Acetylene & MagneGas-2 End-use and Safety Assessment

A comparative end-use environmental impact and safety analysis of acetylene and Taronis' MagneGas-2.

CONTRIBUTORS

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Table of Contents

1 Introduction

This report includes three main sections on the separate safety and end-use assessments of acetylene and MagneGas-2 as well as a comparative summary. The safety sections of the report include information from safety data sheets and literature. The end-use assessments contain the calculations for the carbon dioxide emissions expected from combustion of the gases.

2 Acetylene End-use & Safety Assessment

2.1 Safety

Information regarding safety in proximity to both the manufacturing and use of acetylene was collected from safety data sheets as well as literature.

GHS Classification:	Flammable Gas – 1 Compressed Gas
Hazards:	Extremely Flammable Gas May form explosive mixtures with air Contains gas under pressure; may explode if heated May displace oxygen and cause rapid suffocation
Incompatible Materials:	Oxidizers
Conditions to Avoid:	Avoid all possible sources of ignition (spark or flame). Do not pressurize, cut, weld, braze, solder, drill, grind or expose containers to heat or sources of ignition.

Many of the same threats of the product during production are present during the end-use. There are dangers for both storing the cylinders as well as combustion of the gas. Acetylene is toxic to humans when accumulated so leaks in damaged cylinders can be dangerous if stored indoors. Acute/single exposure to high concentrations of acetylene (>80%) can cause anesthesia, hypertension, and stimulated respiration [1]. According to the same report, there are no studies done for humans with chronic exposure. Deaths have been reported due to inhalation of acetylene [2]. Explosive decomposition of acetylene occurs at relatively low temperatures compared to other gases. It is recommended cylinders are kept below 125 °F. Acetylene cylinders also must be stored at least 20 feet away from oxygen storage or separated by a wall.

Acetylene has very low stability as the pressure and temperature increase. Compared to other fuels, stability is particularly low and there are many precautions taken from both the manufacturing and end-use perspectives.

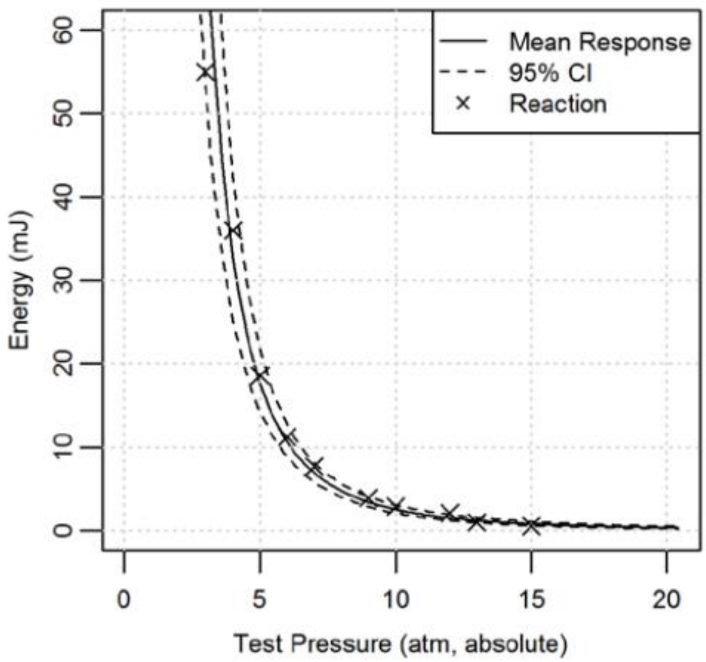

Figure 1. Energy vs. Stability Pressure for Pure Acetylene [3-5]

Figure 1 shows the decomposition energy with respect to stability pressures of acetylene. Acetylene is shown to be instable at as low as 3 atm with 55 mJ of energy.

2.2 End-use

To assess the impact of the combustion of the fuel, the carbon content of the gaseous fuel must be analyzed. For the carbon footprint, the following calculations assume complete combustion (i.e., all carbon is fully oxidized to carbon dioxide and all hydrogen to water vapor). As shown later in the emissions analysis, some of the carbon and hydrogen are present as other trace species (e.g., CO, C_2H_4), the concentration of which varies with temperature of the reactions. With the complete combustion assumption for oxyacetylene combustion, the chemical balance is:

$$C_2H_2(g) + 2.5O_2(g) \longrightarrow 2CO_2(g) + H_2O(g)$$

Carbon, hydrogen, and oxygen have molar masses of $12.01\frac{g}{mol}$, $1.00\frac{g}{mol}$, and $16.0\ \frac{g}{mol}$, respectively. The amount of CO_2 produced on a weight basis can be calculated:

$$\frac{2\ mol\ CO_2 \times 44.01\frac{g}{mol\ CO_2}}{1\ mol\ C_2H_2 \times 26.02\frac{g}{mol\ C_2H_2}} = 3.38\frac{kg\ CO_2}{kg\ C_2H_2}$$

Using this and the density of the gas the expected carbon footprint can be calculated:

$$CF_{end-use} = 3.38\frac{kg\ CO_2}{kg\ C_2H_2} \times 0.033\frac{kg\ C_2H_2}{cu.ft.C_2H_2} = 0.112\frac{kg\ CO_2}{cu.ft.C_2H_2}$$

3 Magnegas-2 End-use & Safety Assessment

3.1 Safety

Safety related information is primarily captured by the available safety data sheet (SDS). There is not significant information in publications on MagneGas to be included in this section.

GHS Classification:

Flammable Gas – 1
Compressed Gas
Acute Toxicity, Inhalation – 4
Skin Corrosion / Irritation – 3
Serious Eye Damage / Eye Irritation – 2B

Hazards:

Extremely Flammable Gas
Contains gas under pressure; may explode if heated
Causes mild skin irritation
Causes eye irritation
Harmful if inhaled
May cause asphyxia
May cause frostbite upon sudden release of compressed gas

Component Exposure Limits:

INGREDIENT:	CAS NO.	OSHA PEL-TLV (ppm; mg/m3)	ACGIH TLV-TWA (ppm)
Hydrogen	1333-74-0	None	Asphyxiant
Carbon Monoxide	630-08-0	50; 55 / 8 hours	25 ppm / 8 hours
Acetylene	74-86-2	None	None
Ethylene	74-85-1	None	200 ppm / 8 hours
Methane	74-82-8	None	1000 ppm / 8 hours
Propylene	115-07-1	None	500 ppm / 8 hours
Carbon Dioxide	124-38-9	5,000; 9,000 / 8 hours	5,000 ppm / 8 hours

Incompatible Materials: Oxidizing Lithium
Halogens
Oxygen
Copper
Silver
Mercury
Brass with >65% Copper

Conditions to Avoid: Storage in excess of 1,000 scf should be outdoors or in well-ventilated area[1,2]. Avoid heat, flames, sparks and other sources of ignition. Minimize contact with material. Containers may rupture or explode if exposed to heat. Cylinders shall not be exposed to direct sunlight outdoors where ambient temperatures exceed 125°F unless designed for use at elevated temperature conditions.

[1] Quantities are to increase 100 percent in buildings equipped throughout with an automatic sprinkler system in accordance with NFPA 13.
[2] Quantities are to increase 100 percent where stored or used in approved, gas cabinets, exhausted enclosures, gas rooms, as appropriate for the material stored.

Analysis of Magnegas-2 has been performed by both WHA International as well as the NASA White Sands Test Facility. These analyses included stability and it was found that MagneGas-2 and MagneGas-Butanol are very stable at higher temperatures and pressures than acetylene.

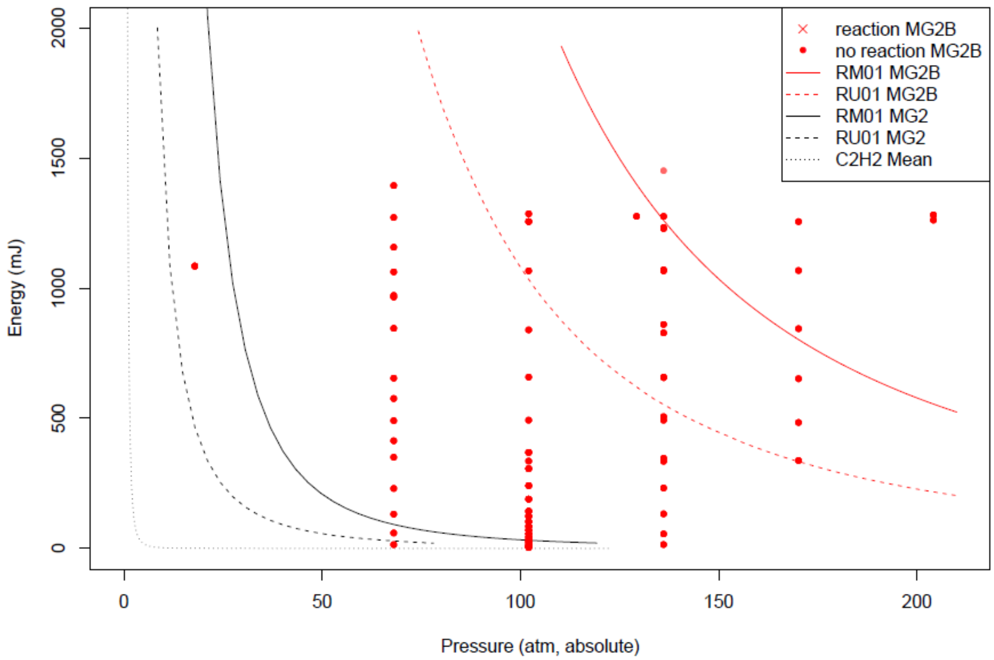

Figure 2. Acetylene/MagneGas-Butanol Comparison Regression Analysis Results with Indicated Ignition Energy [4,5]

Figure 2 shows the decomposition energy with respect to stability pressures of MagneGas-2 (MG2) and MagneGas-Butanol (MG2B), similar to Figure 1 for acetylene. R_{M01} is the 1% predicted ignition probability and R_{U01} is the single-tail 95% confidence interval at that probability.

3.2 End-use

The components of MagneGas-2 were measured and the average values for each component are shown in Table 1. It should be noted that there are more components that exist other than those listed in Table 1, however, those listed make up 99.38% of the total.

Table 1. MagneGas-2 Composition

Chemical Composition	Average %(Vol/Vol)
H_2	51.97
CO	24.56
C_2H_2	11.42
CH_4	6.65
C_2H_4	4.78

To assess the impact of the combustion of MagneGas-2, the values in Table 1 will be used to calculate the CO_2 emissions. For the carbon footprint, the following calculations assume complete combustion (i.e., all carbon is fully oxidized to carbon dioxide and all hydrogen to water vapor). As shown later in the emissions analysis, some of the carbon and hydrogen are present as other trace species (e.g., CO, C_2H_4), the concentration of which varies with temperature of the reactions. With the complete combustion assumption for oxy-MagneGas-2 combustion, the chemical balance is:

$$0.5197H_2 + 0.2456CO + 0.1142C_2H_2 + 0.0665CH_4 + 0.0478C_2H_4 + 0.9446O_2 \longrightarrow 0.8625H_2O + 0.6361CO_2$$

$$CE_{CO2} = \frac{0.6361\, mol\, CO_2}{0.9938\, mol\, fuel} = 0.6401\ \frac{mol\, CO_2}{mol\, fuel}$$

Converting this into a form that is usable for the carbon footprint, $CF_{end\text{-}use}$. First the molar mass of the fuel is calculated:

$$= \frac{1}{0.9938}[[0.5197(2) + 0.1142(2) + 0.0665(4) + 0.0478(4)]\frac{mol\, H}{mol\, fuel} \times 1\frac{g}{mol\, H} + [0.2456(1) + 0.1142(2) + 0.0665(1) + 0.0478(2)]\frac{mol\, C}{mol\, fuel} \times 12.01\frac{g}{mol\, C} + [0.2456(1)]\frac{mol\, O}{mol\, fuel} \times 16\frac{g}{mol\, O}]] = 13.38\frac{g\, fuel}{mol\, fuel}$$

$$CF_{end-use} = \frac{0.6401\ \frac{mol\, CO_2}{mol\, fuel} \times (12 + 32)\frac{g\, CO_2}{mol\, CO_2}}{13.38\frac{g\, fuel}{mol\, fuel}} = 2.105\frac{kg\, CO_2}{kg\, fuel}$$

Then we find the density of the fuel to convert it into a cubic feet basis:

$$\rho_{fuel} = 13.38\frac{g\ fuel}{mol\ fuel} \times 1.195\frac{mol\ fuel}{cu.ft.fuel} \times \frac{1\ kg\ fuel}{1000\ g\ fuel} = 0.016\frac{kg\ fuel}{cu.ft.fuel}$$

Finally, we can calculate the emissions on a cubic feet basis:

$$CF_{end-use} = 2.105\frac{kg\ CO_2}{kg\ fuel} \times 0.016\frac{kg\ fuel}{cu.ft.fuel} = 0.034\frac{kg\ CO_2}{cu.ft.MG}$$

3.3 Emissions Analysis

The MagneGas-2 fuel was oxidized inside a 6-inch diameter stainless steel combustor and the combustion exhaust was characterized with a gas chromatograph. The combustor was lined with a ceramic thermal insulation to minimize the heat loss to the surroundings. This resulted in higher flame and exhaust temperatures. The oxidation was then repeated with the ceramic insulation removed. A schematic of the experimental setup is shown in Fig. 3 below.

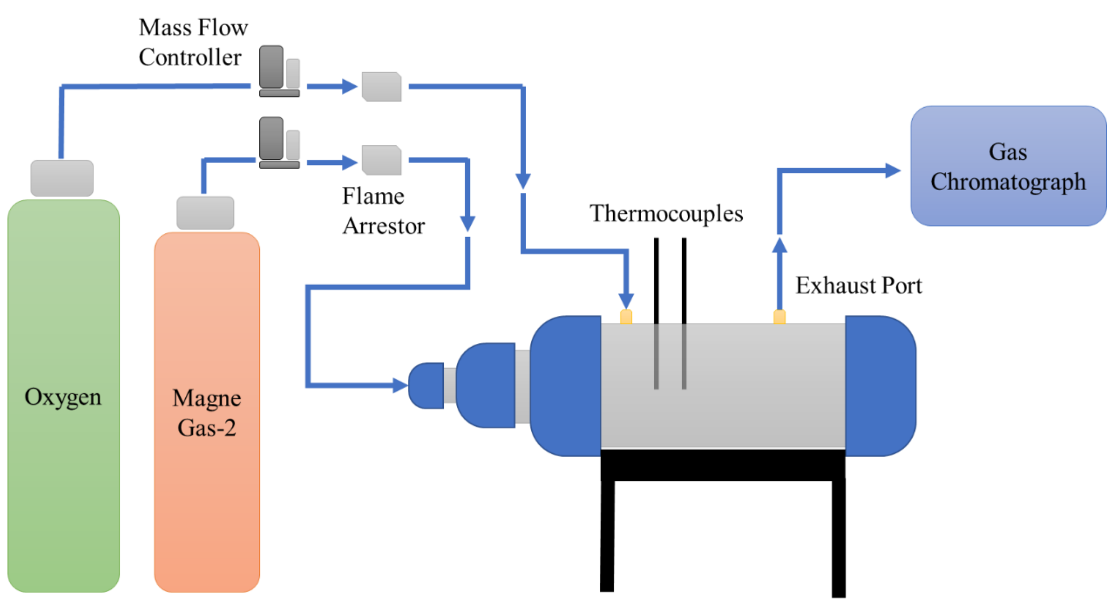

Figure 3. Schematic of the Combustion Characterization Chamber

The gas composition of the MagneGas-2 utilized in the experiment was analyzed by the gas chromatograph and tabulated in Table 2 below. It is important to note that the composition is slightly different than stated in Table 1 above. The operating equivalence ratio, ϕ, was 0.572 with pure oxygen as the oxidant. The flow rates utilized in the experiment are listed in Table 3. The results of the dry exhaust combustion analysis are shown in Table 4 below.

Table 2. MagneGas-2 Composition Utilized in Experiment

Gas Species	**Gas Concentration Mole %**
Methane (CH_4)	6.25
Ethylene (C_2H_4)	3.86
Acetylene (C_2H_2)	11.56
Carbon Monoxide (CO)	30.08
Hydrogen (H_2)	48.25
Total	100.00

Table 3. Equivalence Ratio and MagneGas-2/Oxygen Flow Rates

Equivalence Ratio	**MagneGas-2 (SLM)**	**Oxygen (O_2) (SLM)**
0.572	3.151	5.078

Table 4. Dry Exhaust Composition of the MagneGas-2 Oxidation

Exhaust Species Measured	Gas Concentration Mole % (Insulated)	Gas Concentration Mole % (Non-Insulated)
Methane (CH_4)	0.0004*	0.0047
Ethane (C_2H_6)	0	0.00003*
Ethylene (C_2H_4)	0.0001*	0.0012*
Acetylene (C_2H_2)	0.0003*	0.0026
Propane (C_3H_8)	0	0
Propylene (C_3H_6)	0.0001*	0.0004*
Cyclopropane (C_3H_6)	0	0
n-Butane (C_4H_{10})	0	0
iso-Butane (C_4H_{10})	0	0
iso-Butylene (C_4H_8)	0	0
Trans-2-Butene (C_4H_8)	0	0
Cis-2-Butene (C_4H_8)	0	0
1,3-Butadiene (C_4H_6)	0	0
n-Pentane (C_5H_{12})	0	0
iso-Pentane (C_5H_{12})	0	0
C_6+**	0	0
Carbon Monoxide (CO)	0.0080	0.3473
Oxygen (O_2)	23.9376	21.3749

* - Above/below calibrated range of gas chromatograph. The lower calibrated bound of the gas chromatograph for hydrocarbons is 0.0015% (15 ppm). Interpolation was used to get results.
** - Hydrocarbons that are C_6H_x and greater.

With the equivalence ratio and the measured values of CH_4, C_2H_4, C_2H_2, C_3H_6, and CO, the following reaction balance reaction occurs. The combustion emissions of CO_2 are:

$$0.572(48.25\,H_2 + 30.08\,CO + 11.56\,C_2H_2 + 6.25\,CH_4 + 3.86\,C_2H_4) + 92.145\,O_2 \longrightarrow 0.0004\,CH_4 + 0.0001\,C_2H_4 + 0.0003\,C_2H_2 + 0.0001\,C_3H_6 + 0.008\,CO + 38.412\,CO_2 + 45.775\,H_2O + 39.444\,O_2$$

To calculate an equivalent carbon footprint of the other emissions, assuming complete combustion.

$$0.0004\,CH_4 + 0.0001\,C_2H_4 + 0.0003\,C_2H_2 + 0.0001\,C_3H_6 + 0.008\,CO + 0.0095\,O_2 \longrightarrow 0.0095\,CO_2$$

$$CE_{CO2} = \frac{38.423\,mol\,CO_2}{57.2\,mol\,fuel} = 0.6717\,\frac{mol\,CO_2}{mol\,fuel}$$

Converting this into a form that is usable for the carbon footprint, $CF_{end\text{-}use}$. First the molar mass of the fuel is calculated:

$$= \frac{1}{100}[[48.25(2) + 11.56(2) + 6.25(4) + 3.86(4)]\frac{mol\,H}{mol\,fuel} \times 1.008\frac{g}{mol\,H} + [30.08(1) + 11.56(2) + 6.25(1) + 3.86(2)]\frac{mol\,C}{mol\,fuel} \times 12.01\frac{g}{mol\,C} + [30.08(1)]\frac{mol\,O}{mol\,fuel} \times 16\frac{g}{mol\,O}]] = 14.493\frac{g\,fuel}{mol\,fuel}$$

$$CF_{end-use} = \frac{0.6717\,\frac{mol\,CO_2}{mol\,fuel} \times (12.01 + 32)\frac{g\,CO_2}{mol\,CO_2}}{14.493\frac{g\,fuel}{mol\,fuel}} = 2.0397\frac{kg\,CO_2}{kg\,fuel}$$

Then we find the density of the fuel to convert it into a cubic feet basis:

$$\rho_{fuel} = 14.493\frac{g\,fuel}{mol\,fuel} \times 1.1698\frac{mol\,fuel}{cu.ft.fuel} \times \frac{1\,kg\,fuel}{1000\,g\,fuel} = 0.0170\frac{kg\,fuel}{cu.ft.fuel}$$

Finally, we can calculate the emissions on a cubic feet basis:

$$CF_{end-use} = 2.0397\frac{kg\,CO_2}{kg\,fuel} \times 0.0170\frac{kg\,fuel}{cu.ft.fuel} = 0.035\frac{kg\,CO_2}{cu.ft.MG}$$

4 Summary

Comparing acetylene and MagneGas-2, it has been revealed that MagneGas-2 is significantly more stable at higher pressures and temperatures as well as emits less carbon dioxide upon combustion. A comparative stability graph is shown in Figure 3.

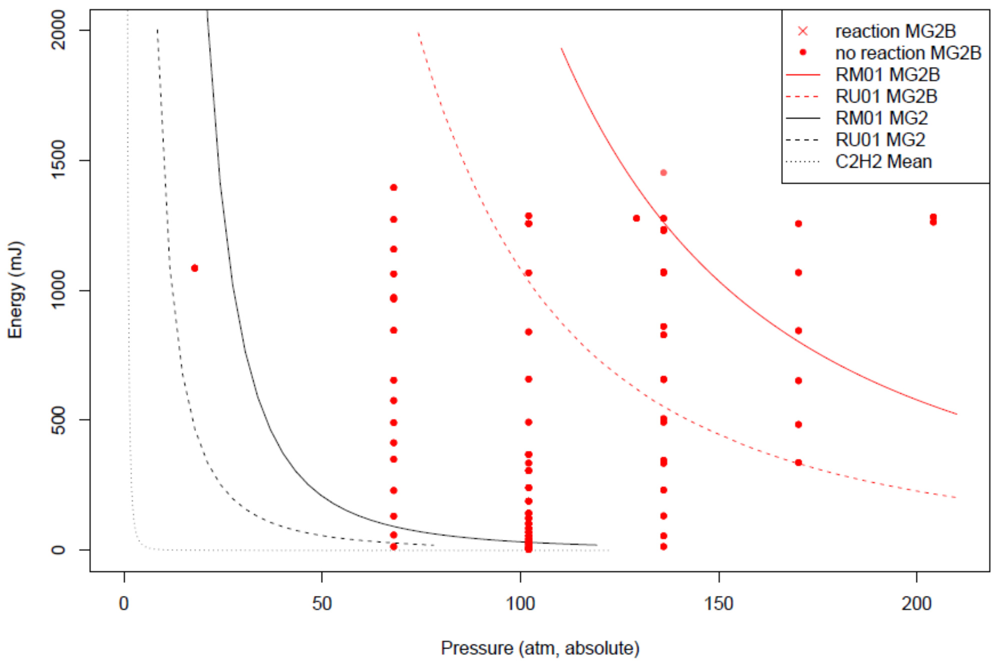

Figure 4. Decomposition Energy vs. Pressure for MagneGas-2 and Pure Acetylene [4,5]

The stability of the gas is indicative of its safety for storage and use. MagneGas-2 has many of the same physical dangers associated in storage and use as acetylene, however, at much more extreme conditions which are unlikely to occur. Acetylene explosions are well documented, happening in both transportation as well as in storage.

The combustion of MagneGas-2 has been shown to have significantly less environmental impactful. It contributes 70% or 0.078 $\frac{kgCO_2}{cu.ft}$ less carbon dioxide than acetylene on a volume basis.

A summary table of the stability and carbon emissions is shown in the following table. At the time of this report, WHA International was performing Gas Stability tests with the MagneGas produced from ethanol feedstock, the same gas that this analysis and tests were performed with. Preliminary testing results indicate that Ignition Energy at 100 atm is also >1,000 mJ.

Table 5. Summary comparison between oxyacetylene and oxy-MagneGas-2

	Oxyacetylene (Calculated)	**Oxy-MagneGas-2 (Calculated)**	**Oxy-MagneGas-2 (Experimental)**
Carbon Footprint	$0.112 \frac{kg\ CO_2}{cu.ft.C_2H_2}$	$0.034 \frac{kg\ CO_2}{cu.ft.MG}$	$0.035 \frac{kg\ CO_2}{cu.ft.MG}$
Safety - Ignition energy at 100 atm	< 5 mJ	NA	>1000 mJ

5 References

[1] Public Health England Toxicology Department. Acetylene Toxicological Overview. Version 1. 2009.

[2] Williams, N. R. and Whittington, R. M. (2001). Death due to inhalation of industrial acetylene. J Toxicol Clin Toxicol 39, 69-71.

[3] Miller, S. (1965). Acetylene: Its Properties, Manufacture and Uses. New York: Academic Press.

[4] Whitehead, J. Linley, N. and Newton, B. (2017). Pressure and Energy Stability Measurements of MagneGas 2™, WHA International, 1-8.

[5] Whitehead, J., Linley, N., and Newton, B. (2017). Pressure and Energy Stability Comparisons between MagneGas 2TM and MagneGas 2BTM, WHA International, 1-4.