	14.112	12.16	1.58	23.84	0.81	27.18	34.43
1767	1.881	58.72	14.064	12.03	1.67	23.86	0.65	27.69	34.10
1780	1.884	58.75	14.044	11.83	1.77	23.51	1.19	28.10	33.61
1792	1.887	58.84	13.988	11.94	1.72	23.43	1.16	27.95	33.80
1805	1.890	58.91	13.952	11.60	1.74	24.31	1.10	27.13	34.12
1817	1.893	58.36	14.277	11.48	1.78	24.81	1.66	26.90	33.38
1830	1.896	59.16	13.830	11.31	1.75	25.56	2.11	26.08	33.20
1842	1.899	59.17	13.822	11.09	1.74	25.77	2.21	26.07	33.12
1854	1.902	59.99	13.343	10.89	1.74	25.77	2.22	26.38	32.99
1867	1.905	59.55	13.586	11.09	1.71	25.02	2.22	26.81	33.16
1879	1.908	59.72	13.488	11.15	1.71	24.72	1.86	27.28	33.29
1892	1.911	60.13	13.263	11.30	1.72	24.51	1.54	27.04	33.89
1904	1.914	60.13	13.267	11.48	1.70	25.38	0.74	26.24	34.46
1917	1.917	60.91	12.847	11.41	1.66	25.95	1.47	25.67	33.84
1929	1.919	60.64	12.993	11.23	1.63	26.87	1.39	25.87	33.02
1942	1.922	61.59	12.483	11.39	1.65	27.31	1.19	25.40	33.07
1954	1.925	62.30	12.126	11.28	1.67	27.03	1.35	25.90	32.77
1967	1.928	63.26	11.619	11.03	1.70	26.66	1.75	26.44	32.41
1979	1.930	62.81	11.854	11.07	1.62	26.30	1.01	26.81	33.19
1992	1.933	62.68	11.919	11.20	1.71	25.83	1.53	26.61	33.12
2004	1.935	63.41	11.567	10.30	1.76	25.75	2.07	26.93	33.20
2017	1.938	64.94	10.804	10.37	1.82	26.12	2.33	26.78	32.59
2029	1.940	64.92	10.814	10.38	1.80	26.37	2.78	26.61	32.06
2042	1.942	64.51	11.006	10.36	2.04	26.32	2.92	26.34	32.01
2055	1.945	64.63	10.953	10.51	2.03	26.12	2.71	26.32	32.32
2067	1.947	65.29	10.639	10.90	1.99	26.75	2.45	26.15	31.76
2080	1.949	65.99	10.309	10.61	1.96	27.79	1.73	25.98	31.92
2092	1.952	66.08	10.269	10.88	1.97	27.76	0.91	26.27	32.21
2105	1.954	66.22	10.204	10.91	1.96	28.64	1.49	26.57	30.42
2117	1.956	67.23	9.762	9.71	2.04	29.35	1.19	27.05	30.67
2130	1.958	67.86	9.482	9.72	2.06	29.28	1.23	27.03	30.69
2143	1.960	68.58	9.166	9.76	2.13	28.53	1.57	27.79	30.23

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
2155	1.962	68.43	9.228	9.39	2.17	28.76	1.73	27.37	30.57
2168	1.964	68.89	9.035	9.46	2.21	28.82	1.52	27.42	30.57
2181	1.966	69.49	8.781	10.77	2.22	28.90	1.63	26.79	29.67
2193	1.968	70.74	8.280	10.71	2.21	28.54	2.68	26.28	29.58
2206	1.970	70.71	8.296	11.07	2.18	29.17	2.53	24.86	30.18
2218	1.972	71.22	8.090	11.19	2.25	29.97	2.38	25.15	29.06
2231	1.974	71.20	8.100	11.29	2.21	30.93	2.12	24.28	29.17
2244	1.975	72.20	7.701	10.89	2.22	30.97	3.65	23.75	28.53
2256	1.977	72.40	7.626	10.83	2.28	31.22	2.93	23.50	29.25
2269	1.979	71.79	7.861	10.97	2.36	31.13	2.58	23.92	29.05
2282	1.980	72.34	7.660	10.61	2.32	29.66	2.97	23.52	30.92
2294	1.982	72.46	7.612	10.86	2.44	29.38	3.02	24.30	30.00
2307	1.984	74.24	6.947	10.74	2.47	29.09	1.62	23.87	32.20
2320	1.985	73.70	7.149	10.31	2.47	29.41	1.40	24.40	32.01
2332	1.987	73.97	7.047	9.93	2.44	29.08	1.45	25.03	32.07
2345	1.988	73.24	7.311	9.79	2.49	29.92	1.69	24.81	31.31
2358	1.990	73.57	7.184	9.17	2.43	27.39	2.98	24.43	33.60
2370	1.991	73.84	7.085	8.38	2.47	28.14	3.27	25.29	32.45
2383	1.993	74.60	6.815	7.93	2.50	28.61	2.98	25.40	32.57
2396	1.995	76.64	6.116	7.31	2.49	28.53	3.55	24.73	33.40
2408	1.996	77.02	5.981	7.80	2.50	28.51	3.67	24.48	33.04
2421	1.997	76.90	6.022	7.48	2.57	31.32	2.10	23.95	32.56
2434	1.998	75.90	6.352	8.06	2.72	30.96	4.02	22.83	31.42
2447	2.000	76.12	5.821	8.87	2.95	30.35	5.84	21.92	30.05

Appendix F. Raman Offgas Data for Experiment 106

As discussed in Appendix A, the Raman readings should be positive and sum to 100% except in cases where there is significant Ar present. Due to the noise in the Raman signal, any raw readings that are less than zero are fixed to zero and then all the gas readings for H₂, NO₂, N₂, O₂, N₂O, and NO are normalized to 100 vol %. Even with these corrections, the Raman readings have noise in them. To reduce this noise, moving averages of the fixed and normalized readings were performed using equation C-1.

These moving averages do not eliminate all the noise but smooth the values so comparisons and calculations can be performed. The fixed, normalized, and moving average Raman gas concentrations are reported in Table F-1. Due to rounding to the nearest hundredth, the numbers in the table may not sum to exactly 100 vol % but all the decimal places were carried in the calculations performed for this report.

Table F-1. Fixed Normalized Moving Average Raman Data for Experiment 106

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
0	0.001	78.14	5.597	0.35	0.25	3.14	1.14	1.93	93.19
11	0.002	78.27	5.556	0.25	0.24	2.84	0.64	1.53	94.50
23	0.003	77.96	5.660	0.33	0.22	3.30	0.64	1.82	93.69
35	0.004	77.93	5.670	0.80	0.21	1.94	0.51	1.55	94.99
46	0.005	77.47	5.820	1.30	0.22	2.00	0.00	4.98	91.50
58	0.006	75.80	6.437	1.84	0.22	2.39	0.22	7.28	88.05
69	0.007	67.15	10.614	2.74	0.19	2.43	0.22	11.65	82.77
81	0.010	52.45	21.894	3.87	0.18	2.51	0.22	16.19	77.03
93	0.015	37.01	39.399	4.52	0.16	3.32	0.22	20.87	70.91
104	0.024	24.16	74.013	5.43	0.10	3.01	0.26	22.53	68.68
116	0.041	17.09	108.088	6.10	0.08	3.57	0.04	25.18	65.03
128	0.065	13.01	134.223	6.60	0.08	3.94	0.04	25.69	63.65
139	0.089	12.26	143.295	7.01	0.08	3.85	0.04	25.65	63.37
151	0.116	11.96	147.538	7.28	0.08	3.97	0.04	26.08	62.54
163	0.145	11.79	149.707	7.22	0.09	4.09	0.00	26.71	61.89
174	0.170	11.55	153.320	7.32	0.09	3.82	0.00	27.01	61.76
186	0.199	11.70	151.100	7.23	0.09	3.77	0.00	26.90	62.01
198	0.228	11.92	148.301	6.98	0.08	3.95	0.00	27.27	61.71
209	0.252	12.83	136.436	7.04	0.08	3.79	0.00	27.38	61.71
221	0.277	15.40	114.449	7.28	0.09	3.77	0.07	25.01	63.78
233	0.296	18.47	92.469	7.21	0.09	3.60	0.07	25.02	64.02
244	0.309	18.48	92.374	7.12	0.09	3.47	0.16	25.07	64.10
256	0.327	18.83	90.664	7.11	0.09	3.40	0.22	25.12	64.08
268	0.346	16.28	106.941	6.98	0.07	3.32	0.22	24.45	64.97
280	0.364	16.79	102.169	6.74	0.06	3.24	0.20	26.43	63.33
291	0.384	14.89	114.486	6.35	0.05	3.25	0.20	25.34	64.81

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
303	0.405	19.95	90.418	5.95	0.05	3.30	0.11	25.49	65.09
315	0.420	20.00	90.004	5.88	0.05	3.23	0.16	25.15	65.52
327	0.434	20.44	86.371	5.92	0.06	3.23	0.16	25.43	65.19
338	0.453	16.16	103.888	5.87	0.06	3.34	0.20	25.15	65.37
350	0.472	16.72	99.659	6.09	0.06	3.50	0.20	25.93	64.20
362	0.490	16.71	99.780	6.47	0.06	3.46	0.20	25.57	64.24
374	0.508	16.82	99.008	6.41	0.05	3.49	0.22	25.95	63.88
385	0.526	16.83	98.937	6.33	0.05	3.57	0.22	25.75	64.08
397	0.544	17.41	94.943	5.94	0.05	3.67	0.21	25.93	64.20
409	0.561	17.45	94.655	6.04	0.05	3.75	0.21	25.76	64.19
421	0.579	20.45	81.487	6.04	0.05	3.93	0.42	25.50	64.05
433	0.593	20.44	81.545	6.08	0.05	3.94	0.29	25.13	64.51
444	0.606	20.85	78.918	6.10	0.05	4.03	0.31	25.02	64.50
456	0.623	18.12	90.384	6.40	0.05	4.06	0.26	24.90	64.32
468	0.639	18.28	89.402	6.20	0.05	4.01	0.26	24.89	64.59
480	0.656	18.47	88.314	6.14	0.05	4.04	0.06	25.07	64.64
492	0.672	18.71	86.885	6.05	0.05	4.22	0.06	25.38	64.26
503	0.687	19.15	84.515	6.00	0.05	4.13	0.04	25.59	64.19
515	0.703	19.18	84.295	5.98	0.04	4.03	0.07	25.83	64.05
527	0.718	19.17	84.356	5.98	0.04	4.18	0.07	26.07	63.65
539	0.734	19.02	85.184	5.97	0.05	3.96	0.10	26.43	63.49
551	0.750	22.12	73.624	5.90	0.05	3.93	0.10	26.40	63.62
563	0.763	22.54	71.392	5.73	0.05	3.96	0.10	26.60	63.56
575	0.775	22.78	70.147	5.57	0.05	4.04	0.03	26.32	63.99
586	0.789	20.10	79.515	5.50	0.05	3.94	0.11	26.27	64.13
598	0.804	20.15	79.238	5.40	0.05	4.03	0.08	25.68	64.76
610	0.818	20.53	77.458	5.35	0.05	3.93	0.24	25.39	65.03
622	0.833	20.54	77.412	5.31	0.05	3.89	0.43	25.18	65.14
634	0.847	20.56	77.310	5.33	0.05	3.88	0.43	25.09	65.22
646	0.862	20.46	77.769	5.26	0.05	4.02	0.35	25.25	65.07
658	0.876	20.84	76.005	5.24	0.05	4.06	0.35	25.53	64.78
670	0.890	20.78	76.321	5.16	0.05	4.14	0.19	25.86	64.60
682	0.904	20.78	76.303	5.21	0.05	4.20	0.00	25.69	64.84
694	0.919	20.88	75.869	5.16	0.05	4.24	0.00	25.83	64.71
706	0.933	23.92	65.529	5.14	0.05	4.16	0.04	25.68	64.93
717	0.943	24.17	64.445	5.17	0.04	4.30	0.04	25.75	64.69
729	0.954	24.25	64.077	5.06	0.04	4.32	0.15	25.57	64.85
741	0.968	22.06	70.701	5.06	0.04	4.53	0.29	25.62	64.47

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
		(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
753	0.981	22.15	70.298	5.06	0.04	4.72	0.29	25.96	63.93
765	0.994	22.19	70.144	5.09	0.05	4.75	0.32	25.77	64.03
777	1.007	22.37	69.449	4.98	0.05	4.90	0.45	25.88	63.74
789	1.020	22.60	68.538	5.20	0.05	5.05	0.34	25.67	63.68
801	1.032	23.05	66.784	5.14	0.05	4.89	0.29	25.89	63.75
813	1.045	23.30	65.910	5.24	0.05	4.78	0.29	25.85	63.80
825	1.057	24.02	63.311	5.39	0.05	4.80	0.31	26.11	63.34
837	1.069	24.07	63.130	5.51	0.05	4.66	0.18	26.05	63.55
849	1.080	24.00	63.370	5.46	0.04	4.54	0.22	26.53	63.21
861	1.093	23.70	64.386	5.61	0.05	4.88	0.24	26.48	62.75
873	1.104	23.95	63.532	5.66	0.05	4.96	0.24	26.40	62.69
885	1.116	24.53	61.615	5.64	0.05	5.29	0.14	26.58	62.31
897	1.128	24.83	60.589	5.65	0.05	5.49	0.14	26.66	62.02
909	1.139	25.46	58.598	5.75	0.06	5.59	0.10	26.57	61.93
921	1.150	25.70	57.890	5.70	0.06	5.59	0.00	26.72	61.94
933	1.160	26.35	55.907	5.60	0.06	5.88	0.00	26.48	61.98
945	1.171	26.10	56.646	5.63	0.06	5.94	0.09	26.22	62.06
957	1.181	26.58	55.312	5.73	0.06	5.97	0.15	26.50	61.60
969	1.192	26.63	55.173	5.78	0.06	6.17	0.15	26.58	61.27
981	1.202	27.19	53.571	5.86	0.06	6.17	0.17	26.34	61.40
993	1.212	27.44	52.940	6.07	0.06	6.09	0.17	26.51	61.10
1006	1.222	27.93	51.632	6.14	0.06	6.02	0.13	26.71	60.94
1018	1.232	28.55	50.058	6.03	0.05	6.06	0.07	27.11	60.68
1030	1.241	28.60	49.931	6.13	0.05	6.10	0.17	26.90	60.64
1042	1.250	28.73	49.615	6.32	0.06	6.31	0.15	27.09	60.06
1054	1.260	28.68	49.737	6.37	0.05	6.43	0.15	27.20	59.81
1066	1.269	29.57	47.732	6.37	0.04	6.78	0.21	27.06	59.55
1078	1.278	30.02	46.694	6.55	0.05	6.88	0.21	26.78	59.53
1090	1.286	30.33	45.973	6.61	0.05	7.18	0.20	27.09	58.87
1102	1.295	29.58	47.638	6.43	0.04	7.13	0.20	27.54	58.66
1114	1.304	29.24	48.407	6.48	0.06	7.47	0.20	27.68	58.12
1127	1.314	29.26	48.362	6.63	0.06	7.40	0.19	27.80	57.91
1139	1.323	30.01	46.707	6.69	0.06	7.59	0.19	27.44	58.03
1151	1.331	30.70	45.171	6.75	0.06	7.59	0.15	27.23	58.22
1163	1.339	31.45	43.601	6.57	0.06	7.66	0.20	26.78	58.72
1175	1.348	31.98	42.570	6.59	0.06	7.52	0.22	27.07	58.53
1187	1.355	31.95	42.631	6.67	0.06	7.68	0.36	27.49	57.73
1199	1.363	31.83	42.859	6.77	0.06	7.99	0.36	27.42	57.40

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
1212	1.372	32.13	42.313	6.84	0.06	8.07	0.39	27.50	57.14
1224	1.380	33.23	40.249	7.22	0.07	8.39	0.41	27.80	56.10
1236	1.387	34.17	38.538	7.43	0.07	8.63	0.39	27.66	55.82
1248	1.394	32.94	40.971	7.53	0.07	8.91	0.16	27.34	55.99
1260	1.402	33.02	40.833	7.57	0.07	8.67	0.16	27.74	55.79
1273	1.411	33.15	40.619	7.67	0.07	8.82	0.24	27.91	55.29
1285	1.418	34.96	37.222	7.73	0.07	8.82	0.24	27.65	55.49
1297	1.425	35.31	36.643	7.77	0.07	9.01	0.24	27.34	55.57
1309	1.431	35.65	36.100	7.73	0.07	8.99	0.30	27.11	55.80
1321	1.438	35.92	35.681	7.84	0.07	9.33	0.41	27.19	55.16
1334	1.445	36.14	35.343	7.83	0.07	9.50	0.24	27.60	54.76
1346	1.452	36.86	34.298	7.85	0.08	9.78	1.00	27.43	53.85
1358	1.458	36.76	34.443	7.88	0.08	9.81	1.01	27.40	53.81
1370	1.465	37.01	34.073	8.20	0.08	9.90	1.00	27.95	52.87
1383	1.472	36.69	34.524	8.26	0.08	9.98	0.96	27.86	52.86
1395	1.478	37.70	33.084	8.42	0.08	10.07	1.01	27.69	52.72
1407	1.484	37.85	32.866	8.68	0.07	10.13	0.18	28.23	52.71
1419	1.490	38.17	32.414	8.82	0.07	10.32	0.17	28.54	52.08
1432	1.497	37.84	32.859	8.64	0.07	10.46	0.19	28.49	52.15
1444	1.503	38.06	32.542	8.65	0.07	10.80	0.12	28.35	52.00
1456	1.509	38.49	31.978	8.61	0.07	10.93	0.06	28.53	51.80
1468	1.515	38.15	32.464	8.68	0.07	11.10	0.18	27.95	52.02
1481	1.521	38.66	31.790	8.82	0.07	11.44	0.18	28.14	51.36
1493	1.527	39.54	30.724	9.04	0.08	11.56	0.24	27.56	51.52
1505	1.533	40.72	29.147	9.45	0.08	11.67	0.24	25.55	53.01
1518	1.539	42.42	27.231	9.76	0.08	12.13	0.24	25.26	52.52
1530	1.544	42.44	27.205	9.74	0.08	12.18	0.12	25.73	52.13
1542	1.549	42.46	27.182	9.52	0.08	11.65	0.12	25.14	53.49
1555	1.554	39.65	30.643	9.48	0.08	11.48	0.00	25.76	53.20
1567	1.560	39.49	30.823	9.26	0.08	11.16	0.10	27.80	51.60
1579	1.566	40.08	30.132	9.19	0.08	10.86	0.16	27.63	52.08
1592	1.572	42.06	27.553	9.26	0.08	10.93	0.18	27.39	52.17
1604	1.577	42.32	27.255	9.56	0.08	11.28	0.18	27.43	51.47
1616	1.582	42.34	27.240	9.53	0.08	11.51	0.18	27.10	51.61
1629	1.588	42.46	27.101	9.67	0.08	11.89	0.11	26.92	51.34
1641	1.593	42.78	26.759	9.62	0.08	11.88	0.11	26.77	51.54
1653	1.598	42.81	26.728	9.71	0.08	11.95	0.10	26.79	51.36
1666	1.603	43.17	26.335	9.79	0.08	12.15	0.10	26.89	51.00

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
1678	1.608	43.10	26.407	9.87	0.08	12.33	0.10	26.92	50.71
1691	1.613	43.43	26.056	9.82	0.08	12.42	0.07	27.00	50.61
1703	1.618	43.58	25.901	9.87	0.08	12.52	0.04	27.27	50.22
1715	1.623	43.96	25.504	9.73	0.09	12.70	0.22	27.16	50.10
1728	1.628	44.57	24.877	9.65	0.08	12.57	0.33	27.42	49.94
1740	1.633	44.65	24.796	9.84	0.08	12.78	0.33	27.03	49.93
1753	1.638	45.30	24.166	9.91	0.08	12.66	0.35	27.19	49.81
1765	1.642	45.37	24.100	9.90	0.09	13.02	0.40	26.71	49.88
1777	1.646	45.82	23.653	10.07	0.09	13.22	0.21	26.39	50.02
1790	1.651	46.10	23.394	10.02	0.10	13.69	0.17	26.16	49.87
1802	1.656	46.62	22.908	9.85	0.10	13.65	0.17	26.03	50.21
1815	1.660	47.28	22.304	9.66	0.10	13.97	0.14	25.72	50.41
1827	1.664	47.25	22.326	9.52	0.10	13.97	0.06	25.83	50.52
1840	1.669	46.95	22.603	9.48	0.10	14.15	0.06	26.13	50.08
1852	1.673	46.83	22.711	9.45	0.10	14.39	0.00	26.15	49.91
1865	1.678	47.63	22.030	9.45	0.10	14.95	0.02	26.33	49.16
1877	1.682	48.41	21.331	9.34	0.10	15.40	0.09	25.90	49.16
1890	1.686	48.82	20.971	9.49	0.11	15.71	0.09	26.04	48.57
1902	1.690	48.45	21.282	9.35	0.11	16.05	0.37	25.80	48.31
1914	1.694	48.61	21.141	9.31	0.11	16.26	0.58	25.62	48.13
1927	1.698	49.15	20.704	9.20	0.11	16.68	0.56	25.25	48.21
1940	1.702	49.57	20.349	9.26	0.11	17.01	0.49	24.82	48.31
1952	1.706	50.52	19.604	9.11	0.10	17.55	0.51	24.67	48.06
1965	1.710	50.60	19.541	9.15	0.10	17.90	0.35	24.66	47.84
1977	1.714	51.33	18.968	9.17	0.11	18.30	0.20	24.26	47.95
1990	1.717	51.44	18.890	9.16	0.12	18.56	0.20	24.55	47.41
2002	1.721	51.91	18.530	9.20	0.12	19.02	0.20	25.15	46.32
2015	1.725	51.85	18.576	9.39	0.12	19.22	0.18	24.99	46.09
2027	1.728	51.81	18.602	9.36	0.12	19.52	0.07	24.93	46.01
2040	1.732	52.57	18.064	9.32	0.12	19.92	0.00	25.36	45.27
2052	1.735	52.55	18.075	9.28	0.11	19.94	0.00	25.79	44.88
2065	1.739	55.86	16.017	9.16	0.11	19.83	0.14	26.06	44.70
2077	1.742	55.55	16.229	8.98	0.11	19.98	0.16	26.24	44.52
2090	1.745	56.09	15.840	9.01	0.11	20.24	0.17	26.04	44.44
2103	1.748	54.25	16.896	9.02	0.11	20.54	0.28	25.33	44.72
2115	1.751	54.90	16.449	9.12	0.11	20.84	0.30	24.96	44.66
2128	1.755	55.45	16.076	9.60	0.11	22.08	0.16	21.17	46.88
2140	1.758	56.70	15.337	9.75	0.11	22.47	0.14	20.89	46.63

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
2153	1.761	56.79	15.279	9.70	0.11	22.55	0.13	21.50	46.00
2165	1.763	57.15	15.043	9.70	0.12	22.90	0.02	22.10	45.16
2178	1.767	56.59	15.361	9.55	0.12	23.12	0.00	22.19	45.02
2236	1.780	57.38	14.867	9.08	0.12	22.47	0.00	25.74	42.59
2248	1.783	58.13	14.409	9.25	0.13	22.90	0.05	25.78	41.88
2260	1.786	58.26	14.330	9.29	0.13	23.24	0.24	25.44	41.66
2272	1.788	58.12	14.413	9.28	0.13	23.26	0.24	25.24	41.85
2283	1.791	58.65	14.109	9.54	0.13	23.51	0.24	24.90	41.69
2294	1.793	58.55	14.170	9.66	0.13	24.01	0.24	25.12	40.84
2306	1.796	59.44	13.650	9.44	0.12	24.17	0.26	25.19	40.82
2317	1.798	59.26	13.755	9.52	0.13	24.76	0.07	24.79	40.73
2328	1.800	60.03	13.318	9.56	0.13	24.95	0.07	24.89	40.40
2339	1.803	59.86	13.414	8.57	0.13	25.34	0.07	25.85	40.03
2351	1.805	60.57	13.027	8.54	0.13	24.72	0.29	25.58	40.75
2362	1.807	60.21	13.220	8.63	0.13	24.91	0.21	25.11	41.01
2373	1.810	60.65	12.979	8.58	0.13	24.59	0.34	25.68	40.68
2384	1.812	60.49	13.064	8.24	0.14	24.42	0.51	26.00	40.69
2396	1.814	60.65	12.977	9.13	0.13	24.46	0.51	25.47	40.29
2407	1.816	60.96	12.814	9.04	0.14	24.80	0.30	25.35	40.38
2418	1.819	61.33	12.616	8.78	0.14	24.75	0.56	25.94	39.83
2430	1.821	61.65	12.442	9.02	0.14	25.83	0.44	23.54	41.02
2441	1.823	62.85	11.850	9.23	0.15	26.54	0.26	22.92	40.91
2453	1.825	63.25	11.644	9.52	0.15	27.35	0.72	20.38	41.88
2464	1.827	64.40	11.063	9.53	0.15	27.66	1.13	20.08	41.45
2475	1.829	63.25	11.632	9.66	0.16	27.88	1.17	19.68	41.46
2487	1.831	63.30	11.606	9.26	0.15	27.51	1.35	21.61	40.11
2498	1.833	63.12	11.691	9.14	0.15	27.00	1.35	22.10	40.25
2509	1.835	63.38	11.561	8.74	0.15	26.59	0.90	24.24	39.38
2521	1.837	63.59	11.455	8.85	0.15	26.61	0.49	24.96	38.95
2532	1.839	64.16	11.187	8.86	0.14	26.66	0.19	24.42	39.72
2543	1.841	64.69	10.920	8.97	0.14	26.51	0.13	24.62	39.63
2555	1.843	64.85	10.842	8.91	0.14	26.78	0.13	23.94	40.10
2566	1.845	64.22	11.145	8.95	0.14	26.66	0.13	24.42	39.70
2577	1.847	61.73	12.506	9.12	0.15	27.55	0.13	22.48	40.57
2589	1.850	62.20	12.286	8.93	0.15	27.55	0.23	23.76	39.39
2600	1.852	62.25	12.258	8.86	0.15	27.58	0.11	23.73	39.57
2612	1.854	64.68	10.927	9.08	0.15	28.05	0.15	23.83	38.73
2623	1.856	64.38	11.067	9.29	0.16	28.45	0.15	21.82	40.13

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
2634	1.858	65.44	10.577	9.01	0.16	27.99	0.15	23.38	39.32
2646	1.859	65.66	10.467	9.48	0.17	29.23	0.06	19.84	41.23
2657	1.861	66.84	9.936	9.43	0.18	30.36	0.06	17.78	42.19
2669	1.863	67.43	9.683	9.34	0.18	30.21	0.40	17.85	42.03
2680	1.865	67.75	9.533	9.11	0.17	29.95	0.40	19.53	40.84
2691	1.866	66.89	9.913	9.12	0.17	29.94	0.76	19.45	40.55
2703	1.868	65.42	10.573	8.82	0.16	29.02	0.75	22.21	39.05
2714	1.870	65.49	10.541	8.83	0.16	28.26	0.75	23.62	38.38
2726	1.872	66.03	10.300	8.84	0.15	28.31	0.63	23.50	38.57
2737	1.874	66.57	10.048	8.95	0.16	28.54	0.80	22.92	38.64
2749	1.876	66.94	9.878	8.98	0.16	28.51	0.50	23.27	38.58
2760	1.877	66.48	10.086	9.23	0.16	29.43	0.50	21.37	39.30
2772	1.879	67.48	9.648	9.11	0.16	29.54	0.77	21.96	38.47
2783	1.881	67.67	9.566	8.98	0.16	29.68	0.70	22.60	37.89
2795	1.883	67.83	9.494	9.08	0.16	30.11	0.59	20.65	39.41
2806	1.884	67.69	9.550	9.03	0.18	30.58	0.66	19.92	39.63
2818	1.886	67.86	9.478	8.75	0.18	29.71	0.82	22.40	38.14
2829	1.888	68.11	9.367	8.93	0.18	29.27	0.54	22.49	38.59
2841	1.889	67.86	9.474	9.19	0.19	30.03	0.35	21.51	38.72
2852	1.891	68.57	9.178	9.01	0.19	30.49	0.55	22.13	37.64
2864	1.893	69.56	8.758	9.18	0.18	31.26	0.71	20.80	37.86
2875	1.894	70.36	8.426	8.99	0.18	31.51	0.56	20.26	38.50
2887	1.896	69.99	8.578	8.76	0.18	33.88	0.56	19.50	37.13
2898	1.897	68.87	9.054	8.72	0.18	33.68	0.56	19.82	37.04
2910	1.899	68.41	9.244	8.72	0.17	32.79	0.30	21.64	36.38
2921	1.901	68.45	9.224	8.66	0.17	32.00	0.25	23.67	35.24
2933	1.902	69.71	8.694	8.87	0.17	31.84	0.61	23.42	35.09
2944	1.904	69.51	8.777	8.89	0.18	30.81	0.66	22.94	36.52
2956	1.905	70.68	8.313	8.74	0.19	31.29	0.66	20.87	38.25
2968	1.907	71.39	8.040	8.78	0.18	31.27	0.75	21.12	37.91
2979	1.908	71.77	7.878	8.94	0.18	32.23	0.68	18.83	39.14
2991	1.910	71.57	7.955	8.66	0.19	33.56	0.52	18.38	38.70
3002	1.911	69.85	8.653	8.67	0.18	32.09	1.08	20.09	37.89
3014	1.913	69.35	8.863	8.48	0.18	31.67	1.08	22.40	36.19
3026	1.914	68.76	9.094	8.21	0.19	31.86	1.14	22.47	36.13
3037	1.916	69.60	8.741	8.20	0.19	31.87	1.82	21.72	36.20
3049	1.918	71.30	8.062	8.47	0.19	31.48	1.79	20.71	37.35
3060	1.919	72.59	7.570	8.63	0.18	32.02	1.18	19.91	38.08

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
3072	1.920	72.96	7.420	9.14	0.19	32.32	1.20	19.03	38.12
3084	1.922	72.73	7.507	9.17	0.21	32.05	1.19	20.14	37.24
3095	1.923	71.37	8.030	8.94	0.20	30.83	0.33	23.33	36.36
3107	1.924	71.14	8.118	8.62	0.20	30.25	0.39	25.11	35.42
3118	1.926	70.74	8.273	8.32	0.22	29.99	0.71	25.55	35.21
3130	1.927	70.88	8.216	7.90	0.21	29.59	0.69	26.12	35.48
3142	1.929	71.38	8.022	7.98	0.19	30.28	0.74	24.63	36.17
3153	1.930	71.54	7.959	8.27	0.20	31.32	0.94	22.33	36.93
3165	1.932	72.49	7.594	8.50	0.20	31.62	1.18	21.94	36.57
3177	1.933	72.69	7.515	8.68	0.20	32.30	0.86	21.04	36.92
3188	1.934	73.14	7.344	8.32	0.20	32.68	0.86	21.27	36.67
3200	1.936	73.29	7.291	8.49	0.22	33.59	0.66	18.83	38.21
3212	1.937	74.63	6.809	8.33	0.20	33.22	0.46	20.50	37.29
3223	1.938	74.74	6.770	8.38	0.21	33.48	0.31	19.00	38.62
3235	1.940	75.46	6.514	8.27	0.20	34.43	0.78	19.90	36.42
3247	1.941	75.11	6.635	8.68	0.22	34.56	0.78	19.02	36.74
3259	1.942	74.74	6.773	8.46	0.21	33.66	0.78	21.16	35.72
3270	1.943	74.14	6.985	8.14	0.22	33.75	1.02	21.87	35.00
3282	1.945	74.04	7.020	8.13	0.23	33.48	0.78	24.21	33.17
3294	1.946	74.92	6.695	8.25	0.23	32.27	0.50	23.97	34.78
3305	1.947	74.94	6.690	8.48	0.23	33.11	0.50	22.20	35.48
3317	1.948	75.84	6.384	8.52	0.22	32.67	1.07	22.76	34.74
3329	1.949	75.17	6.628	8.73	0.23	32.79	1.02	21.42	35.81
3341	1.951	75.10	6.651	9.02	0.22	33.53	1.00	18.81	37.43
3353	1.952	75.24	6.607	9.62	0.23	35.55	0.80	16.48	37.31
3364	1.953	77.02	5.985	8.90	0.22	32.76	0.80	17.74	39.58
3376	1.954	75.92	6.406	8.98	0.22	32.69	0.69	17.34	40.08
3388	1.955	74.92	6.743	8.88	0.22	32.79	0.93	17.35	39.83
3400	1.957	74.18	6.992	8.53	0.23	31.73	0.89	19.08	39.55
3411	1.958	76.08	6.288	8.19	0.23	30.98	1.28	18.96	40.36
3423	1.959	76.94	5.997	8.58	0.24	32.30	1.33	20.57	36.97
3435	1.960	76.55	6.135	8.94	0.25	33.02	0.87	20.62	36.31
3447	1.961	76.86	6.031	9.07	0.25	34.23	0.44	19.24	36.77
3459	1.962	76.99	5.986	9.05	0.26	35.69	0.44	17.33	37.23
3470	1.963	78.33	5.535	8.92	0.26	34.88	0.06	19.88	36.00
3482	1.964	78.44	5.499	9.04	0.26	34.59	0.47	19.56	36.08
3494	1.965	77.83	5.701	8.64	0.26	35.10	0.56	18.73	36.70
3506	1.966	77.17	5.919	8.24	0.25	32.80	0.83	23.50	34.39

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
3518	1.968	75.78	6.404	8.04	0.24	31.39	0.99	24.90	34.43
3530	1.969	75.88	6.368	7.98	0.24	31.40	1.07	24.08	35.23
3541	1.970	76.15	6.278	8.09	0.24	32.96	0.60	22.36	35.75
3553	1.971	77.92	5.669	8.37	0.24	32.39	0.51	22.53	35.97
3565	1.972	78.84	5.369	8.75	0.25	33.00	0.67	18.85	38.49
3577	1.973	78.96	5.331	8.90	0.26	34.07	0.85	17.76	38.16
3589	1.974	79.13	5.276	9.27	0.26	34.96	0.77	20.36	34.38
3601	1.975	79.77	5.080	8.93	0.25	34.40	0.77	21.46	34.18
3613	1.976	79.93	5.029	8.66	0.27	34.65	1.64	21.43	33.34
3625	1.977	79.94	5.026	8.60	0.28	35.44	1.37	21.59	32.72
3637	1.978	79.54	5.148	8.69	0.28	35.58	1.15	21.11	33.18
3649	1.979	80.46	4.858	7.45	0.28	35.10	1.15	20.10	35.93
3660	1.980	80.80	4.752	7.93	0.31	36.88	1.80	20.22	32.86
3672	1.980	81.74	4.472	8.13	0.32	38.21	1.13	19.16	33.04
3684	1.981	82.03	4.385	8.04	0.33	38.27	1.08	18.84	33.43
3696	1.982	81.96	4.408	7.85	0.32	37.29	0.97	21.88	31.69
3708	1.983	80.39	4.888	8.76	0.32	37.36	1.18	21.54	30.84
3720	1.984	79.83	5.056	8.32	0.31	36.05	0.53	22.29	32.51
3732	1.985	80.04	4.992	8.05	0.29	34.22	0.44	23.76	33.24
3744	1.986	80.78	4.758	7.93	0.28	34.31	0.35	25.39	31.74
3756	1.987	81.06	4.673	7.93	0.28	34.94	0.35	24.22	32.28
3768	1.987	81.11	4.657	8.21	0.28	34.71	0.13	23.27	33.39
3780	1.988	81.12	4.655	8.41	0.29	34.49	0.41	23.20	33.19
3792	1.989	78.81	5.415	8.31	0.30	35.20	0.66	22.52	33.02
3804	1.990	79.00	5.359	8.38	0.30	34.82	0.63	23.21	32.66
3816	1.991	79.20	5.299	8.06	0.32	34.78	0.63	23.71	32.50
3828	1.992	81.75	4.467	7.71	0.33	36.32	0.66	23.85	31.12
3840	1.993	82.19	4.336	7.62	0.33	36.06	1.01	23.49	31.50
3852	1.994	82.42	4.265	7.51	0.33	35.80	1.05	24.59	30.71
3864	1.995	82.21	4.328	7.60	0.33	35.63	1.37	23.09	31.98
3876	1.995	82.21	4.330	8.16	0.32	36.85	1.83	18.27	34.57
3888	1.996	82.25	3.964	7.91	0.32	34.55	1.80	19.44	35.98

Appendix G. Raman Offgas Data for Experiment 107

As discussed in Appendix A, the Raman readings should be positive and sum to 100% except in cases where there is significant Ar present. Due to the noise in the Raman signal, any raw readings that are less than zero are fixed to zero and then all the gas readings for H₂, NO₂, N₂, O₂, N₂O, and NO are normalized to 100 vol %. Even with these corrections, the Raman readings have noise in them. To reduce this noise, moving averages of the fixed and normalized readings were performed using equation C-1.

These moving averages do not eliminate all the noise but smooth the values so comparisons and calculations can be performed. The fixed, normalized, and moving average Raman gas concentrations are reported in Table G-1. Due to rounding to the nearest hundredth, the numbers in the table may not sum to exactly 100 vol % but all the decimal places were carried in the calculations performed for this report.

Table G-1. Fixed Normalized Moving Average Raman Data for Experiment 107

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
3	0.0008	87.61	2.841	1.92	5.91	3.83	3.67	3.53	81.14
14	0.0014	87.83	2.783	2.18	5.88	4.09	3.73	4.06	80.05
25	0.002	88.38	2.637	1.90	6.02	5.03	3.53	4.48	79.04
37	0.003	86.95	3.001	1.83	5.67	3.34	2.72	4.00	82.45
48	0.003	87.11	2.962	2.15	4.72	4.16	3.22	4.99	80.75
59	0.004	86.53	3.117	2.44	4.19	3.59	2.94	7.21	79.63
71	0.005	82.30	4.452	2.53	3.35	3.10	2.68	10.66	77.69
82	0.006	68.83	10.955	3.67	2.30	2.96	2.14	14.50	74.44
93	0.009	50.36	25.154	4.41	1.86	3.70	1.63	17.40	71.01
105	0.018	34.20	42.744	5.07	1.46	3.56	1.57	21.10	67.24
116	0.029	24.36	66.228	6.03	0.98	3.76	1.38	22.93	64.91
128	0.048	18.99	91.102	6.90	0.89	4.16	1.22	23.44	63.39
139	0.072	16.83	100.409	7.68	0.99	3.51	0.91	24.42	62.49
150	0.095	16.07	106.008	7.96	1.07	3.90	1.12	25.89	60.07
162	0.120	14.86	122.016	8.60	1.16	4.62	1.01	25.98	58.63
173	0.151	12.57	143.160	9.48	1.29	5.47	0.83	27.30	55.63
185	0.190	14.58	131.046	10.16	1.38	5.50	1.10	27.44	54.42
196	0.215	17.50	102.592	10.38	1.39	5.80	1.10	27.36	53.96
208	0.234	17.73	99.464	10.98	1.40	5.53	1.20	27.01	53.88
219	0.259	17.56	100.189	11.07	1.42	5.09	1.02	27.23	54.17
230	0.284	16.30	108.539	10.63	1.33	4.59	1.18	26.17	56.10
242	0.306	16.88	101.844	10.65	1.38	4.75	0.84	26.78	55.61
253	0.332	15.53	109.467	10.46	1.38	4.82	1.14	26.36	55.84
265	0.359	16.04	105.702	10.23	1.38	4.83	1.18	26.55	55.84
276	0.381	16.74	99.547	10.05	1.38	5.03	1.10	26.21	56.23
288	0.405	16.75	99.478	9.80	1.38	5.10	0.99	25.94	56.79

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
		(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
299	0.428	16.22	103.494	9.46	1.31	4.97	1.06	24.89	58.31
311	0.453	18.72	90.478	9.30	1.29	5.14	0.82	24.89	58.56
322	0.473	18.88	89.343	9.27	1.26	5.26	0.59	24.93	58.69
334	0.492	19.89	82.365	9.37	1.22	4.90	0.63	24.89	58.99
345	0.513	17.79	92.533	9.31	1.17	4.79	0.61	25.07	59.05
357	0.535	17.81	92.352	9.22	1.10	4.64	0.63	25.36	59.04
368	0.556	17.64	93.396	9.17	1.03	4.54	0.59	25.47	59.20
380	0.579	17.60	93.666	8.99	0.97	4.37	0.48	25.55	59.64
391	0.600	18.07	90.836	8.69	0.92	4.51	0.53	25.55	59.80
403	0.622	18.40	88.891	8.62	0.88	4.39	0.51	25.52	60.08
414	0.641	18.99	85.292	8.45	0.84	4.57	0.40	25.70	60.04
426	0.662	19.11	84.669	8.16	0.84	4.46	0.54	25.87	60.13
438	0.682	19.61	82.109	7.96	0.82	4.49	0.65	25.83	60.24
449	0.701	20.10	79.593	7.70	0.79	4.53	0.73	26.12	60.12
461	0.720	20.55	77.328	7.68	0.78	4.65	0.67	26.41	59.81
472	0.737	20.27	78.709	7.54	0.77	4.53	0.72	26.49	59.95
484	0.756	19.94	80.363	7.49	0.76	4.73	0.80	26.56	59.67
495	0.775	20.07	79.766	7.43	0.73	4.81	0.87	26.96	59.20
507	0.794	20.53	77.534	7.37	0.75	4.89	0.81	27.21	58.96
519	0.812	20.85	75.930	7.23	0.75	4.99	0.92	27.47	58.63
530	0.829	20.75	76.418	7.18	0.75	5.15	0.96	28.07	57.89
542	0.848	20.73	76.465	7.18	0.76	5.17	0.90	28.31	57.68
553	0.865	23.98	66.011	7.14	0.79	5.29	0.80	28.89	57.08
565	0.880	24.31	64.518	7.04	0.77	5.21	0.80	29.63	56.56
577	0.895	24.67	62.981	6.92	0.80	5.22	0.82	30.12	56.13
588	0.911	22.06	70.697	6.95	0.81	5.24	0.65	30.39	55.96
600	0.928	22.23	69.959	6.93	0.81	5.27	0.57	31.14	55.29
611	0.943	21.98	71.049	6.86	0.81	5.22	0.67	31.38	55.06
623	0.961	22.16	70.337	8.29	0.81	5.32	0.47	31.03	54.07
635	0.978	21.48	73.377	8.09	0.79	5.44	0.38	31.45	53.84
646	0.994	21.75	72.229	7.94	0.78	5.42	0.68	31.84	53.33
658	1.013	22.06	71.075	8.04	0.78	5.49	0.58	32.02	53.10
670	1.029	23.08	66.760	8.08	0.79	5.69	0.50	32.45	52.49
681	1.044	23.42	65.399	6.81	0.79	5.70	0.59	33.49	52.62
693	1.060	23.30	65.846	6.96	0.80	5.52	0.87	33.71	52.13
705	1.076	23.58	64.851	6.99	0.80	5.57	0.76	34.00	51.89
716	1.090	24.05	63.183	7.05	0.83	5.46	1.03	35.33	50.29
728	1.106	25.06	59.961	7.08	0.82	5.41	1.23	35.58	49.87

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
740	1.120	24.80	60.878	7.05	0.83	5.51	1.49	35.56	49.57
751	1.133	24.79	60.925	7.13	0.85	5.58	1.43	35.67	49.33
763	1.149	24.93	60.518	7.35	0.87	5.64	1.37	35.86	48.91
775	1.163	25.69	57.976	7.26	0.85	5.62	1.34	35.00	49.92
787	1.177	25.90	57.276	7.29	0.87	5.59	1.49	34.90	49.86
798	1.190	25.76	57.673	7.32	0.86	5.63	1.33	34.96	49.89
810	1.204	26.22	56.335	7.74	0.86	5.88	1.14	36.04	48.33
822	1.218	28.07	51.553	7.75	0.86	6.12	1.07	36.12	48.08
833	1.229	28.21	51.156	7.84	0.85	6.35	0.95	36.41	47.61
845	1.241	28.79	49.654	7.88	0.84	6.35	0.78	36.66	47.49
857	1.253	27.65	52.386	7.96	0.86	6.36	1.01	36.55	47.26
869	1.266	28.24	50.875	7.79	0.86	6.15	0.95	35.81	48.44
881	1.279	28.67	49.858	7.76	0.86	6.08	1.06	35.72	48.52
892	1.289	29.43	47.969	7.80	0.90	5.92	1.08	35.72	48.59
904	1.301	29.89	46.912	7.83	0.90	6.10	1.02	35.73	48.42
916	1.312	30.01	46.646	7.99	0.87	6.18	0.61	36.06	48.29
928	1.324	30.39	45.806	8.00	0.87	6.60	0.93	35.95	47.65
939	1.334	31.14	44.271	8.15	0.88	6.16	1.03	36.23	47.55
951	1.345	31.77	42.986	8.26	0.85	6.49	0.93	36.13	47.34
963	1.355	32.11	42.300	8.24	0.87	6.74	0.98	36.02	47.15
975	1.365	32.27	41.981	8.29	0.87	6.89	1.05	35.88	47.02
987	1.376	32.83	40.973	8.29	0.89	6.77	0.82	35.88	47.36
999	1.385	33.66	39.434	8.42	0.84	7.42	0.65	35.66	47.01
1011	1.395	33.66	39.433	8.53	0.85	7.47	0.62	35.72	46.81
1022	1.404	34.05	38.778	8.68	0.85	7.55	0.49	35.60	46.82
1034	1.413	34.20	38.534	8.81	0.88	7.48	0.69	35.44	46.69
1046	1.422	34.32	38.300	8.91	0.68	7.63	0.56	35.57	46.65
1058	1.432	34.61	37.844	9.13	0.76	7.67	0.71	36.12	45.61
1070	1.441	35.65	36.257	9.26	0.77	7.58	0.93	35.50	45.95
1082	1.449	36.40	34.992	9.59	0.75	7.38	0.89	35.37	46.02
1093	1.457	36.48	34.860	9.65	0.76	7.51	0.96	35.15	45.96
1105	1.466	36.31	35.099	9.79	0.94	7.53	1.21	34.46	46.07
1117	1.474	36.79	34.365	9.79	0.91	7.54	0.97	33.48	47.31
1129	1.483	37.17	33.815	10.00	0.90	7.49	1.00	33.46	47.15
1141	1.491	37.54	33.292	10.16	0.92	7.82	0.94	33.22	46.94
1153	1.499	38.32	32.219	10.42	0.90	7.95	0.75	32.89	47.08
1165	1.507	38.54	31.909	10.48	0.90	8.09	0.98	32.59	46.96
1177	1.515	39.12	31.151	10.67	0.91	8.17	1.08	32.36	46.81

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
1189	1.522	39.26	30.968	10.93	0.92	8.34	0.88	31.95	46.98
1200	1.529	40.52	29.384	11.22	0.91	8.22	0.89	31.65	47.10
1212	1.536	40.97	28.845	11.24	0.93	8.10	0.96	31.53	47.24
1224	1.543	41.67	28.000	11.66	0.94	8.20	0.49	31.54	47.18
1236	1.550	42.20	27.415	11.80	0.95	8.44	0.74	31.24	46.84
1248	1.556	43.27	26.255	11.74	0.96	8.74	0.98	31.11	46.47
1260	1.563	44.57	24.898	11.55	0.96	9.13	1.00	30.78	46.57
1272	1.569	45.52	23.942	11.74	0.99	9.42	0.94	30.72	46.19
1284	1.574	45.98	23.497	11.75	0.99	9.37	1.49	30.51	45.89
1296	1.580	46.44	23.071	11.82	0.98	9.44	1.45	30.22	46.08
1308	1.586	47.26	22.343	11.73	0.97	9.69	1.48	29.89	46.23
1320	1.591	48.03	21.648	11.84	0.97	9.47	1.50	29.65	46.57
1332	1.596	48.49	21.248	11.94	0.96	9.44	1.42	29.49	46.74
1344	1.601	48.69	21.083	12.05	0.96	9.65	1.09	28.99	47.25
1356	1.606	49.35	20.541	12.04	1.01	9.99	0.82	28.60	47.54
1368	1.611	49.48	20.426	12.23	1.01	10.05	0.65	28.49	47.58
1380	1.616	50.25	19.823	12.38	1.05	10.44	0.97	28.32	46.84
1392	1.621	50.48	19.639	12.52	1.06	10.85	0.96	27.87	46.73
1404	1.626	51.95	18.508	12.43	1.09	11.04	1.06	27.68	46.71
1416	1.630	51.96	18.506	12.57	1.09	11.01	1.06	27.92	46.35
1428	1.635	52.68	17.977	12.65	1.11	11.34	0.98	27.87	46.05
1440	1.639	52.59	18.035	12.73	1.10	11.29	0.74	27.94	46.20
1452	1.644	53.25	17.562	10.12	1.12	11.69	1.29	28.68	47.11
1464	1.648	54.21	16.919	10.41	1.11	12.07	0.98	28.84	46.58
1476	1.652	54.40	16.787	10.71	1.11	12.22	1.09	28.42	46.46
1488	1.656	54.43	16.766	10.86	1.10	12.46	1.27	28.12	46.19
1500	1.660	53.36	17.481	10.86	1.09	13.02	1.23	27.84	45.95
1512	1.664	53.81	17.175	13.53	1.06	12.89	0.77	26.90	44.85
1524	1.669	54.08	16.990	13.30	1.08	12.92	0.86	26.67	45.16
1536	1.673	54.35	16.804	14.64	1.18	15.06	0.95	29.55	38.62
1549	1.677	57.40	15.065	14.61	1.18	15.15	0.89	29.46	38.71
1561	1.681	57.37	15.086	14.62	1.17	15.32	0.94	29.48	38.48
1573	1.684	57.49	15.007	14.54	1.18	15.85	0.83	29.30	38.29
1585	1.688	54.42	16.751	14.55	1.13	16.38	1.34	28.87	37.73
1597	1.692	54.21	16.898	12.89	1.00	14.66	1.40	25.91	44.14
1610	1.697	54.56	16.662	12.70	1.00	15.11	1.58	25.69	43.92
1622	1.701	54.80	16.507	12.47	0.99	15.72	1.53	25.65	43.65
1634	1.705	55.18	16.249	12.39	0.97	16.06	1.62	25.35	43.60

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
1646	1.709	55.40	16.101	12.41	0.97	16.56	1.16	25.42	43.48
1658	1.713	55.19	16.239	12.42	1.01	17.04	1.11	25.48	42.94
1670	1.717	55.53	16.018	12.39	1.00	17.21	0.86	25.35	43.19
1682	1.721	55.48	16.054	12.65	1.03	16.96	1.03	25.06	43.28
1694	1.725	55.96	15.743	12.81	1.03	17.15	0.95	25.49	42.55
1707	1.729	56.38	15.477	12.73	1.03	17.18	0.97	25.52	42.57
1719	1.732	56.34	15.502	12.74	1.03	17.59	0.86	25.47	42.30
1731	1.736	56.39	15.473	12.93	1.04	17.92	0.89	25.50	41.73
1743	1.740	56.23	15.572	12.85	1.03	18.38	0.74	25.46	41.54
1756	1.744	56.76	15.239	12.60	1.02	18.99	0.69	24.95	41.76
1768	1.748	56.57	15.355	12.53	1.05	19.40	0.75	24.68	41.59
1780	1.752	56.84	15.191	12.39	1.04	19.59	0.90	24.66	41.42
1792	1.755	56.71	15.269	12.12	1.04	19.81	1.02	24.70	41.30
1804	1.759	57.00	15.092	11.94	1.05	20.41	0.90	24.67	41.03
1816	1.763	56.72	15.258	11.96	1.04	20.44	0.95	24.62	40.99
1829	1.767	57.27	14.928	12.08	1.05	20.57	0.89	24.81	40.60
1841	1.770	57.91	14.545	11.98	1.07	20.98	1.05	24.43	40.48
1853	1.774	58.34	14.284	12.15	1.07	21.38	1.01	24.46	39.94
1865	1.777	58.27	14.326	12.00	1.07	21.27	1.22	24.32	40.12
1878	1.781	58.12	14.414	12.16	1.10	21.66	1.21	24.61	39.26
1890	1.785	58.46	14.213	12.07	1.07	22.14	1.44	24.43	38.84
1902	1.788	58.66	14.095	12.15	1.03	22.64	1.04	24.53	38.61
1914	1.792	58.73	14.055	11.94	1.04	22.96	1.35	24.30	38.41
1927	1.795	58.51	14.181	11.88	1.01	24.05	1.24	24.05	37.76
1939	1.799	58.37	14.267	11.64	1.00	24.16	1.39	23.79	38.02
1951	1.802	58.67	14.091	11.59	1.02	24.50	1.37	23.66	37.86
1963	1.806	59.35	13.703	11.60	1.04	24.35	1.65	23.36	38.00
1976	1.809	59.60	13.560	11.72	1.04	24.75	1.24	23.38	37.87
1988	1.813	59.63	13.540	11.78	1.08	24.59	1.50	23.69	37.36
2000	1.816	59.77	13.467	11.78	1.08	24.87	1.47	23.73	37.06
2013	1.819	59.87	13.410	11.67	1.09	25.07	1.27	24.00	36.90
2025	1.823	59.94	13.368	11.67	1.07	25.39	1.14	23.96	36.77
2037	1.826	59.72	13.489	11.44	1.05	25.56	1.31	23.84	36.80
2049	1.829	60.18	13.238	11.54	1.07	25.48	1.36	23.52	37.03
2062	1.833	60.43	13.097	11.59	1.09	25.70	1.26	23.05	37.31
2075	1.836	60.97	12.803	11.63	1.07	25.81	1.36	22.65	37.49
2087	1.839	61.04	12.769	11.93	1.10	25.70	1.28	22.68	37.31
2099	1.842	61.03	12.771	12.03	1.13	25.48	1.24	22.62	37.50

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
(sec)	(M)	(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
2112	1.846	60.78	12.905	11.92	1.12	25.41	1.38	22.75	37.42
2124	1.849	60.91	12.835	11.75	1.11	25.53	1.42	23.11	37.07
2136	1.852	61.37	12.592	11.83	1.12	25.91	1.16	23.27	36.71
2149	1.855	62.05	12.233	11.58	1.13	26.18	1.08	23.40	36.63
2161	1.858	62.29	12.108	11.61	1.16	26.49	1.34	23.11	36.28
2173	1.861	62.29	12.112	11.47	1.19	26.87	0.99	23.03	36.45
2186	1.865	62.19	12.161	11.52	1.20	26.87	1.05	22.96	36.41
2199	1.868	62.11	12.202	11.48	1.25	26.38	1.37	23.04	36.48
2211	1.871	62.57	11.967	11.22	1.24	26.64	1.56	22.86	36.47
2223	1.874	62.38	12.067	10.97	1.21	26.59	1.16	23.31	36.75
2236	1.877	63.03	11.736	11.58	1.24	27.80	1.25	20.32	37.81
2248	1.880	67.35	9.939	11.60	1.24	28.02	1.25	20.10	37.79
2261	1.882	67.77	9.726	11.54	1.21	28.20	1.08	20.09	37.89
2273	1.884	67.55	9.835	11.60	1.24	27.90	1.19	20.41	37.65
2286	1.887	63.55	11.473	11.65	1.28	28.37	1.13	20.30	37.28
2298	1.890	64.05	11.231	11.35	1.24	27.20	1.16	23.38	35.68
2311	1.893	64.46	11.028	11.48	1.29	27.08	0.95	23.53	35.66
2323	1.896	64.66	10.933	11.58	1.30	27.44	1.06	23.54	35.07
2336	1.899	64.73	10.896	11.49	1.31	27.69	1.07	23.41	35.03
2348	1.901	65.08	10.730	11.68	1.28	28.14	1.33	23.48	34.09
2361	1.904	65.57	10.502	11.48	1.27	28.25	1.09	23.50	34.42
2373	1.907	65.85	10.374	11.39	1.25	28.40	1.12	23.46	34.39
2386	1.909	65.74	10.424	11.28	1.23	28.00	1.14	23.58	34.78
2398	1.912	65.69	10.446	11.36	1.21	27.90	1.14	23.85	34.54
2411	1.915	65.99	10.311	11.22	1.23	26.91	1.20	23.87	35.57
2423	1.917	66.57	10.045	11.20	1.25	27.25	1.18	23.68	35.44
2436	1.920	66.70	9.986	11.42	1.27	24.67	1.67	24.20	36.78
2449	1.922	67.52	9.630	11.37	1.30	24.86	1.87	24.16	36.44
2461	1.925	67.29	9.736	11.39	1.29	25.04	1.99	23.81	36.49
2474	1.927	67.22	9.768	11.37	1.29	25.26	1.85	23.68	36.54
2487	1.930	66.49	10.082	11.45	1.31	24.97	2.18	23.74	36.34
2499	1.932	66.77	9.954	11.11	1.31	27.78	2.05	23.00	34.75
2512	1.935	67.33	9.704	10.98	1.30	27.97	1.87	22.81	35.07
2524	1.937	67.52	9.620	10.83	1.35	27.71	2.02	22.87	35.22
2537	1.940	67.89	9.462	10.69	1.38	27.90	2.02	23.02	34.99
2550	1.942	68.27	9.296	10.71	1.41	27.81	1.87	23.22	34.98
2562	1.945	68.64	9.140	10.86	1.44	27.84	1.64	23.66	34.56
2575	1.947	69.34	8.845	10.89	1.46	27.93	1.45	23.85	34.42

Cumulative Reaction Time	Est. Al Conc.	Tracer	Offgas Flow and Concentrations without tracers and water						
		CO ₂ and CO	Total Offgas Flow	H ₂	NO ₂	N ₂	O ₂	N ₂ O	NO
		(vol %)	(cm ³ /min)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)	(vol %)
2587	1.949	69.73	8.685	10.97	1.46	28.18	1.17	24.39	33.83
2600	1.951	69.67	8.711	11.16	1.49	28.19	0.97	24.56	33.64
2613	1.954	69.60	8.738	11.02	1.48	28.15	0.99	24.29	34.07
2625	1.956	69.60	8.738	10.72	1.47	28.24	0.87	24.25	34.45
2638	1.958	69.81	8.650	10.93	1.52	28.50	0.88	23.82	34.34
2651	1.961	69.98	8.583	10.60	1.53	28.84	0.48	23.17	35.38
2663	1.963	69.63	8.725	10.88	1.49	29.18	0.47	22.88	35.09
2676	1.965	70.24	8.475	11.19	1.50	29.57	0.46	22.76	34.52
2689	1.967	70.52	8.365	11.17	1.52	29.64	0.65	22.72	34.30
2701	1.969	71.07	8.142	10.79	1.56	29.47	1.10	22.85	34.23
2714	1.971	71.52	7.967	11.20	1.61	29.23	1.17	22.84	33.96
2762	1.979	71.93	7.807	10.61	1.67	29.06	1.53	22.80	34.33
2774	1.981	72.55	7.566	10.26	1.71	29.34	1.63	22.89	34.17
2786	1.983	73.01	7.396	10.46	1.77	29.07	1.74	22.75	34.21
2797	1.984	73.66	7.154	10.29	1.73	29.44	1.16	22.96	34.43
2808	1.986	74.44	6.868	9.98	1.71	29.55	1.55	22.52	34.68
2820	1.988	74.42	6.875	10.36	1.72	29.50	1.55	22.15	34.72
2831	1.989	74.29	6.924	10.43	1.77	29.69	1.21	22.41	34.50
2842	1.991	74.63	6.803	10.31	1.82	29.91	1.22	22.24	34.50
2854	1.992	75.65	6.443	10.42	1.84	30.32	1.22	22.12	34.09
2865	1.994	76.40	6.179	10.81	1.91	31.12	1.20	22.29	32.68
2876	1.995	76.96	5.990	10.70	1.91	31.49	0.98	22.63	32.30
2887	1.996	77.08	5.998	10.62	1.95	31.89	1.15	22.02	32.36

Distribution:

T. B. Brown, 773-A
M. E. Cercy, 773-42A
D. A. Crowley, 773-43A
D. E. Dooley, 773-A
A. P. Fellingner, 773-42A
S. D. Fink, 773-A
C. C. Herman, 773-A
D. T. Hobbs, 773-A
E. N. Hoffman, 999-W
J. E. Hyatt, 773-A
K. M. Kostelnik, 773-42A
B. B. Looney, 773-42A
D. A. McGuire, 773-42A
T. O. Oliver, 773-42A
F. M. Pennebaker, 773-42A
G. N. Smoland, 773-42A
B. J. Wiedenman, 773-42A
W. R. Wilmarth, 773-A
S. J. Robertson II, 704-2H
K. P. Burrows, 704-24
P. M. Palmer, 704-2H
C. M. Hadden, 704-2H
W. H. Clifton Jr, 704-2H
A. C. Carraway, 211-18H
T. L. Tice, 221-H
J. B. Schaade, 703-H
R. T. Burns, 221-H
S. A. Yano, 704-2H
J. R. Lint, 704-2H
A. D. Meredith, 704-2H
K. J. Usher, 704-2H

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