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Flowsheet Modifications for Sodium Reactor Experiment and Denmark Reactor-3 Used Nuclear Fuel Processing

P. M. Almond

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June 2014

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EXECUTIVE SUMMARY

As part of the H-Canyon Waste (HLW) Minimization Plan, H-Canyon Engineering requested that SRNL evaluate the feasibility of using HB-Line (HBL) column waste streams from AFS-2 processing for the dissolver solution for Used Nuclear Fuel (UNF) processing. The targeted UNF for dissolution using recycled solution are fuels similar to the University of Missouri Research Reactor (MURR) fuel. However, a limited number of the fuel bundles were anticipated to contain uranium silicide fuels similar to the Denmark Reactor (DR-3).

The experiments initially performed to evaluate the use of AFS-2 column waste solution for UNF dissolutions used Al-1100 alloy coupons. The Al-1100 coupons were considered a representative surrogate (based on the fuel bundle and assembly material) that provided an upper bound on the generation of flammable gas during the dissolution process. Experimental results from this work with Al-1100 alloy challenged current assumptions regarding the potential to exceed 60 % of the H_2 lower flammability limit (LFL) in the dissolver off-gas during fuel dissolution. To resolve differences in the previous data that were used for the technical basis, additional experiments were performed as part of an experimental plan to more closely represent the fuels to be dissolved in H-Canyon. This plan included a study of L-Bundle alloy comprised of Al-6061 and U-Al alloys. Guidance for dissolving the remaining Sodium Reactor Experiment (SRE) and DR-3 fuels planned in the Batch 4, 5, and 6 charge plans of the SRE Campaign is provided in this report. Dissolution of the remaining UNF will be addressed in a future report. Flammability calculations are provided for H-Canyon to safely dissolve the fuel assemblies contained in L-Bundles with respect to the H_2 levels in the projected peak off-gas rates for SRE and DR-3 fuels.

The technical basis that has been used for dissolution was established using the experimental work performed to develop a recovery process for highly enriched U fuels discharged from SRS reactors. Large-scale dissolutions were performed by Caracciolo using unirradiated U-Al alloy tubular fuel assemblies and smaller-scale experiments were performed by Schlea using both unirradiated and irradiated coupons from U-Al alloy fuel.

One of the main differences observed in the technical basis data and the Al-1100 data pertained to the H_2 off-gas concentration. The average H_2 concentration of the dissolver off-gas and the H_2 generation profiles (with respect to time) show significant differences. In the earlier work, the H_2 concentration was highest during the initial part of the dissolution and subsequently decreased to a much lower constant value. In the current work, the H_2 concentration with Al-1100 and L-Bundle Al-6061 was observed to be the lowest during the earliest part of the dissolution and generally increased to a constant (or a higher) value during the remaining dissolution. In contrast, when a U-Al alloy was dissolved under the same conditions as Al-1100 and Al-6061 alloys, the off-gas profiles were similar to the original experimental work by Caracciolo, exhibiting high H_2 concentrations initially which decreased with time.

Using impure acid solutions to meet waste minimization needs requires that the Hg catalyst concentration be increased from 0.002 M to 0.012-0.015 M in order to dissolve Al in the presence of the impurities. The results presented herein support using an increased Hg concentration flowsheet for SRE and DR-3 with pure nitric acid dissolving solutions only. A single flowsheet with increased Hg catalyst is under development for dissolver solutions ranging from pure nitric acid to AFS-2 generated impure solutions for future dissolution of other UNF materials. Flammability calculations were also performed to provide guidance for H-Canyon to safely dissolve SRE and DR-3 fuel contained in L-Bundles with respect to the H_2 levels in the projected peak off-gas rates.

Flowsheet parameters for the dissolution of SRE/DR-3 fuel include the following. The Hg catalyst is added gradually after the dissolver has reached temperature to achieve a maximum catalyst concentration of 0.012-0.015 M. The initial nitric acid concentration is in the range of 6-7 M and dependent on the amount of Al, Th, and U to be dissolved, targeting a final nitric acid concentration of 0.5-1.0 M after completion of the dissolution of the last charge. Boric acid (H_3BO_3) or gadolinium nitrate ($Gd(NO_3)_3$) may be used as a nuclear safety poison. Concentrations of up to 2 g/L of B or Gd in surrogate dissolver solutions have been observed to be stable from precipitation.

Hydrogen flammability calculations were performed using the experimental data to determine the conditions that H-Canyon can safely dissolve SRE/DR-3 fuel in L-Bundles with respect to the H_2 levels during the projected peak off-gas rates. To stay under the 60% LFL for H_2, the charges of L-Bundles containing SRE shall be limited to four, where the Hg concentration is added to the recommended 0.012–0.015 M. In order to process the L-Bundles of DR-3 fuel, a minimum of 0.17 M Al must be in solution. This minimum dissolved Al could be reached by first dissolving SRE fuel or by adding $Al(NO_3)_3$ to the dissolver solution. The number of L-Bundles of DR-3 fuel that could be charged successively to the H-Canyon dissolver is dependent on the concentration of U in the U-Al alloy and the dissolved Al concentration. The number of bundles increases as the Al concentration increases in the dissolving solution.

Instructions and limitations regarding the use of this document are provided in the transmittal letter.

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LIST OF ABBREVIATIONS

AD	Analytical Development
AFS-2	Alternate Feed Stock 2
CVAA	Cold Vapor Atomic Absorption
DR-3	Denmark Reactor-3
DSA	Documented Safety Analysis
GC	Gas Chromatography
HLW	High Level Waste
IC	Ion Chromatography
ICP-ES	Inductively Coupled Plasma Emission Spectroscopy
LFL	Lower Flammability Limit
MURR	University of Missouri Research Reactor
SEM	Scanning Electron Microscopy
SRE	Sodium Reactor Experiment
SRNL	Savannah River National Laboratory
TCD	Thermal Conductivity Detector
UNF	Used Nuclear Fuel
XRD	X-ray Diffraction

1.0 Introduction

As part of the H-Canyon High Level Waste (HLW) Minimization Plan,[1] H-Canyon Engineering requested that SRNL evaluate the feasibility of using HB-Line column waste streams from AFS-2 processing for the dissolver solution for Used Nuclear Fuel (UNF) processing. The targeted UNF for dissolution using recycled solution are fuels similar to the University of Missouri Research Reactor (MURR) fuel[2,3] although, a limited number of the fuel bundles are anticipated to contain uranium silicide fuels similar to the Denmark Reactor-3 (DR-3) (DR-3 is a uranium silicide fuel containing Al).

The experiments initially performed to evaluate the use of AFS-2 column waste solution for UNF dissolutions used Al-1100 alloy coupons. The Al-1100 coupons were considered a representative surrogate (based on the fuel bundle and assembly material) that provided an upper bound on the generation of flammable gas during the dissolution process. Experimental results from this work with Al-1100 challenged current assumptions regarding the potential to exceed 60 % of the H_2 LFL in the dissolver off-gas during SRE/DR-3 fuel dissolution. To resolve differences in the previous data that was used for the technical basis, additional experiments were performed as part of an experimental plan[4] to more closely represent the fuels to be dissolved in H-Canyon. This plan included a study of L-Bundle alloy comprised of Al-6061, and various U-Al alloys. The intent of these experiments was to define a dissolution flowsheet that can be used for either AFS-2 impure solutions or pure nitric acid (HNO_3) solutions. A second objective was to tie the current work with previous experimental work used to develop the technical basis for the dissolution of reactor fuels in H-Canyon.

The technical basis that has been used for dissolution was established using the experimental work performed to develop a recovery process for highly enriched U fuels discharged from SRS reactors.[5] Large-scale dissolutions were performed by Caracciolo[5] using unirradiated U-Al alloy tubular fuel assemblies and smaller-scale experiments were performed by Schlea[6] using both unirradiated and irradiated coupons from U-Al alloy fuel. This data provided input for H_2 flammability control for recent site fuels based on calculations by Weitz.[7]

This report presents results from a series of dissolution experiments that were performed to measure and characterize off-gas generation rates that are representative of Sodium Reactor Experiment (SRE) fuels as well as MURR type fuels including DR-3.

2.0 Experimental Procedure

The focus of the dissolution experiments discussed in this report support the continued dissolution of SRE and DR-3 fuel, and therefore, no impurities from the AFS-2 PuO_2 production process were present in the dissolving solutions.

2.1 Dissolving Solutions

Solution ranges used to dissolve Al and U-Al alloy coupons are summarized in Table 2-1.

Table 2-1. Summary of Solution Components and Concentrations.

Element/ Species	Al-1100	L-Bundle (Al-6061)	U-Al Alloy
HNO_3	6.5–7.0 M	7.0 M	7.0 M
Hg	0.002 M, 0.012 M, 0.015 M	0.002 M, 0.012 M	0.012 M
KF	0.1 M	0.05 M, 0.1 M	0.05, 0.1 M
Al	0.0 M, 0.075 M	0.0 M	0.0 M
Th	---	0 g/L, 21.8 g/L	---
U	---	0 g/L, 3.9 g/L	---
Gd	---	0 g/L, 0.48 g/L	---

2.2 Description of Dissolution and Gas Collection Apparatus

The gas generation rates and concentrations were determined using a dissolver apparatus shown in Figure 2-1 that contains a boiling flask with multiple ports, a condenser, an in-line collection bulb, and a water-submerged Tedlar™ bag. The apparatus was assembled in a chemical hood. A second apparatus was placed in a radiological hood for conducting experiments with Th and U. The dissolution vessel and off-gas system use removable glass bulbs to sample and measure the concentration of the gas by gas chromatography (GC). The bulbs are coupled to a gas collection system that fills a Tedlar™ bag which allows measurement of the gas generation rate through water displacement in a graduated column. A second gas collection apparatus was also fabricated to accommodate larger gas generation volumes, if needed.

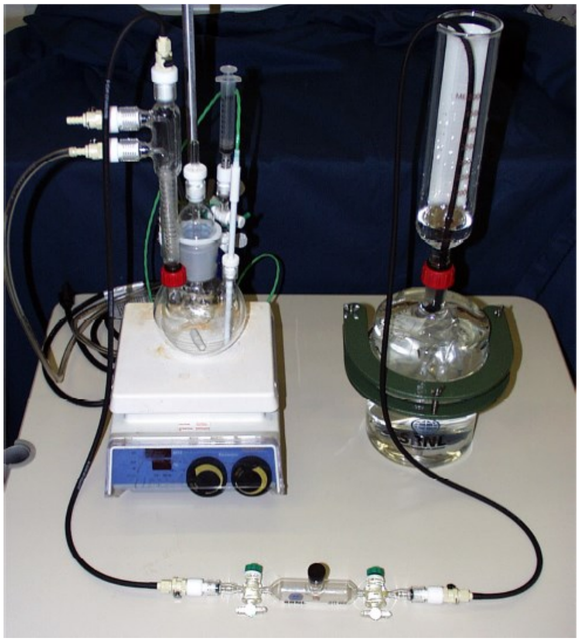

Figure 2-1. Dissolution Vessel and Off-gas Collection System.

Al-1100 alloy coupons were initially used for the dissolution experiments (Experiments 1, 25, 28, and 30). A 150-mL aliquot of 7 M HNO_3 solution was used unless otherwise noted. Four coupons were cut to approximate dimensions of 19 x 11 x 3 mm and each had a 1/16 in. hole drilled for fastening the coupon to glass rods used to lower them into the dissolving solution. The coupons were lightly sanded, washed with soap and water, and then weighed and measured. The coupons weighed about 1.8 g each with a surface area of approximately 6 cm^2. Each coupon was tied by Teflon™ string through the 1/16 in. hole to a glass rod labeled with the coupon position number (for coupon identification). The glass rods penetrated the lid of the boiling flask and were sealed by compressed O-ring fittings. This setup allowed for dissolution of all 4 coupons without breaking the gas-sealed system by lowering each glass rod sequentially over the duration of the experiment. The experiments targeted a nominal 1.7 M final dissolved Al concentration.

Nominally 150 mL of solution was weighed and added to the flask containing a Teflon™ stir bar, and then the flask was sealed. The dissolution vessel and off-gas collection system (including 8 gas sample bulbs) were leak checked by filling the system with Ar to inflate the Tedlar™ bag and observing a constant water column height over several minutes. The stir bar rotation was set at 325 rpm. The solution was then heated to 100 °C. The off-gas system was vented to relieve pressure (to zero the off-gas collection system), and a stopwatch was started as the first coupon was lowered into the solution. Time versus water displacement was manually recorded until the coupon was visually observed to have dissolved completely. For each coupon dissolution, a gas sample was taken generally at 450 mL of off-gas volume (about half of total gas produced for each coupon) and a second sample was taken after the coupon had completely dissolved. The collected gas was then purged at the gas bulb connection from the Tedlar™ bag, leaving residual gas in the remainder of the void space of the apparatus. The procedure was repeated for the dissolution of coupons 2 through 4, producing a total of 4 off-gas generation rate data sets (1 per coupon), and 8 gas samples (2 per coupon) for each experiment that spanned the range of Al concentrations in solution.

L-Bundle (Al-6061) coupons were used for a second series of experiments. The coupons were cut from the side of an actual L-bundle end cap provided by H-Canyon Engineering. Four L-Bundle coupons were used with nominal dimensions of 20 x 13 x 2 mm and each had a 1/16 in hole drilled for fastening the coupon to a glass rod. The coupons had a mass of about 1 g each. A solution volume of 90 mL was used in the boiling flask to achieve a final Al concentration near 1.6 M. Eight gas samples (2 per coupon) were collected during each dissolution experiment.

Coupons prepared from a 30 wt % or a 68.8 wt % U-Al alloy were used in a third series of experiments. These coupons were used to model the dissolution of DR-3 fuel assemblies. The 30 wt % U-Al coupons were cut to a nominal size of 20 x 10 x 4.65 mm giving a mass of 2.3–2.7 g. Three coupons were used for the 30 wt % U-Al alloy dissolutions resulting in 6 gas samples (2 per coupon) giving a final Al concentration near 1.4 M. In a separate experiment, a single coupon from a 68.8 wt % U-Al alloy was dissolved measuring 20 x 8 x 3 mm and having a mass of 2.3 g resulting in final Al concentration of 0.17 M. Three Al-6061 coupons were dissolved following the dissolution of the 68.8 wt % U-Al alloy resulting in a final Al concentration of 0.88 M. Two gas samples were collected during the dissolution of each coupon.

2.3 Sample Analyses by Analytical Development

Gas, solid, and liquid samples were submitted to Analytical Development (AD) for analysis. Results are archived in the AD LIMS system.

2.3.1 Gas Analysis

Off-gas samples were submitted to AD for analysis by GC. Samples were analyzed within 1 day of gas collection. Calibration was carried out prior to and after the sample analyses, as well as calibration verification using an air blank. Samples were run in duplicate for confirmation of results. Argon carrier gas was used. A 1 vol % H_2 standard was used for determining the response factor for H_2. Blank air was used for calibration of N_2 and O_2. All responses are assumed to be linear at the concentrations measured.

2.3.2 Solids Analysis

A portion of the solids remaining after dissolution were submitted for characterization by X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM) as needed. The remaining filtered solids were submitted to AD for dissolution using the aqua regia digestion method. The vessel was sealed and placed in a drying oven for 2 hours at 115 °C and then cooled. The solution was filtered through a 0.2 µm filter. The pressure vessel and the filter were rinsed with several 2–3 mL portions of de-ionized water which were then passed through the filter. The dissolved solids were sent for ICP-ES, IC, and CVAA Hg analysis.

2.3.3 Liquids Analysis

Liquid solutions were sampled before and after the dissolution experiments, and liquids were also generated from dissolution of solids using the aqua regia digestion method. The solutions were analyzed for Free Acid, ICP-ES, IC, and CVAA Hg to confirm makeup values and identify any experimental concerns.

3.0 Results and Discussion

3.1 Solution Compositions

The solutions containing HNO_3, Hg, KF, and Al for Al-1100 alloy dissolution experiments are listed in Table 3-1. Experiment 1 was used as a benchmark to the current recommended MURR flowsheet.[2,3] Baseline experiments 25 and 28 were used to compare to dissolution experiments performed with impurities in the dissolving solution using 0.012 M Hg. Experiment 30 provides data to support using a Hg concentration range of 0.012–0.015 M for the modified flowsheet recommendations.

Table 3-1. Composition of Dissolving Solutions.

Element/ Species	Experiment 1	Experiment 25	Experiment 28	Experiment 30
HNO_3	7.00 M	7.00 M	6.65 M	6.51 M
Hg	0.002 M	0.012 M	0.012 M	0.015 M
K	0.1 M	0.1 M	0.1 M	0.1 M
F	0.1 M	0.1 M	0.1 M	0.1 M
Al	0.075 M	0.075 M	0.0 M	0.0 M

3.2 Precipitated Solids

Upon completion of the dissolution experiments, the solutions were cooled to room temperature and then filtered using a 0.45 µM cellulose filter. Filtered solids were subsequently rinsed with deionized water and allowed to dry. Al-1100 experiments 1, 25, 28, and 30 produced gray solids identified by XRD as elemental silicon. Aluminum nitrate was identified in the unrinsed filtered solids from Experiment 1. Experiments 35 and 36 with L-Bundle Al-6061 alloy produced white amorphous solids (unidentifiable by XRD). No observable solids were generated for the U-Al alloys used in Experiments 41 and 42.

Table 3-2. XRD Results of Precipitated Solids

Experiment	XRD
1	Si, $Al(NO_3)_3(H_2O)_6$*
25	Si
28	Si
30	Si
35	amorphous
36	amorphous
41	no observable solids
42	no observable solids

*identified from un-rinsed filtered solid

3.3 Peak Off-gas Rates – Baseline Solutions used to Dissolve Al-1100

Al-1100 alloy dissolutions were performed with the solutions in Table 3-1 to provide a comparison with dissolutions performed using minimum and maximum impurity solutions. Off-gas rates were measured for the Al-1100 coupons. The off-gas volume generated per coupon is tracked by recording height changes in the water column of the Tedlar™ Bag system in the experimental setup. The water column heights then translate into volumes of gas generated. The volumes of gas generated are then corrected for the slight pressure created by the rising water column above the Tedlar™ bag collection system as well as the tubing volume that is submerged in the water column. As described in Section 2.1, each experiment consisted of four sequentially dissolved Al coupons. This technique resulted in four sequential peak off-gas rate measurements for Experiment 1 of 121, 24, 18, and 13 $cm^3/min/cm^2$ as the dissolved Al concentration increased (Table 3-3). The off-gas generation rates from the experiment are presented in Figure 3-1.

Table 3-3. Measured Peak Off-gas Rates and Al Concentrations for Baseline Solutions 1–4 Used to Dissolve Al-1100.

Coupon No.	**Experiment 1 Peak Off-gas ($cm^3/min/cm^2$)**	**Initial [Al] (M)**	**Experiment 28 Peak Off-gas ($cm^3/min/cm^2$)**	**Initial [Al] (M)**
Coupon 1	121.2	0.075	74.3	0
Coupon 2	24.1	0.49	64.0	0.39
Coupon 3	17.7	0.903	46.6	0.78
Coupon 4	13.0	1.32	33.5	1.17
All Coupons	---	1.72	---	1.56
Coupon No.	**Experiment 25 Peak Off-gas ($cm^3/min/cm^2$)**	**Initial [Al] (M)**	**Experiment 30 Peak Off-gas ($cm^3/min/cm^2$)**	**Initial [Al] (M)**
Coupon 1	90.1	0.075	66.2	0
Coupon 2	60.6	0.49	69.5	0.41
Coupon 3	41.6	0.91	70.9	0.79
Coupon 4	35.6	1.32	32.9	1.17
All Coupons	---	1.73	---	1.53

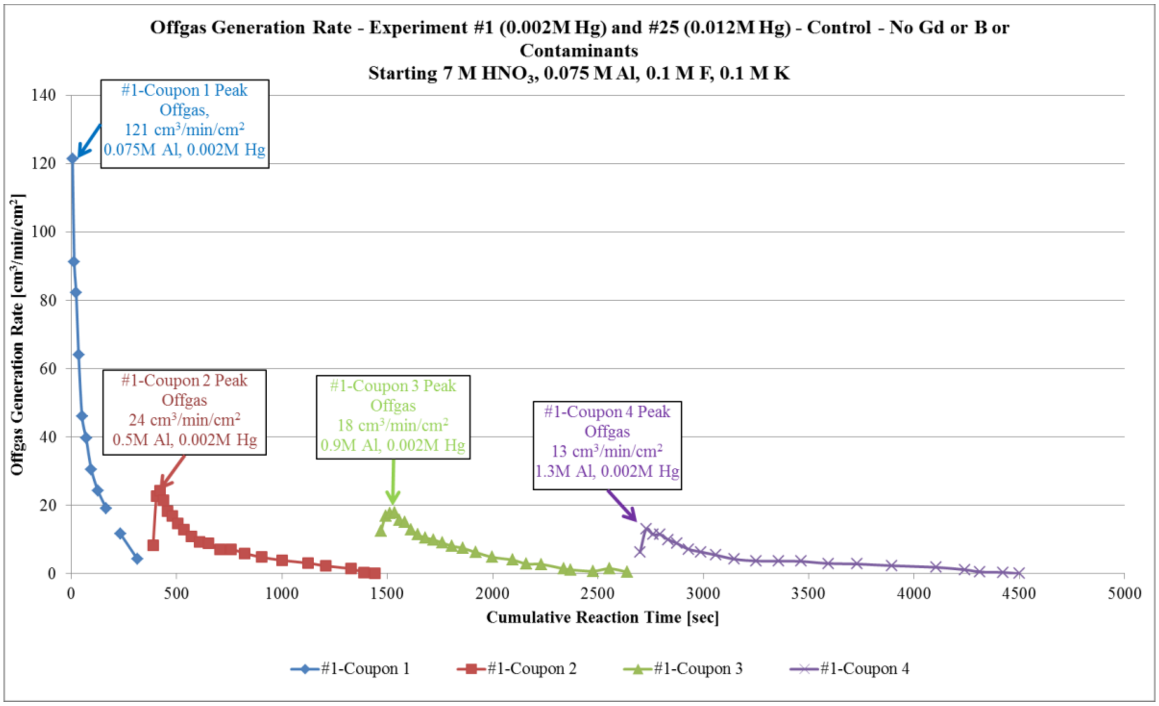

Figure 3-1. Experiment 1 Off-gas Generation Rates at 0.002 M Hg for Al-1100.

Experiment 25 repeated Experiment 1 with the initial Hg increased to 0.012 M and off-gas rates were compared to Experiment 1 at 0.002 M Hg (Figure 3-2). The initial off-gas rate for Experiment 1 of 121 $cm^3/min/cm^2$ was larger than for Experiment 25 at 90 $cm^3/min/cm^2$. However, the effect of the increased Hg became apparent as the dissolved Al concentrations increased, since the peak off-gas rates for coupons 2 through 4 increased by approximately three times.

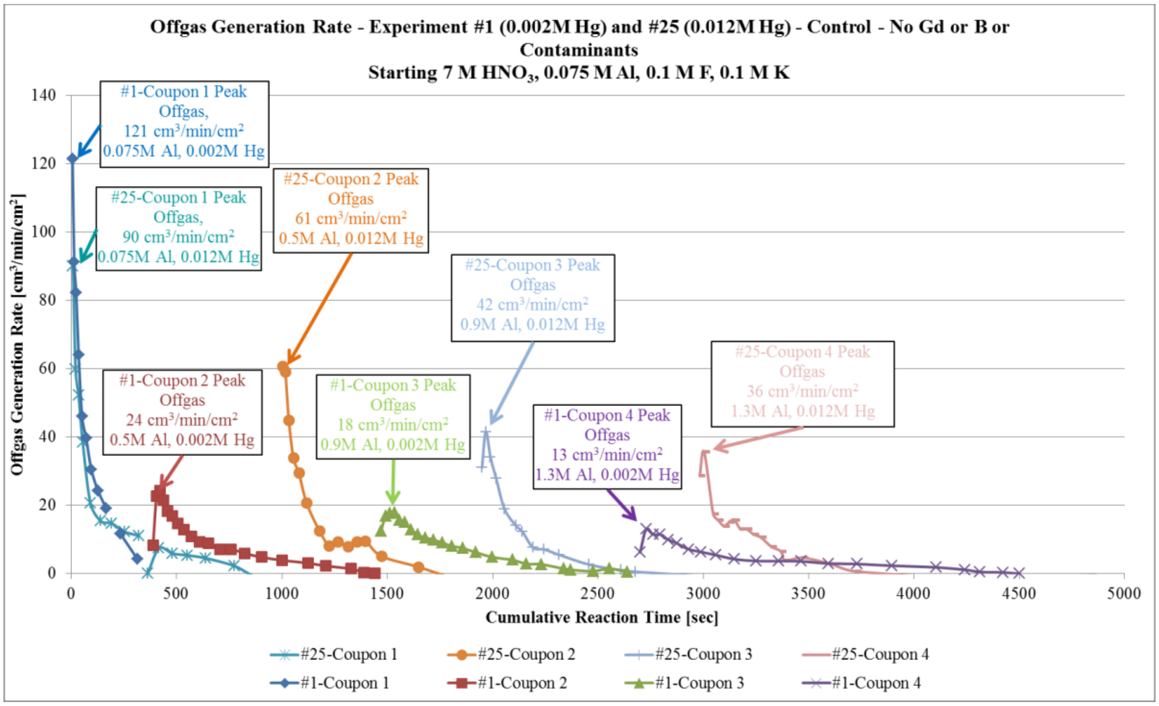

Figure 3-2. Comparison of Experiment 1 and 25 Off-gas Generation Rates for Al-1100.

Experiments 28 and 30 were also performed at elevated Hg concentrations of 0.012 and 0.015 M, respectively. Plots of Experiment 28 and 30 off-gas generation rates are shown in Figure 3-3 and Figure 3-4, respectively. The off-gas rates for Experiment 30 (0.015 M Hg) are similar to the rates for Experiment 28 (0.012 M Hg). The off-gas rates for Experiments 28 and 30 are not 6 and 7.5 times the off-gas rate for Experiment 1, respectively, based on the assumption that the off-gas rate increases proportionally to the Hg concentration.[6]

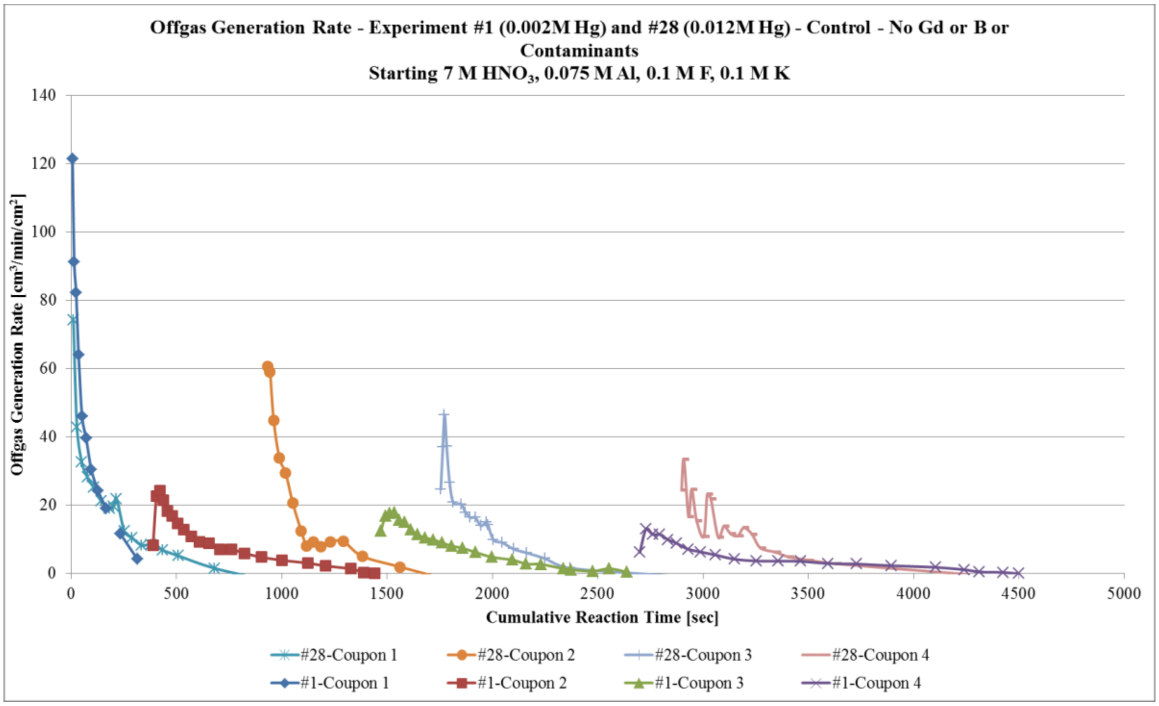

Figure 3-3. Comparison of Experiment 1 and 28 Off-gas Generation Rates for Al-1100

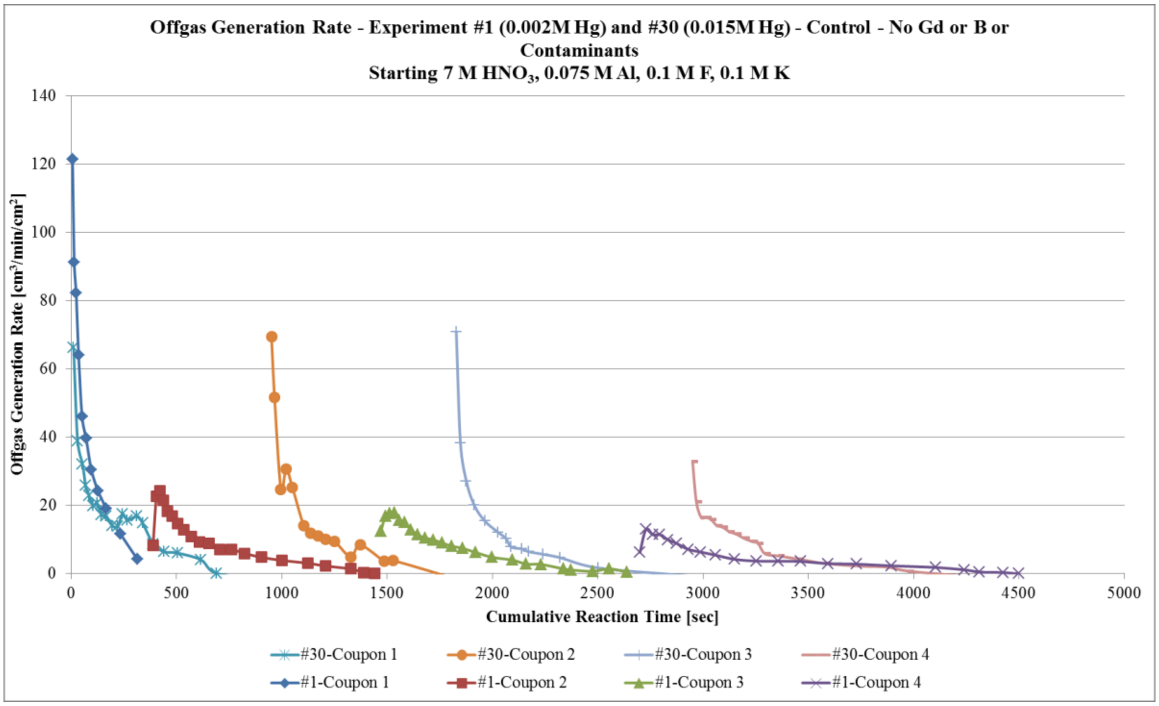

Figure 3-4. Comparison of Experiment 1 and 30 Off-gas Generation Rates for Al-1100

For comparison, the peak off-gas rate at four dissolved Al concentrations is reported in Table 3-3 for Experiments 1, 25, 28, and 30. For the initial Al coupon dissolved in each experiment, increasing the Hg from 0.002 M (Experiment 1) to 0.012 or 0.015 M did not result in greater initial peak off-gas rates, as anticipated. The maximum off-gas rate was observed with the initial coupon for Experiment 1 at 0.002 M Hg. Experiment 30, which used 0.015 M Hg maintained a near constant peak off-gas rate for coupons 1 through 3 of about 70 $cm^3/min/cm^2$. The data from these experiments indicate that increasing the Hg concentration 6- to 7.5-fold does not increase initial peak off-gas rates proportionately. However, while initial peak off-gas rates are similar at the range of Hg concentrations studied from 0.002 to 0.015 M, increasing the Hg concentration above 0.002 does raise the off-gas rate (albeit disproportionally) at higher dissolved Al concentrations. These results correlate with observations by Wymer et al.[9] that increasing Hg did not scale with Al dissolution rate at Hg concentrations greater than 0.005 M (Section 3.4).

3.4 Baseline Aluminum Dissolution Rates for Al-1100

The Al and HNO_3 concentrations throughout the experiments are estimated based on the actual initial concentrations and the assumption that 3.75 moles of HNO_3 are used per mole of Al dissolved, as discussed in prior work[10] and shown below:

$$(1) \qquad Al_{(s)} + 3.75\ HNO_3 \rightarrow Al(NO_3)_3 + 0.225\ NO_{(g)} + 0.15\ N_2O_{(g)} + 0.1125\ N_{2(g)} + 1.875\ H_2O_{(g)}$$

The corresponding dissolved Al concentration for each gas sample was estimated based on the actual initial concentrations and the final dissolved concentrations once the coupon had completely dissolved. The HNO_3 concentration is based on the Al concentration deducting 3.75 mole of HNO_3 from the solution per mole of Al dissolved. From the above chemical reaction, the amount of off-gas generated is directly related to the rate at which Al is being dissolved. Therefore, the Al concentration can be tied to the amount of off-gas being generated at any point in time. Between the initial and final Al concentrations for each coupon, the intermediate Al concentrations are estimated based on the percent of total gas volume generated per coupon dissolved. These intermediate Al concentrations are shown in Appendix A. The gas volume per coupon is tracked by recording height changes in the water column of the Tedlar™ bag system in the experimental setup. The water column heights then translate into volumes of gas generated. The volumes of gas generated are then corrected for the slight pressure created by the rising water column above the Tedlar™ bag collection system as well as the volume of the submerged tubing in the water column. The percent of total corrected gas volume generated per coupon is then calculated by:

$$(2) \qquad \%\ \text{of total corrected gas volume generated} = \frac{\text{Gas Generated at Specific Height}}{\text{Total Gas Generated per Coupon}}$$

Where:

% of total corrected gas volume generated – the percent of total gas volume generated at a specific water height
Gas Generated at Specific Height – the gas volume generated at a specific water height corrected for pressure from water column height above where gas is collected in the Tedlar™ bag
Total Gas Generated per Coupon – the total gas volume generated from dissolving the coupon completely corrected for pressure from water column height above where gas is collected in the Tedlar™ bag

The intermediate Al concentrations then become:

(3) Est. Al [M] = % of total corrected gas volume generated *(Final Al [M] – Init Al [M]) + Init Al [M]

Where:

Est. Al [M] – the estimated dissolved Al molarity at % of total corrected gas volume generated for each coupon
Final Al [M] – the final dissolved Al molarity based on the total mass of coupons dissolved
Init Al [M] – the initial dissolved Al molarity based on the total mass coupons dissolved at the start of a coupon dissolution

The estimated Al molarity may start out at zero or some non-zero value and continues to increase as each coupon is dissolved. The above estimation of Al molarity allows the tracking of the dissolved Al across the dissolution of multiple coupons.

Based on the estimated dissolved Al concentrations, the HNO_3 concentration can be estimated by the following equations:

$$(4) \qquad Est.HNO_3Consumed_t[mole] = (Al_t[M] * Vol_t[L] - Al_{t-1}[M] * Vol_{t-1}[L]) * \frac{3.75 \text{ mole } HNO_3 \text{ Consumed}}{\text{mole Al Dissolved}}$$

$$(5) \qquad Est.HNO_{3_t}[M] = \frac{(Est.HNO_{3_{t-1}}[M] * Vol_{t-1}[L]) - Est.HNO_3Consumed_t[mole]}{Vol_t[L]}$$

Where:

Est. HNO_3 Consumed (t) – the estimated moles of HNO_3 consumed at time t
Al(t) – the dissolved Al molarity at time t
Al(t-1) – the dissolved Al molarity at time t-1 or previous time step
Vol(t) – the solution volume at time t which is assumed constant unless additions or removals are made
Vol(t-1) – the solution volume at time t-1 or previous time step
Est. HNO_3 (t) – the estimated HNO_3 molarity at time t
Est. HNO_3 (t-1) – the estimated HNO_3 molarity at time t-1 or previous time step

Al dissolution rates for Experiments 1 and 25 performed at 0.002 and 0.012 M Hg, respectively, were calculated from off-gas data as described above for comparison (Figure 3-5). Maximum dissolution rates for Al-1100 at 0.002 and 0.012 M Hg were approximately three times U-Al dissolution rates of 180 mg/min/cm^2 reported in the literature[8] and measured in this work (Section 3.7). However, the initial Al dissolution rate for Al-1100 measured directly was 130 mg/min/cm^2 at 0.004 M Hg (Figure 3-6). The calculated Al dissolution rates for experiments 1 and 25 were similar despite the difference in Hg concentration.

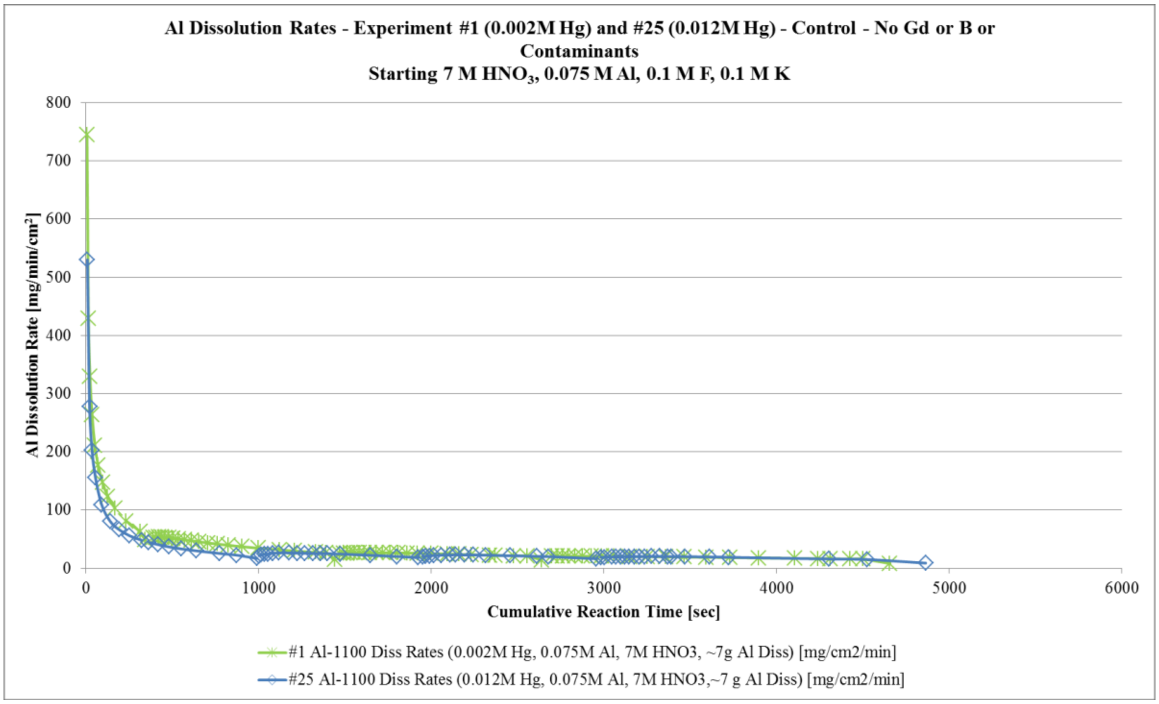

Figure 3-5. Comparison of Al-1100 Dissolution Rates as a Function of Aluminum Concentration.

Wymer et al.[9] presented similar observations for 15 wt % extruded U-Al alloy, where increasing the Hg concentration from 0.002 to 0.005 M increased the maximum dissolution rate only ~5–10% at 7 M HNO_3 at no dissolved Al. Furthermore, increasing Hg concentrations above 0.005 M at 8 M HNO_3 and 0 M Al did not show any significant increase in dissolution rate. Aluminum dissolution rates were measured with Al-1100 at two Hg concentrations using solutions initially containing 0 M Al, 0.004 M Hg, 7 M HNO_3, 0.1 M KF, and 0 M Al, 0.015 M Hg, 6.5 M HNO_3, 0.1 M KF. For each experiment, a fresh coupon of known mass and dimensions was dropped in the hot dissolving solution momentarily and then extracted. The change in coupon mass and dimensions were measured and used to calculate Al dissolution rates in mg/min/cm^2. These two new sets of data are plotted with the data from Wymer's manuscript in Figure 3-6. The trend observed for the Al-1100 dissolution rate as a function of the Hg concentration in this work correlates with Al dissolution rates for U-Al alloy observed by Wymer.[9] These results help explain the similar initial peak off-gas rates observed over the range of Hg concentrations used in the dissolving solutions.

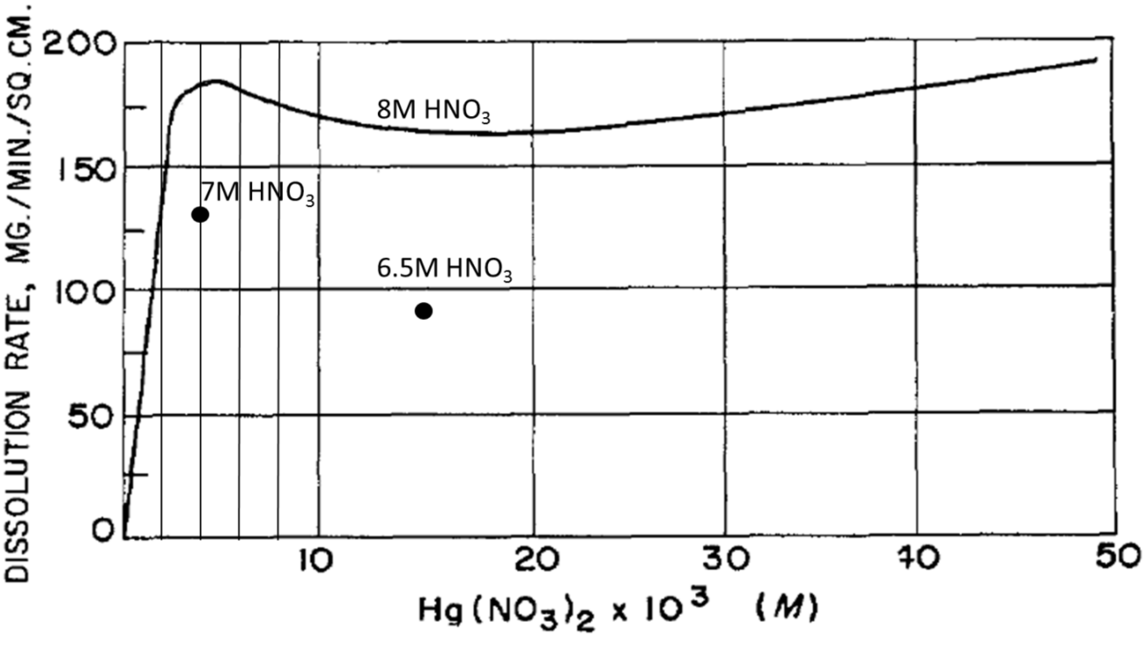

Figure 3-6. Comparison of Al-1100 Dissolution Rates for Wymer et al. (solid line) and This Work as a Function of Hg Concentration.

3.5 H_2 Gas Concentrations – Al-1100 Dissolution Experiments

Eight off-gas samples were collected sequentially (1-8) during each Al-1100 experiment as described in Section 2.1 (two samples were collected for each of four coupons dissolved). The gas samples were analyzed by GC, quantitatively for H_2, O_2, and N_2. For Experiments 1, 25, 28, and 30, the measured H_2 concentrations by GC are provided in Table 3-4.

Table 3-4. Measured H_2 Concentrations Analyzed by GC for Al-1100 Dissolution.

Gas Sample	Experiment 1 H_2 [vol %]	Experiment 25 H_2 [vol %]	Experiment 28 H_2 [vol %]	Experiment 30 H_2 [vol %]
1	1.6	0.3	*	0.3
2	1.5	0.3	0.4	0.4
3	6.6	1.2	1.0	0.9
4	7.1	1.0	0.8	1.1
5	6.0	1.6	1.2	1.3
6	6.1	1.5	1.5	0.9
7	6.9	1.2	0.8	1.5
8	6.9	1.7	1.5	1.8

*air leak during sample analysis

The analyzed concentrations of the off-gas species from the Al metal dissolutions were corrected to account for dilution from gas in the dissolution vessel, condenser, Viton® tubing, and sample bulb. To calculate the adjusted concentrations, ideal mixing of the gases in the void space was assumed and the effect of temperature variations in the gas was assumed negligible. For H_2 or any other component of the off-gas, the adjusted concentration is calculated by material balance,

(6) $$C_{gen} V_{gen} = C_{measured} (V_{void} + V_{bulb} + V_{gen}) - C_{initial} V_{void}$$

Where:

C_{gen} – the concentration of an off-gas component in the generated gas (vol %)
$C_{measured}$ – the concentration of an off-gas component measured in a gas sample (vol %)
$C_{initial}$ – the concentration of an off-gas component before the sample collection (vol %)
V_{gen} – the volume of gas collected in the Tedlar™ collection bag (cm^3)
V_{void} – the void volume of dissolution vessel, condenser, and Viton® tubing (cm^3)
V_{bulb} – the volume of the gas sample bulb (cm^3)

The corrected gas concentrations for each gas sample are provided in Table 3-5 and plotted in Figure 3-7. Some values could not be calculated based on the raw GC data.

Table 3-5. Corrected Gas Concentrations for H_2 – Alloy Al-1100.

Gas Sample	Experiment 1 H_2 [vol %]	Experiment 25 H_2 [vol %]	Experiment 28 H_2 [vol %]	Experiment 30 H_2 [vol %]
1	2.8	0.5	nc	0.4
2	1.6	0.4	nc_2	0.6
3	10.6	1.9	1.5	1.3
4	9.0	0.9	0.7	1.5
5	5.8	2.1	1.6	1.5
6	7.3	1.7	2.2	0.4
7	8.0	1.1	0.4	2.0
8	8.2	3.6	2.6	2.6

nc = not calculated due to poor measured data,
nc_2 = not calculated due to the previous data point was unavailable as input for equation 6.

Hydrogen gas concentrations corrected for dilution are plotted in Figure 3-7. The maximum corrected H_2 concentration was 10.6 vol % of the total off-gas for Experiment 1, where the corrected H_2 concentration ranged from 1.6 to 10.6 vol %. It was observed that increasing the Hg in the dissolving solutions from 0.002 M to 0.012 M (or 0.015 M) decreased the maximum H_2 percentage in general, giving a maximum of 3.6 vol % (Figure 3-7). In general, a H_2 profile of low to high was observed during the Al-1100 alloy dissolutions.

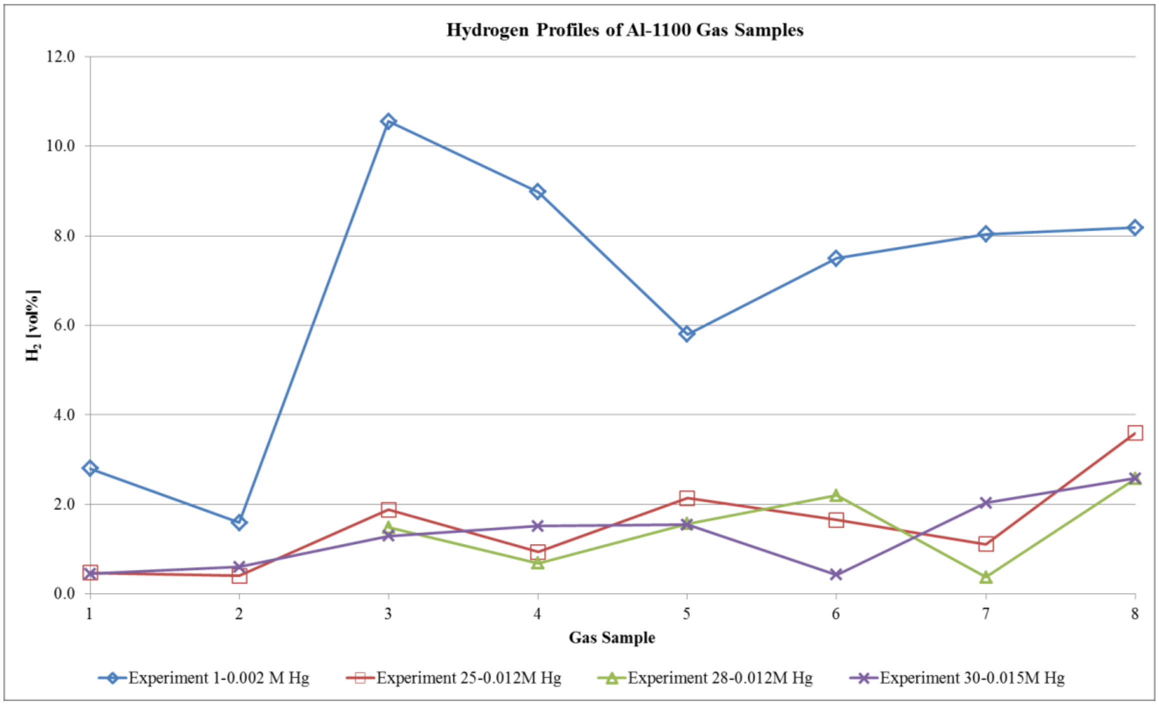

Figure 3-7. Comparison of H_2 for Al-1100 Experiments with Increasing Mercury.

3.6 Dissolution Experiments with Other Al-containing Alloys

The initial experiments performed to evaluate the use of AFS-2 column waste solution for UNF dissolutions used Al-1100 alloy coupons. The Al-1100 coupons were considered a representative surrogate (based on the fuel bundle and assembly materials) that provided an upper bound on the generation of flammable gas during the dissolution process. However, when the flammability calculations were performed for Al-1100, it was observed that the peak off-gas rates combined with the H_2 concentration challenged current assumptions regarding the potential to exceed 60% of the H_2 LFL in the dissolver during fuel dissolution (Appendix B). Particularly, the second coupon for Experiment 1 gave a combination of high off-gas rate and H_2 concentration. Secondly, the H_2 concentration profile of low-to-high for Experiment 1 contrasted to that of Caracciolo's H_2 profile of high-to-low (See Figure 3-8). The Al-1100 H_2 concentration profiles were in agreement with Long's reporting that as the concentration of the reacting acid decreases, the dissolution mechanisms shift toward reactions that consume less acid (i.e. reactions that produce H_2 over NOx gases).[8]

Additional experiments were performed as part of an experimental plan[4] to more closely represent the fuels to be dissolved in H-Canyon in an effort to better understand the data and allow for increasing the number of bundles that can be dissolved together throughout the dissolver charge plan. The experiments outlined in the next sections included a study of L-Bundle alloy comprised of Al-6061 and a 30 wt % and 68.8 wt % U-Al alloy. The U-Al alloys were used to model the dissolution of DR-3 fuel assemblies.

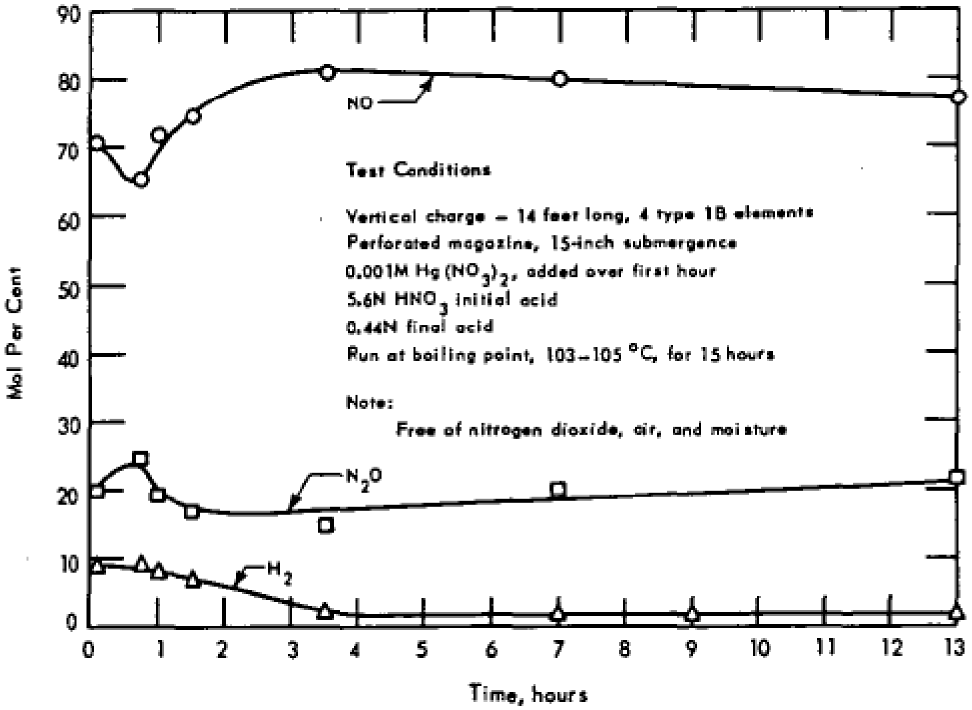

Figure 3-8. Caracciolo Off-gas Profiles.[5]

3.7 Evaluation of L-Bundle Alloy Dissolution Representative of SRE

SRE fuel meat is comprised of a Th-U alloy, and its reactivity and off-gas behavior were measured in previous work.[10] The L-Bundle serves as the outer container for the fuel and Al tubes and confinement can for dissolution. L-bundle off-gas rate and H_2 concentration data were collected for use as input for flammability calculations applicable to SRE fuel to be dissolved in L-Bundles. Coupons cut from an actual L-Bundle comprised of Al-6061 alloy were prepared to understand its reactivity and gas generation behavior versus the Al-1100 dissolution behavior. Experiment 35 using L-Bundle coupons was performed to compare to Experiment 1 that used Al-1100. Experiment 36 targeted replicating an initial charge of fuel to a dissolver where the L-Bundle is initially lowered into the HNO_3 solution at ambient temperature and the Hg is slowly metered into the dissolver. Experiment 36 differed from Experiment 35 in that the Hg was metered in using a syringe rather than having the Hg initially present, and the coupon from Experiment 36 was submerged in the dissolving solution prior to heating the solution. Experiment 40 was conducted to evaluate SRE dissolution at a higher Hg concentration.

Experiment 35 was performed with L-Bundle Al-6061 alloy to compare and contrast results of Experiment 1 with Al-1100. The dissolving solution consisted of 0.002 M Hg, 7 M HNO_3, and 0.1 M KF, and 0 Al (Experiment 1 had 0.075 M Al initially). The peak off-gas rates for Experiment 35 using L-Bundle coupons were 162, 36, 14, and 7 $cm^3/min/cm^2$ for the first, second, third, and fourth coupons, respectively. The Al concentration in solution increased as each coupon dissolved. Figure 3-9 plots off-gas rates for Experiment 1 and 35, showing a small increase in peak off-gas for the first 2 coupons dissolved during Experiment 35. This observation may be partially explained by the difference in the initial Al concentration. This data shows that the peak off-gas and dissolution rates for L-bundle and Al-1100 are similar.

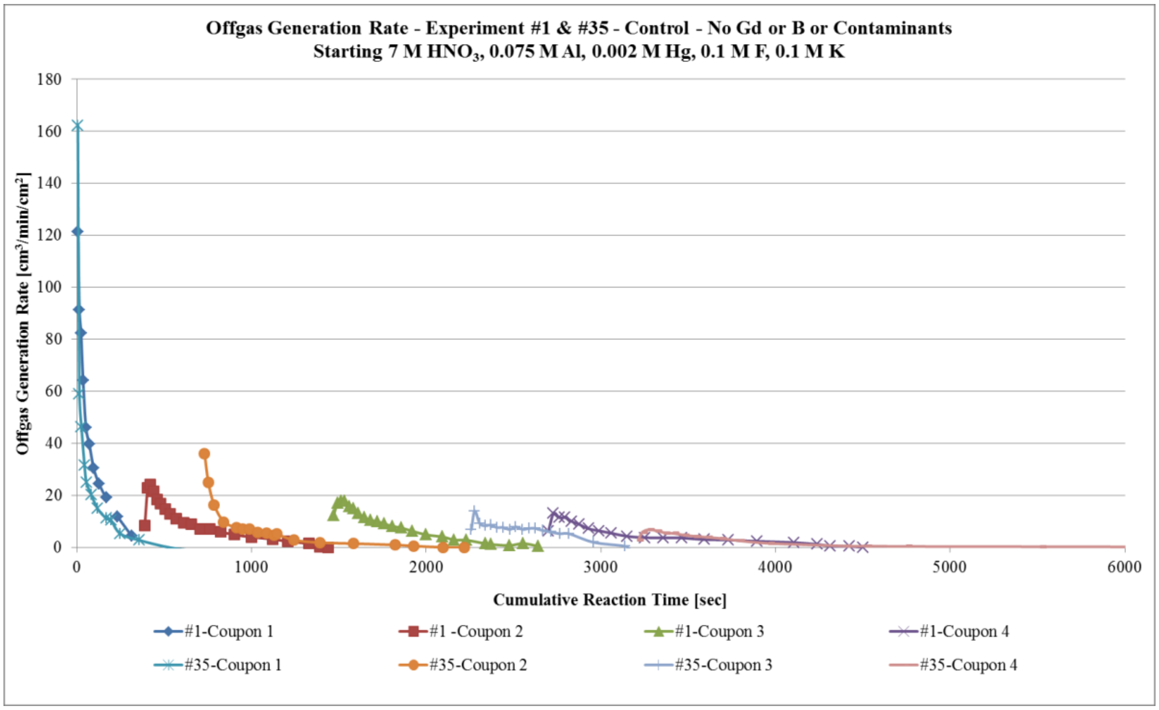

Figure 3-9. Comparison of L-Bundle and Al-1100 at 0.002 M Hg.

Experiment 36 targeted replicating an initial charge of fuel to a dissolver. It used the same solution matrix that was used for Experiment 35, but it differed from Experiment 35 in that the Hg was metered in rather than having the Hg initially present, and the coupon was submerged in the dissolving solution prior to heating the solution to temperature. After reaching 100 °C, the Hg was added in three equal additions by syringe (initially, at 60 s, and at 120 s) to achieve a 0.002 M Hg concentration. Figure 3-10 shows that metering in Hg reduces the peak off-gas during the dissolution of the initial coupon. The peak off-gas of 162 $cm^3/min/cm^2$ for Experiment 35 was reduced to 37 $cm^3/min/cm^2$ in Experiment 36 (Figure 3-10 and Table 3-6).

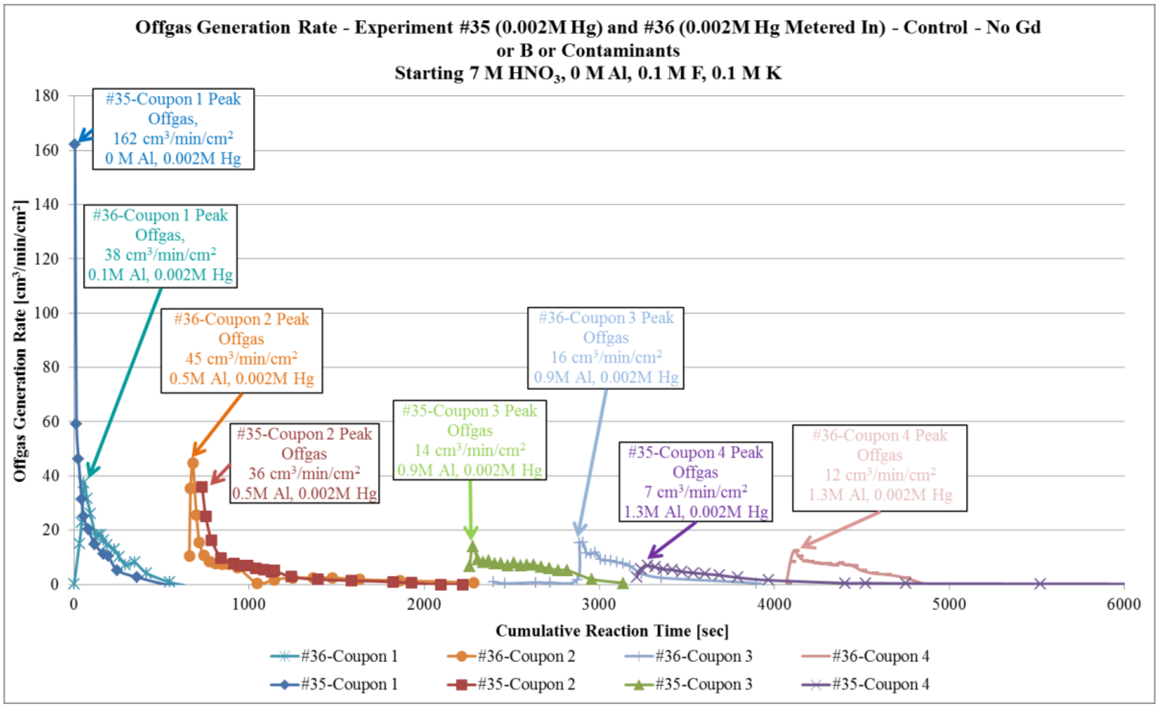

Figure 3-10. Comparison of L-Bundle Off-gas Rate – Metering in Hg (Experiment 36) vs Hg Initially Present (Experiment 35).

Table 3-6. Peak Off-gas Rates and Al Concentrations for Experiments 35, 36, and 40 with L-Bundle Alloy Al-6061.

Coupon No.	**Experiment 35 Peak Off-gas ($cm^3/min/cm^2$)**	**Initial [Al] (M)**	**Experiment 36 Peak Off-gas ($cm^3/min/cm^2$)**	**Initial [Al] (M)**	**Experiment 40 Peak Off-gas ($cm^3/min/cm^2$)**	**Initial [Al] (M)**
Coupon 1	162.2	0	37.3	0	68.4	0
Coupon 2	35.9	0.416	44.8	0.415	31.4	0.412
Coupon 3	14.0	0.831	15.6	0.821	28.5	0.818
Coupon 4	6.9	1.270	12.5	1.229	26.5	1.222
All Coupons	---	1.602	---	1.602	---	1.593

Calculated Al dissolution rates (described in Section 3.3) show a marked decrease in initial rate for Experiment 36 versus Experiment 35 (Figure 3-11).

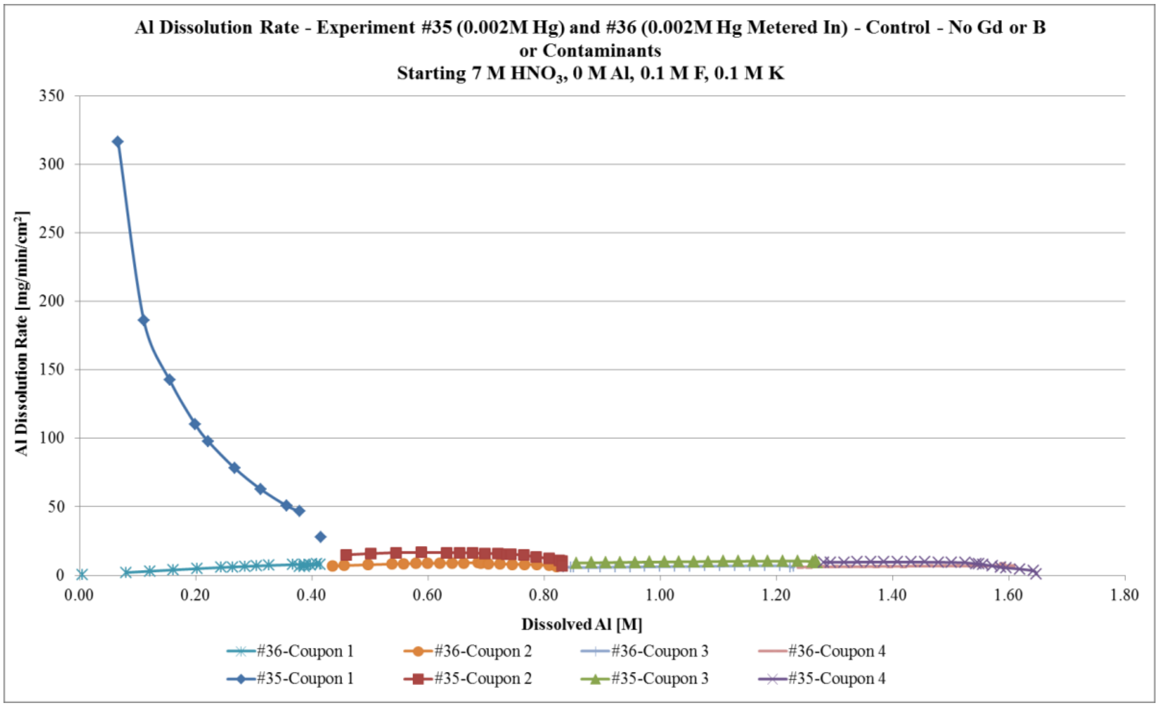

Figure 3-11. Comparison of L-Bundle Dissolution Rate with Metering in Hg (Experiment 36) vs Hg initially Present (Experiment 35).

Experiment 40 was performed with L-Bundle alloy to measure and compare the effects of increased Hg in combination with the effects of dissolved U, Th, and Gd in solution. The solution initially contained 3.9 g/L U and 21.8 g/L Th, 0.48 g/L Gd, 7 M HNO$_3$, 0.012 M Hg, and 0.05 M KF. The peak off-gas rates for Experiment 40 were 68, 31, 29, and 27 cm^3/min/cm^2 for coupons 1 through 4, respectively (Figure 3-12 and Table 3-6). The presence of the impurities in Experiment 40 had a suppressive effect on the initial off-gas rate of 68 cm^3/min/cm^2 versus 162 cm^3/min/cm^2 for Experiment 35. The phenomenon of off-gas rate reduction in the presence of impurities has also been observed with Waste Minimization simulants (which contain impurities), to be presented in a future report. The increased Hg concentration used in Experiment 40 is credited for increasing the off-gas rate at higher dissolved Al concentrations, similar to Experiments 25, 28, and 30 with Al-1100. Aluminum dissolution rates for Experiment 40 are provided in Figure 3-13.

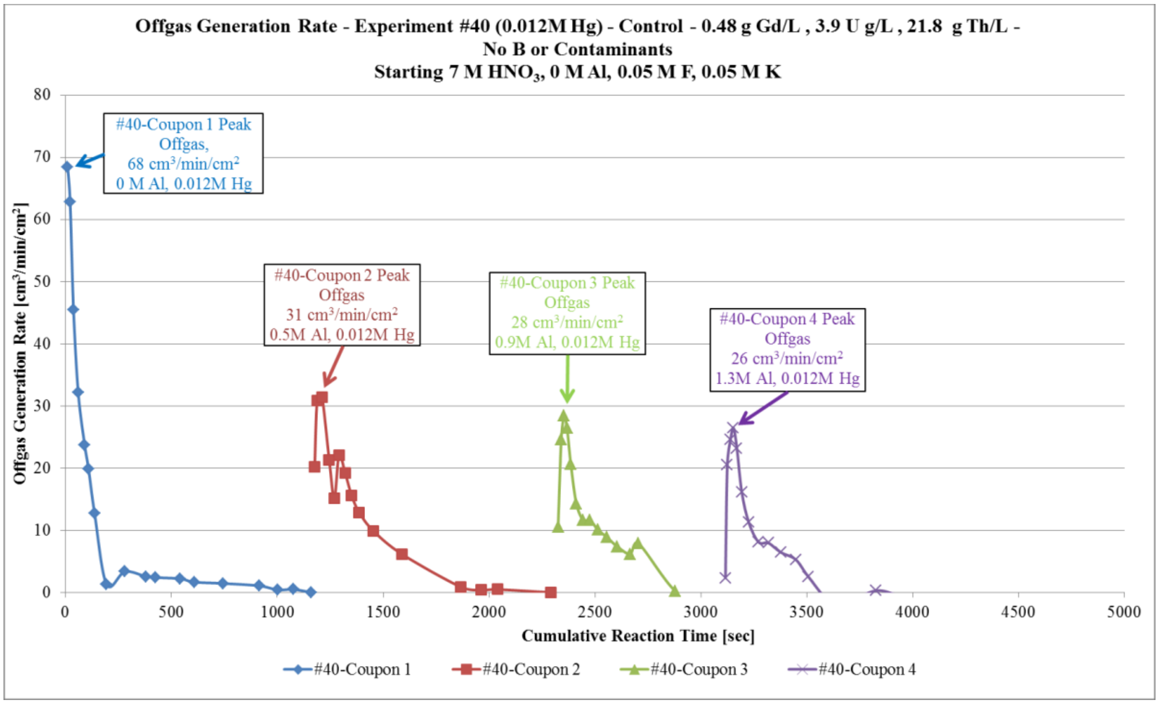

Figure 3-12. Experiment 40 Off-gas Generation Rates at 0.012 M Hg and 3.9 g/L U, 21.8 g/L Th, and 0.48 g/L Gd.

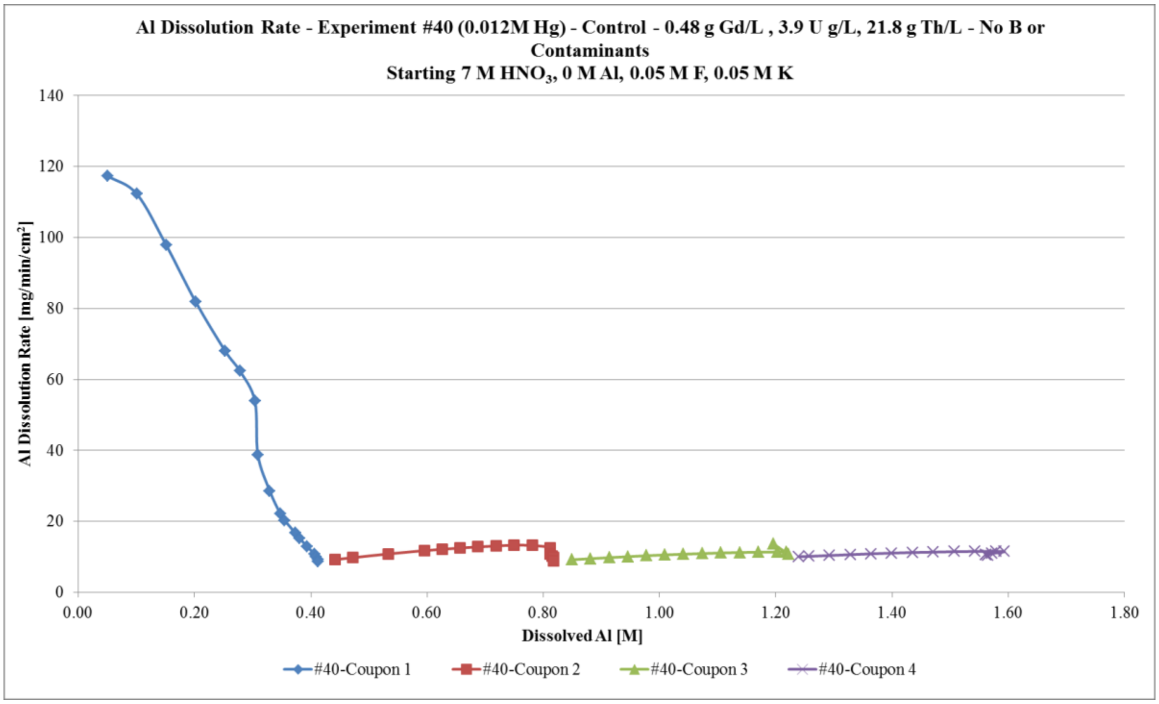

Figure 3-13. Experiment 40 Al Dissolution Rates at 0.012 M Hg and 3.9 g/L U, 21.8 g/L Th, and 0.48 g/L Gd.

3.7.1 H_2 Off-gas Concentrations for Experiments with L-Bundle Alloy

Hydrogen gas concentrations corrected for dilution (Equation 6) for experiments with L-Bundle alloy are provided in Table 3-7. Experiment 35 had a peak H_2 concentration measured in gas sample 4 taken at the end of the second coupon dissolution. Additionally, a mass balance corrected value of 19.4% H_2 was observed for the final gas sample. The high final H_2 concentration is attributed to the solution becoming acid deficient for this experiment.[8] Free acid measurements of the final solution were < 0.05 M, where they are typically > 0.5 M. Experiment 36, performed with the same solution composition (other than the Hg was metered in) gave a peak H_2 concentration of 10.6 vol % for gas sample 6 taken at the end of the third coupon dissolution. The final H_2 measurement was 4.6 vol % (vs 19.4 vol % for experiment 35) and the free acid of the final solution was measured at 0.4 M. Experiment 40 initially produced very little H_2, yet the final coupon produced H_2 concentrations of 11.4 vol % and 11.5 vol %. The increase in H_2 in this experiment is not attributed to acid deficiency, as the final free acid was measured at 0.9 M. A H_2 concentration profile of low-to-high was observed for L-Bundle alloy similar to Al-1100.

Table 3-7. Corrected Gas Concentrations for H_2 – L-Bundle

Gas Sample	Experiment 35 H_2 [vol %]	Experiment 36 H_2 [vol %]	Experiment 40 H_2 [vol %]
1	3.4	4.4	0.8
2	2.5	0.3	0.5
3	6.9	4.8	1.5
4	10.4	7.1	1.5
5	0.0*	2.3	2.9
6	2.3	10.6	2.4
7	8.8	3.9	11.4
8	19.4	4.6	11.5

*Corrected H_2 less than 0 vol %

3.8 Evaluation of U-Al Alloy Dissolution Representative of DR-3 Assemblies

A third series of experiments was performed using U-Al alloys to more closely represent the DR-3 fuels to be dissolved in H-Canyon. Experiment 41 was performed with a 30 wt % U-Al alloy using a solution containing 7 M HNO_3, 0 M Al, and 0.1 M KF. A total of three coupons were sequentially dissolved in the solution giving final estimated dissolved U and Al concentrations of 0.066 M and 1.36 M, respectively (Table 3-8). Peak off-gas rates of 113, 31, and 15 $cm^3/min/cm^2$ were measured for coupons 1 through 3, respectively (Table 3-8 and Figure 3-14). In Figure 3-15, off-gas rate data show that Experiment 41 had similar peak off-gas rates to Experiment 1. (Experiment 1 had peak off-gas rates of 121, 24, and 18 $cm^3/min/cm^2$ for the initial three coupons, respectively.)

Table 3-8. Measured Peak Off-gas Rates and Al Concentrations for U-Al Alloys

Coupon No.	Experiment 41 Peak Off-gas (cm^3/min/cm^2)	Initial [Al] (M)	Experiment 42 Peak Off-gas (cm^3/min/cm^2)	Initial [Al] (M)
Coupon 1	113.1	0	20.8	0
Coupon 2	30.5	0.439	---	---
Coupon 3	15.3	0.893	---	---
All Coupons	---	1.358	---	0.18

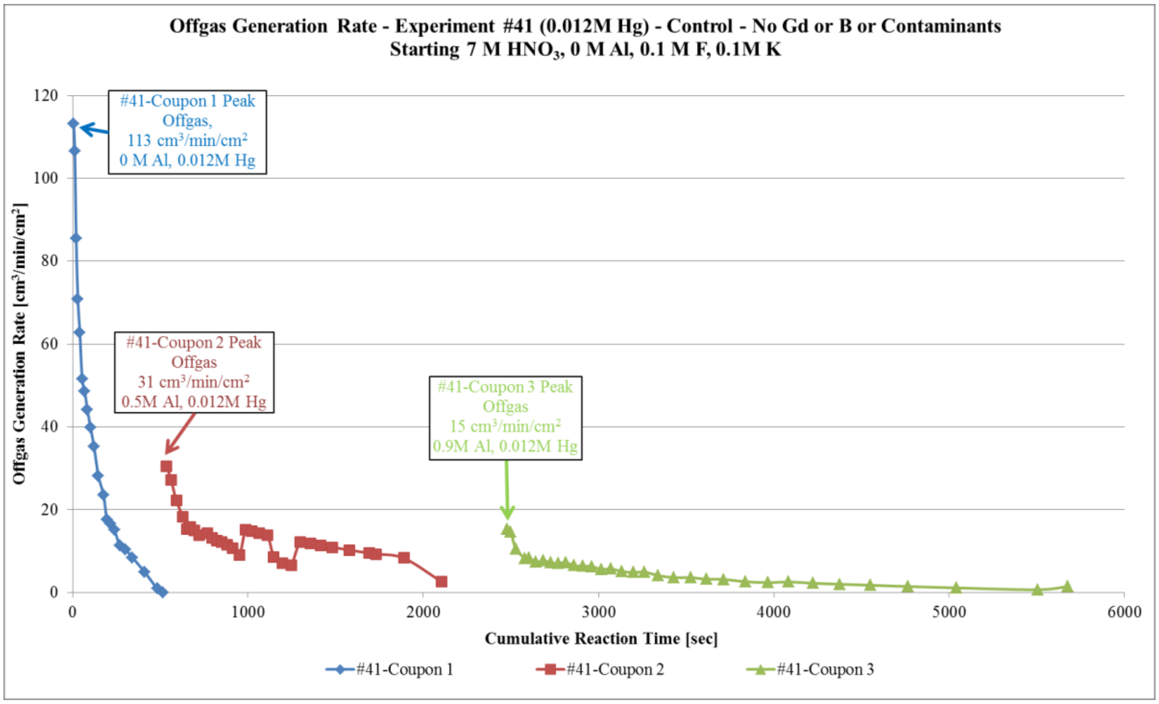

Figure 3-14. Experiment 41 Off-gas Generation Rates at 0.012 M Hg for 30 wt % U-Al Alloy

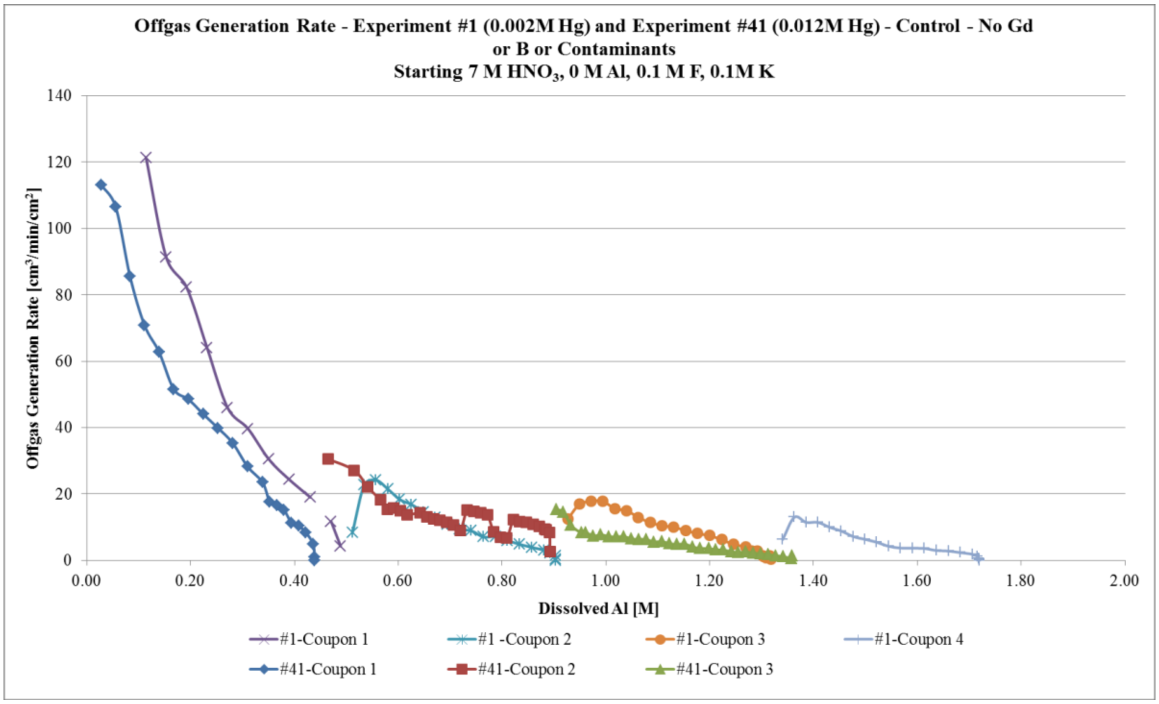

Figure 3-15. Comparison of Off-gas Generation Rates for Experiment 41 (30 wt % U-Al and 0.012 M Hg) and Experiment 1 (Al-1100 and 0.002 M Hg).

Aluminum dissolution rates were calculated as described in Section 3.3, and plotted in Figure 3-16. The initial rate is comparable to the peak U-Al dissolution rate of 180 mg/min/cm^2 reported in the literature.[8]

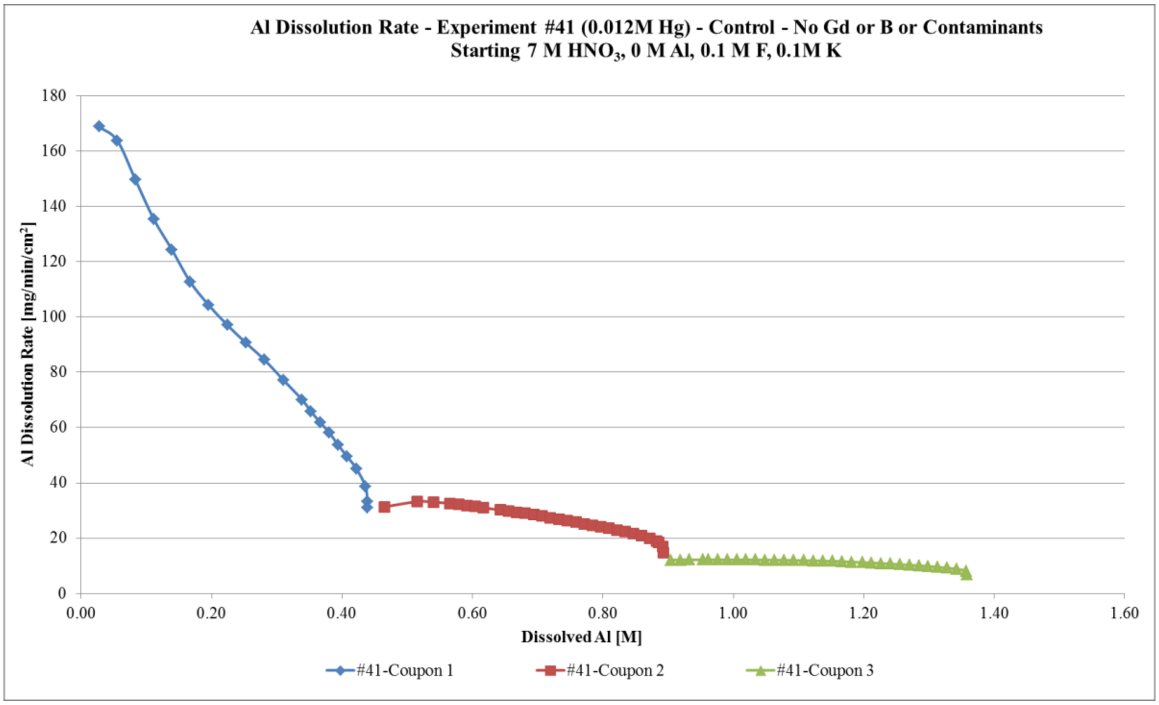

Figure 3-16. Experiment 41 Al Dissolution Rates of 30 wt % U-Al Alloy at 0.012 M Hg.

Experiment 42 was performed by dissolving a 68.8 wt % U-Al coupon in a 0.012 M Hg and 7 M HNO_3 solution. The off-gas generation rates for Experiment 42 and 41 are shown in Figure 3-17. The 68.8 wt % U-Al alloy had a peak off-gas rate of 21 $cm^3/min/cm^2$ which is much smaller than the peak off-gas rate for Experiment 41 of 113 $cm^3/min/cm^2$ (Table 3-8). The Al dissolution rates for Experiment 42 and 41 (initial coupon only) are shown in Figure 3-18 for comparison. The off-gas rate and dissolution rate of the 68.8 wt % U-Al is much less than the 30 wt % U-Al, most likely due to the difference in the percentage of U as well as differences in the structure and fabrication of the alloys. The 68.8 wt % U-Al alloy is the intermetallic compound UAl_4. The 30 wt % U-Al alloy is comprised of a U-Al intermetallic dispersed in a continuous Al matrix. Therefore, in terms of H_2 production and off-gas rate, the 68.8 wt % U-Al alloy is bounded by the 30 wt % U-Al alloy. The 30 wt % U-Al alloy off-gas rate and H_2 concentrations were used for the flammability calculations pertaining to DR-3 fuel dissolutions.

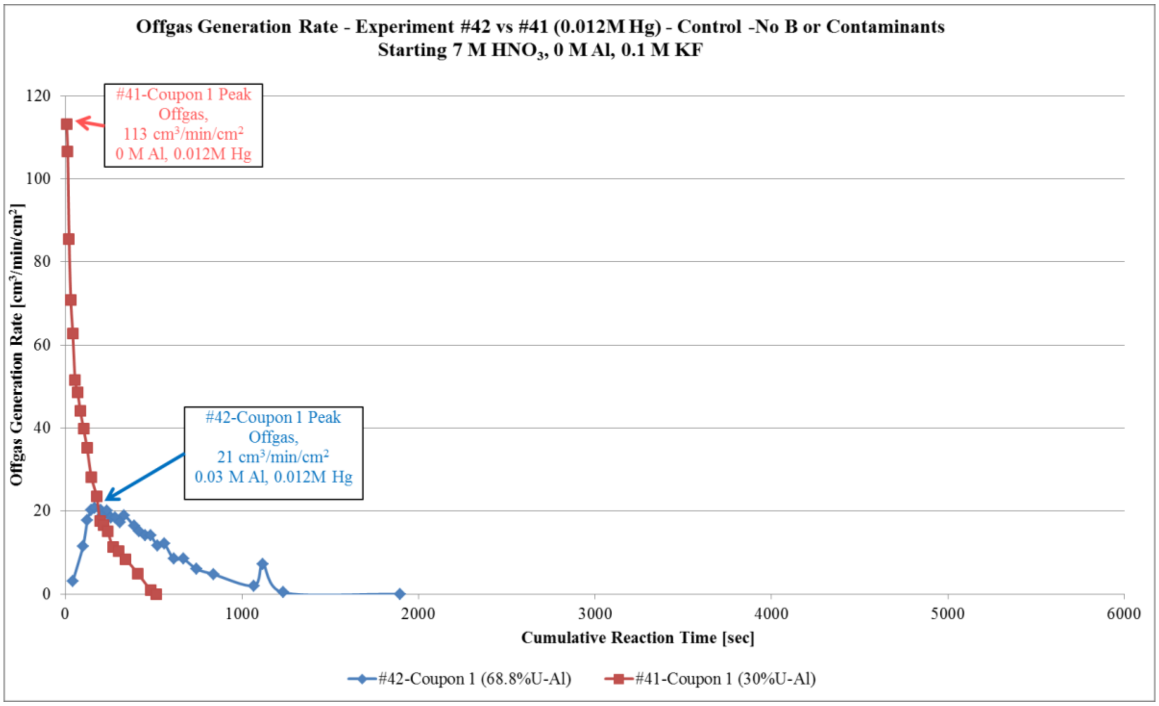

Figure 3-17. Comparison of Off-gas Generation Rates for Experiment 42 (68.8 wt % U-Al) and Experiment 41 (30 wt % U-Al) at 0.012 M Hg.

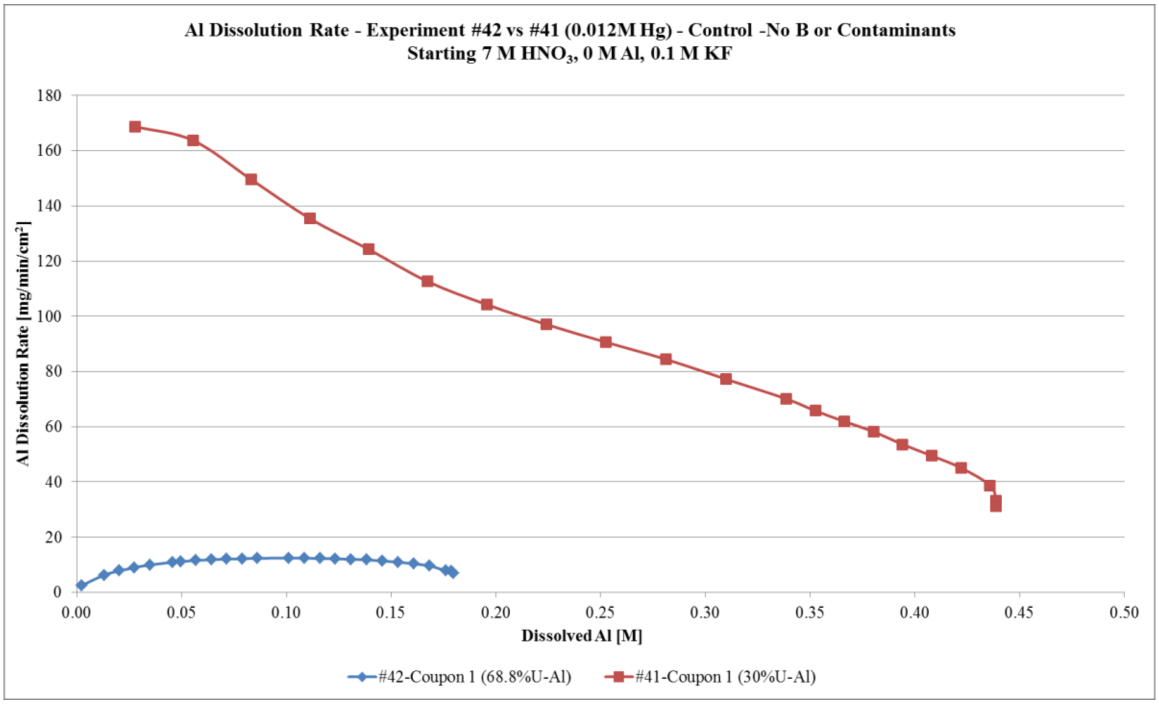

Figure 3-18. Comparison of Al Dissolution Rates for Experiment 42 (68.8 wt % U-Al) and Experiment 41 (30 wt % U-Al) at 0.012 M Hg.

3.8.1 H_2 Off-gas Concentrations for 30 wt % U-Al alloy

Hydrogen gas concentrations corrected for dilution for the dissolution of the 30 wt % U-Al alloy (Experiment 41) are provided in Table 3-9. Experiment 41 had a peak H_2 concentration initially, for gas sample 1, and the H_2 trended downward to 5.2 vol % at the end of the dissolution of the third coupon. The H_2 concentration profile throughout the experiment went from high-to-low which is different from the profile observed for both the Al-1100 and L-Bundle alloy (i.e. H_2 concentration trended low-to-high). When compared to Caracciolo's work, the same trend is observed. The H_2 concentration profile from Caracciolo's dissolution of a 16 wt % U-Al tubular assembly displayed the same high-to-low tendancy (Figure 3-19). The H_2 concentrations are very similar at low Al concentrations. However, Caracciolo's H_2 concentrations dropped to near 2 vol % at high dissolved Al near the end of the dissolution. In Experiment 41 the H_2 concentration drops to approximately 5 vol % at high Al concentrations. This divergence may be explained as an artifact of scaling from a large-scale to lab-scale experiment (13 h dissolution vs 2 h dissoluton, respectively), difference in solution impurities, difference in Hg concentration (0.001 M vs 0.012 M Hg), or the difference in the U percentage in the alloy, or alloy fabrication method.

Figure 3-20 compares Al dissolution rates from Experiment 41 with Caracciolo's semiworks dissoution of 16 and 25 wt % U-Al at 0.001 M Hg. This data demonstrate that dissolution rates for Experiment 41 that used a 30 wt % U-Al are consistent with Caracciolo's data from the dissolution of a 25 wt % U-Al alloy. The reduction in dissolution rate for Caracciolo's experiment observed in the initial portion of the fuel dissolution can be explained by the metered addition of mercury. Kyser's estimated rate at 0.001 M Hg for dissolution of 16 wt % U-Al with and without metering mercury is also plotted for comparison to Caracciolo's 16 wt % U-Al alloy data.[2,3]

Based on a review of off-gas generation rates and measured H_2 concentrations from this study, and a comparison of Al dissolution rates from the work performed by Caracciolo with this study, it was determined that the dissolution of 30 wt % U-Al alloy is bounding for H_2 generation rates expected from DR-3 fuels ranging from nominally 16 wt % to 68.8 wt % U. This conclusion is first based on a comparison of the off-gas generation rates and H_2 concentrations measured for the 30 wt % and 68.8 wt % U-Al alloys. Figure 3-17 shows a significant reduction in off-gas generation rates for the 68.8 wt % alloy. The corrected H_2 concentrations from the dissolution of the 68.8 wt % alloy were also much less. Hydrogen concentrations of 2.5 and 3.7 vol % are lower than concentrations measured for the dissolution of the 30 wt % alloy which ranged from 5.2 to 10.1 vol % (Table 3-9). At U concentrations less than 30 wt %, Figure 3-20 shows that the Al dissolution rate (which is generally proportional to off-gas generation rate) for 16 wt % and 25 wt % U-Al alloys are approximately equal to the dissolution rate of the 30 wt % U-Al alloy. The H_2 concentration profile from Caracciolo's dissolution of the 16 wt % U-Al alloy was also very similar to the profile from the dissolution of the 30 wt % U-Al alloy (Figure 3-19); although, the H_2 concentrations at the end of Caracciolo's dissolution were less (nominally 2 vs 5 vol %). Therefore, the H_2 generation rate from the 30 wt % alloy would be equivalent or greater than the rate calculated from the Caracciolo data. No data are available for the dissolution of U-Al alloys with U concentrations less than 16 wt %; however, a conservative evaluation of the flammable gas generation from alloys in this concentration range was performed using existing data from the dissolution of Al-1100 and 30 wt % U-Al alloys. The evaluation, including guidance for the number of L-Bundles which can be charged to the H-Canyon dissolver, is provided in Section 3.9.

Table 3-9. Corrected Gas Concentrations for H_2 – 30 wt % U-Al Alloy.

Experiment	**Gas Sample**	**H_2 [vol %]**
41	1	10.1
41	2	8.3
41	3	5.8
41	4	6.7
41	5	6.0
41	6	5.2

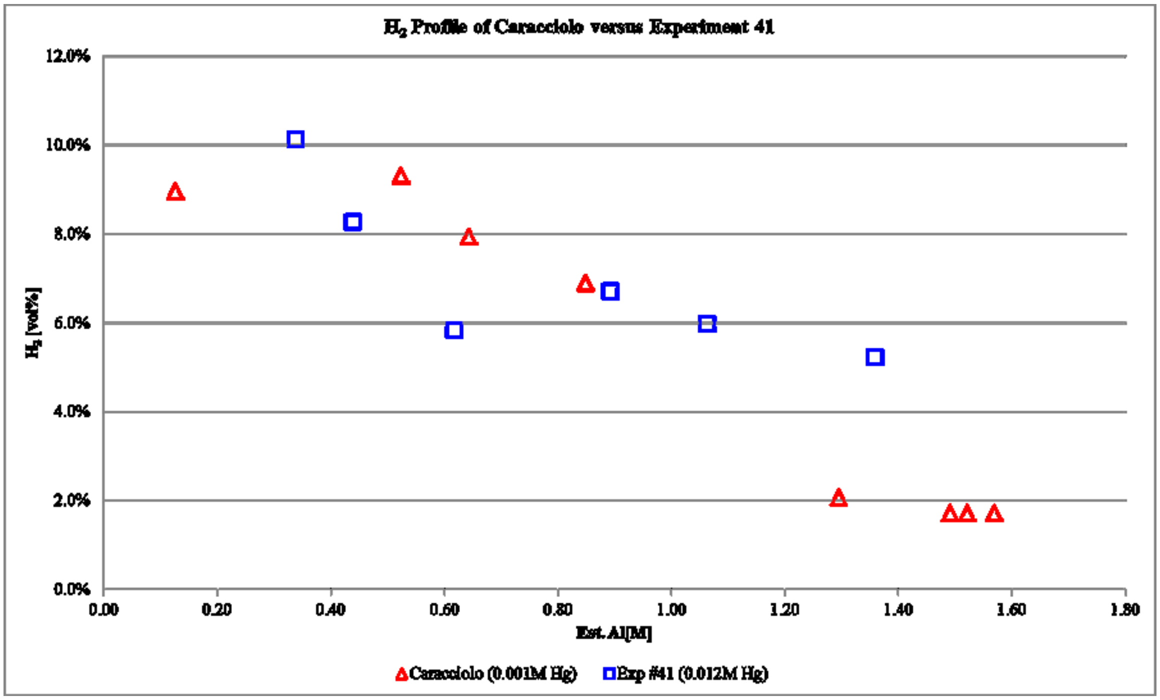

Figure 3-19. H_2 Profile for Experiment 41 (30 wt % U-Al) vs Caracciolo's Semiworks Dissolution of 16 wt % U-Al Alloy.

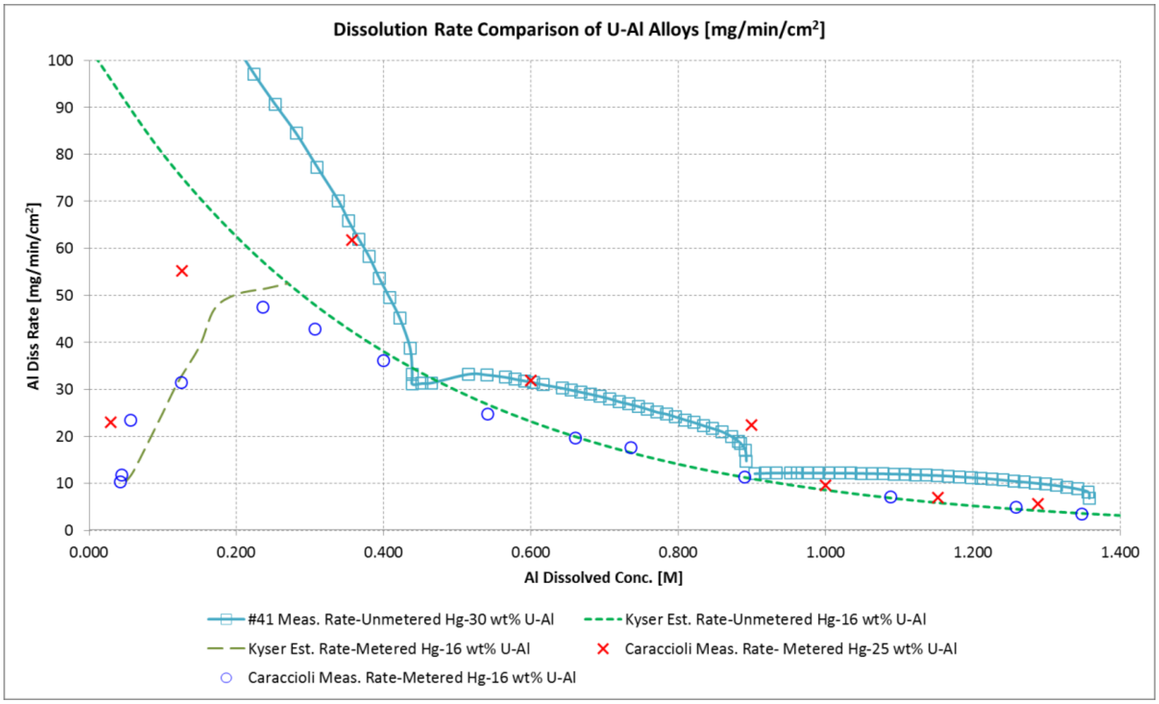

Figure 3-20. Aluminum Dissolution Rate Comparison for Experiment 41 (30 wt % U-Al), Caracciolo's Semiworks Dissolution of 16–25 wt % U-Al Alloy, and Kyser's Estimated Rates for 16 wt % U-Al Alloy

3.9 Off-gas Rate

To dissolve the SRE and DR-3 fuel assemblies in the H-Canyon dissolver without exceeding the 60% LFL limit on H_2, calculations were performed using the off-gas rate and mass balance corrected H_2 concentration data discussed in prior sections of this report and surface area calculations discussed in reference 10. The off-gas rates and H_2 concentrations measured for Experiment 36 were used to simulate the dissolution of the L-Bundle containing the SRE fuel since the L-Bundle material has to be dissolved first and has the largest surface area and off-gas generation compared to the SRE fuel.[10] The off-gas rates and H_2 concentrations measured for Experiment 41 are from the dissolution of a 30 wt % U-Al alloy. The off-gas generation data from Experiment 41 were similar to data from the dissolution of the L-Bundle material; therefore, the data from Experiment 41 were used to represent the dissolution of the L-Bundle containing the DR-3 fuel assemblies.

A criterion of 60% of the H_2 LFL value at 200 °C was used for the SRE and DR-3 fuel dissolution calculations in this report as was done in earlier studies.[2] The H_2 LFL at 200 °C was chosen due to the iodine reactor in the off-gas stream of the H-Canyon dissolver being heated to 200 °C. The H_2 LFL values come from data reported by Scott et al. (at 28 °C)[11] based on measurements using an air, H_2, N_2O, and NO mixture. The Scott data is broken down into three data sets based on the NO/N_2O molar ratio as shown in Table 3-10. The flammable points in Table 3-10 have an asterisk beside them and the other points did not propagate a flame. Although the NO and N_2O volume percent data measured in these experiments were only estimated values, the NO/N_2O ratios were lower than 2.57 and often closer to 0.33 than to 1.0 or 2.57. A plot of the Scott H_2 LFL's versus air volume percent for NO/N_2O ratios of 0.33, 1.0 and 2.57 are shown in Figure 3-21. The flammable points in Figure 3-21 have a red fill and the non-flammable points have no fill. Based on the estimated NO/N_2O ratios in the current experiments and that the H_2 LFL for the NO/N_2O ratio of 0.33 is more conservative than the higher ratios, the LFL data at an NO/N_2O ratio of 0.33 was used for the flammability calculations.

Table 3-10. H_2 Lower Flammability Limit from Scott Data.

NO/N_2O Ratio:	2.57	1.00	0.33
Air [vol %]	**Scott H_2 LFL[vol %]**	**Scott H_2 LFL[vol %]**	**Scott H_2 LFL[vol %]**
1.5	6.2*	---	---
4.6	6.4*	---	---
6.2	5.9	---	---
21.7	6.4*	---	---
29	---	6.3*	---
34	---	---	5.3*
34.5	6.1	---	---
46	---	---	4.5
50	---	5.1	6.3*
52	---	---	4.5
52.6	7.2*	---	---
54	---	7.0*	---
58		5.9	
59	---	---	5.6*
60.8	5.5	---	---
61	---	6.9*	---
63	---	---	4.1
66.8	6.6*	---	---
69	---	6.3*	---
74.1	4.3	---	---
81	---	4.2	---

*propagated flame

In order to use the Scott flammability data at an NO/N_2O ratio of 0.33, all the data points in Table 3-10 (including points that did and did not propagate a flame) were fit to an equation. The fitted equation for the Scott H_2 LFL data for the NO/N_2O ratio of 0.33 for varying air concentrations is:

$$(7) \qquad H_2 \text{ LFL vol\%} = 0.01 * \left(1.636 + \frac{284.242}{Air\% * 100} - \frac{5485.518}{(Air\% * 100)^2}\right)$$

Where:

H_2 *LFL vol%* – the H_2 lower flammability limit in volume percent
Air% – the volume percent of air in the gas mixture

The fitted equation was used to predict the H_2 LFL limits for the dissolver L-Bundle calculations and is shown in Figure 3-21 along with the original Scott data for the points which propagated a flame.

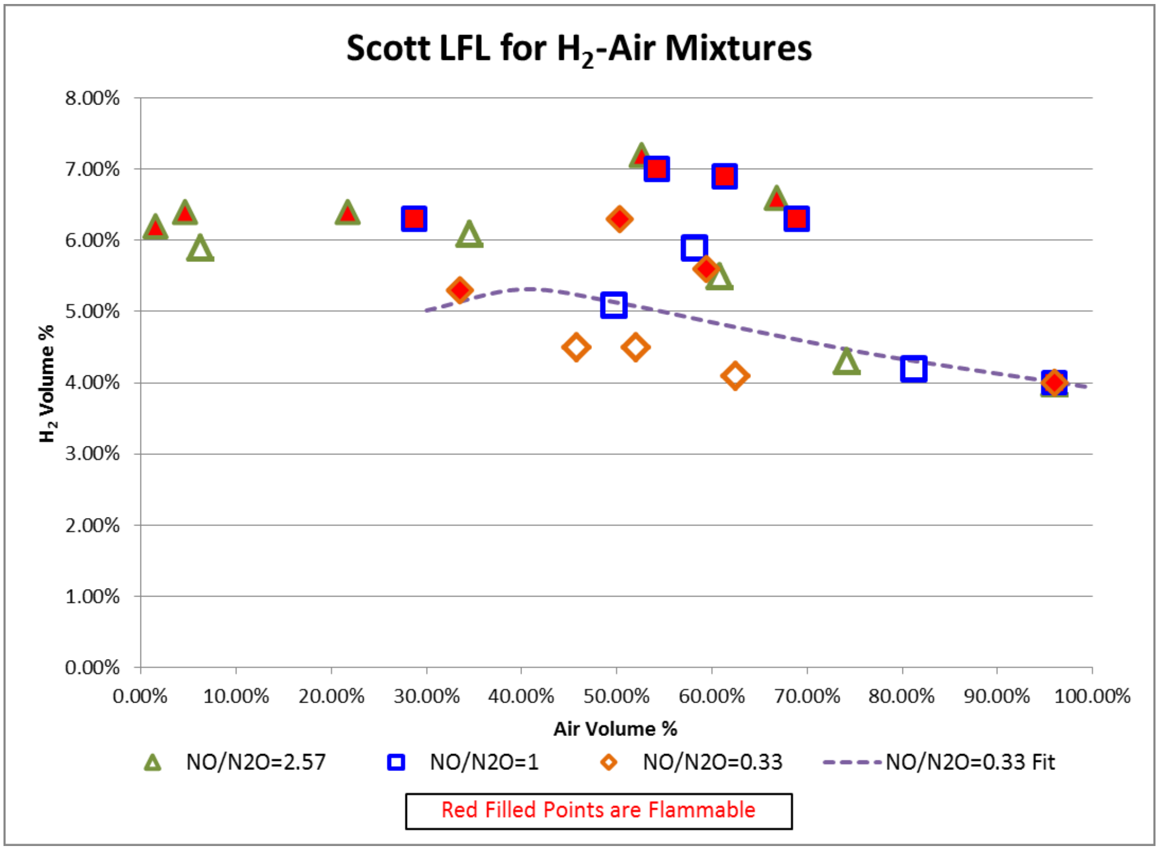

Figure 3-21. Scott Lower Flammability Limits for H_2–Air Mixtures.

The 28 °C Scott data was corrected to 200 °C using a temperature correction from Dyer's work:[12]

(8) $LFL_T = LFL_{ref}*(1 - A*(T-T_{ref}))$

Where:

LFL_T – the LFL at Temperature T (°C)
LFL_{ref} – the LFL at Reference Temperature T (°C)
A – the empirical coefficient (Zabetakis attenuation factor) = 0.0011
T – the temperature (°C) at which LFL is to be evaluated

For the 28 °C Scott data the correction to 200 °C becomes:

(9) $LFL_{200} = LFL_{28}*(1 - 0.0011*(200-28)) = LFL_{28}*0.811$

The next step in the flammability calculation is to pick the measured peak off-gas rate from the appropriate dissolution experiments and its associated mass balance corrected H_2 concentration. The way the experiments were performed, a gas sample was taken after the dissolution of approximately one-half of a metal coupon and another gas sample taken when the coupon was completely dissolved. For Experiment 36, four L-Bundle coupons were dissolved giving eight gas samples. For Experiment 41, three 30 wt % U-Al coupons were dissolved giving six gas samples. For each gas sample, a peak off-gas rate was selected from the measured off-gas rates during which time the gas sample was collected. This peak off-gas rate is used in conjunction with the measured H_2 concentration for each gas sample that is mass balance corrected for sample dilution. For Experiments 36 and 41 the maximum off-gas rates and associated H_2 concentrations are shown in Table 3-11.

The peak off-gas rate for an L-Bundle containing a fuel assembly is based on the outer surface area of the L-Bundle since it has the greater surface area and is dissolved initially as shown in reference 10.

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 ft^2. Therefore the predicted peak off-gas rate per L-Bundle is calculated by:

(10) Predicted Peak Off-gas Rate per Bundle [scfm] = Estimated or Max Peak Off-gas Rate [scfm/ft^2] *L-Bundle Outer Surface Area [ft^2]

For 54 in. immersion in the dissolver, the calculation becomes:

(11) Predicted Peak Off-gas Rate per Bundle [scfm] = Estimated or Max Peak Off-gas Rate [scfm/ft^2] *6.4546 ft^2

Depending on the desired number of L-Bundles to be charged to the dissolver, the Total Predicted Peak Off-gas Rate is calculated by:

(12) Total Predicted Peak Off-gas Rate [scfm] = Predicted Peak Off-gas Rate per Bundle [scfm] * Number of Bundles

Therefore the Predicted Peak H_2 Off-gas rate based on the total predicted peak off-gas rate is calculated by:

(13) Predicted Peak H_2 Off-gas Rate [scfm] = Total Predicted Peak Off-gas Rate [scfm]* Peak Measured/Mass Balance H_2 Concentration [Vol%]

Using the Predicted Peak H_2 Off-gas rate and the H-Canyon Air Purge rate, the predicted H_2 concentration with the air purge is calculated by:

$$\text{(14)} \quad \text{Predicted H}_2\text{ Concentration with air dilution [vol\%]} = \frac{\text{Predicted Peak H}_2\text{Off−gas rate [scfm]}}{\text{Total Predicted Peak Off−gas rate [scfm] + Air Purge Rate [scfm])}}$$

For the nominal H-Canyon dissolver air purge of 40 scfm, the calculation becomes:

$$\text{(15)} \quad \text{Predicted H}_2\text{ Concentration with air dilution [vol\%]} = \frac{\text{Predicted Peak H}_2\text{ Off−gas rate [scfm]}}{\text{Total Predicted Peak Off−gas rate [scfm] + 40 [scfm])}}$$

The predicted H_2 Concentration with air dilution is then compared with 60% of the calculated H_2 LFL for the air concentration to see if it is less than this value.

The dissolver off-gas calculations for Experiment 36 (Table 3-11) showed that for SRE fuel in L-Bundles, four bundles could be charged at any given time based on the peak off-gas rates (Appendix B). Based on Experiment 41, DR-3 assemblies (modeled using the 30 wt % U-Al alloy in L-Bundles) would exceed 60% of the H_2 LFL if four L-Bundles are dissolved. A conservative approach was used for the flammability calculations where the peak off-gas rate was used during the time a gas sample was collected. It has been reported in multiple past experiments that as the dissolved Al increases in the HNO_3 solution, the dissolution reaction slows down.[2,5] From the experiments performed in this work, the Al dissolution rate slows down as the dissolved Al concentration increases as shown in Figure 3-11 and Figure 3-16. The off-gas generation rate also decreases as the dissolved Al increases.

Table 3-11. L-Bundle Calculations Based on Peak Off-gas Rates for Dissolver Charges of SRE and DR-3 Fuel Assemblies.

Experiment	Bundles	Alloy	Est. Initial HNO_3 [M]	Est. Initial Al Conc [M]	Hg [M] (assume constant)	Gas Sample	Peak Measured/ Mass Bal H_2 [vol%]	Meas Peak off-gas rate [scfm/ft2]	Total Predicted Peak Off-gas Rate [scfm]	Predicted Peak H2 Off-gas rate [scfm]	Predicted H_2 vol% with air dilution	60% of Dyer Corrected LFL [vol%]	Check Pred H_2 with dilution ≤ 60% LFL
36	4	L-Bundle	7.01	0.00	0→0.002	1	4.38%	1.19	30.72	1.35	1.90%	2.41%	OK
36	4	L-Bundle	5.65	0.33	0→0.002	2	0.32%	0.41	10.62	0.03	0.07%	2.12%	OK
36	4	L-Bundle	5.31	0.42	0→0.002	3	4.76%	1.43	36.86	1.76	2.28%	2.47%	OK
36	4	L-Bundle	4.42	0.62	0→0.002	4	7.07%	0.24	6.07	0.43	0.93%	2.04%	OK
36	4	L-Bundle	3.59	0.82	0→0.002	5	2.33%	0.50	12.85	0.30	0.57%	2.16%	OK
36	4	L-Bundle	2.35	1.08	0→0.002	6	10.46%	0.26	6.71	0.70	1.50%	2.05%	OK
36	4	L-Bundle	1.77	1.22	0→0.002	7	3.87%	0.40	10.28	0.40	0.79%	2.11%	OK
36	4	L-Bundle	0.89	1.46	0→0.002	8	3.98%	0.23	5.93	0.24	0.51%	2.03%	OK
---	---	---	---	---	---	---	---	---	---	---	---	---	---
41	4	30%U-Al	7.16	0.00	0.012	1	10.14%	3.61	93.09	9.44	7.10%	2.44%	FAIL
41	4	30%U-Al	5.89	0.34	0.012	2	8.27%	0.56	14.47	1.20	2.20%	2.18%	Marginal
41	4	30%U-Al	5.52	0.44	0.012	3	5.84%	0.97	25.11	1.47	2.25%	2.34%	OK
41	4	30%U-Al	4.85	0.62	0.012	4	6.71%	0.48	12.50	0.84	1.60%	2.15%	OK
41	4	30%U-Al	3.67	0.89	0.012	5	5.98%	0.49	12.58	0.75	1.43%	2.15%	OK
41	4	30%U-Al	3.03	1.06	0.012	6	5.24%	0.20	5.15	0.27	0.60%	2.02%	OK

Since four bundles of the 30 wt % U-Al alloy (which is applicable to the DR-3 fuel) could not be charged to the dissolver without exceeding 60% of the H_2 LFL using the peak off-gas approach, the less conservative method of choosing the off-gas rate associated with a specific dissolved Al concentration was examined. In order to use the off-gas rate associated with a specific dissolved Al concentration, the measured off-gas rates and their associated mass balance corrected H_2 concentrations were correlated with the dissolved Al as shown in Table 3-12. The dissolved Al concentrations are estimated as explained in Section 3.3.

Using the off-gas rates associated with the dissolved Al concentrations in Experiment 41, the dissolver off-gas calculations for the 30 wt % U-Al alloy fuels in L-Bundles (i.e., DR-3 fuel) show that a graded approach is needed to permit dissolution of these fuel assemblies. For this graded approach, a fit of the off-gas rate data for Experiment 41 in terms of dissolved Al was performed that was continuous over the dissolved coupon range. The fit of the data from TableCurve 2D (Systat software)[13] was:

(16) Est. Off-gas rate [scfm/ft^2] = 4.3284227 - 22.654108*(Est. Al [M]) + 50.208105*(Est. Al [M])^2 - 52.740289*(Est. Al [M])^3 + 25.89167*(Est. Al [M])^4 - 4.7808848*(Est. Al [M])^5

Where:

Est. Off-gas rate [scfm/ft^2] – the estimated off-gas rate per surface area from fit across all coupons
Est. Al [M] – the estimated dissolved Al concentration

This empirical fit of the off-gas rate data is shown along with the measured data in Figure 3-22. The flammability calculations used the corrected H_2 concentrations corresponding to the dissolved Al concentration ranges (Table 3-12). Results from the flammability calculations are provided in Table 3-13.

To illustrate how the H_2 lower flammability calculations were performed for Table 3-13, a sample calculation is shown for Experiment 41 at an estimated 0.18 M Al concentration. Initially, the estimated off-gas rate for 0.18 M Al is determined using Equation (16) above:

(17) Est. Off-gas rate [scfm/ft^2] = 4.3284227 - 22.654108*(0.18) + 50.208105*(0.18)^2 - 52.740289*(0.18)^3 + 25.89167*(0.18)^4 - 4.7808848*(0.18)^5 = 1.60 [scfm/ft^2]

Next the predicted peak off-gas rate per L-Bundle for Experiment 41 at 0.18 M Al is calculated using Equation 18:

(18) Predicted Peak Off-gas Rate per Bundle [scfm] = 1.60 [scfm/ft^2] *6.4546 ft^2 = 10.30 [scfm]

Assuming 1 L-Bundle is to be charged to the dissolver, the total predicted peak off-gas rate is then calculated using Equation 19:

(19) Total Predicted Peak Off-gas Rate [scfm] = 10.30 [scfm] * 1 = 10.30 [scfm]

Now based on the corrected H_2 concentration for Experiment 41 gas sample 1 of 10.1 vol % from Table 3-9, the predicted peak H_2 off-gas rate for 1 L-Bundle is calculated using Equation 20:

(20) Predicted Peak H_2 Off-gas Rate [scfm] = 10.30 [scfm]* 10.1 [Vol %] = 1.04 [scfm]

The predicted H_2 concentration with air dilution is then calculated using Equation 21:

(21) $$\text{Predicted } H_2 \text{ Concentration with air dilution [vol\%]} = \frac{1.04 \text{ [scfm]}}{10.30 \text{ [scfm]} + 40 \text{ [scfm]})} = 2.08 \text{ [vol \%]}$$

To calculate the lower flammability limit of H_2 based on Scott's data, calculate the volume percent of air during the peak off-gas rate using Equation 22:

(22) $$\text{Predicted air concentration with air dilution [vol\%]} = \frac{40 \text{ [scfm]}}{10.30 \text{ [scfm]} + 40 \text{ [scfm]})} = 79.5 \text{ [vol \%]}$$

Then Equation 23 is used to calculate the lower flammability limit of H_2 based on the air percent assuming a NO/N_2O ratio of 0.33:

(23) $$H_2 \text{ LFL vol\%} = 1.636 + \frac{284.242}{79.5} - \frac{5485.518}{(79.5)^2} = 4.34 \text{ vol \%}$$

This lower flammability limit of H_2 is then adjusted from 28 °C to 200 °C using the Dyer correction from Equation 24:

(24) LFL_T = 4.34 vol %*0.811 = 3.52 vol %

The safety limit is defined as 60% of the H_2 lower flammability limit at 200 °C, therefore take 60% of the Dyer corrected value:

(25) Safety Limit = 3.52 vol %*0.60 = 2.11 vol %

Sixty percent of the Dyer corrected H_2 lower flammability limit at 200 °C for Experiment 41 at 0.18 M Al is 2.11 vol %. The predicted H_2 concentration with air dilution for Experiment 41 at 0.18 M Al is 2.08 vol % which is less than the 60% of the Dyer corrected H_2 LFL of 2.11 vol%, so 1 L-Bundle may be charged as shown in Table 3-13.

The calculations in Table 3-13 show the number of bundles that can be charged with increasing Al concentration without violating 60% of the H_2 LFL for U-Al alloys ranging from 16–68.8 wt % U. Table 3-13 shows for less than or equal to 0.17 M dissolved Al that no L-Bundles of a U-Al alloy (i.e., DR-3 fuel assemblies) can be dissolved without exceeding 60% of the H_2 LFL. If the dissolved Al concentration is greater than 0.17 M but less than or equal to 0.30 M then 1 L-Bundle of a U-Al alloy can be charged. As the dissolved Al concentration continues to increase, the number of L-Bundles that can be dissolved also increases. The maximum number of L-Bundles containing a U-Al alloy (i.e., DR-3 fuel assemblies ranging from 16–68.8 wt % U) which can be charged as a function of the Al concentration is summarized in Table 3-14.

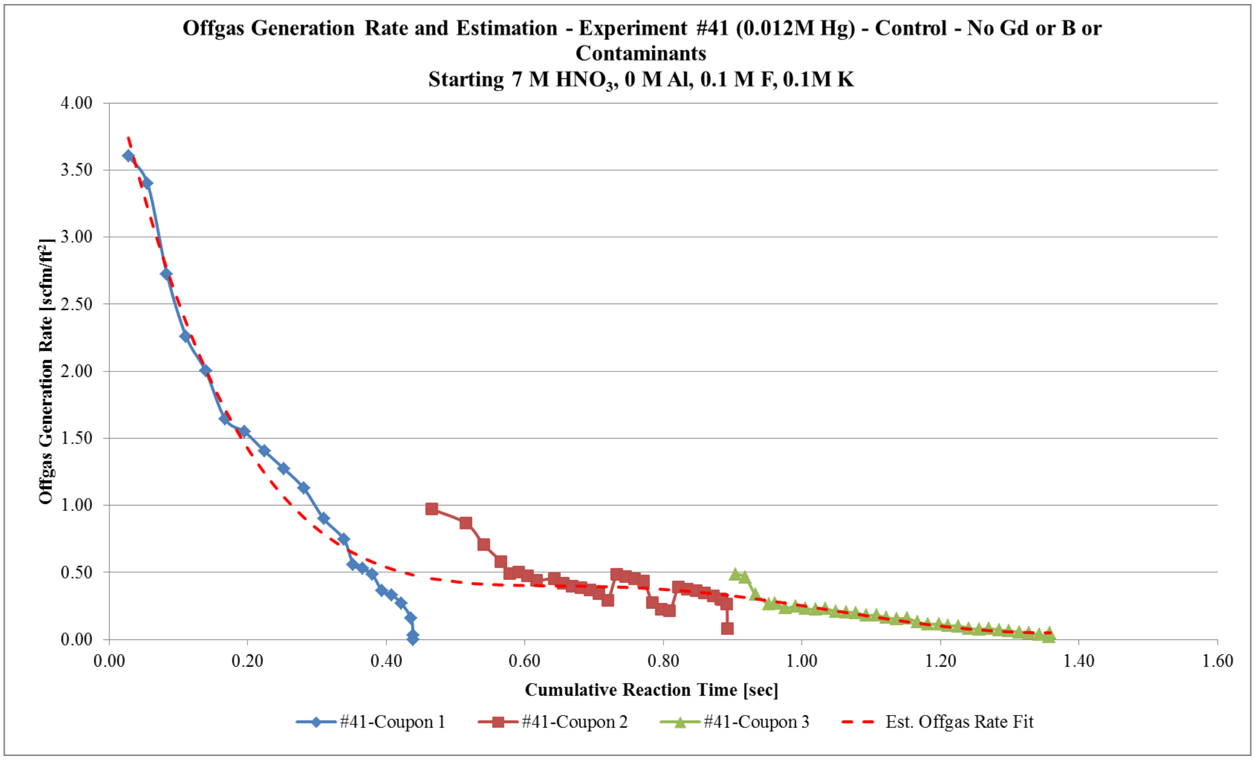

Figure 3-22. Off-gas Rates and Estimated Fit for Flammability Calculations

Table 3-12. Corrected H_2 Concentrations for 30 wt % U-Al Assemblies.

Dissolved Al [M]	Corrected H_2 Concentrations [vol%]
0< [Al] ≤ 0.34	10.14%
0.34 < [Al] ≤ 0.44	8.27%
0.44 < [Al] ≤ 0.62	5.84%
0.62 < [Al] ≤ 0.89	6.71%
0.89 < [Al] ≤ 1.06	5.98%
1.06 < [Al] ≤ 1.36	5.24%

Table 3-13. L-Bundle Calculations Based on Correlation of Off-gas Rate with Dissolved Al Concentration for Dissolver Charges of DR-3 Fuel Assemblies Ranging from 16–68.8 wt % U-Al Alloy.

Experiment	Bundles	Alloy	Est. HNO_3 [M]	Est. Al Conc [M]	Hg [M] (assume constant)	Gas Sample	Measured/ Mass Bal H_2 [vol%]	Est. Off-gas rate [scfm/ft^2]	Total Predicted Peak Off-gas Rate [scfm]	Predicted Peak H2 Off-gas rate [scfm]	Predicted H_2 vol% with air dilution	60% of Dyer Corrected LFL [vol%]	Check Pred H_2 with dilution ≤ 60% LFL
41	0	30%U-Al	6.79	0.10	0.012	1	10.14%	2.51	0.00	0	0.00%	1.91%	OK
41	0	30%U-Al	6.52	0.17	0.012	1	10.14%	1.69	0.00	0	0.00%	1.91%	OK
41	1	30%U-Al	6.49	0.18	0.012	1	10.14%	1.60	10.30	1.04	2.08%	2.11%	OK
41	1	30%U-Al	6.04	0.30	0.012	1	10.14%	0.83	5.33	0.54	1.19%	2.02%	OK
41	2	30%U-Al	6.00	0.31	0.012	1	10.14%	0.78	10.13	1.03	2.05%	2.11%	OK
41	2	30%U-Al	5.89	0.34	0.012	1	10.14%	0.68	8.80	0.89	1.83%	2.09%	OK
41	3	30%U-Al	5.85	0.35	0.012	2	8.27%	0.65	12.63	1.04	1.98%	2.15%	OK
41	3	30%U-Al	5.70	0.39	0.012	2	8.27%	0.56	10.79	0.89	1.76%	2.12%	OK
41	4	30%U-Al	5.66	0.40	0.012	2	8.27%	0.54	13.90	1.15	2.13%	2.18%	OK
41	4	30%U-Al	5.51	0.44	0.012	2	8.27%	0.48	12.39	1.02	1.96%	2.15%	OK
41	7	30%U-Al	5.47	0.45	0.012	3	5.84%	0.47	21.18	1.24	2.02%	2.29%	OK
41	7	30%U-Al	4.69	0.66	0.012	4	6.71%	0.399	18.02	1.21	2.08%	2.24%	OK
41	8	30%U-Al	4.65	0.67	0.012	4	6.71%	0.398	20.56	1.38	2.28%	2.28%	OK
41	8	30%U-Al	4.01	0.84	0.012	4	6.71%	0.36	18.47	1.24	2.12%	2.25%	OK
41	9	30%U-Al	3.97	0.85	0.012	4	6.71%	0.35	20.50	1.38	2.27%	2.28%	OK
41	9	30%U-Al	3.86	0.88	0.012	4	6.71%	0.34	19.58	1.31	2.20%	2.26%	OK
41	10	30%U-Al	3.82	0.89	0.012	5	5.98%	0.33	21.38	1.28	2.08%	2.29%	OK
41	10	30%U-Al	2.10	1.35	0.012	6	5.24%	0.05	3.26	0.17	0.39%	1.98%	OK

Table 3-14. Maximum L-Bundles of DR-3 Assemblies Containing 16–68.8 wt % U-Al Alloy Generating < 60% of the H_2 LFL

Dissolved Al [M]	Max DR-3 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] ≤ 1.35	10

To conservatively evaluate the number of L-Bundles containing U-Al alloy fuel assemblies with a U concentration less than 16 wt %, flammable gas generation calculations were performed using off-gas generation rates from Al-1100 alloy (Experiment 28) and the H_2 concentration profile for the 30 wt % U-Al alloy (Experiment 41). The off-gas generation rate during dissolution of Al-1100 is expected to provide a bounding value when compared to the dissolution of alloys containing concentrations of U less than 16 wt %. Likewise, the H_2 concentration profile measured during the dissolution of the 30 wt % U-Al alloy is expected to provide bounding values for the H_2 concentration in the off-gas from the dissolution of these materials. The 30 wt % U-Al alloy had the highest H_2 values for all dissolved Al concentrations. To use the off-gas generation from Experiment 28, the data were fit to a three parameter exponential decay using SigmaPlot 12[14] to smooth the data where coupons two, three, and four were added to the dissolving solution.

$$\text{Est. Off-gas rate}\left[\frac{\text{scfm}}{\text{ft}^2}\right] = 0.464 * \exp\left(\frac{0.11}{\text{Est. Al [M]} + 0.034}\right) \tag{26}$$

Where:

Est. Off-gas rate [scfm/ft^2] – the estimated off-gas rate per surface area from fit across all coupons
Est. Al [M] – the estimated dissolved Al concentration

This empirical fit of the off-gas rate data is shown along with the measured data in Figure 3-23. The flammability calculations used the corrected H_2 concentrations from Experiment 41 which correspond to dissolved Al ranges (Table 3-12). Results from the flammability calculations are provided in Table 3-15.

The calculations in Table 3-15 show the number of bundles that can be charged to the H-Canyon dissolver with increasing Al concentration without exceeding 60% of the H_2 LFL during dissolution of U-Al alloys with U concentrations less than 16 wt %. No bundles of DR-3 fuel with U concentrations less than 16 wt % can be charged to the dissolver for Al concentrations less than or equal to 0.17 M (consistent with Table 3-14). If the dissolved Al concentration is greater than 0.17 M but less than or equal to 0.34 M then 1 L-Bundle containing fuel with U in this concentration range can be charged. As the dissolved Al concentration continues to increase, the number of L-Bundles that can be dissolved also increases. The maximum number of DR-3 bundles containing a 0–16 wt % U-Al alloy which can be charged as a function of the Al concentration is summarized in Table 3-16. For dissolver charges containing assemblies with both 0–16 wt % and 16–68.8 wt % U-Al alloys, the number of L-Bundles allowed by Table 3-16 applies.

The uncertainties associated with the number of bundles of SRE/DR-3 fuel which can be charged to the H-Canyon dissolver were not calculated; however, the largest uncertainty associated with the calculations is from the H_2 analysis. The uncertainty in the H_2 analysis was reported as ± 20 %. Therefore, the uncertainty in the bundle calculation is driven by this value.

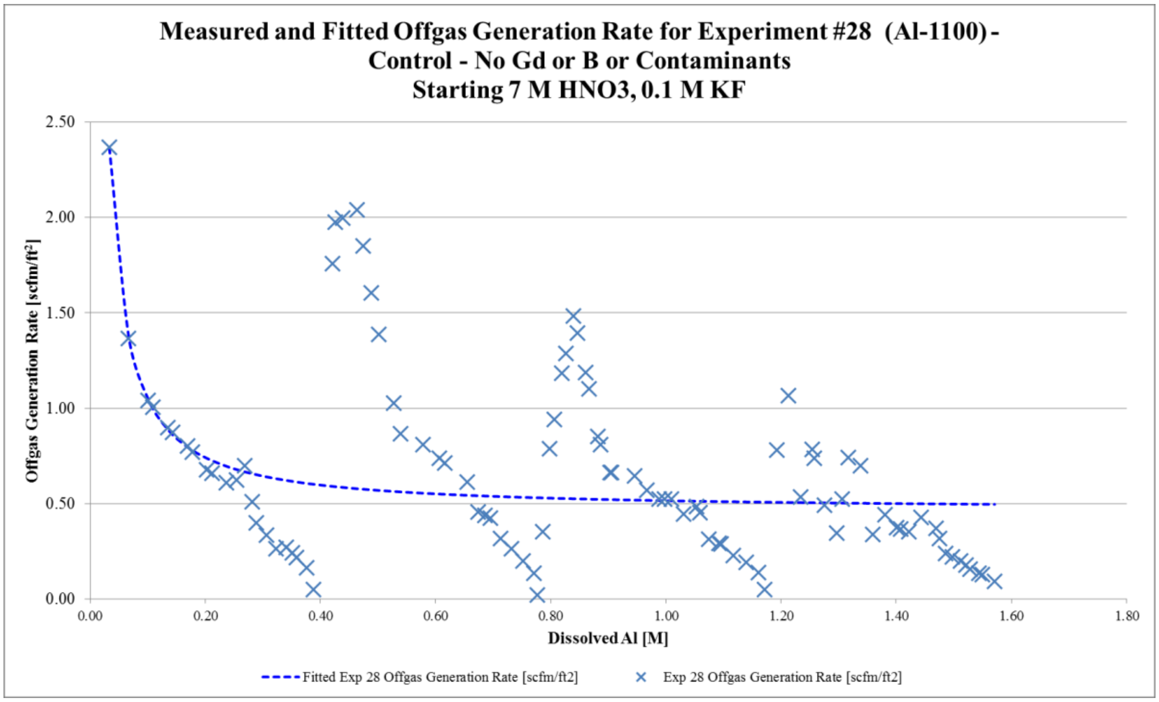

Figure 3-23. Off-gas Rates and Estimated Fit for 0–16 wt % U-Al Alloy Flammability Calculations

Table 3-15. L-Bundle Calculations Based on Experiment 28 Off-gas Rate Correlation and Experiment 41 H_2 Concentrations for Dissolver Charges of DR-3 Fuel Assemblies from 0–16 wt % U-Al Alloy

Experiment	Bundles	Alloy	Est. HNO_3 [M]	Est. Al Conc [M]	Hg [M] (assume constant)	Gas Sample	Measured/ Mass Bal H_2 [vol%]	Est. Off-gas rate [scfm/ft^2]	Total Predicted Peak Off-gas Rate [scfm]	Predicted Peak H_2 Off-gas rate [scfm]	Predicted H_2 vol% with air dilution	60% of Dyer Corrected LFL [vol%]	Check Pred H_2 with dilution ≤ 60% LFL
28/41	0	0-16%U-Al	6.79	0.10	0.012	1	10.14%	1.05	0.00	0.00	0.00%	1.91%	OK
28/41	0	0-16%U-Al	6.52	0.17	0.012	1	10.14%	0.80	0.00	0.00	0.00%	1.91%	OK
28/41	1	0-16%U-Al	6.49	0.18	0.012	1	10.14%	0.78	5.01	0.51	1.13%	2.01%	OK
28/41	1	0-16%U-Al	5.89	0.34	0.012	1	10.14%	0.62	4.02	0.41	0.93%	1.99%	OK
28/41	2	0-16%U-Al	5.85	0.35	0.012	2	8.27%	0.62	7.98	0.66	1.37%	2.07%	OK
28/41	2	0-16%U-Al	5.51	0.44	0.012	2	8.27%	0.59	7.55	0.62	1.31%	2.06%	OK
28/41	3	0-16%U-Al	5.47	0.45	0.012	3	5.84%	0.58	11.28	0.66	1.28%	2.13%	OK
28/41	3	0-16%U-Al	4.24	0.78	0.012	4	6.71%	0.53	10.28	0.69	1.37%	2.11%	OK
28/41	4	0-16%U-Al	4.20	0.79	0.012	4	6.71%	0.53	13.69	0.92	1.71%	2.17%	OK
28/41	4	0-16%U-Al	3.86	0.88	0.012	4	6.71%	0.52	13.51	0.91	1.69%	2.17%	OK
28/41	7	0-16%U-Al	3.82	0.89	0.012	5	5.98%	0.52	23.61	1.41	2.22%	2.32%	OK
28/41	7	0-16%U-Al	3.19	1.06	0.012	5	5.98%	0.51	23.18	1.39	2.19%	2.31%	OK
28/41	8	0-16%U-Al	3.15	1.07	0.012	6	5.24%	0.51	26.47	1.39	2.09%	2.36%	OK
28/41	8	0-16%U-Al	2.10	1.35	0.012	6	5.24%	0.50	25.94	1.36	2.06%	2.35%	OK

Table 3-16. Maximum L-Bundles of DR-3 Assemblies Containing 0–16 wt % U-Al Alloy Generating < 60% of the H_2 LFL

Dissolved Al [M]	Max DR-3 Bundles
$[Al] \leq 0.17$	0
$0.17 < [Al] \leq 0.34$	1
$0.34 < [Al] \leq 0.44$	2
$0.44 < [Al] \leq 0.78$	3
$0.78 < [Al] \leq 0.88$	4
$0.88 < [Al] \leq 1.06$	7
$1.06 < [Al] \leq 1.35$	8

3.10 Comparison of Caracciolo Study with Current Experimental Data

The previous work by Caracciolo supporting the technical basis for fuel dissolution was based on large-scale experiments. The lab-scale experimental data provided in this report are generally consistent with the work by Caracciolo and expands upon his work. This report provides alloy-specific, detailed off-gas and H_2 concentration profiles relevant to dissolving SRE and DR-3 fuels at increased Hg concentrations. When the U-Al alloys were dissolved, the H_2 concentration profiles were similar to Caracciolo's data. Hydrogen concentrations were observed to be the highest at the beginning of the dissolution and they trended downward consistent with Caracciolo’s work. A comparison of Caracciolo's Al dissolution rate for a 25 wt % U-Al alloy fuel tube to the dissolution rate measured in this work using a 30 wt % U-Al alloy were similar, except at the beginning of the dissolution. This difference in rates was due to the slow addition of Hg during the initial fuel tube dissolution in Caracciolo’s work.

The H_2 flammability calculations performed using Caracciolo’s data when compared to calculations performed with data from the current study are different due to the assumptions which were used. In the past, an average H_2 concentration of 7 vol % was used for all flammable gas calculations based on the Caracciolo data (which peaked at 10 vol % at the beginning of dissolution) with an allowance made for the slow addition of Hg to reduce the dissolution rate. The peak off-gas rates used for flammability calculations were also estimated from the Caracciolo data. In contrast, the calculations in this report use discrete H_2 concentrations for specific dissolved Al ranges where peak off-gas is observed.

4.0 Conclusions

Hydrogen flammability calculations were performed using the experimental data to provide guidance for H-Canyon to safely dissolve SRE fuel followed by DR-3 fuel assemblies with respect to the H_2 concentrations in the off-gas at projected peak rates. To stay under the 60% LFL for H_2, the initial and subsequent charges of L-Bundles containing SRE fuel shall be limited to four bundles in a charge. The L-Bundles containing DR-3 fuel may be processed based on the dissolved Al concentration as shown in Table 4-1 (for 16–68.8 wt % U-Al alloy) and Table 4-2 (for 0–16 wt % U-Al alloy). For dissolver charges containing assemblies with both 16–68.8 wt % and 0–16 wt % U-Al alloys, the number of L-Bundles allowed by Table 4-2 applies. Based on an immersion depth of 54 in. and an air purge rate of 40 scfm in the H-Canyon dissolver, the dissolved Al must be greater than 0.17 M before even one L-Bundle of DR-3 may be dissolved. Once a higher dissolved Al concentration is reached, the number of L-Bundles of DR-3 can be processed at the rates provided in the tables. Results from the experiments indicate that increasing the Hg concentration from 0.002 M to the range of 0.012–0.015 M generally reduced the off-gas H_2 concentrations.

Table 4-1. Maximum L-Bundles of DR-3 Assemblies Containing 16–68.8 wt % U-Al Alloy Generating < 60% of the H_2 LFL

Dissolved Al [M]	Max DR-3 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] ≤ 1.35	10

Table 4-2. Maximum L-Bundles of DR-3 Assemblies Containing 0–16 wt % U-Al Alloy Generating < 60% of the H_2 LFL

Dissolved Al [M]	Max DR-3 Bundles
[Al] ≤ 0.17	0
0.17 < [Al] ≤ 0.34	1
0.34 < [Al] ≤ 0.44	2
0.44 < [Al] ≤ 0.78	3
0.78 < [Al] ≤ 0.88	4
0.88 < [Al] ≤ 1.06	7
1.06 < [Al] ≤ 1.35	8

Based on a review of off-gas generation rates and measured H_2 concentrations from this study, and a comparison of Al dissolution rates from the work performed by Caracciolo with this study, it was concluded that the dissolution of 30 wt % U-Al alloy is bounding for H_2 generation rates expected from DR-3 fuels ranging from nominally 16–68.8 wt % U-Al alloy (Table 4-1). For DR-3 fuels containing less than nominally 16 wt % U-Al alloy, bounding H_2 generation rates were calculated using the off-gas rate from the dissolution of Al-1100 alloy and the H_2 concentration profile for the dissolution of the 30 wt % U-Al alloy.

The time required to completely dissolve a charge of SRE or DR-3 fuel using the modified flowsheet is expected to be shorter than the previously used flowsheet (i.e. 48 hours). The increase in the Hg concentration from 0.002 M to 0.012–0.015 M will result in increased dissolution rates, especially at higher Al concentrations. Therefore, dissolution times may be adjusted based on field observations.

5.0 Recommendations

This report describes how to process SRE and DR-3 fuels in the H-Canyon dissolver beginning with the remaining Batch 4 bundles. Prior to charging the remaining 12 DR-3 bundles in Batch 4 the Hg concentration should be increased to 0.012–0.015 M. Charging of the remaining DR-3 bundles can then proceed using Table 4-1. The dissolution of SRE fuels was covered by prior research which indicated that the limiting factor in processing the Th fuel (associated with H_2 gas generation) was the L-Bundle (Al-6061/6063) alloy containing the Th fuel slugs.[10]

The basic conditions for the SRE/DR-3 flowsheet recommendations for the H-Canyon dissolver for Batches 5 and 6 are:

- 54 in. immersion of L-Bundle
- 40 scfm air purge
- Nominal initial solution composition:
    - 6–7 M HNO_3 (based on material charged)
    - 0.05–0.10 M F^-
    - 0–0.5 g/L Gd
- Metering in to 0.012–0.015 M Hg as described in Procedure 221-H-4101, Rev. 62[15]
- Final HNO_3 > 0.5 M

The higher Hg concentration of 0.012–0.015 M is being recommended to handle the case of maximum contaminants from the recycle of the AFS-2 HNO_3 stream from anion exchange. The Hg should be added slowly to the dissolver over a six-hour time period after charging fuel using the same procedures as currently used for the SRE/DR-3 campaign.

The results from dissolution experiments with Al-1100 and L-Bundle alloys indicated that a maximum of four L-Bundles of SRE may be processed at any time in the batch charge plan which is consistent with prior recommendations[3]. In order to process the L-Bundles of DR-3 fuel based on the recent experiments with U-Al alloys, a minimum of 0.17 M Al must be in solution. This minimum dissolved Al could be reached by first dissolving SRE fuel or by adding $Al(NO_3)_3$ to the dissolver solution. The number of L-Bundles of DR-3 fuel that could be charged successively to the H-Canyon dissolver is dependent on the dissolved Al as shown in Table 4-1 for 16–68.8 wt % U-Al alloy and in Table 4-2 for 0–16 wt % U-Al alloy.

6.0 Future Work

Recommended future work will entail improvements in experimental design such as off-gas analysis and improvements to better represent the large-scale dissolution process at H-Canyon, for example increasing lab scale and control of experimental parameters such as Hg addition. Improvements in gas analysis, such as online Raman spectroscopy and mass spectrometry, are currently under development to advance the ability to characterize off-gas species and remove conservatism associated with gas sampling, mixing and dilution. Raman spectroscopy has the capability to measure all nitrogen oxides (NO_2, NO, and N_2O) as well as H_2. Determination of more accurate NO:N_2O ratios may allow use of higher H_2 LFL data for calculating flammability limits. Long-term objectives are to perform larger scale dissolution experiments with samples of unirradiated fuel and to develop and demonstrate continuous off-gas monitoring for the H-Canyon dissolver.

7.0 References

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Appendix A. Off-gas and Al Dissolution Rate Data

Table A-1. Off-gas and Al Dissolution Rate Data.

Experiment	Coupon	Cumulative Reaction Time [sec]	Off-gas Generation Rate [$cm^3/min/cm^2$]	Est. Al [M]	Al Dissolution Rate [$mg/min/cm^2$]
1	1	6.13	121.40	0.11	745.18
1	1	14.31	91.32	0.15	428.67
1	1	23.42	82.31	0.19	329.06
1	1	35.16	64.11	0.23	264.07
1	1	51.57	46.04	0.27	210.75
1	1	70.69	39.66	0.31	176.24
1	1	95.65	30.49	0.35	146.93
1	1	127.09	24.30	0.39	123.19
1	1	167.38	19.03	0.43	103.14
1	1	233.14	11.70	0.47	80.97
1	1	314.21	4.28	0.49	62.40
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1	2	388.46	8.29	0.51	52.77
1	2	404.84	22.72	0.53	52.89
1	2	420.24	24.21	0.56	53.12
1	2	437.62	21.49	0.58	53.10
1	2	458	18.36	0.60	52.74
1	2	480.29	16.82	0.63	52.20
1	2	505.96	14.64	0.65	51.37
1	2	535.29	12.83	0.67	50.28
1	2	569.98	10.87	0.69	48.84
1	2	610.53	9.32	0.72	47.11
1	2	653	8.91	0.74	45.46
1	2	706.77	7.05	0.76	43.32
1	2	759.84	7.16	0.79	41.52
1	2	823.65	5.96	0.81	39.43
1	2	902.48	4.84	0.83	37.02
1	2	999.56	3.94	0.86	34.36
1	2	1122.96	3.10	0.88	31.42
1	2	1207.04	2.28	0.89	29.62
1	2	1328.92	1.42	0.90	27.22
1	2	1390.25	0.31	0.90	26.05
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1	3	1469.85	12.40	0.93	25.29
1	3	1491.85	16.94	0.95	25.52
1	3	1512.85	17.78	0.97	25.77
1	3	1533.85	17.81	0.99	26.01
1	3	1557.85	15.62	1.02	26.19
1	3	1582.85	15.02	1.04	26.36

Experiment	Coupon	Cumulative Reaction Time [sec]	Off-gas Generation Rate [cm^3/min/cm^2]	Est. Al [M]	Al Dissolution Rate [mg/min/cm^2]
1	3	1611.85	12.97	1.06	26.45
1	3	1644.85	11.42	1.09	26.47
1	3	1680.85	10.49	1.11	26.45
1	3	1718.85	9.96	1.13	26.40
1	3	1760.85	9.02	1.15	26.30
1	3	1807.85	8.08	1.18	26.12
1	3	1858.85	7.46	1.20	25.90
1	3	1919.85	6.25	1.22	25.56
1	3	1998.85	4.83	1.25	25.02
1	3	2093.85	4.03	1.27	24.32
1	3	2160.85	2.86	1.28	23.79
1	3	2230.85	2.74	1.29	23.25
1	3	2337.85	1.43	1.30	22.34
1	3	2371.85	1.13	1.30	22.06
1	3	2476.85	0.73	1.31	21.20
1	3	2554.85	1.48	1.32	20.67
1	3	2639.85	0.45	1.32	13.85
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1	4	2699.85	6.27	1.34	20.17
1	4	2728.85	13.01	1.36	20.29
1	4	2761.85	11.45	1.39	20.38
1	4	2794.85	11.47	1.41	20.46
1	4	2832.85	9.98	1.43	20.52
1	4	2875.85	8.84	1.45	20.53
1	4	2928.85	7.18	1.48	20.47
1	4	2988.85	6.36	1.50	20.37
1	4	3058.85	5.46	1.52	20.21
1	4	3148.85	4.25	1.54	19.93
1	4	3251.85	3.72	1.57	19.58
1	4	3356.85	3.66	1.59	19.25
1	4	3463.85	3.60	1.61	18.92
1	4	3592.85	2.99	1.64	18.50
1	4	3729.85	2.82	1.66	18.08
1	4	3894.85	2.35	1.68	17.55
1	4	4105.85	1.84	1.71	16.88
1	4	4239.85	1.16	1.72	16.43
1	4	4312.85	0.53	1.72	16.18
1	4	4423.85	0.35	1.72	15.79
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25	1	8.25	90.07	0.11	530.35
25	1	20.73	59.77	0.14	277.21
25	1	35.07	52.21	0.18	203.11
25	1	54.61	38.46	0.21	155.73
25	1	90.98	20.74	0.25	108.72
25	1	140.05	15.43	0.28	80.57

Experiment	Coupon	Cumulative Reaction Time [sec]	Off-gas Generation Rate [cm^3/min/cm^2]	Est. Al [M]	Al Dissolution Rate [mg/min/cm^2]
25	1	191.54	14.76	0.32	66.20
25	1	253.56	12.30	0.35	55.54
25	1	322.37	11.13	0.39	48.05
25	1	348.82	0.00	0.00	0.00
25	1	363.95	0.00	0.40	44.50
25	1	415.78	7.42	0.42	40.65
25	1	480.88	5.92	0.44	36.62
25	1	552.69	5.37	0.46	33.15
25	1	637.96	4.53	0.47	29.83
25	1	774.16	2.27	0.49	25.32
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25	2	1003.13	60.58	0.53	21.18
25	2	1015.81	59.03	0.57	22.47
25	2	1032.52	44.96	0.61	23.65
25	2	1054.81	33.84	0.65	24.66
25	2	1080.55	29.41	0.69	25.55
25	2	1117.44	20.60	0.73	26.15
25	2	1178.1	12.57	0.77	26.17
25	2	1225.34	8.09	0.79	25.82
25	2	1266.34	9.34	0.81	25.62
25	2	1315	7.89	0.83	25.29
25	2	1356.67	9.23	0.85	25.11
25	2	1397.37	9.46	0.87	24.96
25	2	1472.88	5.11	0.89	24.24
25	2	1647.96	1.99	0.91	22.11
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25	3	1949.56	31.05	0.95	19.64
25	3	1967.56	41.56	1.00	20.41
25	3	1989.56	34.13	1.05	21.13
25	3	2016.56	27.92	1.09	21.78
25	3	2056.56	18.91	1.14	22.28
25	3	2110.56	14.06	1.19	22.61
25	3	2141.56	12.28	1.21	22.73
25	3	2191.56	7.63	1.23	22.65
25	3	2245.56	7.08	1.26	22.53
25	3	2314.56	5.55	1.28	22.28
25	3	2458.56	2.66	1.31	21.36
25	3	2610.56	1.01	1.32	20.27
25	3	2677.56	0.57	1.32	19.79
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25	4	2982.56	28.66	1.36	18.37
25	4	3003.56	35.62	1.41	18.85
25	4	3046.56	17.46	1.45	19.18
25	4	3070.56	15.69	1.48	19.33
25	4	3097.56	13.97	1.50	19.45

Experiment	Coupon	Cumulative Reaction Time [sec]	Off-gas Generation Rate [cm^3/min/cm^2]	Est. Al [M]	Al Dissolution Rate [mg/min/cm^2]
25	4	3122.56	15.12	1.52	19.59
25	4	3146.56	15.78	1.54	19.73
25	4	3175.56	13.08	1.57	19.84
25	4	3204.56	13.10	1.59	19.95
25	4	3237.56	11.54	1.61	20.03
25	4	3273.56	10.60	1.64	20.09
25	4	3321.56	7.96	1.66	20.08
25	4	3368.56	6.52	1.68	20.02
25	4	3388.56	3.83	1.68	19.96
25	4	3470.56	4.68	1.70	19.75
25	4	3610.56	2.74	1.73	19.25
25	4	3723.56	0.68	1.73	18.71
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35	1	4.99	162.24	0.07	316.58
35	1	14.18	59.01	0.11	186.03
35	1	25.96	46.21	0.15	142.53
35	1	43.33	31.45	0.20	109.99
35	1	54.3	24.97	0.22	97.62
35	1	81.37	20.30	0.27	78.32
35	1	118.49	14.86	0.31	62.86
35	1	168.24	11.13	0.36	50.69
35	1	194.96	10.39	0.38	46.52
35	1	248.21	5.22	0.40	0.00
35	1	358.9	2.71	0.42	27.69
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35	2	730.94	35.89	0.46	14.92
35	2	752.47	25.00	0.50	15.86
35	2	785.6	16.31	0.55	16.50
35	2	840.91	9.81	0.59	16.65
35	2	911.63	7.70	0.63	16.50
35	2	950.53	7.02	0.65	16.37
35	2	989.57	7.00	0.68	16.25
35	2	1036.38	5.85	0.70	16.02
35	2	1085.78	5.56	0.72	15.77
35	2	1127.13	4.65	0.74	15.52
35	2	1143.32	5.10	0.74	15.44
35	2	1241.66	2.80	0.76	14.64
35	2	1391.97	1.84	0.79	13.44
35	2	1583.45	1.44	0.81	12.15
35	2	1823.45	0.92	0.83	10.78
35	2	1926.45	0.54	0.83	10.26
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35	3	2258.45	6.79	0.86	8.90
35	3	2277.45	13.96	0.88	9.09
35	3	2306.45	9.16	0.91	9.23

Experiment	Coupon	Cumulative Reaction Time [sec]	Off-gas Generation Rate [cm^3/min/cm^2]	Est. Al [M]	Al Dissolution Rate [mg/min/cm^2]
35	3	2338.45	8.32	0.93	9.36
35	3	2369.45	8.60	0.96	9.48
35	3	2404.45	7.63	0.98	9.59
35	3	2439.45	7.65	1.01	9.70
35	3	2478.45	6.88	1.03	9.79
35	3	2512.45	7.90	1.06	9.89
35	3	2551.45	6.90	1.08	9.97
35	3	2588.45	7.29	1.11	10.06
35	3	2625.45	7.30	1.13	10.15
35	3	2667.45	6.44	1.16	10.22
35	3	2713.45	5.90	1.19	10.26
35	3	2765.45	5.22	1.21	10.29
35	3	2817.45	5.23	1.24	10.31
35	3	2958.45	1.93	1.26	10.03
35	3	3137.45	0.46	1.27	9.51
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35	4	3214.45	2.77	1.28	9.43
35	4	3237.45	5.80	1.29	9.45
35	4	3276.45	6.85	1.32	9.50
35	4	3318.45	6.37	1.34	9.55
35	4	3366.45	5.58	1.36	9.57
35	4	3416.45	5.37	1.39	9.59
35	4	3473.45	4.72	1.41	9.60
35	4	3536.45	4.28	1.43	9.58
35	4	3606.45	3.86	1.46	9.55
35	4	3685.45	3.42	1.48	9.49
35	4	3791.45	2.56	1.50	9.37
35	4	3965.45	1.56	1.53	9.10
35	4	4405.45	0.49	1.54	8.29
35	4	4520.45	0.47	1.55	8.11
35	4	4750.45	0.36	1.56	7.75
35	4	5520.45	0.25	1.57	6.74
35	4	6564.45	0.16	1.59	5.72
35	4	7042.45	0.23	1.60	5.36
35	4	8557.45	0.18	1.62	4.48
35	4	12653.45	0.07	1.64	3.07
35	4	14041.45	0.04	1.65	0.82
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36	1	919	0.07	0.01	0.13
36	1	949.3	15.08	0.04	0.00
36	1	962	22.81	0.08	1.98
36	1	976.09	37.33	0.12	2.93
36	1	992.8	31.59	0.16	3.89
36	1	1013.18	26.00	0.20	4.78
36	1	1043.58	17.50	0.24	5.64

Experiment	Coupon	Cumulative Reaction Time [sec]	Off-gas Generation Rate [cm^3/min/cm^2]	Est. Al [M]	Al Dissolution Rate [mg/min/cm^2]
36	1	1058.21	18.23	0.26	6.03
36	1	1072.77	18.35	0.28	6.41
36	1	1089.15	16.34	0.30	6.77
36	1	1107.52	14.60	0.33	7.11
36	1	1149.21	12.90	0.37	7.72
36	1	1175.77	10.15	0.39	7.97
36	1	1213.49	7.16	0.41	8.14
36	1	1265.33	8.10	0.41	7.92
36	1	1333.58	4.17	0.40	7.22
36	1	1464.27	0.86	0.39	6.40
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36	2	1577.18	10.36	0.43	6.77
36	2	1584.72	35.54	0.46	7.05
36	2	1596.72	44.78	0.50	7.63
36	2	1617.72	25.69	0.54	8.15
36	2	1635.27	15.41	0.56	8.37
36	2	1660.34	10.81	0.58	8.55
36	2	1692.68	8.39	0.60	8.69
36	2	1727.72	7.76	0.62	8.81
36	2	1764.72	7.37	0.64	8.91
36	2	1801.72	7.38	0.66	9.01
36	2	1853.72	6.31	0.69	9.09
36	2	1966.72	0.48	0.69	8.62
36	2	2060.72	1.75	0.70	8.37
36	2	2169.72	2.52	0.72	8.19
36	2	2285.72	2.37	0.75	8.00
36	2	2395.72	2.50	0.77	7.85
36	2	2550.72	1.78	0.79	7.57
36	2	2780.72	1.44	0.81	7.13
36	2	3202.72	0.68	0.82	6.29
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36	3	3314.72	0.94	0.83	6.07
36	3	3382.72	0.39	0.83	5.97
36	3	3557.72	0.75	0.85	5.76
36	3	3639.72	0.64	0.85	5.67
36	3	3792.72	1.73	0.88	5.60
36	3	3806.72	15.15	0.90	5.71
36	3	3823.72	15.62	0.92	5.84
36	3	3846.72	11.57	0.95	5.97
36	3	3870.72	11.11	0.97	6.09
36	3	3896.72	11.83	1.00	6.21
36	3	3925.72	9.22	1.02	6.32
36	3	3955.72	8.93	1.05	6.43
36	3	3986.72	8.66	1.08	6.54
36	3	4019.72	8.15	1.10	6.64

Experiment	Coupon	Cumulative Reaction Time [sec]	Off-gas Generation Rate [cm^3/min/cm^2]	Est. Al [M]	Al Dissolution Rate [mg/min/cm^2]
36	3	4054.72	7.70	1.13	6.74
36	3	4094.72	6.75	1.15	6.83
36	3	4162.72	3.98	1.18	6.87
36	3	4272.72	2.46	1.21	6.84
36	3	4816.72	0.45	1.23	6.18
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36	4	4987.72	0.71	1.24	5.96
36	4	5009.72	8.33	1.25	6.01
36	4	5030.72	12.49	1.28	6.11
36	4	5055.72	10.51	1.31	6.20
36	4	5085.72	8.77	1.33	6.29
36	4	5116.72	8.51	1.36	6.37
36	4	5149.72	8.01	1.38	6.45
36	4	5183.72	7.79	1.41	6.52
36	4	5218.72	7.58	1.43	6.60
36	4	5255.72	7.18	1.46	6.67
36	4	5289.72	7.83	1.48	6.74
36	4	5326.72	7.21	1.51	6.81
36	4	5365.72	6.85	1.54	6.88
36	4	5417.72	5.15	1.56	6.93
36	4	5483.72	4.06	1.59	6.96
36	4	5556.72	3.68	1.61	6.98
36	4	5664.72	2.49	1.64	6.95
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40	1	10.39	68.44	0.05	117.35
40	1	21.76	62.78	0.10	112.28
40	1	37.51	45.49	0.15	97.88
40	1	59.89	32.13	0.20	81.90
40	1	90.33	23.71	0.25	68.00
40	1	108.51	19.91	0.28	62.33
40	1	136.98	12.74	0.30	53.91
40	1	193.89	1.28	0.31	38.73
40	1	280.64	3.35	0.33	28.53
40	1	380.29	2.56	0.35	22.21
40	1	425.89	2.40	0.36	20.27
40	1	541.48	2.21	0.37	16.75
40	1	607.1	1.67	0.38	15.25
40	1	743.26	1.45	0.39	12.88
40	1	913.39	1.07	0.41	10.82
40	1	1001.48	0.42	0.41	9.93
40	1	1075.73	0.49	0.41	9.30
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40	2	1176.1	20.18	0.44	9.25
40	2	1187.79	30.80	0.47	9.79
40	2	1210.76	31.44	0.53	10.84

Experiment	Coupon	Cumulative Reaction Time [sec]	Off-gas Generation Rate [cm^3/min/cm^2]	Est. Al [M]	Al Dissolution Rate [mg/min/cm^2]
40	2	1244.79	21.30	0.60	11.76
40	2	1268.85	15.11	0.63	12.13
40	2	1291.04	22.05	0.66	12.51
40	2	1319.69	19.25	0.69	12.82
40	2	1351.04	15.56	0.72	13.08
40	2	1386.88	12.84	0.75	13.29
40	2	1453.63	9.89	0.78	13.21
40	2	1589.76	6.13	0.81	12.56
40	2	1865.43	0.89	0.81	10.70
40	2	1963.43	0.38	0.82	10.21
40	2	2039.43	0.48	0.82	9.87
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40	3	2325.43	10.53	0.85	9.22
40	3	2340.43	24.61	0.88	9.50
40	3	2353.43	28.45	0.91	9.79
40	3	2367.43	26.47	0.95	10.07
40	3	2385.43	20.63	0.98	10.33
40	3	2411.43	14.31	1.01	10.55
40	3	2443.43	11.65	1.04	10.75
40	3	2475.43	11.67	1.07	10.94
40	3	2512.43	10.11	1.11	11.10
40	3	2554.43	8.92	1.14	11.23
40	3	2605.43	7.36	1.17	11.33
40	3	2666.43	6.17	1.20	11.37
40	3	2704.43	7.90	1.22	11.36
40	3	2879.43	0.22	1.22	10.70
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40	4	3115.43	2.33	1.24	10.04
40	4	3124.43	20.50	1.26	10.16
40	4	3139.43	24.63	1.29	10.39
40	4	3153.43	26.44	1.33	10.63
40	4	3169.43	23.18	1.36	10.86
40	4	3192.43	16.16	1.40	11.06
40	4	3225.43	11.28	1.44	11.23
40	4	3271.43	8.11	1.47	11.35
40	4	3318.43	7.95	1.51	11.46
40	4	3376.43	6.45	1.54	11.53
40	4	3447.43	5.28	1.58	11.56
40	4	3506.43	2.55	1.59	11.47
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41	2	5.98	113.11	0.03	168.78
41	2	12.35	106.59	0.06	163.76
41	2	20.32	85.51	0.08	149.58
41	2	29.98	70.82	0.11	135.43
41	2	40.92	62.77	0.14	124.26

Experiment	**Coupon**	**Cumulative Reaction Time [sec]**	**Off-gas Generation Rate [cm^3/min/cm^2]**	**Est. Al [M]**	**Al Dissolution Rate [mg/min/cm^2]**
41	2	54.29	51.55	0.17	112.60
41	2	68.54	48.55	0.20	104.25
41	2	84.29	44.08	0.22	97.06
41	2	101.76	39.89	0.25	90.62
41	2	121.57	35.31	0.28	84.44
41	2	146.45	28.22	0.31	77.25
41	2	176.45	23.49	0.34	70.07
41	2	195.67	17.58	0.35	65.76
41	2	215.98	16.67	0.37	61.92
41	2	238.35	15.16	0.38	58.23
41	2	268.29	11.35	0.39	53.62
41	2	300.98	10.41	0.41	49.49
41	2	341.45	8.43	0.42	45.11
41	2	410.79	4.93	0.44	38.74
41	2	482.45	0.95	0.44	33.20
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41	3	536.61	30.51	0.47	31.37
41	3	561.39	27.15	0.52	33.21
41	3	591.83	22.19	0.54	33.04
41	3	629.08	18.20	0.57	32.54
41	3	651.23	15.35	0.58	32.14
41	3	672.89	15.72	0.59	31.79
41	3	695.76	14.92	0.60	31.40
41	3	720.54	13.79	0.62	30.97
41	3	768.58	14.27	0.64	30.23
41	3	794.86	13.08	0.66	29.82
41	3	822.58	12.42	0.67	29.38
41	3	851.04	12.12	0.68	28.94
41	3	881.01	11.53	0.69	28.49
41	3	913.51	10.65	0.71	27.99
41	3	951.67	9.09	0.72	27.36
41	3	986.20	15.19	0.73	26.87
41	3	1023.54	14.76	0.75	26.35
41	3	1065.39	14.27	0.76	25.76
41	3	1111.42	13.76	0.77	25.12
41	3	1147.73	8.55	0.78	24.72
41	3	1195.39	7.04	0.80	24.11
41	3	1246.01	6.64	0.81	23.49
41	3	1297.11	12.21	0.82	22.92
41	3	1355.36	11.77	0.83	22.27
41	3	1414.89	11.36	0.85	21.66
41	3	1481.98	10.92	0.86	20.98
41	3	1579.17	10.25	0.87	19.98
41	3	1692.44	9.49	0.88	18.86
41	3	1730.44	9.25	0.88	18.50

Experiment	Coupon	Cumulative Reaction Time [sec]	Off-gas Generation Rate [cm^3/min/cm^2]	Est. Al [M]	Al Dissolution Rate [mg/min/cm^2]
41	3	1888.44	8.31	0.89	17.07
41	3	2104.44	2.60	0.89	14.75
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41	4	2477.74	15.29	0.90	12.06
41	4	2498.74	14.59	0.92	12.15
41	4	2527.74	10.58	0.93	12.19
41	4	2579.74	8.28	0.95	12.21
41	4	2601.74	8.40	0.96	12.21
41	4	2643.74	7.35	0.98	12.20
41	4	2683.74	7.73	0.99	12.20
41	4	2726.74	7.20	1.01	12.18
41	4	2770.74	7.05	1.02	12.16
41	4	2813.74	7.23	1.03	12.15
41	4	2861.74	6.49	1.05	12.11
41	4	2910.74	6.37	1.06	12.07
41	4	2960.74	6.25	1.08	12.03
41	4	3016.74	5.59	1.09	11.97
41	4	3071.74	5.71	1.11	11.92
41	4	3133.74	5.07	1.12	11.84
41	4	3198.74	4.85	1.14	11.75
41	4	3262.74	4.93	1.15	11.67
41	4	3339.74	4.11	1.17	11.55
41	4	3427.74	3.60	1.18	11.39
41	4	3524.74	3.60	1.20	11.23
41	4	3613.74	3.21	1.21	11.08
41	4	3714.74	3.15	1.23	10.91
41	4	3836.74	2.62	1.24	10.69
41	4	3964.74	2.39	1.26	10.47
41	4	4084.74	2.55	1.27	10.28
41	4	4221.74	2.24	1.28	10.05
41	4	4375.74	2.00	1.30	9.81
41	4	4551.74	1.75	1.31	9.54
41	4	4764.74	1.45	1.33	9.21
41	4	5042.74	1.11	1.34	8.80
41	4	5502.74	0.67	1.36	8.15
41	4	5677.74	1.43	1.36	6.84
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42	1	41.74	3.17	0.00	2.48
42	1	99.11	11.55	0.01	6.27
42	1	124.05	17.75	0.02	7.80
42	1	145.93	20.27	0.03	9.01
42	1	167.27	20.82	0.03	9.94
42	1	200.14	20.32	0.05	10.92
42	1	211.86	19.04	0.05	11.14
42	1	234.11	20.08	0.06	11.57

Experiment	Coupon	Cumulative Reaction Time [sec]	Off-gas Generation Rate [cm^3/min/cm^2]	Est. Al [M]	Al Dissolution Rate [mg/min/cm^2]
42	1	258.30	18.51	0.06	11.84
42	1	282.64	18.43	0.07	12.06
42	1	308.68	17.26	0.08	12.18
42	1	333.27	18.88	0.09	12.34
42	1	388.24	16.42	0.10	12.41
42	1	418.30	15.06	0.11	12.37
42	1	450.39	14.13	0.12	12.27
42	1	482.61	14.10	0.12	12.19
42	1	521.64	11.66	0.13	11.96
42	1	559.27	12.12	0.14	11.79
42	1	613.18	8.47	0.15	11.34
42	1	667.02	8.50	0.15	10.96
42	1	742.68	6.06	0.16	10.33
42	1	838.58	4.79	0.17	9.57
42	1	1065.96	2.02	0.18	7.87
42	1	1119.46	7.18	0.18	7.62
42	1	1232.99	0.39	0.18	6.94

Appendix B. Sample Calculation and Verification of H_2 LFL for Each Experiment

To illustrate how the H_2 lower flammability calculations were performed as illustrated in Table B-1, a sample calculation will be shown for Experiment 1 gas sample 1. First, the measured peak off-gas rate for gas sample 1 is 3.87 scfm/ft^2 as shown in Table B-1. Therefore the predicted peak off-gas rate per L-Bundle for Experiment 1 gas sample 1 is calculated using Equation 27:

(27) Predicted Peak Off-gas Rate per Bundle [scfm] = 3.87 [scfm/ft^2] *6.4546 ft^2 = 24.9793 [scfm]

Assuming that there are 4 L-Bundles to be charged to the dissolver, the total predicted peak off-gas rate is then calculated using Equation 28:

(28) Total Predicted Peak Off-gas Rate [scfm] = 24.9793 [scfm] * 4 = 99.9172 [scfm]

Now based on the measured/mass balance H_2 concentration for Experiment 1 gas sample 1 of 2.8% from Table 3-5, the predicted peak H_2 off-gas rate for 4 L-Bundles is calculated using Equation 29:

(29) Predicted Peak H_2 Off-gas Rate [scfm] = 99.9172 [scfm]* 2.8 [Vol%] = 2.7977 [scfm]

The predicted H_2 concentration with air dilution is then calculated using Equation 30:

(30) $$\text{Predicted H}_2\text{ Concentration with air dilution [vol\%]} = \frac{2.7977\text{ [scfm]}}{99.9172\text{ [scfm]} + 40\text{ [scfm])}} = 2.0\text{ [vol\%]}$$

To calculate the lower flammability limit of H_2 based on Scott's data, first calculate the volume percent of air during the peak off-gas rate using Equation 31:

(31) $$\text{Predicted air concentration with air dilution [vol\%]} = \frac{40\text{ [scfm]}}{99.9172\text{ [scfm]} + 40\text{ [scfm])}} = 28.59\text{ [vol\%]}$$

Now use Equation 32 to calculate the lower flammability limit of H_2 based on the air percent assuming a NO/N_2O ratio of 0.33:

(32) $$\text{H}_2\text{ LFL vol\%} = 0.01 * \left(1.636 + \frac{284.242}{28.59} - \frac{5485.518}{(28.59)^2}\right) = 4.89\text{ [vol\%]}$$

This lower flammability limit of H_2 is then adjusted from 28° to 200°C using the Dyer correction Equation 33:

(33) LFL_T =4.89 [vol%]0.811 = 3.95 [vol%]

The safety limit is defined as 60% of the H_2 lower flammability limit at 200°C so take 60% of the Dyer corrected value:

(34) Safety Limit = 3.95 [vol%]0.60 = 2.37 [vol%]

So 60% of the Dyer corrected H_2 lower flammability limit at 200 °C for Experiment 1 gas sample 1 is 2.37 vol %. The predicted H_2 concentration with air dilution for Experiment 1 gas sample 1 is 2.0 vol % which is less than the 60% of the Dyer corrected H_2 LFL of 2.37 vol % so 4 L-Bundles may be charged as shown in Table B-1.

Table B-1. H_2 LFL Check for 4 Bundles for Each Experiment.

Experi-ment	Bun-dles	Alloy	Contam-inants	Initial HNO_3 [M]	Initial Al Conc [M]	Hg [M] (assume constant)	Gas Sample	60% of Dyer Corrected H_2 LFL	Predicted vol % H_2 with air dilution	U [g/L]	Th [g/L]	Max off-gas rate per SA [scfm/ft^2]	Check Pred H_2 with dilution ≤ 60% LFL
1	4	Al-1100	None	6.99	0.075	0.002	1	2.37%	2.00%	0.00	0.00	3.87	OK
1	4	Al-1100	None	6.99	0.075	0.002	2	2.34%	0.61%	0.00	0.00	0.97	OK
1	4	Al-1100	None	6.99	0.075	0.002	3	2.27%	3.51%	0.00	0.00	0.77	FAIL
1	4	Al-1100	None	6.99	0.075	0.002	4	2.03%	1.15%	0.00	0.00	0.23	OK
1	4	Al-1100	None	6.99	0.075	0.002	5	2.19%	1.56%	0.00	0.00	0.57	OK
1	4	Al-1100	None	6.99	0.075	0.002	6	2.04%	1.00%	0.00	0.00	0.24	OK
1	4	Al-1100	None	6.99	0.075	0.002	7	2.12%	1.70%	0.00	0.00	0.41	OK
1	4	Al-1100	None	6.99	0.075	0.002	8	1.97%	0.56%	0.00	0.00	0.11	OK
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25	4	Al-1100	None	7.00	0.075	0.012	1	2.57%	0.31%	0.00	0.00	2.87	OK
25	4	Al-1100	None	7.00	0.075	0.012	2	2.15%	0.09%	0.00	0.00	0.47	OK
25	4	Al-1100	None	7.00	0.075	0.012	3	2.56%	1.04%	0.00	0.00	1.93	OK
25	4	Al-1100	None	7.00	0.075	0.012	4	2.11%	0.19%	0.00	0.00	0.40	OK
25	4	Al-1100	None	7.00	0.075	0.012	5	2.44%	0.99%	0.00	0.00	1.32	OK
25	4	Al-1100	None	7.00	0.075	0.012	6	2.11%	0.33%	0.00	0.00	0.39	OK
25	4	Al-1100	None	7.00	0.075	0.012	7	2.39%	0.47%	0.00	0.00	1.14	OK
25	4	Al-1100	None	7.00	0.075	0.012	8	2.10%	0.69%	0.00	0.00	0.37	OK
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28	4	Al-1100	None	6.65	0	0.004	1	2.59%	0.00%	0.00	0.00	2.37	OK
28	4	Al-1100	None	6.65	0	0.004	2	2.24%	0.22%	0.00	0.00	0.70	OK
28	4	Al-1100	None	6.65	0	0.004	3	2.57%	0.84%	0.00	0.00	2.04	OK
28	4	Al-1100	None	6.65	0	0.004	4	2.21%	0.19%	0.00	0.00	0.61	OK
28	4	Al-1100	None	6.65	0	0.004	5	2.48%	0.77%	0.00	0.00	1.48	OK
28	4	Al-1100	None	6.65	0	0.004	6	2.15%	0.52%	0.00	0.00	0.48	OK
28	4	Al-1100	None	6.65	0	0.004	7	2.37%	0.15%	0.00	0.00	1.07	OK
28	4	Al-1100	None	6.65	0	0.004	8	2.13%	0.56%	0.00	0.00	0.43	OK
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30	4	Al-1100	None	6.47	0	0.015	1	2.57%	0.26%	0.00	0.00	2.11	OK
30	4	Al-1100	None	6.47	0	0.015	2	2.18%	0.16%	0.00	0.00	0.56	OK
30	4	Al-1100	None	6.47	0	0.015	3	2.58%	0.76%	0.00	0.00	2.21	OK
30	4	Al-1100	None	6.47	0	0.015	4	2.10%	0.30%	0.00	0.00	0.38	OK
30	4	Al-1100	None	6.47	0	0.015	5	2.58%	0.91%	0.00	0.00	2.26	OK
30	4	Al-1100	None	6.47	0	0.015	6	2.08%	0.07%	0.00	0.00	0.33	OK
30	4	Al-1100	None	6.47	0	0.015	7	2.36%	0.82%	0.00	0.00	1.05	OK
30	4	Al-1100	None	6.47	0	0.015	8	2.06%	0.40%	0.00	0.00	0.28	OK
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33	4	Al-1100	None	7.03	0	0.0012	1	2.49%	1.38%	3.90	26.60	1.51	OK
33	4	Al-1100	None	7.03	0	0.0012	2	2.08%	0.28%	3.90	26.60	0.33	OK
33	4	Al-1100	None	7.03	0	0.0012	3	2.03%	0.62%	3.90	26.60	0.22	OK
33	4	Al-1100	None	7.03	0	0.0012	4	1.95%	0.11%	3.90	26.60	0.07	OK
33	4	Al-1100	None	7.03	0	0.0012	5	1.93%	0.03%	3.90	26.60	0.04	OK
33	4	Al-1100	None	7.03	0	0.0012	6	1.94%	0.04%	3.90	26.60	0.04	OK

Experi-ment	Bun-dles	Alloy	Contam-inants	Initial HNO_3 [M]	Initial Al Conc [M]	Hg [M] (assume constant)	Gas Sample	60% of Dyer Corrected H_2 LFL	Predicted vol % H_2 with air dilution	U [g/L]	Th [g/L]	Max off-gas rate per SA [scfm/ft^2]	Check Pred H_2 with dilution ≤ 60% LFL
33	4	Al-1100	None	7.03	0	0.0012	7	1.97%	0.13%	3.90	26.60	0.11	OK
33	4	Al-1100	None	7.03	0	0.0012	8	1.92%	0.01%	3.90	26.60	0.02	OK
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34	4	Al-1100	None	7.03	0	0.002	1	2.59%	0.80%	3.90	26.60	2.60	OK
34	4	Al-1100	None	7.03	0	0.002	2	2.29%	1.91%	3.90	26.60	0.82	OK
34	4	Al-1100	None	7.03	0	0.002	3	2.22%	1.68%	3.90	26.60	0.65	OK
34	4	Al-1100	None	7.03	0	0.002	4	2.03%	0.20%	3.90	26.60	0.22	OK
34	4	Al-1100	None	7.03	0	0.002	5	2.20%	1.68%	3.90	26.60	0.61	OK
34	4	Al-1100	None	7.03	0	0.002	6	2.02%	0.71%	3.90	26.60	0.21	OK
34	4	Al-1100	None	7.03	0	0.002	7	2.14%	1.82%	3.90	26.60	0.46	OK
34	4	Al-1100	None	7.03	0	0.002	8	1.97%	0.55%	3.90	26.60	0.11	OK
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35-4	4	L-Bundle	None	7.01	0	0.002	1	1.77%	2.65%	0.00	0.00	5.17	FAIL
35-4	4	L-Bundle	None	7.01	0	0.002	2	2.08%	0.43%	0.00	0.00	0.33	OK
35-4	4	L-Bundle	None	7.01	0	0.002	3	2.39%	2.92%	0.00	0.00	1.14	FAIL
35-4	4	L-Bundle	None	7.01	0	0.002	4	2.03%	1.30%	0.00	0.00	0.22	OK
35-4	4	L-Bundle	None	7.01	0	0.002	5	2.13%	-0.01%	0.00	0.00	0.44	OK
35-4	4	L-Bundle	None	7.01	0	0.002	6	2.03%	0.30%	0.00	0.00	0.23	OK
35-4	4	L-Bundle	None	7.01	0	0.002	7	2.03%	1.08%	0.00	0.00	0.22	OK
35-4	4	L-Bundle	None	7.01	0	0.002	8	1.94%	0.60%	0.00	0.00	0.05	OK
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36-2	4	L-Bundle	None	7.01	0	0→0.002	1	2.41%	1.90%	0.00	0.00	1.19	OK
36-2	4	L-Bundle	None	7.01	0	0→0.002	2	2.12%	0.07%	0.00	0.00	0.41	OK
36-2	4	L-Bundle	None	7.01	0	0→0.002	3	2.47%	2.28%	0.00	0.00	1.43	OK
36-2	4	L-Bundle	None	7.01	0	0→0.002	4	2.04%	0.93%	0.00	0.00	0.24	OK
36-2	4	L-Bundle	None	7.01	0	0→0.002	5	2.16%	0.57%	0.00	0.00	0.50	OK
36-2	4	L-Bundle	None	7.01	0	0→0.002	6	2.05%	1.50%	0.00	0.00	0.26	OK
36-2	4	L-Bundle	None	7.01	0	0→0.002	7	2.11%	0.79%	0.00	0.00	0.40	OK
36-2	4	L-Bundle	None	7.01	0	0→0.002	8	2.03%	0.51%	0.00	0.00	0.23	OK
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37	4	L-Bundle	None	4.25	0	0.002	1	2.56%	3.63%	0.00	0.00	2.98	FAIL
37	4	L-Bundle	None	4.25	0	0.002	2	2.11%	0.62%	0.00	0.00	0.39	OK
37	4	L-Bundle	None	4.25	0	0.002	3	2.34%	0.15%	0.00	0.00	0.97	OK
37	4	L-Bundle	None	4.25	0	0.002	4	2.12%	0.85%	0.00	0.00	0.41	OK
37	4	L-Bundle	None	4.25	0	0.002	5	2.07%	0.62%	0.00	0.00	0.30	OK
37	4	L-Bundle	None	4.25	0	0.002	6	1.96%	-0.09%	0.00	0.00	0.09	OK
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40	4	L-Bundle	None	7.16	0	0.012	1	2.58%	0.44%	3.90	21.8	2.18	OK
40	4	L-Bundle	None	7.16	0	0.012	2	1.97%	0.03%	3.90	21.8	0.11	OK
40	4	L-Bundle	None	7.16	0	0.012	3	2.35%	0.57%	3.90	21.8	1.00	OK
40	4	L-Bundle	None	7.16	0	0.012	4	2.24%	0.46%	3.90	21.8	0.70	OK
40	4	L-Bundle	None	7.16	0	0.012	5	2.32%	1.07%	3.90	21.8	0.91	OK
40	4	L-Bundle	None	7.16	0	0.012	6	2.10%	0.46%	3.90	21.8	0.37	OK
40	4	L-Bundle	None	7.16	0	0.012	7	2.30%	3.99%	3.90	21.8	0.84	FAIL

Experiment	Bundles	Alloy	Contaminants	Initial HNO_3 [M]	Initial Al Conc [M]	Hg [M] (assume constant)	Gas Sample	60% of Dyer Corrected H_2 LFL	Predicted vol % H_2 with air dilution	U [g/L]	Th [g/L]	Max off-gas rate per SA [scfm/ft^2]	Check Pred H_2 with dilution ≤ 60% LFL
40	4	L-Bundle	None	7.16	0	0.012	8	2.04%	1.61%	3.90	21.8	0.25	OK
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41	4	30%U-Al	None	7.16	0	0.012	1	2.44%	7.10%	0.00	0.00	3.61	FAIL
41	4	30%U-Al	None	7.16	0	0.012	2	2.18%	2.20%	0.00	0.00	0.56	FAIL
41	4	30%U-Al	None	7.16	0	0.012	3	2.34%	2.25%	0.00	0.00	0.97	OK
41	4	30%U-Al	None	7.16	0	0.012	4	2.15%	1.60%	0.00	0.00	0.48	OK
41	4	30%U-Al	None	7.16	0	0.012	5	2.15%	1.43%	0.00	0.00	0.49	OK
41	4	30%U-Al	None	7.16	0	0.012	6	2.02%	0.60%	0.00	0.00	0.20	OK
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42	4	68.8%U-Al	None	7.16	0	0.012	1	2.23%	1.11%	0.00	0.00	0.66	OK
42	4	68.8%U-Al	None	7.16	0	0.012	2	2.17%	0.62%	0.00	0.00	0.52	OK
42	4	68.8%U-Al	None	7.16	0	0.012	3	2.50%	0.00%	0.00	0.00	1.56	OK
42	4	68.8%U-Al	None	7.16	0	0.012	4	2.03%	0.01%	0.00	0.00	0.22	OK
42	4	68.8%U-Al	None	7.16	0	0.012	5	2.38%	0.60%	0.00	0.00	1.10	OK
42	4	68.8%U-Al	None	7.16	0	0.012	6	2.00%	0.00%	0.00	0.00	0.17	OK
42	4	68.8%U-Al	None	7.16	0	0.012	7	2.32%	0.53%	0.00	0.00	0.91	OK
42	4	68.8%U-Al	None	7.16	0	0.012	8	1.95%	0.00%	0.00	0.00	0.06	OK
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22	4	Al-1100	Min	7.00	0.075	0.012	1	2.57%	0.00%	0.00	0.00	2.92	OK
22	4	Al-1100	Min	7.00	0.075	0.012	2	2.15%	0.30%	0.00	0.00	0.47	OK
22	4	Al-1100	Min	7.00	0.075	0.012	3	2.36%	1.67%	0.00	0.00	1.04	OK
22	4	Al-1100	Min	7.00	0.075	0.012	4	2.06%	0.62%	0.00	0.00	0.29	OK
22	4	Al-1100	Min	7.00	0.075	0.012	5	2.24%	0.80%	0.00	0.00	0.70	OK
22	4	Al-1100	Min	7.00	0.075	0.012	6	2.02%	0.77%	0.00	0.00	0.20	OK
22	4	Al-1100	Min	7.00	0.075	0.012	7	2.16%	1.19%	0.00	0.00	0.50	OK
22	4	Al-1100	Min	7.00	0.075	0.012	8	1.98%	0.38%	0.00	0.00	0.13	OK
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24	4	Al-1100	Min	7.01	0.075	0.012	1	2.59%	1.41%	0.00	0.00	2.53	OK
24	4	Al-1100	Min	7.01	0.075	0.012	2	2.13%	0.06%	0.00	0.00	0.43	OK
24	4	Al-1100	Min	7.01	0.075	0.012	3	2.38%	2.32%	0.00	0.00	1.10	OK
24	4	Al-1100	Min	7.01	0.075	0.012	4	2.10%	-0.70%	0.00	0.00	0.37	OK
24	4	Al-1100	Min	7.01	0.075	0.012	5	2.24%	2.03%	0.00	0.00	0.71	OK
24	4	Al-1100	Min	7.01	0.075	0.012	6	2.04%	0.53%	0.00	0.00	0.25	OK
24	4	Al-1100	Min	7.01	0.075	0.012	7	2.18%	0.90%	0.00	0.00	0.54	OK
24	4	Al-1100	Min	7.01	0.075	0.012	8	1.99%	0.35%	0.00	0.00	0.14	OK
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31	4	Al-1100	Min	7.00	0	0.015	1	2.58%	0.32%	0.00	0.00	2.75	OK
31	4	Al-1100	Min	7.00	0	0.015	2	2.12%	0.24%	0.00	0.00	0.41	OK
31	4	Al-1100	Min	7.00	0	0.015	3	2.42%	2.60%	0.00	0.00	1.22	FAIL
31	4	Al-1100	Min	7.00	0	0.015	4	2.11%	1.02%	0.00	0.00	0.39	OK
31	4	Al-1100	Min	7.00	0	0.015	5	2.23%	1.25%	0.00	0.00	0.66	OK
31	4	Al-1100	Min	7.00	0	0.015	6	2.04%	0.76%	0.00	0.00	0.25	OK
31	4	Al-1100	Min	7.00	0	0.015	7	2.16%	1.09%	0.00	0.00	0.50	OK
31	4	Al-1100	Min	7.00	0	0.015	8	2.00%	0.24%	0.00	0.00	0.17	OK

Experi-ment	Bun-dles	Alloy	Contam-inants	Initial HNO_3 [M]	Initial Al Conc [M]	Hg [M] (assume constant)	Gas Sample	60% of Dyer Corrected H_2 LFL	Predicted vol % H_2 with air dilution	U [g/L]	Th [g/L]	Max off-gas rate per SA [scfm/ft^2]	Check Pred H_2 with dilution ≤ 60% LFL
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38	4	L-Bundle	Min	7.01	0.075	0.012	1	2.16%	3.39%	0.00	0.00	4.43	Fail
38	4	L-Bundle	Min	7.01	0.075	0.012	2	1.95%	0.27%	0.00	0.00	0.06	OK
38	4	L-Bundle	Min	7.01	0.075	0.012	3	2.23%	1.18%	0.00	0.00	0.67	OK
38	4	L-Bundle	Min	7.01	0.075	0.012	4	1.94%	0.12%	0.00	0.00	0.06	OK
38	4	L-Bundle	Min	7.01	0.075	0.012	5	2.04%	0.63%	0.00	0.00	0.24	OK
38	4	L-Bundle	Min	7.01	0.075	0.012	6	1.93%	0.05%	0.00	0.00	0.04	OK
38	4	L-Bundle	Min	7.01	0.075	0.012	7	1.94%	0.19%	0.00	0.00	0.06	OK
38	4	L-Bundle	Min	7.01	0.075	0.012	8	1.94%	0.00%	0.00	0.00	0.05	OK
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43	4	30%U-Al	Min	7.16	0.075	0.012	1	2.57%	5.95%	0.00	0.00	2.07	Fail
43	4	30%U-Al	Min	7.16	0.075	0.012	2	2.14%	1.20%	0.00	0.00	0.46	OK
43	4	30%U-Al	Min	7.16	0.075	0.012	3	2.28%	2.17%	0.00	0.00	0.80	OK
43	4	30%U-Al	Min	7.16	0.075	0.012	4	2.01%	0.51%	0.00	0.00	0.18	OK
43	4	30%U-Al	Min	7.16	0.075	0.012	5	2.18%	1.65%	0.00	0.00	0.56	OK
43	4	30%U-Al	Min	7.16	0.075	0.012	6	1.98%	0.33%	0.00	0.00	0.12	OK
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20	4	Al-1100	Max	7.01	0.075	0.012	1	2.44%	1.37%	0.00	0.00	1.32	OK
20	4	Al-1100	Max	7.01	0.075	0.012	2	2.16%	0.37%	0.00	0.00	0.50	OK
20	4	Al-1100	Max	7.01	0.075	0.012	3	2.32%	0.67%	0.00	0.00	0.91	OK
20	4	Al-1100	Max	7.01	0.075	0.012	4	2.11%	0.52%	0.00	0.00	0.40	OK
20	4	Al-1100	Max	7.01	0.075	0.012	5	2.26%	0.71%	0.00	0.00	0.75	OK
20	4	Al-1100	Max	7.01	0.075	0.012	6	2.08%	0.21%	0.00	0.00	0.32	OK
20	4	Al-1100	Max	7.01	0.075	0.012	7	2.21%	0.52%	0.00	0.00	0.62	OK
20	4	Al-1100	Max	7.01	0.075	0.012	8	2.03%	0.33%	0.00	0.00	0.23	OK
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23	4	Al-1100	Max	7.00	0.075	0.012	1	2.59%	1.76%	0.00	0.00	2.62	OK
23	4	Al-1100	Max	7.00	0.075	0.012	2	2.20%	0.81%	0.00	0.00	0.59	OK
23	4	Al-1100	Max	7.00	0.075	0.012	3	2.28%	0.65%	0.00	0.00	0.79	OK
23	4	Al-1100	Max	7.00	0.075	0.012	4	2.07%	0.43%	0.00	0.00	0.31	OK
23	4	Al-1100	Max	7.00	0.075	0.012	5	2.23%	0.78%	0.00	0.00	0.67	OK
23	4	Al-1100	Max	7.00	0.075	0.012	6	2.04%	0.35%	0.00	0.00	0.24	OK
23	4	Al-1100	Max	7.00	0.075	0.012	7	2.17%	0.60%	0.00	0.00	0.54	OK

Distribution:

S. L. Marra, 773-A
T. B. Brown, 773-A
D. H. McGuire, 999-W
S. D. Fink, 773-A
C. C. Herman, 773-A
E. N. Hoffman, 999-W
F. M. Pennebaker, 773-42A
W. R. Wilmarth, 773-A
J. B. Schaade, 704-2H
P. B. Andrews, 704-2H
M. J. Lewczyk, 221-H
K. P. Burrows, 704-2H
K. J. Gallahue, 221-H
J. E. Therrell, 704-2H
K. J. Usher, 704-2H
S. L. Hudlow, 221-H
W. H. Clifton, Jr. 704-2H
S. L. Garrison, 704-2H
P. M. Almond, 773-A
K. P. Crapse, 773-A
W. E. Daniel, 999-W
E. A. Kyser, 773-A
T. S. Rudisill, 773-A
R. A. Pierce, 773-A
J. M. Duffey, 773-A
K. M. Taylor-Pashow, 773-A
M. C. Thompson, 773-A
P. E. O’Rourke, 773-A
R. J. Lascola, 773-41A
P. R. Jackson, 703-46A
J. L. Bodkin, 221-H
P. M. Palmer, 221-H
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