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Design of a Gas Conditioning System for the Second Generation Union College Areogel Lab Catalytic Test Bed

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Design of a Gas Conditioning System for the Second Generation Union College Areogel Lab Catalytic Test Bed

By

Tom Swanton

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of the requirements for
Honors in the Department of Mechanical Engineering

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ABSTRACT

SWANTON, THOMAS Design of a gas conditioning system for the second Generation Union College Areogel Lab catalytic test bed

ADVISOR: Professor Bradford Bruno, Ph.D.

The goal of this project was to design and fabricate a system which could deliver artificially created test gas to the heating section at a specified composition, flow rate, and humidity, while additionally simulating the transient conditions found in automobile exhaust. It will make up one subsystem of the Union College Aerogel Lab's second generation catalytic test bed. The test bed will be used to test the viability of catalytic aerogels as three way catalysts for automotive exhaust. To date a system for mixing test based on partial pressure has been fabricated and is operational, a system for generating transient conditions using solenoid valves and two gas mixtures has been designed and the parts sourced, and several viable humidification designs have been evaluated.

Table of Contents:

1. Background

2. Previous Work

5. Gas Mixing System

7. Gas Switching System

8. Humidification of the Test Gas

9. Global System Design

Attachments

1. Background

1.1 Exhaust and Common Pollutants

Gasoline powered internal combustion engines are a dominant driver of transportation in the world today and are unlikely to be replaced any time in the near future. An ideal engine would burn fuel completely, at the proper stoichiometric ratio with oxygen. The only products of this combustion would be water and carbon dioxide. This scenario proves impossible in an actual engine due to the unstable and transient nature of internal combustion. Instead engine combustion is characterized as either rich or lean. A rich burn has an excess of fuel in the charge and thus a shortage of air while a lean burn has a shortage of fuel and too much air. The relative amounts of air and fuel in the charge can be described with the air fuel ratio (AFR) which is defined in equation 1.

$$AFR = \frac{m_{Air}\ (kg)}{m_{Fuel}\ (kg)} \tag{1}$$

The air fuel ratio for the stoichiometric combustion of gasoline is 14.7. An AFR above 14.7 would describe a lean burn while an AFR below 14.7 describes a rich burn. An automobiles engine management system works to keep the AFR as close to stoichiometric as possible. While the major exhaust components of either burn remain water and carbon dioxide, other products are produced in smaller quantities. These products can cause serious health and environmental problems. The three primary pollutants found in automobile exhaust are carbon monoxide (CO), unburned hydrocarbons (UHCs), and oxides of nitrogen (NO_x). Figure 1.1

shows a plot of the levels of these pollutants, as well as water (H_2O), carbon dioxide (CO_2), and oxygen (O_2), with respect to the air fuel ratio.

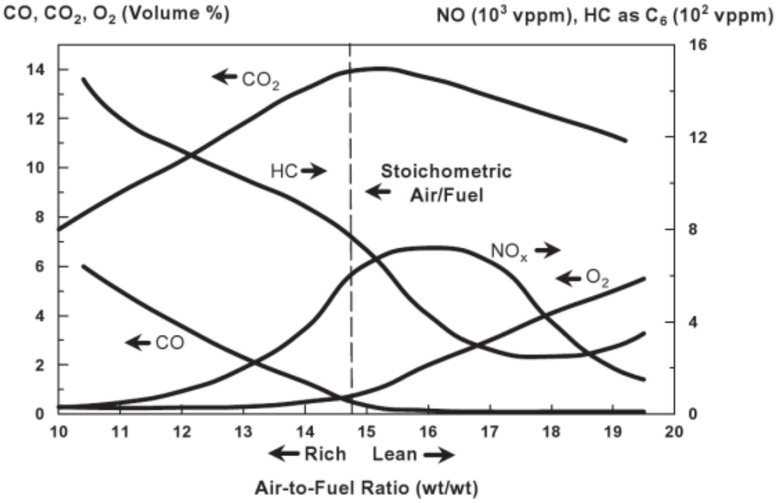


Figure 1.1 The relative levels of exhaust components with respect to the air fuel ratio

(Image Source: Heck et al, *Catalytic Pollution Control,* pp. 104)

Oxides of nitrogen describe a group of combustion products including nitric oxide (NO) and nitrogen dioxide (NO_2). In a gasoline engine the vast majority of NO_x production is in the form of NO. In a diesel a larger portion, up to 30%, may be NO_2. Nitrogen oxides are formed at very high temperatures in lean combustion environments by the combustion of atmospheric nitrogen. The reactions leading to their formation are described by the three revisable reactions of the Zeldovitich Mechanism:

$$O + N_2 \leftrightarrow NO + N$$

$$N + O_2 \leftrightarrow NO + O$$

$$N + OH \leftrightarrow NO + H$$

As combustion continues and the cylinder pressure increases temperatures of the gases behind the flame front are further raised higher than combustion temperatures. Most NO_x found in the exhaust is formed in this region. During the expansion stroke of the engine cycle temperatures drop quickly and NO_x levels are frozen at levels far higher than equilibrium. This freezing occurs much earlier in a lean mixture than a rich one. Therefore NO_x Levels are far higher for lean burns than rich ones. Efforts to limit NO_x production in engines generally focus on lowering combustion chamber temperatures. [1]

Oxides of Nitrogen have significant health and environmental effects. While generally non toxic on its own, NO will oxidize into NO_2, a far more deadly gas which can cause severe lung damage and death in relatively small concentrations. [1]. On a larger scale, NO_x in the atmosphere is oxidized to form the nitric acids found in acid rain. Acid rain contributes to forest damage and the acidification of fresh water sources. [1]

Carbon monoxide is generated inside the combustion chamber as one of the intermediate reactions in the oxidation of a hydrocarbon. The CO is then oxidized into CO_2, one of the final products of combustion. The rate of oxidation of CO is dependent on the available oxygen in the chamber. In rich burns a shortage of oxygen results in portions of un-oxidized CO passing into the exhaust. Engine designers work to minimize CO production by leaning the burn and improving the uniformity of the charge. [1]

Carbon monoxide has an affinity for the hemoglobin in human blood which is 240 times higher than that of oxygen. High concentrations of CO in the blood prevent cells from receiving oxygen, causing loss of consciousness and eventually death. The danger of CO is greatly increased by the fact that it is colorless and odorless. [1]

Unburned hydrocarbons are portions of the fuel from the charge and lubricants leaked into the combustion chamber which are not completely burned before leaving in the exhaust. Gasoline is made up of a variety of complex hydrocarbons. During combustion the long chains in these hydrocarbons are broken down in a series of intermediate reactions before being completely oxidized. It is therefore possible to have a wide range of hydrocarbons in the exhaust even if the fuel used is very pure. One of the main factors influencing UHC levels is quenching, where heat is lost to the piston and cylinder walls, stopping further combustion. Since the cylinder walls cannot sustain combustion level temperatures without melting some level of quenching is unavoidable. During cold start, before the engine warms up, quenching is particularly prevalent. A rich mixture will also result in an excess of UHCs as there is not enough oxygen in the combustion chamber to burn them [1] Unburned hydrocarbons are less acutely toxic than either NO_x or CO but when released can react with other pollutants in the atmosphere to form photochemical smog and low level ozone. [2]

Because combustion varies widely by location within the combustion chamber, all of these pollutants may be found in the exhaust simultaneously. As figure 1.1 shows there is an inherent trade-off between the pollutants, with NO_x dominant in lean burns while CO and UHCs dominate fuel rich burns. This makes it very difficult to eliminate pollutants from the combustion products.

1.2 Transient Compositions in Automobile Exhaust

The task of managing combustion in a modern automobile engine is left to the engine management system (EMS). On the most basic level the EMS in a spark ignition is responsible for adding an appropriate amount of fuel for the amount of air entering the engine. The airflow is governed by the throttle which is controlled by the driver. The controller for the fuel system receives feedback from the oxygen sensor, also known as the λ sensor, which can determine if the exhaust leaving the cylinders is composed of the products of a lean or rich burn. This closed loop control system is shown in figure 1.2.

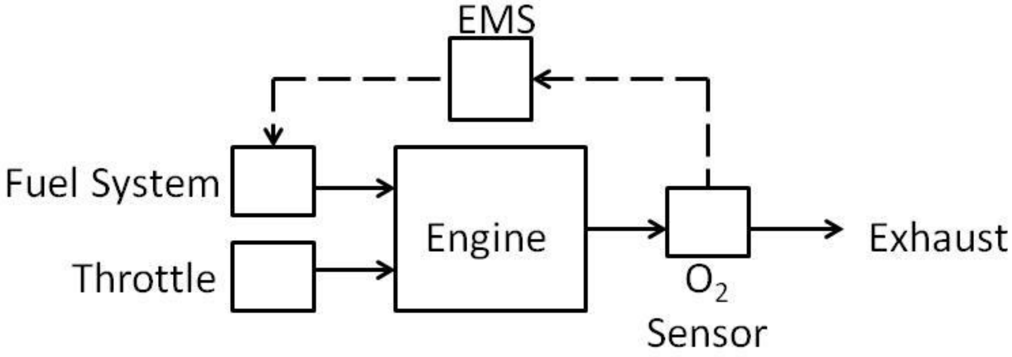


Figure 1.2 A diagram showing the simplified control system in an automobile engine

Overall the EMS does a very good job at regulating engine combustion and keeping combustion stoichiometric. Its ability to maintain combustion stability is limited by the amount of time it takes air to pass through the engine. For if the O_2 sensor reads that the engine is running slightly lean then the EMS will increase the amount of gasoline added almost instantaneously. While the richer mixture runs through the intake manifold, valves, four cycles of combustion, and finally into the exhaust headers the sensor will continue to show a lean burn and the EMS continues to add more fuel. After the rich exhaust reaches the sensor the EMS signals the fuel system to reduce the fuel added and the cycle repeats itself. Therefore the composition of the exhaust will continuously oscillate between a slightly lean and a slightly rich composition. [3]

The frequency of this cycle is limited by the time it takes the charge to travel from the fuel system to the O_2 sensor and the time it takes for the engine management system to take a reading from the sensor and enact a change in the fuel system. Since the EMS is electronic its response time is generally small compared to the time it takes air move through the engine. The overall time is called the time lag and is denoted τ_L. The frequency for the oscillations is called the limit cycle and is found from equation 2. [3]

$$f_{LC} = \frac{1}{4\tau_L} \tag{2}$$

Figure 1.3 shows the relationship between the exhaust composition, as read by the sensor and the controller output from the EMS.

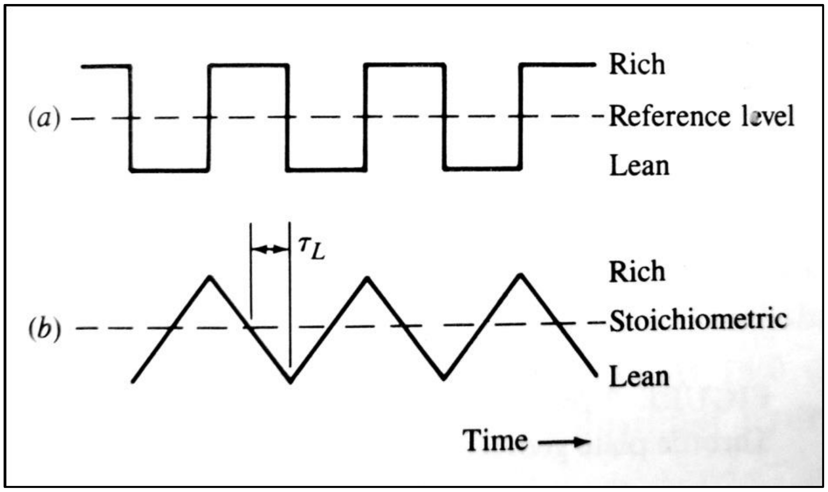


Figure 1.3 A comparison of a) the signal from the oxygen sensor to (b) the controller output voltage relative to the lag time τ_L. Image source: Heywood, John B *Internal Combustion Engine Fundamentals* pg 303

This represents the simplest possible model for exhaust composition transients as a result of the engine management system. For the purposes of this project the frequency of the limit cycle is assumed to be 1 Hz.

1.3 Three Way Catalysts

While it is the goal of engine designers to create increasingly cleaner burning engines through optimizing systems such as combustion chamber shapes and fuel injection, it has so far proved impossible to eliminate the production of all pollutants. Therefore, in order to meet increasingly stringent pollution regulations, it is generally necessary to introduce some form of exhaust after-treatment system.

In contemporary automotive exhaust systems this is done by adding a “three way catalyst” between the engine and tailpipe. These catalysts are made up of precious metals and alumina supports which are wash coated onto a ceramic honeycomb structure to maximize the surface are of catalyst exposed to the exhaust. [2]. Figure 1.4 shows a cut away of a typical catalytic converter.

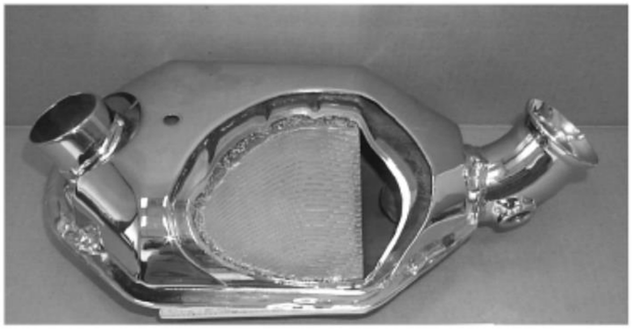


Figure 1.4 Photograph showing a cutaway of a catalytic converter. The innermost layer is the ceramic honeycomb wash coated with catalyst.

(Image Source: Heck et al, *Catalytic Pollution Control,* pp. 111)

The three way catalyst breaks down the three main pollutants into carbon dioxide, water and nitrogen according to the following reactions [2]

$$C_yH_n + (1 + .25n)O_2 \rightarrow yCO_2 + .5nH_2O$$

$$CO + .5\,O_2 \rightarrow CO_2$$

$$CO + H_2O \rightarrow CO_2 + H_2$$

$$NO + CO \rightarrow .5\,N_2 + H_2O$$

$$(2 + .5n)NO + C_yH_n \rightarrow (1 + .25n)N_2 + yCO_2 + .5n\,H_2O$$

The three way catalyst both oxidizes CO and UHCs and reduces NO_x simultaneously. The catalyst's effectiveness is dependent on high temperatures. Since the catalytic converter is heated by the hot engine exhaust, there is a period of warm-up time before catalytic activity begins. The temperature at which the reactions are initiated is called the light-off temperature. [2]

The three way catalysts found in automobiles are very expensive relative to the total cost of the vehicle. The primary catalytic materials used are platinum and palladium, both of which command very high prices and are very environmentally damaging to mine and purify. This makes the cost of catalytic converters very dependent on precious metal prices and valuable to the point of catalytic converters being cut out of automobiles by thieves for their metal value. In addition the processes used to coat the catalytic material on the substrate are closely guarded industrial secrets and generally expensive as well. A lower cost catalytic converter would provide direct cost reduction to consumers and reduce the need for environmentally damaging precious metal mining.

2. Previous Work

2.1Previous Work and Current Test bed

In recent years it has been shown [4] [5] that catalytic aerogel materials (CAMs) can act as an effective three way catalyst without the need of precious metals. These aerogels are produced in the Union College Aerogel Lab using the novel rapid super-critical extraction (RSCE) method. When used as three way catalysts, CAMs can achieve significant reductions pollutants found in automotive exhaust.

The effectiveness of these materials at reducing emissions is determined using a catalytic test bed. The test bed generates simulated exhaust and passes it over a sample of catalytic material at temperatures representative of those in an automobile's catalytic converter. The sample is located in the test chamber. The effectiveness of the aerogel is determined by analyzing the reduction of pollutants at the outlet. Figure 2.1 shows an operation schematic of the current catalytic testbed.

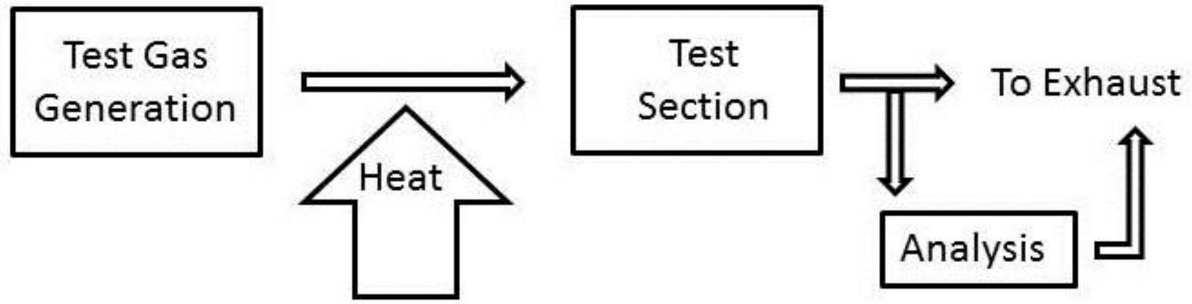


Figure 2.1 A general schematic of a catalytic test bed

The idea for Union's first generation test-bed was first proposed by Michael Bono in 2008 as part of his senior project. His testing setup used an emissions blend specified by the California Bureau of Automotive Repair (BAR). Designated BAR 97 Blend 32, the blend contains known concentrations of the three common pollutants found in automobile exhaust. The composition of the emissions blend is specified in table 2.1.

Table 2.1 Composition of BAR 97 Blend 32 calibration gas

(Source: Airgas Special Applications: Environmental Monitoring)

BAR 97 Blend 32	
Propane	200 ppm
Carbon Monoxide	0.50%
Carbon Dioxide	6.00%
Nitrogen Monxide	300 ppm
Nitrogen	Balance (93.45%)

The purpose of this blend is to aid in the calibration of emissions testing equipment. Bono mixed the blend with air from a compressed air line to generate a test gas with concentrations of CO, UHCs, and O_2 representative of typical automotive exhaust at a stoichiometric burn. At the time the gas analyzer used in testing was incapable of measuring of concentrations of NO but it was determined that the levels were within those typical for a gasoline engine. [4]

This proved an adequate solution because the blends were readily available from local gas suppliers as opposed to ordering custom blends at a far greater cost. The gas to air ratio was set using rotameters and control valves to set the air and emissions blend flow rates independently. The mixed gas was then flowed into the test chamber, consisting of a metal tube with screens to retain the sample. The test section was heated using heating tape controlled by a proportional voltage controller. The outlet measurements were taken using a 4 gas analyzer similar to those found in repair garages for automobile inspections. The final setup is shown in figure 2.2. While initial testing showed the system was functional it was found that the temperatures exiting the test chamber were about 300°C, far short of the desired temperature of 500° C. [4]

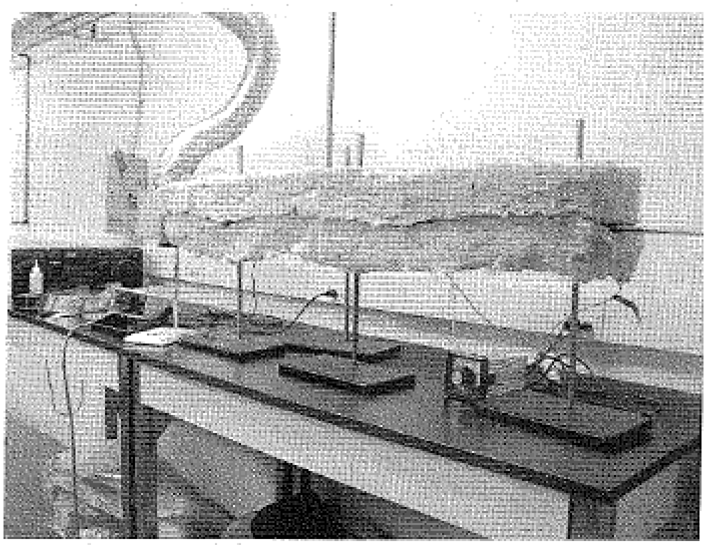


Figure 2.2 The final setup as designed by Michael Bono in 2008

(Image source: Bono 2009)

Over the next few years several students continued to develop the test bed. The bulk of this work focused on the heating and test sections. The method of using two rotameters to mix emissions blend and compressed air remained through every iteration. The most significant modification to the test gas delivery system was the addition of a dedicated compressed air line by Justin Rodriguez as part of his senior project in 2011. This allowed the heating system to reach steady state with just air flowing through the lines to avoid wasting the emissions blend. This flow was controlled with a dedicated rotameter attached to the air line. Figure 2.3 shows the updated gas delivery system.

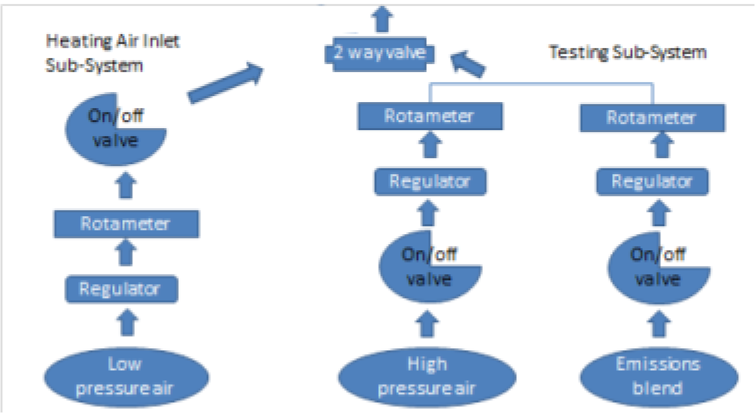


Figure 2.3 Gas delivery system as updated by Justin Rodriguez to include an auxiliary air line for heat up (Image source: Rodriguez 2011)

The current test bed is made up of three primary systems. The gas delivery system mixes the emissions blend and the compressed air into the required flow rate by the hand adjustment of rotameters. The test gas is then passed through an inline heater into the test section which is wrapped in heating tape and insulation. The CAM sample is located in the test section between two screens. After the gas passes through the test section it is sampled by a 5 gas analyzer of the type found in automotive repair shops. Unlike the 4 gas analyzer used in previous experiments this instrument can also detect concentrations of NO. Since the initial composition of the test gas entering the chamber is known it is possible to determine the effectiveness of the cam from the outlet measurements. Finally the flow is directed to the exhaust port where it is vented safely out of the building. Figure 2.4 shows a picture of the current catalytic test bed.

Figure 2.4 The current catalytic test bed. The probe for the 5 gas analyzer is hanging on the left side of the frame beneath the detector. The emissions blend tank is located to the right of the image. (Image courtesy of Dave Carabis)

2.2 Second Generation Test Bed

While the current system has proved adequate for proving the viability of CAMs as three way catalysts it is the goal of the second generation test bed to expand the range of experiments which may be performed, increase the level of automation in control and data collection, while at the same time making it easier to operate and maintain safely. Another goal of the project is to give the user better control of the composition and state of the gas mixture entering the system as well as be able to model transient conditions in addition to the steady state case allowed by the current test bed. This will require the construction of a new test bed.

This project will be funded by a portion the NSF grant awarded to the Union College Aerogel Lab to continue their research into catalytic aerogel materials. Approximately $75,000 has been allotted to the design and construction of the new test bed. [6]

3. Design Requirements

The scope of this project is all the sub-systems in the new test bed up to the heating sub-system. This includes the mixing, metering, and humidification of the test gas, as well as simulating the transient compositions found in automotive exhaust. Another senior, Paul Brockman is responsible for the heating and test sections.

The current source of test gas comes from premixed disposable gas cylinders purchased from a local gas supplier. The tanks are a certified blend used to calibrate emissions testers. These tanks are expensive and have a large lead time when ordered. The new system should be able to create custom blends to expand the scope of testing. This offers a reduction in cost and increased flexibility in mixture composition.

Once the test gas can be generated in the appropriate compositions, the next step is to meter it to the system effectively. For good repeatability between tests it is important to know how much gas is entering the system and be able to control that flow precisely. The first generation test bed utilizes rotameters to control the flow into the test bed. This is a very user intensive process which introduces a good deal of uncertainty into the test. We would like to overhaul the metering system with one that is both more user friendly and consistent. The system should be able to meter out gas to be able to support test section temperatures from 100°C to 800°C and range of flow rates based on reactor conditions.

The ability to simulate transient conditions in the new test bed is an important expansion of its capabilities. The composition of exhaust components is determined by the burn conditions in the cylinder. The burn conditions are in turn controlled by the vehicles engine management system. The goal of the system is to keep the burn in the cylinder stoichiometric. Due the limitations of the engine management system the exhaust composition tends to oscillate between slightly lean and slightly rich burn conditions with a frequency of about 1 Hz. This means that the composition of the exhaust going into the three way catalyst is not constant. The second generation test bed must be able to replicate this behavior.

Another expansion of test bed capabilities is humidification. The current system uses exclusively dry gas. This is not reflective of actual conditions found inside a catalytic converter. Water is a very significant product of hydrocarbon combustion and large quantities of it are present in automotive exhaust. Additionally it is an unreasonable assumption that air entering an engine is at zero relative humidity, and any water in the initial charge must be carried to the exhaust. Therefore it is crucial that the second generation test bed be able to humidify the test gas to levels which may be found in typical engine exhaust.

An overarching goal for the second generation test bed is that it be easier to use and more reliable. This means introducing a significant degree of automation. On the current test bed it takes a skilled operator several hours to test a single sample. The final goal for the system is complete automation, with a user loading the sample and selecting the test parameters from a unified interface and then sitting back and focusing on the results rather than franticly turning switches and knobs. In the context of my project this means ensuring that all of the hardware and sensors used have the potential for complete automation.

A final and paramount concern is user safety. The test bed will employ high pressures and temperatures, toxic gases and large voltages. It is important to incorporate redundant safety features as well as detailed protocol to ensure safe use.

In conclusion, the goal of my project is to design and fabricate a system which can deliver simulated test gas to the heating section at a specified composition, flow rate, and humidity, while additionally simulating the transient conditions found in automobile exhaust. This system must have the potential for full automation and be safe and easy to use.

4. Units and Flow Rates

Flow rates in catalytic reactors are generally described in terms of a space velocity. Space velocity is defined in equation 3.

$$s = \frac{\dot{V}}{V_t} \tag{3}$$

Where $\dot{V}$ is the volumetric flow rate of the gas entering the test chamber, V_T is the internal volume of the test chamber, and s is the space velocity with units of 1/s. Space velocity is important because it is the inverse of residence time, or the amount of time a theoretical gas particle spends in the test chamber exposed to the catalyst. Lower space velocities are advantageous to catalytic activity there is more time for the catalytic reactions to occur. The space velocities in an automotive catalytic converter are governed by the engine speed and displacement controlling the flow rates and spatial considerations limiting the size of the converter.

Further complicating the matter is the fact that as test gas is heated it expands, changing the volumetric flow rate as the gas moves through the heating section. Therefore it is convenient to describe the flow rate of test gas as a mass flow rate, which is constant when the system is at steady state. The mass flow rate may be calculated from the space velocity and the test section temperature using previous equation and the ideal gas law. Rearranging the space velocity equation yields an expression for the volumetric flow rate.

$$\dot{V} = sV_t \tag{4}$$

The volumetric flow rate is related to the mass flow rate by density.

$$\dot{m} = \rho\dot{V} \tag{5}$$

If the test gas is assumed to be ideal, its density can be found from a modified form of the ideal gas law.

$$\rho = \frac{P}{RT} \tag{6}$$

Where P is the pressure in the test section, assumed to be atmospheric. R is the specific gas constant of the test gas, assumed to be equal to that of air and T is the temperature of the test section in Kelvin. The resulting density, ρ, has units of kg.m^3. These equations are combined to get a mass flow rate as a function of the reactor temperature and space velocity.

$$\dot{m} = \frac{sV_tP}{RT} \tag{7}$$

Figure 4.1 is a plot showing the relationship of mass flow, space velocity and reactor temperature. A sample calculation for the mass flow rate from a temperatures and space velocity is presented in attachment A.

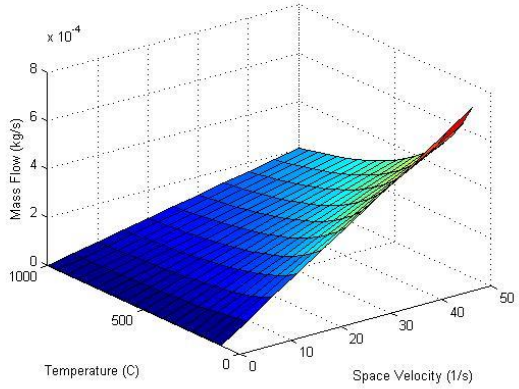


Figure 4.1 Plot showing the mass flow rate as a function of reactor temperature and space velocity

When volumetric flow rates are described in this paper it should be assumed that the test gas is at standard temperature and pressure unless specified otherwise. The abbreviation SLM describes a flow in l/min under standard conditions.

Through these calculations there is a reoccurring assumption that the test gas may be modeled using the ideal gas law. This is a very powerful assumption not only because it eases the calculation of the gas conditions at various states, but because it simplifies calculations with regard to the gases' composition. In a mixture of ideal gases the volume fraction is equivalent to the mole fraction is equivalent to the partial pressure fraction. This can be verified by the ideal gas law. The volume fraction is useful for computing volumetric flow rates when sourcing controllers. The molar fraction is helpful when looking at chemical reactions between components. Finally the partial pressure fraction is useful in mixing gases. Being able to switch between these without conversion factors is very helpful.

The question then becomes how good is this assumption? The test gas used is mostly nitrogen and carbon dioxide. These two components make up over 95% of the gas going into the test section. Since both of these gases behave as ideal gases it is a reasonable assumption that the mixture will act as an ideal gas. Because the composition of the test gas is so similar to that of air it is further assumed in some calculations that the test gas shares the thermodynamic properties of air as these properties are readily available. Overall these assumptions are acceptable for the purposes of designing the systems and sourcing parts however a more detailed analysis should be used to set testing parameters.

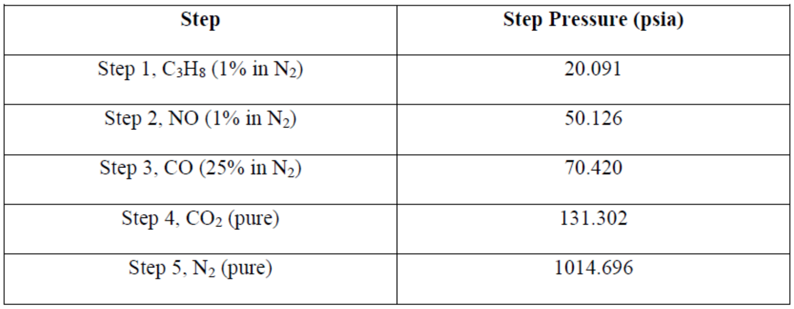
5. Gas Mixing Sub-System

5.1 Motivation and Principle

The gas mixing system (GMS) is a stand-alone system which will mix cylinders of test gas from individual tanks of gas components. The ability to mix test gas in-house would be extremely beneficial to future research. Not only does it represent a significant cost reduction over purchasing disposable cylinders from a gas supplier but it also allows for the formation of custom exhaust blends to suit testing needs.

The GMS operates on the principle of partial pressures. Partial pressure is the pressure a component of a gas mixture would exert on the container if were the sole component. The sum of the partial pressures is equal to the total pressure in the container. For an ideal gas mixture the proportion of partial pressure to total pressure of a component is equal to its percent concentration. Therefore it is possible to fill a container with the proper mixture by stepping the partial pressure of its components to reach its final pressure. It is important that these steps be carried out with regard to absolute pressure. Table 2 shows the pressure steps for mixing a 1000psig tank of BAR 97 Blend 32 test gas. [7]

Table 5.1: Step pressures for filling a tank with 1000psig of BAR 32 blend (note that 1000 psig = 1014.7 psia) (Source: Carabis 2012, pp. 18)



Step	Step Pressure (psia)
Step 1, C_3H_8 (1% in N_2)	20.091
Step 2, NO (1% in N_2)	50.126
Step 3, CO (25% in N_2)	70.420
Step 4, CO_2 (pure)	131.302
Step 5, N_2 (pure)	1014.696

5.2 Design

The majority of the design work on the GMS was completed by Dave Carabis in the summer of 2012. He calculated the necessary partial pressure steps and carried out the uncertainty analysis to determine the pressure transducers and regulators needed. As part of his project he sourced the component gases, required regulators, and vacuum pump, as well as the appropriate hardware to connect them. He also developed a schematic of the systems plumbing and designed a stainless steel face plate to mount the regulators on. [7]

One of the initial phases of the current project was to take over the GMS project from Dave and carry it through to completion. This process can be broken down into three general parts. The first was the final design of the manifold plumbing. A comparison of the two designs is shown in figure 5.1. A larger version of the final schematic is presented in Attachment J.

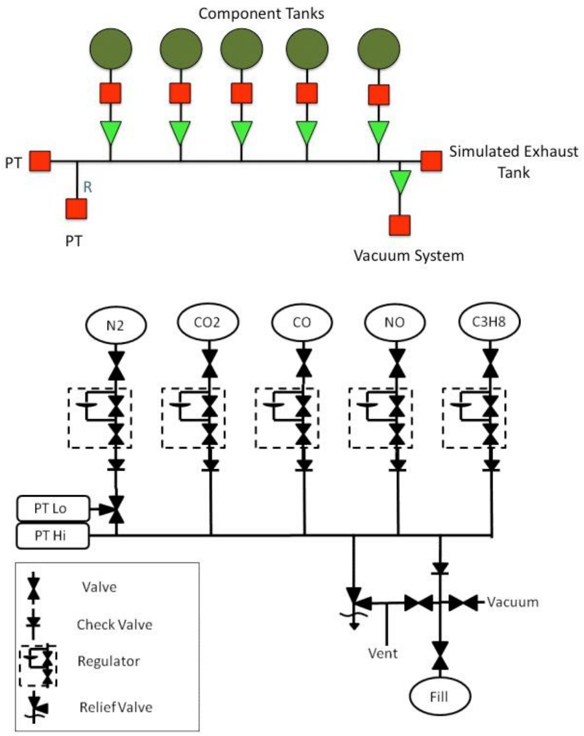


Figure 5.1a Manifold schematic proposed be Dave Carabis, **b** final schematic

The manifold is designed to connect each component tank one at a time to the fill tank and pressure transducer. A typical fill step would start by venting and pulling a vacuum on the manifold with the fill tank and the component tank both closed off. The component tank would then be opened and the manifold raised to the appropriate step pressure before opening the fill tank. The pressures are measured with the pressure transducers and set with the regulators. When the pressures equalized, tanks would be closed off and the process repeated for the next component. Check valves are employed throughout to prevent back flow at any stage in the process.

The primary difference between the two systems is the treatment of the low pressure transducer. Since this device was only designed to measure pressures up to 150 psia, there needs to be some means of isolating it from the manifold during the nitrogen fill stage where manifold pressures reach over 1000 psia. Originally the low pressure transducer was protected by a separate switch and last resort relief valve. The final design utilizes a three way valve to prevent the nitrogen tank and low pressure transducer from being attached to the manifold at the same time. The pressure relief valve was then resprung and mounted to the main manifold to act as a redundant safety measure to vent the entire manifold in the event of dangerously high pressures.

The next major step of the finishing the GMS was to source the remaining components and build the final system. The additional parts purchased included the fill tanks and the alarm system. The alarm recommendations are presented in Attachment P. The fill tanks are size 200 (200 standard cubic feet of standard air at max pressure). Each size 200 tank at 1000 psig holds over 13 times more test gas than the disposable tanks currently in use. These tanks are fitted with a specific type of valve connection, called a cga, to prevent them from being mistakenly attached to any other equipment in the lab. Additionally framing was fabricated from 80/20 stock and a stainless steel backing plate was designed to provide mechanical support to the plumbing. The frame sets the controls six inches back from the hood sash. This ensures that the sash may be closed at any time and that any leaks from the regulators would be safely contained within the hood. Figure 5.2a shows a profile of the GMS within the hood.

The GMS as well as the Carbon Monoxide, Propane, and Nitric Oxide bottles are mounted inside of a fume hood to contain any potential leaks. Due to their size the Carbon Dioxide, Nitrogen, and fill bottles are secured in the space between the hood and the wall. The vacuum pump is also pulled outside of the hood to prevent sparks from the electric motor from igniting any flammable gases around the GMS. In order to prevent any leaks into the lab the outlet of the vacuum pump was routed back into the hood with steel pipe. Figure 5.2b shows the global layout of the GMS relative to the tanks and the hood. Access to the tanks and the hood was provided by cutting holes in the side of the hood to run lines. These air gaps were reduced through the use of rubber grommets. The holes should not affect the operation of the hood as they represent a small amount of open area compared to the gap between the sash and sill of the hood. The vent line of manifold runs directly to the hood vent to minimize the possibility of vented gas from escaping the hood. The manifold is connected by ¼ in stainless tubing secured with Swagelok ® compression fittings. The tanks are connected using flexible stainless steel reinforced lines. Figure 5.2c shows the completed plumbing of the GMS.

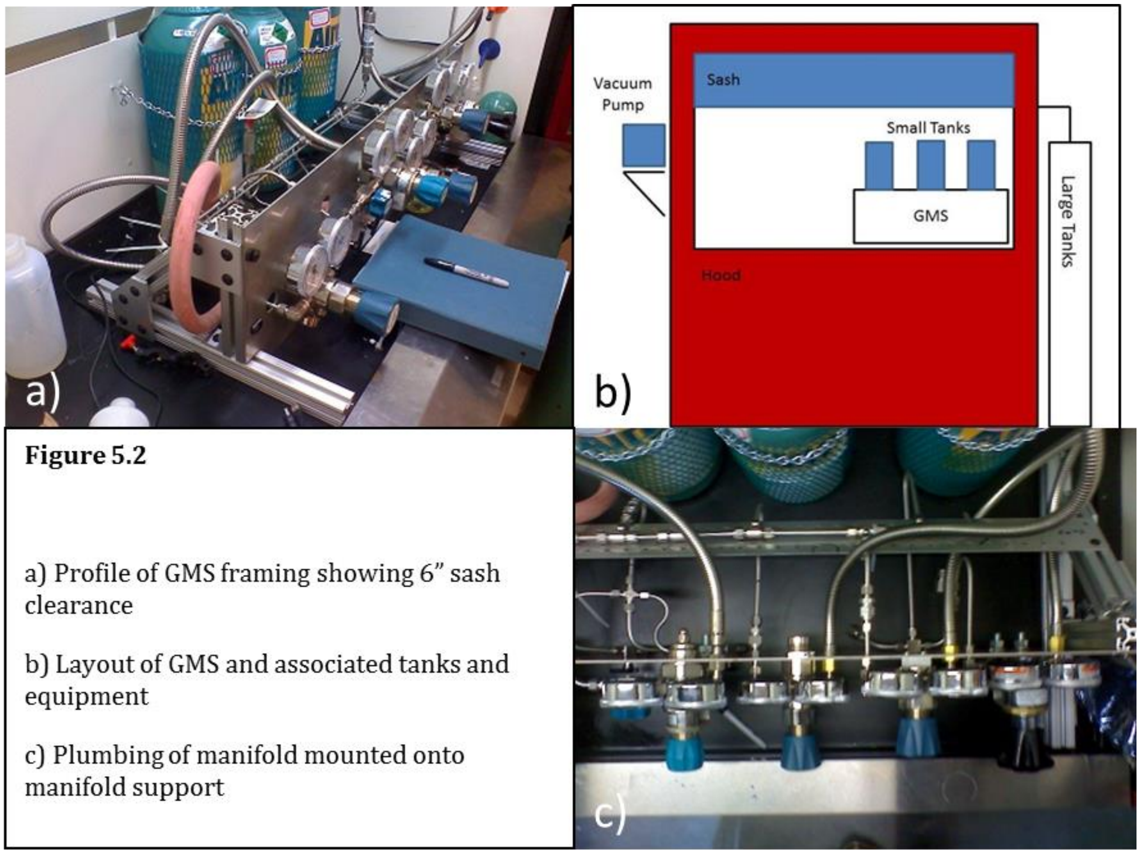


Figure 5.2

a) Profile of GMS framing showing 6" sash clearance

b) Layout of GMS and associated tanks and equipment

c) Plumbing of manifold mounted onto manifold support

5.3 Leak Testing and Current Use

Before any bottles of test gas could be produced the GMS had to be thoroughly leak tested with a non toxic gas. The first step was to identify the different parts of the system which would need to be tested independently. If the check valves work properly they will isolate the regulator lines from the main manifold. While this is desirable for safe filling, it necessitates testing each of those lines separately with the non toxic test gas. Another important step was to tie down the loose gas hoses. In the event of a high pressure leak the hoses must be secured to prevent injury. This function would normally be provided by the weight of the secured cylinders but since they were not yet attached, the flexible lines were secured to the frame using cable ties.

The leak testing was done using a tank of pressurized nitrogen delivered to different parts of the manifold through an intermediate regulator. Beginning from a low pressure (5 psig) the manifold was tested in small increments of pressure until the manifold pressure reached 150 psig. The final leak testing was performed on the manifold without the intermediate regulator to reach pressures up to 1500 psig. The relief valve was tested and adjusted during this phase.

At this moment the manifold and regulator panel are mounted and assembled with all tanks and lines in place. The vacuum pump has been modified and a stand to mount on the hood fabricated (figure 5.3). Alarms for CO, flammable gases, and NO have been purchased and are installed outside the hood. The first bottle of test gas was mixed in December of 2012. At this point the GMS is completely operational currently waiting to be inspected.

Figure 5.3 Mock-up of modified gas pump with stand

5.4 Adding Oxygen in GMS: Equilibrium Calculations

The Bar 97 Emissions Blend 32 purchased from the gas supplier is conspicuously missing one component typically found in exhaust, oxygen. In the current test bed, and additional rotameter is used to mix in compressed air to create a final blend with a small concentration of oxygen. This system is undesirable for two reasons. The first is that the composition of the compressed air from the lab is not regulated thereby introducing the potential for contamination of the test gas. The second is that adding air in the test bed requires a very precise flow meter which is both expensive and difficult to use.

A far more convenient solution would be to add oxygen to the blend in the GMS. Regulators are far cheaper than flow meters, and adding oxygen would be a simple matter of adding a pressure step to the GMS instructions. At this point the question becomes: why was this not done in the first place, by the gas supplier?

Part of the reason for this is that mixing oxygen and fuel, in this case carbon monoxide and propane, at high pressures is considered extremely dangerous. In the high enough concentrations the container would effectively become a bomb. This issue was partially addressed in the initial design phases of the GMS. A calculation was performed to determine how much energy would be released if all of the NO were to instantly oxidize the CO in the tank. The propane was ignored because NO would be the limiting reactant. It was found that the resulting heat would only raise the pressure 17.6 psi which is considered safe in a tank rated for over 2500 psi. [7] This suggests that adding small amounts of oxygen to the tank would not result in an unstable mixture likely to combust and rupture the tank. One situation where dangerous mixtures could still be generated is though operator error on the GMS.

Another reason for not mixing oxygen into the initial tanks is the potential that it will oxidize the NO. This reaction will happen in engines at low speeds. Oxidation can also occur at standard conditions resulting in the conversion of NO into its far more deadly relative NO_2. [1] The additional safety hazard of the resulting NO_2 is not likely significant because the same reactions would occur if NO were released directly into the atmosphere. What would be problematic is that the resulting composition would no longer resemble automobile exhaust. In addition the assumption that the contents of the tank are known would no longer be reasonable if the contents change with time. This would render the tank effectively useless.

In both cases it is important to remember that automobile exhaust is not at chemical equilibrium. Most of the pollutants found in exhaust are results of intermediate reactions frozen by the rapid cooling during the expansion stroke. While this temperature reduction slows reaction rates it does not stop them completely. Even when sitting in the tank the blend will continue to shift towards its equilibrium concentrations. To answer the question of adding oxygen using the GMS it is important to know where this equilibrium is. The chemical equilibrium of a mixture is the point where the concentrations no longer change with time. At this point the forward and reverse reactions in the mixture occur at the same rates.

In order to find the equilibrium concentrations it was first necessary to identify the initial concentrations which would result from mixing oxygen into the tank. The goal is to generate the same mixture which is produced by mixing the emissions blend with air. The ratio of emissions blend to air is 1: 0.017. The compositions of the emissions blend, air and the final mix are presented in table 5.2.

Table 5.2 The generation of test gas by mixing emissions blend and air.

BAR 97 Blend 32				Air (assumed)				Final Mixture	
Propane	200 ppm			Nitrogen	78.67%			Nitrogen	93.20%
Carbon Monoxide	0.50%			Oxygen	20.94%			Carbon Dioxide	5.91%
Carbon Dioxide	6.00%	x 1	+	Carbon Dioxide	0.39%	x 0.017	=	Carbon Monoxide	0.49%
Nitrogen Monxide	300 ppm							Oxygen	0.35%
Nitrogen	Balance (93.45%)							Nitrogen Monoxide	0.03%
								Propane	0.02%

The column labeled *Final Mixture* represents the initial mole fractions for the test gas which goes on to enter the test section. This is also the composition which would result by mixing oxygen into the mixture with the GMS to avoid blending it with air.

To find the equilibrium concentrations for this tank, the potential products in the final mix need to be identified. This is important because any products not identified will not show up in the final composition even if they would actually be formed. In addition to the components found in the initial tank, 5 additional components were considered. These were water (H_2O), Ethane (C_2H_6), Methane (C_4H_6), and Hydrogen (H_2).

The equilibrium mixture will minimize the free energy in the system. This state is identified using equilibrium constants. The equilibrium constant describes the bias of a reaction in one direction or the other. By identifying the equilibrium constants for reactions containing the components identified in the final mixture it is possible to create a system of non linear equations governing how the products are distributed at equilibrium. This system is bounded by conserving the molar amounts of the elements in the container. The reactions in the tank are strictly chemical; therefore the each atom must retain its identity regardless of the molecule it makes up.

The identifying the necessary equilibrium reactions and their constants were identified. The resulting system of equations will be solved using computer aided numerical methods using the initial concentrations as a starting point. To date the numerical model has been unsuccessful. The end result would have been the equilibrium concentration of the theoretical tank. If the final composition is significantly different from the initial, than we would need to consider the reaction rates to identify a shelf life for the tank. The partial MATLAB script for the equilibrium calculations is presented in Attachment G.

5.5 Final Design for Oxygen Addition

Given the potential of decomposition in the tank and the risks associated with user error in having an oxygen cylinder on the GMS the decision was made not to add oxygen to the test gas bottles, but rather add oxygen in the gas conditioning system as the system runs. This is similar to the way the system is currently run, with a small portion of oxygen containing air into the test gas flow.

The amount of oxygen which will need to be added to the test gas is determined by the equivalence ratio of the burn. The quantity of oxygen in the exhaust relative to the equivalence ratio is shown in figure 1.1 from the first section.

Engines generally run with an equivalence ratio between 0.9 and 1.2 [3]. Newer, fuel injected engines should operate well inside this range. These limits represent extreme cases such as a mistuned engine or a faulty fuel system where the engine is running, but well outside of its normal conditions. That translates into an Oxygen mole fraction between 0.005 and 0.025, a range of over an order of magnitude.

Adding pure oxygen in these quantities is problematic on several levels. First, pure oxygen is very dangerous to use. Second, the flow rates for these concentrations are so small they are nearly impossible to meter accurately. Finally for different tests there is such a large range of potential flow rates between the lean and rich extremes. All of these problems could be addressed by using mixtures of Oxygen and Nitrogen. Mixtures between 1% and 20% Oxygen are readily available from gas suppliers at a variety of calibration levels. Therefore a large range of Oxygen flow rates could be generated with a very narrow range of mixture flow rates.

6. Real Time Mixing and Mass Flow Controllers

It would be ideal to mix the different exhaust components in real time and thus eliminate the need for the GMS entirely. Such a system would also allow for these concentrations of this mixture to be changed during tests to create the transient conditions in actual catalytic converters.

In a real time gas mixing setup each component gas cylinder would be connected to the test bed by a separate mass flow controller. Since the mixture is produced on demand and immediately there is no risk of a change in composition over time in the mixture. A schematic of the proposed system is shown in 6.1. This is the design originally put forward in the grant proposal. [6]

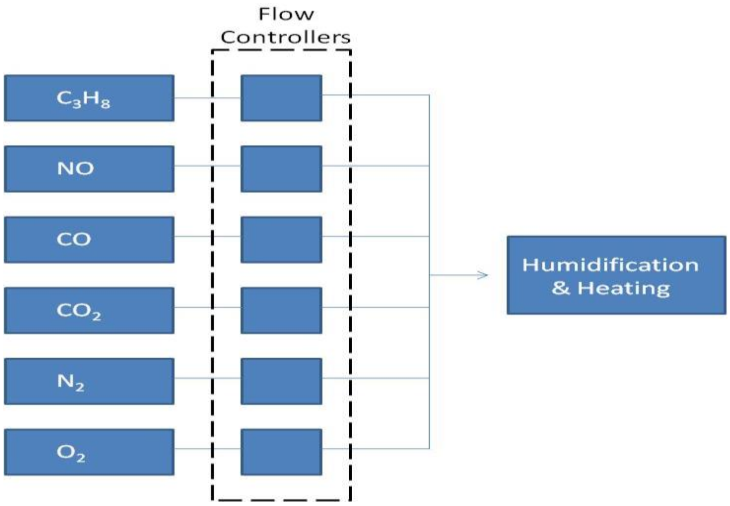


Figure 6.1 Schematic of proposed real time mixing system with an independent controller for each component gas

Gas flows in these contexts are generally regulated by thermal mass flow controllers. These devices are comprised of a thermal mass sensor connected to a proportional valve by a control circuit. The mass flow sensor contains a bypass which diverts a small amount of the flow through a separate loop. The separated portion passes through two heating elements in series which are supplied with fixed power and contain and thermocouples to measure the temperature at each point. The parts of a thermal mass flow controller are shown in figure 6.2a. At zero flow the coils will be at the same temperature. As the flow rate increases the temperatures will drift apart due to the cooling effects of the flow. This drift is scaled with calibration factors into the flow measurement. This temperature drift is shown in figure 6.2b.

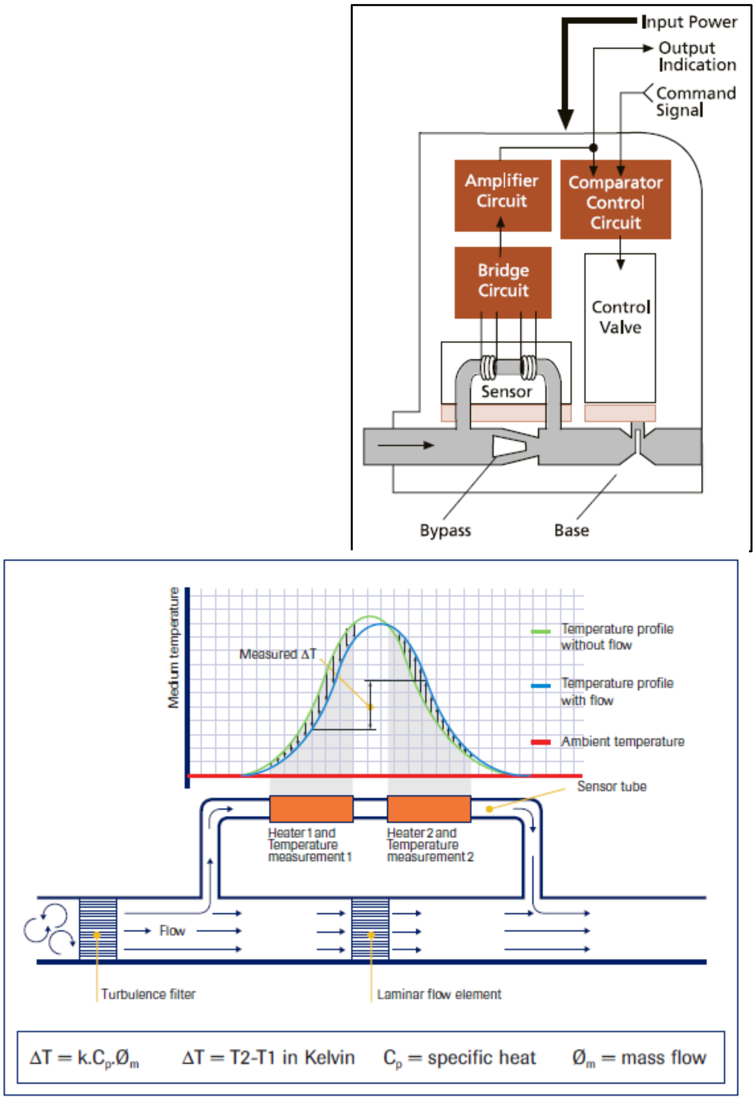


Figure 11 a) schematic of mass flow controller showing bypass and control valve **b)** temperature drift under non-steady flow
Image sources:
http://www.advanced-energy.com/upload/File/White_Papers/SL-MFCFUND-270-01.pdf
http://www.bronkhorstusa.com/en/products/gas_flow_meters_and_controllers/elflow_select/

While elegant in its simplicity, a real time gas mixing system has significant drawbacks. The first is cost. Mass flow controllers, especially those for very low flow rates, are very expensive, on the order of thousands of dollars for each controller. A real time mixing system would require at least six of these controllers. In addition the response time for most thermal mass flow controllers is on the order of 1 second, which is equivalent to the desired switching frequency. By the time the controllers were able to set the correct flow rate, the system would already be on the next oscillation. This is impractical from a control point of view. The final consideration is safety. Mixing the exhaust components in real time would require that all of the component cylinders be connected to the test bed at all times. This creates an increased risk of exposure to the concentrated pollutants to the user.

With these considerations in mind the real time mixing system is not an acceptable solution to the design requirements.

7. Gas Switching System

7.1 Switching as an Alternative to Real Time Mixing

A strong alternative to real time mixing is to generate the transient compositions required by using switch to alternate between different mixtures. In order to simulate the transition between slightly lean and slightly rich burns, the source of the flow will be switched between a tank containing exhaust components representative of a rich burn and one of a lean burn. The frequency of this switch will be approximately 1 Hz to best represent the response time of the engine control system. The switching would create alternating “slugs” of the mixtures in the line. Figure 7.1 shows a potential configuration for such a system.

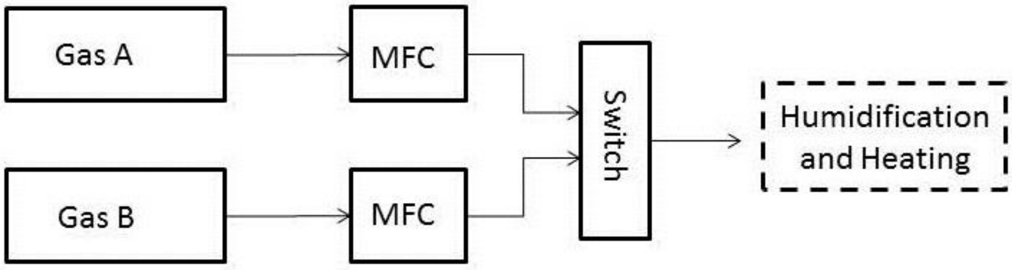


Figure 7.1 A proposed schematic for a gas switching system where the flows of two mixtures, A and B are metered out at flow rates equal to ½ the total flow rate while the switch alternates between them.

This configuration addresses many of the problems with the real time mixing system. Since the two tanks are premixed the risk of dangerous leaks of concentrated gas during regular testing is eliminated. Also since there are only two flow sources, a maximum of two flow controllers would be needed, the total cost is reduced. Finally, the transient conditions are driven by the switch while the controllers ideally remain in steady state, so the system is not limited by the response time of the controllers.

7.2 Slug Length and Mixing

Despite these advantages the gas switching approach is not without its own problems. The first concern which presented itself was mixing between the slugs. Since the slugs are made up of gas, the mechanisms of diffusion and the no slip condition at the wall will cause some mixing between the adjacent slugs.

Mixing is undesirable because it smoothes out the transient conditions in the gas composition going into the test chamber. With infinite mixing the gas entering the test chamber would be a perfect average of the lean and rich compositions. This entirely defeats the purpose of the two mixtures and the switching and effectively turns the system back into a steady state one.

Since this mixing occurs only at the border between two slugs, longer slugs will generally result in less mixing. The first step was to calculate the length of the slugs for the range of mass flow rates at which the test bed would be used. The slug length is equal to the slug volume divided by the cross sectional area of the pipe it is in.

$$l = \frac{V}{A_{CS}} \tag{8}$$

The volume of the slug is the volumetric flow rate divided by the frequency of switching. The volumetric flow rate can be found by taking the mass flow rate and dividing it by the density of the fluid. In this case the density in both cases is assumed to be equal to that of air at standard conditions.

$$V = \frac{\dot{V}}{2f} = \frac{\dot{m}}{2\rho f} \tag{9}$$

Combined, these two equations yield the slug length equation.

$$l = \frac{\dot{m}}{2\rho f A_{CS}} \tag{10}$$

There are a couple important observations taken from this equation. The first is that the slug length is proportional to the mass flow rate and inversely proportional to the cross sectional area. Since the cross sectional area of a tube is proportional to the square of its diameter, halving the diameter of the tube would quadruple the slug length. Of course this approach is complicated by the increased wall effects in narrow tube compared to a wide one but it does show the importance of the tube diameter on slug length.

An excel chart and MATLAB script were used to create determine the slug length for a variety of mass flow rates and tube diameters. The plot of the MATLAB results is shown in figure 7.2 and the excel calculations are included in Attachment H. A sample calculation for slug length is presented in Attachment B.

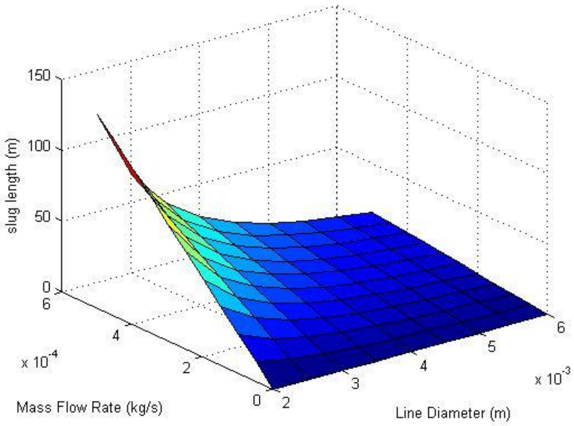


Figure 7.2 Slug lengths as a function of mass flow rate and line diameter.

These calculations show that for standard ¼ inch steel tubing, with a space velocity of 15 1/s and a test section temperature of 500° C, the slug length is over 2 meters. This is very long compared to the diameter of the tube and on the order of the estimated length of tube in the whole test bed. Therefore the mixing between slugs will likely not be significant and the slug length considerations should not be the primary factor driving the design.

7.3 Pressure Transients and Controller Stability

Another design complication with the gas switching system is the effects of the switching on the stability of the mass flow controllers. Consider again the schematic presented in figure 7.1. While the switch is closed for gas A and open for gas B, the mass flow controller on gas A's line is pumping gas into a closed line. This increases the back pressure on the line and forces the controller to compensate by adjusting the control valve. When the switch changes positions, all of this pressure is released and the controller's pressure differential is returned to its original state. Since both the response time of a thermal mass flow controller and the switching frequency are on the order of seconds it is unlikely that the controller would be able to keep up. These effects have the potential to create large errors in the mass flow, rendering the controllers useless.

There are several means of addressing the effects of pressure transients on the mass flow controllers. The first would be to maximize the volume of tube between the switch and the controller. In theory, gas added at a mass constant flow rate an infinitely long tube closed on one end would never increase the pressure in the tube. In practice, a sufficiently long tube would cushion the controller from the effects of the switch on the other end.

Another option would be to use what is known as a *pressure transient immune* mass flow controller. The key to these devices is using choked flow. Under normal conditions the flow rate through a nozzle dividing regions of high and low pressures increases with the pressure differential. At a certain point, the velocity of the gas through the nozzle will reach the speed of sound and the flow becomes choked. No matter how much the downstream pressure is reduced the flow rate will remain the same. Thus the flow is governed by upstream pressure alone. In the context of the PTIMFC the control valve is moved upstream of the flow meter and a restriction plate is placed downstream. The flow is controlled by regulating the pressure upstream of the flow restrictor with the control valve. The control valve also helps to isolate the flow sensor from upstream pressure transients. [8]

In order to evaluate these options an estimate of the magnitude of the pressure transients had to be made. To do this the line between the MFC and the valve was considered to be a fixed control volume at atmospheric pressure. It was then assumed that the MFC added air at a constant mass flow rate to the sealed line. The maximum pressure was calculated by using the ideal gas law assuming a constant temperature process. This does not take into account the fast pressure transients caused by rapidly cycling the air in and out of the line but it does give a conservative estimate of the pressure change in the line while the switch is closed. For a space velocity of 15 1/s and a test bed temperature of 500°C in 1m of ¼ in tubing the pressure rise was estimated to be about 30psi, or 2 atmospheres. This calculation is presented in Attachment C. This is far too large of a pressure gain for even a pressure transient immune MFC to handle and requires a rethinking of the system structure.

7.4 Bypass Configurations

A more fundamental solution to the problem of pressure transients is to design the switching system in such a way that the flow is never blocked and therefore always steady. One way to do this is to divert the flow during switching rather than simply switching it "off." This way unwanted gas bypasses the line entirely rather than building up upstream of the switch. As long as the switching time is small relative to the frequency of switching, any pressure transients generated should be minimal. Figure 7.3 shows a 3 way valve acting as a bypass.

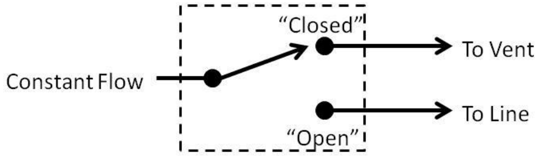


Figure 7.3: 3 way valve acting as a bypass on/off

Within the context of the gas switching system this is called the "single bypass configuration." It is made up of two bypass valves, each attached to one flow of test gas. Figure 7.4 shows the single bypass gas switching configuration.

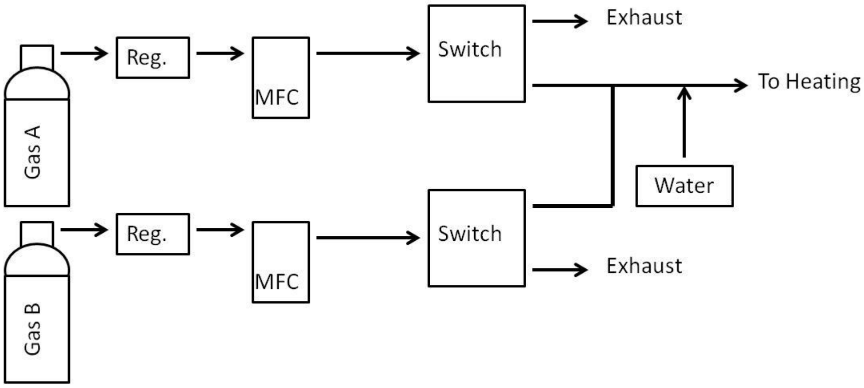


Figure 7.4: Single Bypass gas switching configuration

The primary disadvantage of the single bypass configuration is that one half of the test gas is wasted by being vented to the exhaust. An alternative to venting the bypass gas would be to collect it into another line. The bypass line, like the main line, would then be made up of alternating slugs each test gas composition. The slugs in the bypass line would be exactly 1 cycle out of phase with the main line so that when a slug of gas A entered the main line, a slug of gas B would enter the bypass line. Therefore the result would be the creation of two parallel gas flows. Since they are out of phase, it would prove impractical to try to combine these flows back into a unified flow. A more reasonable application of the bypass flow would be to supply a second test chamber so that two experiments may be run at the same time. This configuration, shown in figure 7.5, is called the "double bypass configuration."

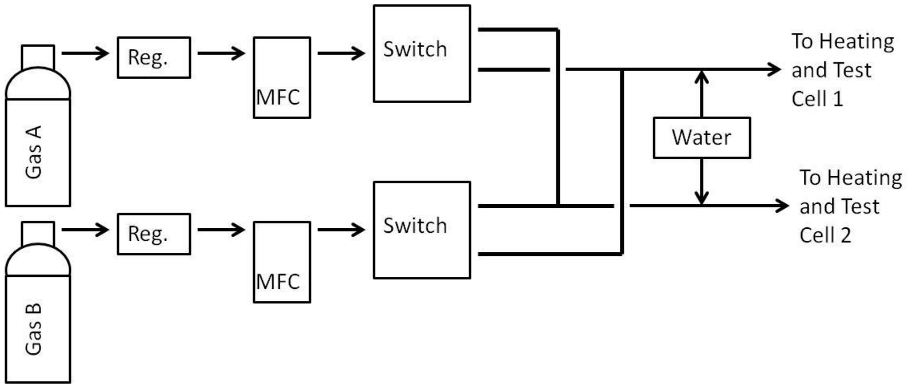


Figure 7.5: Double Bypass configuration

While the double bypass configuration has the advantage of conserving the gas which would otherwise be be vented with the single bypass and greatly increases the capability of the system by adding a second test cell, it is not without problems. The first and most obvious is cost. The double bypass configuration effectively uses the same switching hardware as the single bypass but adding the second line requires the addition of an additional humidification system and test cell, doubling the cost of the downstream hardware.

The second major challenge with the double bypass system is evenly splitting the test gas flow between the two lines. Theoretically, if each line is identical from the switch to the final exhaust port, than exactly one half of the test gas will travel down one line as the other. With real plumbing this is not a practical assumption. Without precise knowledge of how much gas ends up in each line it is impossible to know the flow rate or composition in the test cell, making the initial flow control completely useless. The solution to this problem is careful measurement and calibration of the final product. Any imbalances in flow may be addressed by adding an additional flow obstruction, such as an adjustable needle valve to the line which has more flow.

7.5 Solenoid Valves for Switching

Up to this point the discussion of the gas switching system has been focused mainly on the controllers, their specifications, and potential problems. Besides the controllers, the valves make up the other major components in either bypass system. So far the valves have only been considered in the ideal sense, instantaneously switching, with pressure loss. Since this is clearly not the case with real valves it is necessary to lay out specific design requirements for the valves so that appropriate hardware could be selected.

The bypass valves must be in the 3-2 configuration, meaning that they have three ports with two possible positions. In this case the valves would have one inlet which can be connected to either of two outlets. Each of the outlets should allow for equal flow of test gas to ensure an even distribution between the two lines. The overall system must be able to operate at a 1 Hz switching frequency, meaning that the valves must be able to switch positions every 0.5s. Since a continuous, steady, flow of gas is desired, the response time of the valve should be small compared to the time it remains in each position. Additionally since the valve will be actuated 120 times a minute, it must be rated for a large number of high frequency cycles to ensure longevity. Finally, these valves must be easy to operate remotely with an electronic signal.

Solenoid valves adhere to these design requirements well. These devices use an electromagnetic coil to move a plunger up and down to expose and cover different valve ports. Unlike motor actuated ball valves, solenoid valves have very small response times, typically on the order of tens of milliseconds. This means that the response time is an order of magnitude smaller than the switching duration. There are two common arrangements for solenoid valves, as determined by their internal plumbing. A direct acting solenoid valve controls the entire flow with the solenoid plunger while in a pilot operated valve the flow solenoid controls a smaller passage which toggles a pressure differential across a diaphragm controlling the main flow. Pilot operated valves are used in high flow, high pressure situations. Figure 7.6 shows cutaways of a direct acting and pilot operated valve.

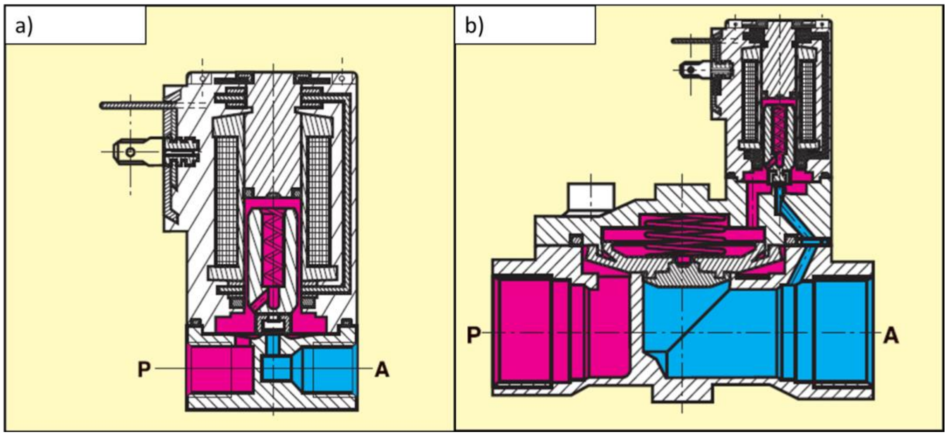


Figure 7.6: Cutaways of an a) direct acting and b)pilot operated valve

Image source: http://www.omega.com/Green/pdf/VALVE_TECH_REF.pdf

Of the two arrangements, the mechanical simplicity of the direct acting valve is better suited to the gas switching system given the relatively low flow rates and pressures involved. A final consideration when selecting a solenoid valve is whether it is normally open, normally closed, or universal. A universal valve is the most flexible arrangement as it functions regardless of which port pressure is applied to.

ASCO Long Life Solenoid Valves (Model 8320G174Q) were chosen for this configuration. These valves use a diaphragm to open and close the ports of the valve. Unlike a pilot operated valve, the diaphragm is operated directly by the solenoid. A cutaway diagram of this setup is shown in figure 7.7.

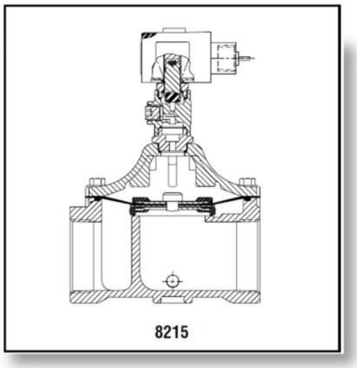


Figure 7.7: Cutaway of an ASCO Long Life Solenoid Valve (2 way valve shown)

Image source: http://www.ascovalve.com/Common/PDFFiles/Product/LongLifeR2.pdf

The diaphragm isolates the solenoid from the gas passing through the valve as well as eliminating the need for metal to metal contact inside the solenoid, dramatically increasing the lifetime of the valve. The particular valves selected are rated for 20 million cycles (one cycle being on-off-on), translating into over 500 hours of run time at the desired 1 Hz switching frequency. The valves are universal with an orifice size of 3/32in for both outlets. The valve documentation is included in Attachment S.

The ASCO valves employ coils which operate on 120 VAC single phase power. The current to these valves must be controlled using a digital I/O signal from a PC. This required the design of a control circuit. The final circuit design is presented in figure 7.8 as well as Attachment K.

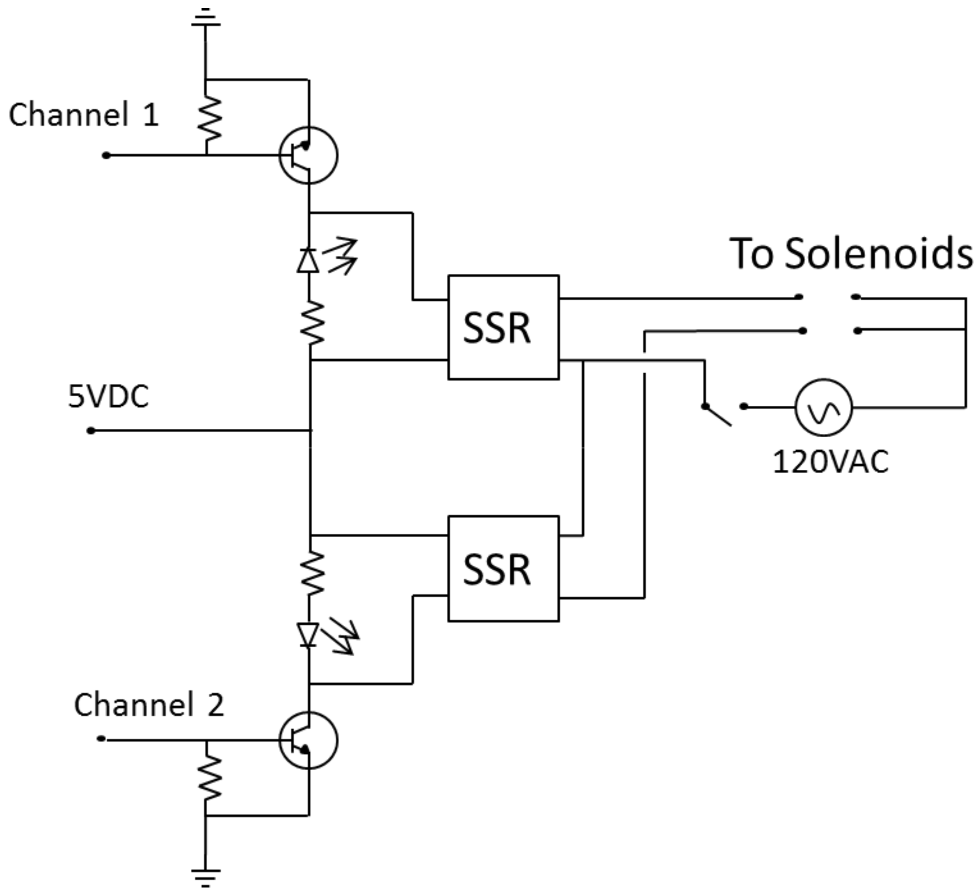


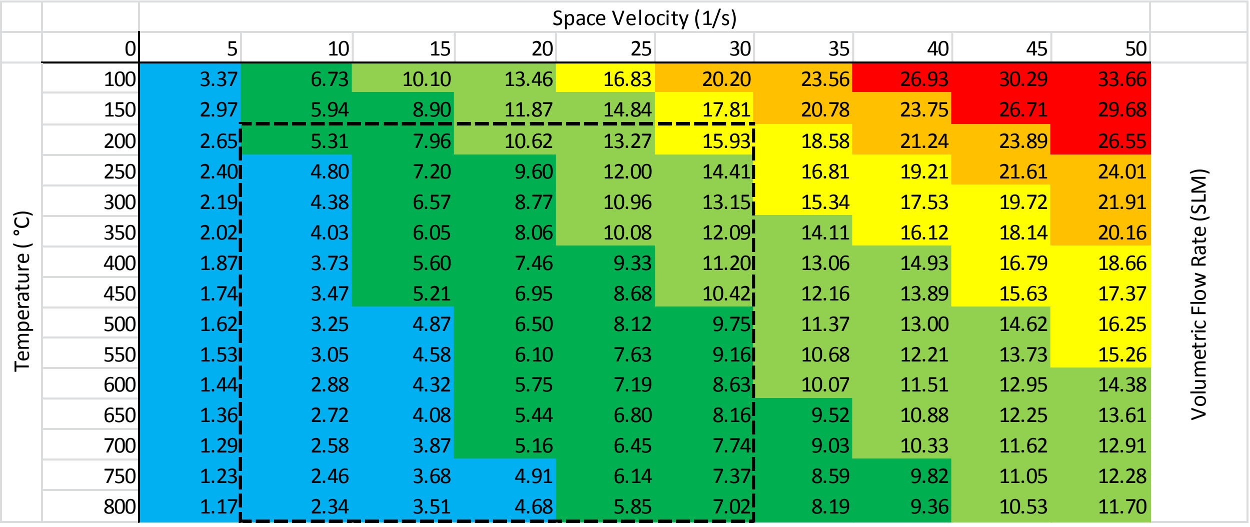
Figure 7.8: Control circuit for solenoid valves

The control circuit is actually two identical circuits, one for each solenoid. This was done to allow for the possibility of overlap during valve switching as an additional calibration variable. The main feature of the circuit is the VDC to VAC solid state relay sourced from Omega Engineering. The solid state relay works in a similar way to a standard relay, with a small control current regulating a much larger line current. Unlike a mechanical relay, the solid state device has no moving parts and is therefore is more reliable and responds faster. The specification for the relays used in this circuit may be found in Attachment T. The 0-5VDC control voltage switching the relay is in turn controlled by a transistor switch operated by the digital control signal. A LED circuit is placed in parallel with the solid state relay to indicate its position. The end result is two AC powered solenoid valves run independently by two digital I/O channels.

7.6 Concerns with Scaling

The final concern with the gas switching system is one of range. Mass flow controllers are rated for certain flow rates (generally given in SLM) with a rated accuracy given as a percent of a full scale reading. The test bed is a unique application for these controllers because of the wide variation in flow rates required to meet different test conditions. In order to source the flow meters the mass flow rates initially calculated from the space velocities and test section temperatures. This resulted in a range of flow rates from 1 to 34 SLM. These flow rates are shown in table 4. This means that if a flow controller were selected to capture the high end within 1% full scale accuracy, the percent error at the lowest flow rates would be over 30%. This situation is obviously unacceptable for the test bed. The first step is to reexamine the design constraints. The initial design requirements called for the test section to work with space velocities from 5 to 50 1/s and test section temperatures from 100 to 800 °C. After further consideration, it was proposed these requirements were reduced to space velocities from 10 to 30 1/s and 200 to 800°C. This in turn would reduce the flow rates required to a range of flow rates down to a range of 2 to 16 SLM. With fairly small changes to the initial design criteria the required turndown ratio could be reduced from 34:1 to 8:1. The dashed line on table 7.1 shows the proposed boundaries.

Table 7.1 Flow rates in SLM for different space velocities and test section temperatures, dashed line indicates proposed boundaries. Colors indicate the magnitude of the flow rate.



		Space Velocity (1/s)										
	0	5	10	15	20	25	30	35	40	45	50	
Temperature (°C)	100	3.37	6.73	10.10	13.46	16.83	20.20	23.56	26.93	30.29	33.66	Volumetric Flow Rate (SLM)
	150	2.97	5.94	8.90	11.87	14.84	17.81	20.78	23.75	26.71	29.68	
	200	2.65	5.31	7.96	10.62	13.27	15.93	18.58	21.24	23.89	26.55	
	250	2.40	4.80	7.20	9.60	12.00	14.41	16.81	19.21	21.61	24.01	
	300	2.19	4.38	6.57	8.77	10.96	13.15	15.34	17.53	19.72	21.91	
	350	2.02	4.03	6.05	8.06	10.08	12.09	14.11	16.12	18.14	20.16	
	400	1.87	3.73	5.60	7.46	9.33	11.20	13.06	14.93	16.79	18.66	
	450	1.74	3.47	5.21	6.95	8.68	10.42	12.16	13.89	15.63	17.37	
	500	1.62	3.25	4.87	6.50	8.12	9.75	11.37	13.00	14.62	16.25	
	550	1.53	3.05	4.58	6.10	7.63	9.16	10.68	12.21	13.73	15.26	
	600	1.44	2.88	4.32	5.75	7.19	8.63	10.07	11.51	12.95	14.38	
	650	1.36	2.72	4.08	5.44	6.80	8.16	9.52	10.88	12.25	13.61	
	700	1.29	2.58	3.87	5.16	6.45	7.74	9.03	10.33	11.62	12.91	
	750	1.23	2.46	3.68	4.91	6.14	7.37	8.59	9.82	11.05	12.28	
	800	1.17	2.34	3.51	4.68	5.85	7.02	8.19	9.36	10.53	11.70	

A further option to capture the range of needed flow rates is to use multiple controllers for different scales. This is an option best avoided as it would at least double the cost of the controllers and require another level of flow switching between the multiple controllers. Several controller manufacturers claim to have multi-range controllers which carry multiple calibration curves to rescale the controllers while attached to the system.

The ability to rescale and recalibrate the controller from a computer means that the controllers range is only limited by the physical size of its components. Since the rescaling must occur through a computer interface these controllers are exclusively digital and generally more expensive than their analog counterparts. They also generally have the ability to store multiple calibration curves for different gas compositions, another useful ability for this application. It is highly recommended that these multi gas, multi scale controllers be implemented in the final design. Quotes for two of these controllers may be found in Attachments Q and R.

8. Humidification of the Test Gas

8.1 Water as a Component of Exhaust

Adding water to the test gas is problematic because water is a liquid at room temperature. Air at 25° C can only hold 1.96% water vapor by mass before becoming saturated [9]. At 100° C a mixture of 100% water will theoretically remain gaseous. Both of these values assume the mixture is at atmospheric pressure. The concentration of water in the humidified mixture will fall somewhere between these extremes. It is therefore necessary to add heat to the test gas to raise its temperature and hold the needed water vapor. It is further necessary to design the system to ensure that this water does not condense at any point in the system. The first step in designing the humidification system was to figure out how much water is produced in to automobile exhaust as a result of combustion.

The test gas will be manufactured to match the composition of dehumidified automobile exhaust. By adding the appropriate amount of water the final composition will reflect actual automotive exhaust. In order to find out the quantity of water needed, the equation for the stoichiometric combustion of octane was balanced.

$$C_8H_{18} + 12.5O_2 \rightarrow 9H_2O + 8CO_2$$

This equation gives the relationship between the molar amounts of fuel and air burned to water and carbon dioxide produced. The stoichiometric air fuel ratio for octane is 14.7:1. The air fuel ratio is a ratio of masses (equation 1), so it was divided by the inverse of the molar weights of air and fuel, to get the molar ratio (equation 11).

$$Molar\ Ratio\ =\ AFR\ \left(\frac{M_{Fuel}}{M_{Air}}\right) \tag{10}$$

The molar ratio was used to determine that the composition of the charge, listed in table 7.2.

Table 7.2 Composition of charge for a stoichiometric burn of octane in air

Component	Fraction
Nitrogen (N_2)	0.7766
Oxygen (O_2)	0.2064
Octane (C_8H_{16})	0.0170
Total:	1.000

Using the balanced equation for the mole fraction of water in the exhaust can be approximated by removing the octane and oxygen components and distributing them into water and carbon dioxide at a 9 to 8 ratio. This ratio comes from the balanced chemical reaction. The composition of the stoichiometric exhaust is shown in table 7.3.

Table 7.3 Composition of exhaust for Stoichiometric burn of octane in air

Component	Fraction
Nitrogen (N_2)	0.7766
Carbon Dioxide (CO_2)	0.1051
Water (H_20)	0.1183
Total:	1.000

The MATLAB Calculations for the charge and stoichiometric compositions are presented in Attachment I. These numbers are an over-simplification of the exhaust composition. The since the combustion is non-stoichiometric, there are trace amounts of fuel oxygen and other pollutants in the exhaust which are accounted for in the test gas. These quantities are small relative to the three primary exhaust components and do not have significant impact on the overall humidity of the test gas. What this calculation does provide is an approximate fraction of water which should be present in the humidified test gas.

Determining the Flow Rate of Liquid Water

The next step is to use the overall test section flow rates to convert the molar concentration of water in representative automobile exhaust into a flow rate of water which must be added to the test gas in the humidification system. This is done by first calculating the molar mass of each of the component molecules. The mass fraction for a given component can then be calculated according to equation 12.

$$(Mass\ Fraction) = \frac{(Mole\ Fraction)(Molar\ Mass)}{\sum[(Mole\ Fraction)(Molar\ Mass)]} \qquad 13$$

These calculations are outlined in greater detail in Attachment D. The overall result is that the final flow of test gas should be approximately 7.5% water by mass.

When describing mixtures of water vapor in gas, there are a few common terms from the field of psychometrics which the reader should be familiar with. The first is absolute humidity, denoted ω, which is defined as the mass ratio of water to dry gas. In this case the absolute humidity of the mixture entering the heating system should be 0.081. A second important property for a humidified mixture is relative humidity which is denoted by φ. This quantity is defined as the partial pressure of water vapor relative to the saturated vapor pressure of the vapor at that temperature. A relative humidity of 100% indicates that the gas is saturated and will accept no more water vapor, whereas a relative humidity of 0 indicates that the gas is completely dry. As the gas rises in temperature it will accept more water vapor and therefore its relative humidity will drop for a given absolute humidity. In the context of the humidification sub-system relative humidity is important because the humidified test gas in the lines must be kept at a temperature such that the relative humidity is much less than 100% so that water will not condense out of the mixture. The temperature at which a mixture with a given absolute humidity reaches a 100% relative humidity is called the dew point. This is because as the temperature continues to drop, liquid water will begin to condense out of the mixture. The dew point of the humidified test gas flow will be about 49°C. A general sense of the relationships between absolute humidity, relative humidity, and dew point in air at atmospheric pressure may be seen in a psychometric chart like the one pictured in figure 8.1.

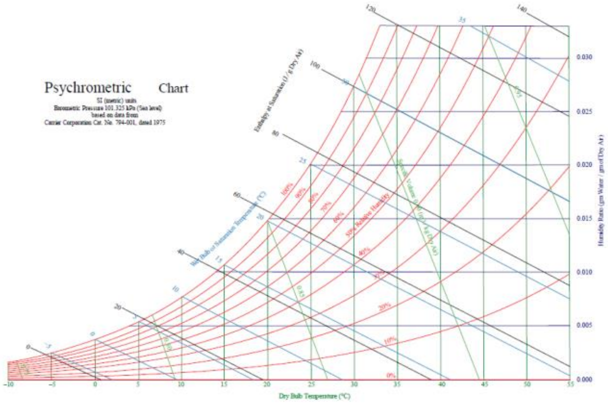


Figure 8.1 A psychometric chart for air at atmospheric pressure with temperature on the x axis, absolute humidity on the y axis. The curved lines indicate constant relative humidity with φ = 100% making up the upper border

The desired mass flow rate of water is equal to the mass fraction of water multiplied by the total mass flow rate. The flow rate of dry gas from the switching system is then equal to the difference of the total mass flow rate and the water mass flow rate. For the calculations in this paper water is assumed to be an incompressible fluid. Given the relatively low pressures involved and the limited precision of the overall calculations, this is a reasonable assumption. It is important to observe that both the dry gas flow rate and the water flow rate are directly proportional to the overall flow rate.

Heating Power Required

In addition to adding the correct amount of water to the line one must also add enough heat to evaporate that water in order to achieve proper line humidification. The first step in this calculation is to set up a control volume around the humidifier and define the flows of mass and energy in and out of it. Since the partial pressure of water is low it is reasonable to assume it as an ideal gas. This allows the components to be treated separately, with the test gas assumed to be nitrogen modeled as an ideal gas and the properties of the water taken from the steam tables. [10] The first law of thermodynamics can then be applied to the system determine the amount of heat which would need to be added in order to bring each component from its initial to its final state. A more detailed treatment of this calculation is presented in Attachment E. The resulting heat required was calculated to be approximately 28W. When sizing heaters for this application it is important to remember that it is simple to reduce electric heater output by reducing the voltage, but it is impossible to safely exceed it. Therefore it is advantageous to select a heater with a maximum power well above the target.

While the thermodynamic calculations to determine the quantities of water and heat needed by the flow to bring it to the desired humidity are fairly basic, accomplishing this in an actual system is a more complex problem. There are two basic methods commonly used to humidify a gas flow to a desired level. The first is controlled evaporation, or adding a precise amount of water to the heated gas flow. The second is called a bubble humidifier, and involves pushing bubbles of dry gas through a heated reservoir of water in order to achieve the desired humidity.

8.2 Method of Controlled Evaporation

The method of controlled evaporation relies on precisely metering the amount of water added to the flow. Sufficient heat is then added such that the water completely evaporates and mixes with the test gas creating the desired humidified flow. Figure 8.2 shows a schematic of a controlled evaporation system.

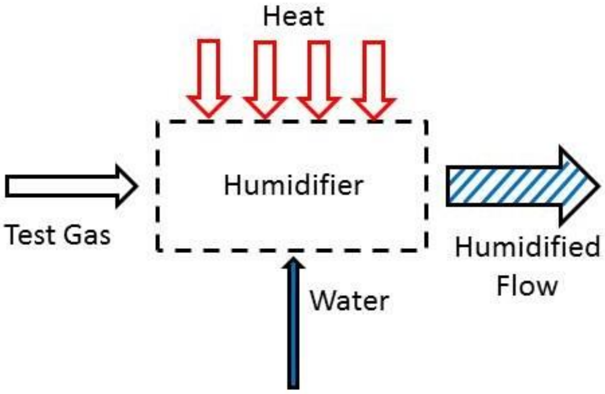


Figure 8.2 Schematic of the controlled evaporator. The mass flows of gas and water are parameters which may be controlled by the user. The heat added is sufficient to ensure the complete evaporation of the water in the test gas.

This method has several distinct advantages. The first is that the only variable which requires precise system control is the mass flow rate of the water entering the line. As long as sufficient heat is added to evaporate the water, there is no risk of over-heating or over humidification especially because the humidified flow will be pumped into the heating section which will raise the temperature of the line to hundreds of degrees Celsius. Since all the water added to the line is quickly evaporated, the overall system tends to be very stable over long periods of time, provided no water condenses out of the mixture. The end result is a very simple and robust humidification system.

The disadvantage to the controlled evaporation system is the difficulties in precisely controlling small flows of liquid. Since the desired flow rate of water is proportional to the overall flow rate, the same scaling issues present in controlling the test gas flow are present in the water flow controls. Three common options are available to meter out water in the desired quantities.

Liquid Mass Flow Controllers

The first is to use a thermal mass flow controller for liquids. These operate on the same basic principles as the mass flow controllers for gas and tend to occupy the same price range, on the order of thousands of dollars. Unlike the mass flow controllers for gases described earlier, there are currently no liquid MFCs available which can be rescaled for different flow rates. An additional concern is that the water supply would have to be pressurized in order to overcome the head loss of the controller and the tubing. This is a trivial issue for gases as they are generally already stored in pressurized vessels. For liquids this requires the addition of an additional system to pressurize the liquid reservoir like the one shown in figure 8.3. The need for additional pressurization drives up the potential cost and complexity of the humidification sub-system.

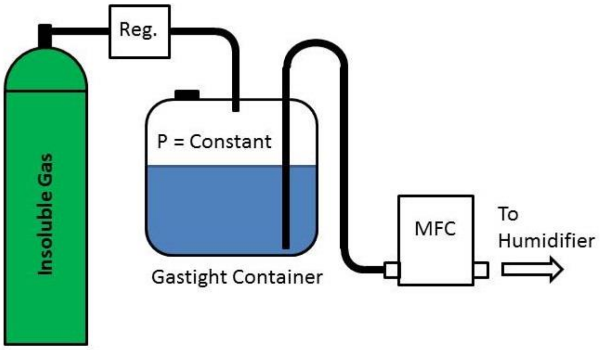


Figure 8.3 Reservoir pressurization setup required to move water through flow controller into humidifier

Positive Displacement Pumps

An alternative to using a mass flow controller to meter out the desired water flow is to use a positive displacement micro pump instead. A positive displacement pump moves a fixed volume of fluid from its inlet to its outlet with each cycle. Since water can be assumed to be an incompressible fluid, a given number of pump cycles will add a known quantity of water to the line. In addition no pressurization of the water reservoir is needed. Like the liquid MFCs the problem with using micro-pumps to control the water flow into the line is one of cost. Very small pumps are specialized products which must be manufactured to exceptionally stringent tolerances. In addition, advanced controllers must be employed to precisely control pump movement and monitor volumetric flow rate. Figure 8.4 shows a typical micro pump which could be used in these applications.

Figure 8.4 An example of a positive displacement pump used to meter low flows of liquid, this model is configured to operate four separate channels. Image source: http://www.coleparmer.com/Product/Ismatec_low_speed_planetary_gear_driven_pump_4_channels_115_230_VAC/EW-78001-00

The quoted price for this pump with a digital control is $3,290[1]. This particular pump, the Ismatec low speed planetary gear pump (model # EW-78001-00), is advantageous because it can support up to four channels though a single device eliminating the need for a separate pump for each humidified line.

Syringe Pumps

A different approach to pumping small quantities of liquid is to use a syringe pump. A typical syringe pump is pictured in figure 8.5.

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[1] Price Source: http://www.coleparmer.com/Product/Ismatec_low_speed_planetary_gear_driven_pump_4_channels_115_230_VAC/EW-78001-00

Figure 8.5 A syringe pump used for metering liquids. Image Source: http://www.katsci.com/products/ne-300-just-infusion-syringe-pump.aspx

Syringe pumps use carefully controlled motors to drive a piston into a cylinder of known dimensions. One significant advantage to syringe pumps is that multiple syringes can be operated by a single pump to provide equal flow rates. The linear position of the piston is proportional to the quantity of water added to the line while its velocity is proportional to the mass flow rate. Unlike mass flow controllers or positive displacement pumps, syringe pumps cannot operate continuously. The maximum operating time is limited by the volume of the syringe. Since the maximum desired flow rate is approximately 100mL/ hour, a volume of 0.5L would be needed to sustain a five hour test. This capacity far exceeds that of the vast majority of commercially available syringe pumps which typically have capacities on the order of tens of milliliters. The few pumps which are available are designed for high pressure applications and are extremely costly.

This leaves the option of designing a custom syringe pump for this specific application. This is not an unreasonable proposition. Figure 8.6 shows the basic components of a syringe pump, all of which are fairly basic.

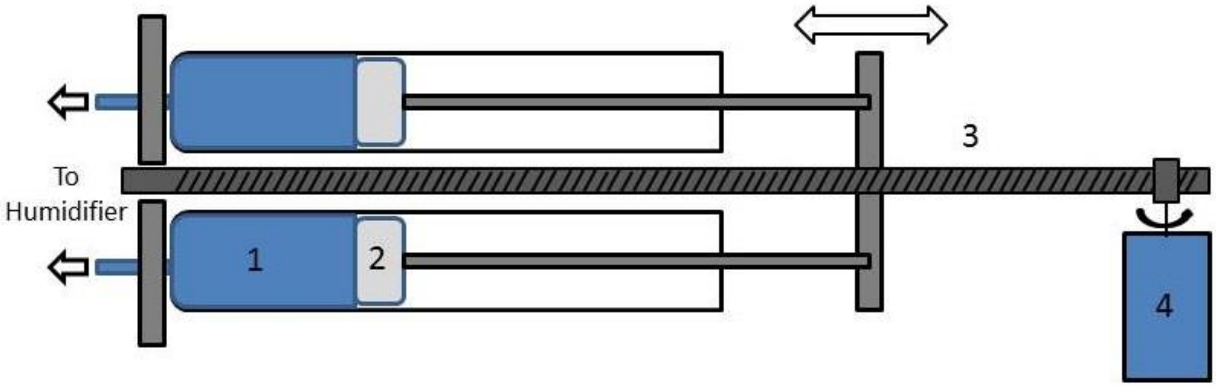

Figure 8.6 A diagram of a two channel syringe pump which could be used to provide water to the humidification subsystem showing: 1.syringe cylinder, 2. syringe plunger, 3. Screw drive 4. motor actuator

The overall accuracy of a custom syringe pump would depend most heavily on the ability to accurately and precisely control the servo motor. This would require the addition of a closed loop control system to control its position. The feasibility of the syringe pump to meter water into a controlled evaporation system depends on the cost of the pump components and controller relative to the other options.

8.3 Bubble Humidifier

The traditional method used to create a humidified gas flow is to use a device called a bubble humidifier. These are most often used in medicine to humidify oxygen for patients. A diagram showing the components of a bubble humidifier is shown in figure 8.7.

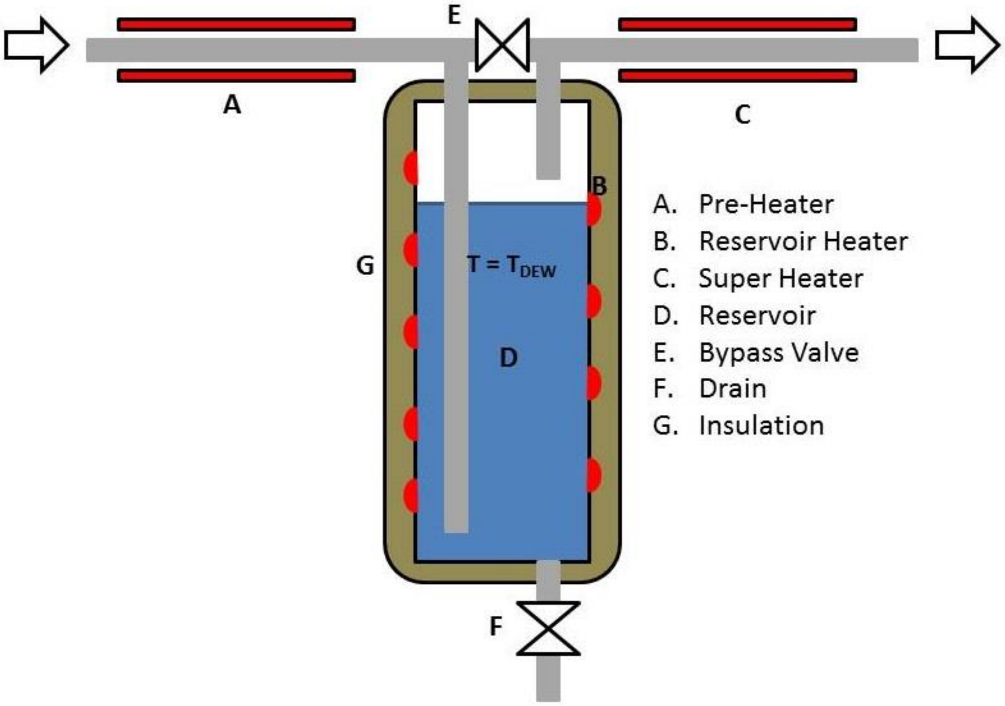

Figure 8.7 Diagram of a bubble humidifier. Test gas enters from the left and exits into the heating system on the right

The reservoir is kept at the dew point for the desired absolute humidity. Therefore if a bubble of dry test gas was kept in the humidifier indefinitely it would eventually reach equilibrium with its surroundings by becoming saturated with water vapor. At this point it would have a relative humidity of 100% and an absolute humidity equal to the desired absolute humidity. This process occurs as the bubble floats to the top of the fluid column. As the bubbles exit the humidifier they are again heated by the super-heater to minimize the risk of condensation in the lines. In order to minimize the required column height, the test gas would be preheated to the reservoir temperature before it reached the inlet.

The key design considerations for a bubble humidifier are the water column dimensions. A larger volume of fluid is more stable with respect to temperature but also has more thermal inertia and therefore would take longer to reach steady state. The height of the column determines the residence time of the bubble in the reservoir. The longer this time is, the more likely the bubble is to become saturated with water vapor.

The main advantage to the bubble humidifier is that the precise flow rates of test gas and water are largely unimportant. Water only needs to be added to the system to maintain the approximate level in the humidifier. A proposed leveling system using conductive sensors is presented in Attachment M. As long humidifier is large enough so that the bubbles leave it saturated with water vapor the flow rate of the test gas theoretically has no effect on the absolute humidity of the mixture. Therefore a bubble humidifier should be able to escape many of the scaling concerns inherent in the controlled evaporator design.

The main disadvantage of the bubble humidifier is that it requires careful control of the resevoir's temperature and pressure to ensure that the saturated test gas leaving it is at the appropriate relative humidity. This presents a very challenging control problem. Additionally bubble humidifiers tend to have poor long term stability. [11] These factors limit the potential accuracy and precision of the bubble humidifier as a means of humidifying the test gas.

Solubility of Test Gas in the Humidifier

An additional problem which presented itself with the bubble humidifier option is the potential for components in the test gas mixture to dissolve into the reservoir and change the composition of the outgoing mixture in a way which could not be measured. Since the concentration of each component of the test gas in the bubble is higher than that of the water there is the potential for an exchange across the boundary of the bubble. The longer the bubble remains in the reservoir, the more gas is likely to dissolve. This exchange is shown in figure 8.8.

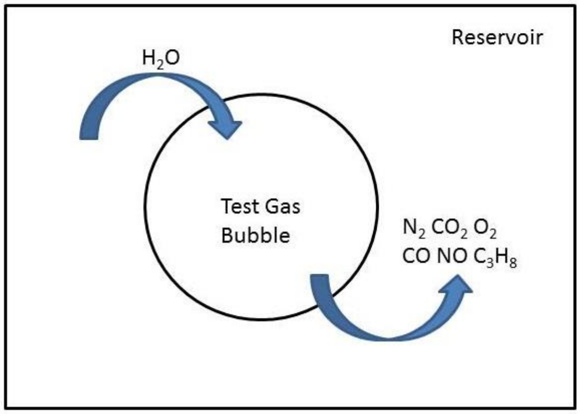

Figure 8.8 The component exchange between a bubble of test gas in the humidifier and the surrounding test gas. The bubble, initially made up of dry gas takes on water vapor. At the same time, some of the mixture components dissolve into the surrounding reservoir.

There are two potential scenarios in which this would not pose a problem. The first is that all of the gas components are insoluble in water. The second is that though some components are soluble in water, the amount of each component it would take to saturate the reservoir is small compared to the amount of that component in the reservoir at any given time. In this case reservoir would quickly become saturated with each component and the system would reach steady state in a short time.

The ability of a gas to dissolve into water is called its solubility, and it is described in terms of moles of gas which can dissolve into a liter of water (mol/L). The solubility of each of the test gas components is presented in table 8.2. [12]

Table 8.2 Solubility of test gas components in water. All data for water at 25°C, 1atm. Data not available for all components at higher temperatures

	Solubility ($x10^3$ mol/L)		
Component	**Highest**	**Average**	**Lowest**
C3H8	1.50	1.40	1.40
CO	7.40	2.00	0.82
CO2	45.00	35.00	31.00
NO	1.90	1.50	0.00
N2	0.65	0.63	0.61
O2	1.30	1.30	1.20

Of these components CO_2 has solubility an order of magnitude higher than the next component, thus eliminating the possibility of the first scenario.

In order to address the possibility of the second scenario two quantities need to be compared: the moles of each component which could dissolve into a humidifier of a given volume, and the moles of test gas present in the humidifier at any given time. These calculations are formally presented in Attachment F. The first quantity is derived by simply multiplying the volume of the humidifier by the solubility of each component. This makes the component costs for the bubble humidifier design considerably lower than the controlled evaporator design.

The calculation of the second quantity is slightly more involved. The key quantity to calculate is the volume of the test gas in the humidifier at a given point in time. This was done by multiplying the volumetric flow rate of the test gas by the residence time of the gas in the humidifier. The residence time was taken to be the time taken by a single bubble to reach the top of the humidifier; a quantity which depends on the velocity of the bubble and the height of the humidifier. The velocity of the bubble was estimated using stokes solution which models the bubble as a buoyant sphere with a density equal to that of air. [13] While this model makes a number of assumptions, it provides a reasonable order of magnitude estimate of the bubbles velocity. Most importantly it states that the velocity is proportional to the square of the bubble size. These equations were used to calculate the volume of gas in the humidifier which was then multiplied by the volume fractions of each component to arrive at the molar quantity for each component.

When these calculations were performed for each component results presented in table 8.3 were generated.

Table 8.3 Potental losses of each component of the test gas to a 1L reservoir with a .3m height. The bubble size was specified to be 1mm. Take, for example, the potential losses of CO_2. The humidifier could hold up to 240 times more CO_2 by volume as is in it at any given time.

Relative Potential Losses (Capacity/ Component Volume $x10^{-3}$)			
Component	**Highest**	**Average**	**Lowest**
C3H8	2.43	2.27	2.27
CO	0.48	0.13	0.05
CO2	0.24	0.19	0.17
NO	2.06	1.62	0.00
N2	0.00	0.00	0.00
O2	0.12	0.12	0.11

The quantities in the table represent the ratio of the molar amount of each component which it would take to saturate the humidifier relative to the amount that is in it at any given time. In order for the system to quickly reach steady state this number should be very low. Unfortunately this is not the case, meaning that the second scenario is unlikely. One key observation is that the gas components most likely to present solubility problems are not necessarily those with the highest solubility, gases with low concentrations also have high potential solubility losses. It is important to note that this calculation does nothing to address the rate at which the gas could dissolve into the humidifier, which would be the logical next step in determining the potential losses due to solubility. Additionally this calculation does not take into account any interactions between the dissolved components. That is it assumes each component is dissolving into a completely degassed volume of water.

Conclusions and Current Work

For the reasons outlined above there are many potential problems with using a bubble humidifier. Since the extent of these problems is very difficult to determine analytically, the best course of action would be to gather experimental data regarding a bubble humidifier's effectiveness. Figure 8.9 shows a bubble humidifier constructed from basic lab ware which can be used to measure several humidifier parameters.

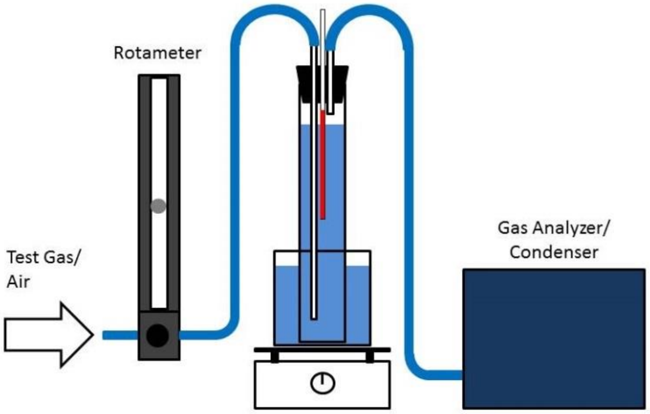

Figure 8.9 Glassware humidifier test setup

The setup uses a rotameter to distribute test gas to a humidifier constructed from a graduated cylinder. The temperature of the humidifier is measured using a thermometer and heat is added by immersing the graduated cylinder in beaker filled with water resting on a hot plate.

There are two important experiments which could be performed using such a setup. The first would be to measure the ability of the humidifier to humidify gas. This would be done by attaching a condenser to the outlet. By measuring the volume of water exiting the condenser it would be possible to determine the humidification load of the bubbler for a given temperature and gas flow rate. The other experiment would be to flow a premixed bottle of test gas through the bubble humidifier and use the five gas analyzer to determine the reduction of the different pollutants over time. This would give the experimenter an indication of how long it would take the system to reach steady state or whether the solubility losses are even measurable by the lab's instrumentation.

Another design option worth perusing is designing a large capacity syringe pump to drive a controlled evaporation humidifier. The proposed pump would be fairly simple to design and price out, potentially offering a cost effective solution.

9. Global System Design

9.1 Global Schematic

While investigating the designs of the individual gas conditioning subsystems it is also useful to consider the layout of the global system as well. This helps identify additional components which will be needed but are not native to any particular sub-system. Additionally looking at the system from a global perspective helps the designer identify any potentially problematic interactions between subsystems. Finally, this process starts a discussion on the overall power and process control requirements for the system.

An overall schematic for the gas conditioning system is presented in figure 9.1. A larger version of this figure is located in Attachment N. This design will evolve as a final design for the humidification system is developed.

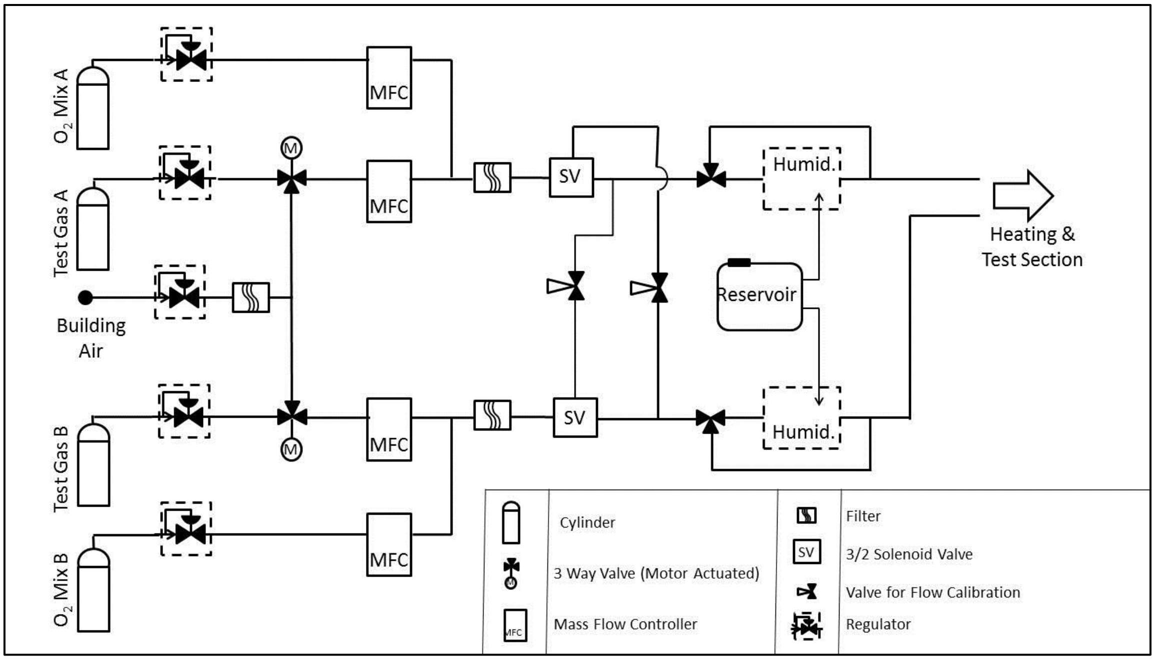

Figure 9.1 A schematic of the gas conditioning system.

9.2 Layout of Subsystems and Compressed Air Line

The order in which the subsystems are arranged is an important consideration in the overall design. In this schematic the order is as follows, 1) the test gas and oxygen mixture are metered and mixed, 2) the transient compositions are generated by the gas switching sub-system, 3) the gas is humidified. Humidification should occur last because both the solenoid valves and the mass flow controllers are temperature sensitive and the controllers are not rated for humidified flows. A case could be made for placing the humidification system before the switching system. This would eliminate potential slug mixing within the humidification system. The problem with this approach is that due to the rapid pressure changes large wetted area in the solenoid valves it would be very difficult to prevent damaging condensation without heating the entire valve. The oxygen addition must occur before the switching subsystem because each oxygen mixture must be added to the correct test gas mixture. To do so after the switching subsystem would necessitate the switching of the oxygen flows as well.

Another major addition in the global schematic is the building compressed air line, which is connected to each test gas line by a 3 way valve. On the current test bed the compressed air line serves three important functions: it provides the needed oxygen to be mixed into the test gas, it allows the heating system to reach steady state without wasting test gas, and it provides a cooling flow to the heating system after testing is finished.

With the exception of the oxygen addition, which is provided for by separate cylinders, it is desirable to retain these capabilities. Air can also be used to purge the downstream lines of moisture after testing or service. In the current design, when the compressed air line is in use both of the three way valves will be open to the air flow and the switching subsystem will be turned off. Then the flow in each line can be controlled by the test gas flow controllers. Oxygen addition is not needed during this time so those flow controllers can be set to zero flow. The humidification subsystem would continue to run through this process.

Since air must be run through the lines between each step in the temperature sweep, the three way switches should be motor actuated and digitally controlled. In the event of a power failure the switches should fail with the air inlet open to minimize the risk of a dangerous leak of test gas into the lab.

At some point during the lifetime of the test bed it may become necessary to replicate tests from the previous test bed. Therefore it should be possible for the new gas conditioning system to replicate the behavior of the old one. This could be done by using a single switching line and attaching the filtered compressed air line to the O_2 mixture MFC. The switching system would then be left in a single position to not interrupt the flow. Finally a bypass valve would be installed for the humidification system so that dry gas at would run into the heating system.

9.3 Filtration Needs

Thermal mass flow controllers are very sensitive to particulate contamination. Any dust or oil which gets into the bypass section of the controller can cost costly damage and lengthy system downtime. Therefore it is necessary to create a “clean zone” around the controllers to protect them from contamination. This is done using filters.

The major source for potential contamination of the controllers is the compressed air line from the building. Therefore it is necessary to filter that flow immediately after the pressure regulator. A second potential source of contamination is backflow from the switching and humidification sub systems. Adding a filter between the flow controllers and those components has the additional advantage of muffling pressure waves created by the solenoid valves and increasing the stability of the flow controllers. The recommended filter placements are shown in figure 9.1 from the first section. So far the mixture tanks have been considered to be free of contaminants. While this is a good assumption, it does not account for dust entering the lines while the tanks are being replaced.

When selecting a filter to protect the flow controllers the primary concern is the pore size which determines what size particles the filter can remove from the flow. The appropriate pore size should be determined according to the MFC manufacturer's specifications. There is a basic tradeoff between a filter's ability to remove contaminants and the amount which it impedes fluid flow. An additional consideration is the ability to service the filter element without removing the filter body from the line.

9.4 Relationship between Flow Rates

Throughout the conditioning system the flow rates vary widely in different lines and components. Therefore it is important to understand the relationship between the different flow rates. When comparing flow rates between different systems and components it mass flow rates should be used.

The flow rate calculated from section 4 is the *global* flow rate. This is the mass flow rate entering into the heating section for a given set of test chamber conditions. The *dry gas* flow rate is the flow going through each switch and in each switched line. It is equal to the global mass flow rate minus the water mass flow rate in the humidification system. It is also equal to the sum of the test gas and oxygen flow rates. Equation 14 and 15 shows the relationship between these quantities.

$$(global) = (test\ gas) + (oxygen\ addition) + (water\ addition) \tag{14}$$

$$(dry\ gas) = (test\ gas) + (oxygen\ addition) \tag{15}$$

These flow rates are used to source the different components in the system. Figure 9.2 shows the global schematic highlighted according to the flow rate in the line.

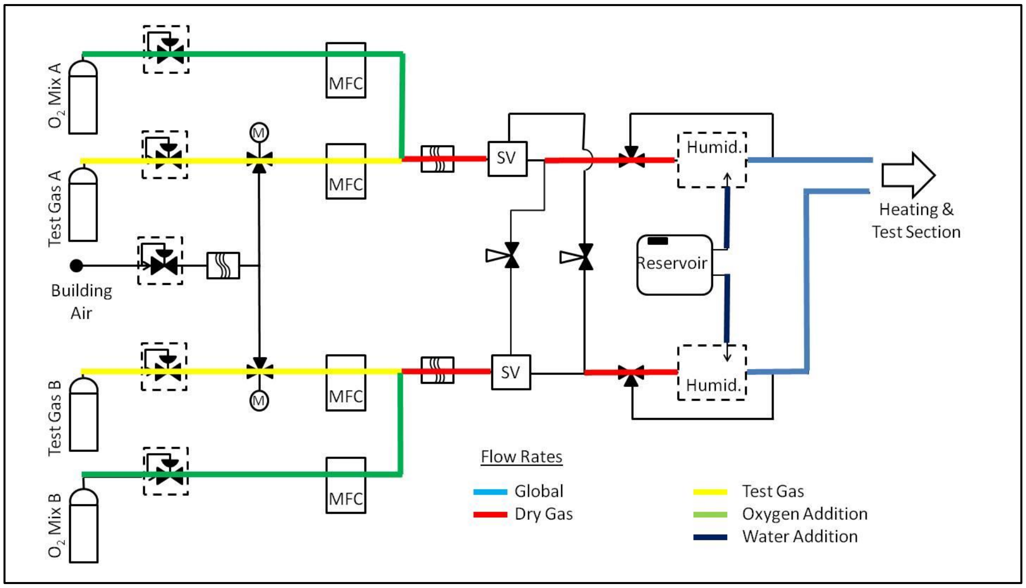

Figure 9.2 The global schematic with the different flow rates highlighted on their respective lines. Note that each outlet of the solenoid valve outputs one half of the dry gas flow rate.

9.5 Power and Control Systems

The gas conditioning system contains many different electrical components. Broadly speaking, they can be divided into two categories: AC and DC powered. The AC components include the solenoid valves, the motor actuated 3 way valves, and likely the heater elements in the humidification system. The DC components include the flow controllers and any powered control circuits. Therefore both an AC and DC power supply will be necessary.

The end goal of the project is to have the potential for the system completely controlled from a computer. Some of the components, such as the mass flow controllers, will already be set up for digital control. This is usually in the form of a

RS-232 cable and computer software provided by the manufacturer. Alternatively, since several of the controllers will be used, it may be advantageous to set up a device network such as DeviceNet or a similar proprietary network to simplify wiring and have a single interface.

It will also be necessary to monitor conditions such as temperature and pressure at different points in the system during testing. This will require the installation of pressure transducers and thermocouples at different points along the lines. A data acquisition system will be needed to monitor these instruments and compile results onto a computer. Many data acquisition systems also have a digital I/O output which can be used to drive control circuits for components.

9.6 Safety Measures

Operator safety is the paramount concern of the design. The gas conditioning system contains AC wiring, high pressure cylinders, heating elements, and toxic gases. Each of these things can be potentially deadly to the operator. The final system will require a grounded enclosure to protect the user from burns and show while the system is in use. Additionally an emergency stop switch should be incorporated into the wiring and computer protocol which completely shuts down the system and purges it with compressed air.

10. Future Goals for Project

While this report covers many of the preliminary design steps for the gas conditioning system, there remains a good deal of work to be done before the project is finished. The first step is to prove the viability of the switching sub-system. This means building a mockup of the system and ensuring that it operates according to the models outlined in the switching section. Of particular importance is the valve's ability to split the flow evenly and generate distinct slugs of gas in the line. Additionally a humidifier design needs to be selected and fabricated. The continued humidification experiments will play a large role in that decision. When all of the subsystems have been tested and proven individually the full gas conditioning system may be assembled and tested.

11. Acknowledgements

My work so far on this project would not have been possible without the valuable help and advice of several people. First and foremost I would like to thank my advisor, Professor Bruno, as well as Professors Anderson and Carroll from the Aerogel Lab. Both Stan Gorski and the Union College Machine shop were enormously helpful with their fabrication skills and technical advice. Additionally cannot thank our department secretary, Rhonda Becker, enough for her help and patience in coordinating purchases and other logistics. Finally I would like to thank Dave Carabis, Travis Barker, Paul Brockmann, Jose Madero, and Professor Hodgeson for their insight throughout the design process. This project was funded by NSF Grant #059375584.

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Attachments

I. Calculations
    A. Mass Flow Rate
    B. Standard Slug Length
    C. Pressure Rise Due to Switching
    D. Humidification
    E. Heat Addition Requirement
    F. Solubility in Bubbler Humidifier
II. MATLAB Scripts
    G. Equilibrium Calculation Setup
    H. Flow Rate and Slug Length Calculation and Figures
    I. Humidification Calculation
III. Designs
    J. GMS Final Schematic
    K. Control Circuit for Switching
    L. Designs for Bubbler Humidifier
    M. Leveling System for Bubbler Humidifier
    N. Global Schematic
IV. Product Specifications
    O. GMS Tank Quote
    P. Alarm Recommendations
    Q. Bronkhorst MFC Quote
    R. Brooks MFC Quote
    S. Solenoid Valve Specifications
    T. Solid State Relay Specifications

A. Mass Flow Rate

This calculation determines the overall mass flow rate in the conditioning system based on the conditions in the test section. The flow rate depends on the space velocity, test section temperature, and the volume of the test section.

$$\dot{m} = \frac{sV_tP}{RT_t}$$

Variable	Quantity	Value	Units	Notes and Assumptions
ṁ	Mass Flow Rate		$^{kg}/_{s}$	
s	Space Velocity	15	s^{-1}	Given
V_t	Test Section Volume	$1.51\text{x}10^{-5}$	m^3	0.85" diameter by 1.62" height
P	Pressure	101.3	kPa	Assumed atmospheric
R	Specific Gas Constant	0.287	$^{kJ}/_{kg\text{-}K}$	Air as an ideal gas
T_t	Test Section Temperature	500	°C	Given

$$\dot{m} = \frac{(15\ s^{-1})(1.51\text{x}10^{-5}\text{m})(101.3\ kPa)}{(.287\ ^{kJ}/_{kg-K})(500 + 273.15\ K)}$$

$$\dot{m} = 1.034\ x10^{-4}\ ^{kg}/_{s}$$

Convert to SLM

$$\frac{1.034\ x10^{-4}\ kg}{1s}\ \frac{m^3}{1.275\ kg}\ \frac{1000\ L}{1m^3}\ \frac{60\ s}{1\ min} = 4.866\ \frac{L}{m}\ at\ standard\ conditions$$

(Assumes test gas is air $\rho = 1.275\ ^{kg}/_{m3}$)

B. Standard Slug Length

The slug length is the length of a single unit of gas in the line of a given composition. A long slug length relative to the line diameter indicates that there is a low risk of mixing between the slugs. The slug length is proportional to the mass flow rate and inversely proportional to the switching frequency. Each cycle of the switching frequency consists of the generation of two slugs.

$$l = \frac{\dot{m}}{2\rho A f}$$

Variable	Quantity	Value	Units	Notes and Assumptions
l	Slug Length		m	
ṁ	Mass Flow Rate	1.034 x10^{-4}	$^{kg}/_{s}$	From previous section
ρ		1.275	$^{kg}/_{m3}$	Assumes air at STP
A	Line Cross Section Area		m^2	Standard SS ¼ in tubing
f	Switching Frequency	1	Hz	Given

$$l = \frac{(1.034\, x10^{-4}\, kg/s)}{2(1.275\ \ kg/m^3)(\,1.91\, x10^{-5}\, m^3)(1Hz)}$$

$$l = 2.122\, m$$

C. Pressure Rise Due to Switching

The goal of this calculation is to estimate the rise in pressure in the line when the valve is closed and the flow controller continues to add a constant mass flow rate. The test gas is assumed to be air at a constant temperature acting as an ideal gas. The line is treated as a fixed control volume initially at atmospheric pressure. The sample calculation is for test section conditions

Starting with the ideal gas law solved for pressure to find the pressure in the line given the mass of the gas inside of it:

$$P = \frac{mRT}{V}$$

Variable	Quantity	Value	Units	Notes and Assumptions
P	Pressure		kPa	
m	Mass		kg	
R		0.287	$^{kJ}/_{kg\text{-}K}$	Assumes air at STP
T	Temperature	300	K	Assume constant room temp
V	Volume	2.24 x10^{-5}	m^3	1m of standard SS ¼ in tubing

The mass added while the valve is closed is depends on the mass flow rate and the switching frequency.

$$m_{added} = \frac{\dot{m}}{2f}$$

Variable	Quantity	Value	Units	Notes and Assumptions
$\mathbf{m}_{\mathbf{added}}$	Mass Added to Line		kPa	
$\dot{\mathbf{m}}$	Mass Flow Rate	1.034 x10^{-4}	$^{kg}/_{s}$	s= 15 T_t= 500°C
f	Switching Frequency	1	Hz	Given

$$P_{max} = \frac{\left(\rho V + \frac{1}{2}\dot{m}f^{-1}\right)RT}{V}$$

The total mass in the system the instant before the valve opens is the sum of the mass originally in the line and the mass added. The initial density is for air at standard conditions:

$$P_{max} = \frac{\left[(1.275\,kg/m^3)(2.24\,x10^{-5}m^3) + \frac{1}{2}(1.034\,x10^{-4})(1Hz)^{-1}\right](0.287\,kJ/kg\cdot k)(300K)}{(2.24\,x10^{-5}\,m^3)}$$

$$P_{max} = 308.5\,kPa = 44.74\,psia$$

D. Humidification

The goal of the humidification calculation is to take the global mass flow rate in the conditioning system and known information about combustion in engines to come up with a mass flow rate of water. The MATLAB script in attachment I takes the balanced equation for the combustion of octane (below) in air and returns the mole fractions of each component in the exhaust, shown in the first table.

$$C_8H_{18} + 12.5O_2 \rightarrow 9H_2O + 8CO_2$$

Component	**Mol Fraction**
N2	0.777
CO2	0.105
H2O	0.118
Total	1.000

These mole fractions are turned into mass fractions using the molar mass of each component and the equation below.

$$(Mass\ Fraction) = \frac{(Mole\ Fraction)(Molar\ Mass)}{\sum[(Mole\ Fraction)(Molar\ Mass)]}$$

Component	**M**		**Number**		**Total**	
Nitrogen (N_2)						
N_2	14.01	x	2	=	28.02	
					28.02	**kg/kmol**
Carbon Dioxide (CO_2)						
C	12.01	x	1	=	12.01	
O_2	16	x	2	=	32	
					44.01	**kg/kmol**
Water (H_2O)						
H_2	1.008	x	2	=	2.016	
O	16	x	1	=	16	
					18.016	**kg/kmol**

As a sample calculation the mass fraction of CO_2 is solved for below:

$$(Mass\ Fraction\ CO_2) = \frac{(0.105\ kmol)(44.01\frac{kg}{kmol})}{(28.517kg)}$$

$$(Mass\ Fraction\ CO_2) = 0.162$$

The remaining components are solved for below:

Component	kMol	kg/Kmol	kg	kg/kg
N2	0.78	28.02	21.76	0.76
CO2	0.11	44.01	4.63	0.16
H2O	0.12	18.02	2.13	0.07
Total	1.000		28.517	1.000

Since water makes up 0.07kg of every kilogram of mass leaving the confiditioning system the mass flow rate for water can be calculated as follows.

$$\dot{m}_{water} = \dot{m}_{global}(mass\ fraction\ of\ water)$$

This equation is solved for test section conditions of s = 15 1/s and T_t = 500°C:

$$\dot{m}_{water} = (1.034\ x10^{-4}\ kg/s)(0.0745)$$

$$\dot{m}_{water} = 7.708\ x10^{-6}\ kg/s$$

Convert to g/hr:

$$\frac{7.78\ x10^{-6}\ kg}{s}\ \frac{3600s}{hr}\ \frac{1000}{kg} = \frac{27.75g}{hr}$$

The amount of dry gas making up the remaining flow is equal to the global mass flow rate minus the water flow rate.

$$\dot{m}_{dry\ gas} = (1.034\ x10^{-4}\ kg/s) - (7.708\ x10^{-6}\ kg/s)$$

$$\dot{m}_{dry\ gas} = 9.569\ x\ 10^{-5}\ kg/s$$

Finally the absolute humidity of the mixture, ω, is calculated.

$$\omega = \frac{\dot{m}_{water}}{\dot{m}_{dry\ gas}}$$

$$\omega = \frac{(7.78\ x10^{-6}\ kg/s)}{(9.569\ x10^{-5}\ kg/s)}$$

$$\omega = 0.081$$

E. Heat Addition Requirement

This calculation determines a baseline for the amount of heat which must be added to the test gas and water in order to form the vapor mixture which will be pumped into the heating assembly. The mixture is assumed to be an ideal gas as the water represents a low partial pressure in the mixture. Therefore the water and test gas, assumed to be nitrogen, can be treated separately in the calculation. Additionally the enthalpy of water can assumed only to be dependent on temperature such that the enthalpy is equal to the saturated vapor enthalpy at that temperature. Each component is brought from 1atm and 20°C to 100° C with no change in pressure. Though the dew point of the mixture was estimated to be close to 49°C, additional heat should be added to minimize the risk of condensation. The case of a s= 15 1/s and T_t= 500°C was again chosen for this calculation. The equation used is simply a first law energy balance for a control volume.[2]

$$\dot{Q} = \dot{m}_{water}\left(h_{water,f} - h_{water,i}\right) + \dot{m}_{test\ gas}\left(h_{test\ gas,f} - h_{test\ gas,i}\right)$$

Variable	Quantity	Value	Units	Notes and Assumptions
$\dot{Q}$	Heat flux into humidifier		W	
$\dot{m}_{water}$	Mass flow of water	7.78 x10^{-6}	kg/s	from above
$h_{water,f}$	Enthalpy of water at outlet	2676	kJ/kg	T=100°C, x= 1 (CATT 3)
$h_{water,i}$	Enthalpy of water at inlet	84.03	kJ/kg	T=20°C, P = 1atm (CATT 3)
$\dot{m}_{test\ gas}$	Mass flow of test gas	9.57 x10^{-5}	kg/s	from above
$h_{test\ gas,f}$	Enthalpy of gas at outlet	-5.197	kJ/kg	T=100°C, P = 1atm (CATT 3)
$h_{test\ gas,i}$	Enthalpy of gas at inlet	78.05	kJ/kg	T=20°C, P = 1atm (CATT 3)

$$\dot{Q} = (7.78\ x10^{-6}\ kg/s)[(2676\ kJ/kg) - (84.03\ kJ/kg)] + (9.57\ x10^{-5})[(78.05\ kJ/kg) - (-5.197\ kJ/kg)]$$

$$\dot{Q} = .0281\ kJ/s$$

$$\dot{Q} = 28.1\ W$$

---

[2] Borgankke, Claude and Richard E. Sonntag. *Fundementals of Thermodynamics: 7th Edition*. Hoboken: John Wiley & Sons, 2009. print

F. Solubility in Bubbler Humidifier

The goal of this calculation is to compare the amount of a gas mixture component which can dissolve into the humidifier to the amount of gas which is in it at any given point. The volume which can dissolve in the humidifier is simple the solubility multiplied by the humidifier volume.

$$(mol\ lost)_i = K_i V_H$$

Variable	Quantity	Value	Units	Notes and Assumptions
(mol lost)$_i$	molar quantity of component i dissolved in humidifier		kmol	
K$_i$	Solubility of component i	4.5 x10^{-2}	mol/L	given
V$_H$	Water volume of humidifier	1	L	assumed

This calculation was carried out for CO_2

$$(mol\ lost)_{CO_2} = (4.5\ x10^{-2}\ mol/L)(1L)(10^{-3}kmol/mol)$$

$$(mol\ lost)_{CO_2} = 4.5\ x10^{-5}\ kmol$$

In order to find the molar amount of CO_2 in the humidifier, the volume of gas in the bubbles had to be estimated using the equation below. A figure showing the different quantities is included at the end of the calculation.

$$V_{gas} = \dot{V}t$$

Variable	Quantity	Value	Units	Notes and Assumptions
$\boldsymbol{V_{gas}}$	Volume of gas in Humidifier		L	
$\dot{V}$	Volumetric flow rate	15	L/min	Approximate maximum dry flow
t	Residence time of gas		s	Equal to bubble rise time

The residence time of a single unit of gas in the humidifier is estimated as the time it takes it to travel the height of the humidifier in the form of a bubble. To do this the two equations below are used. The second is the Stokes solution for the terminal velocity of a gas bubble in a liquid.[3]

$$t = \frac{h}{u_\infty}$$

---

[3] Talaia, Mario A. R. "Terminal Velocity of a Bubble Rise in a Liquid Column." *World Academy of Science, Engineering and Technology* Vol. 28, (2007) online

$$u_\infty = \frac{1}{18}\frac{gd^2(\rho_{water} - \rho_{gas})}{\mu_{water}}$$

Variable	Quantity	Value	Units	Notes and Assumptions
h	Height of humidifier	0.3	m	Assumed (estimate)
u_∞	Terminal velocity of bubble	15	$^{m}/_{s}$	Given
g	Gravitational constant	9.81	$^{m}/_{s2}$	Assumed atmospheric
d	Bubble Diameter	0.001	$^{kJ}/_{kg\text{-}K}$	Air as an ideal gas
ρ_{water}	Density of water	1000	$^{kg}/_{m3}$	Water at normal conditions
ρ_{gas}	Density of test gas	1.275	$^{kg}/_{m3}$	Air at STP
μ_{water}	Viscosity of water	0.543 x10^{-3}	$^{N\text{-}s}/_{m2}$	Water at 20° C[4]

Solving for the terminal velocity of a 1mm bubble in water:

$$u_\infty = \frac{1}{18}\frac{(9.81\, m/s^2)(0.001m)^2[(1000\, kg/m^3) - (1.225\, kg/m^3)]}{(0.547\, x10^{-3}\, N \cdot s/m}$$

$$u_\infty = 0.994\, m/s$$

Using this value for the bubble velocity, the volume of gas in the 0.3m tall humidifier can be calculated:

$$t = \frac{0.3m}{0.994m/s}$$

$$t = .301s$$

The total volume of the gas in the humidifier can then be estimated:

$$V_{gas} = (15\, L/min)(0.301s)(\frac{1\, min}{60\, s})$$

$$V_{gas} = \ 0.0753\, L$$

Finally the proportion of CO_2 must be found and converted into a molar quantity. Recall that the molar fraction of an ideal gas is equal to its volume fraction. Therefore the volume of CO_2 can be found with the mole fraction and converted to a molar quantity using the density and molar mass.

$$(kmol)_i = V_{gas}\, \rho_i\, (vol\, fraction)_i\, (molar\, mass)^{-1}$$

---

[4] Source: EngineeringToolbox.com

$$(kmol)_{CO_2} = (0.0753\,L)(1.8420\,kg/m^3)(0.0587\,L_{CO_2}/L_{mix})(44.01\,kg/kmol)(0.001\,m^3/L)$$

$$(kmol)_{CO_2} = 1.850\,x10^{-7}\,kmol$$

By comparing the two molar quantities the relative losses can be calculated:

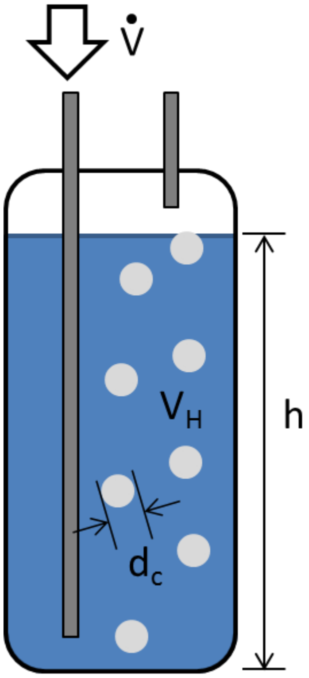
$$Relative\ Losses = \frac{(moles\ lost)}{(total\ moles\ in\ humidifier)}$$

$$Relative\ Losses = \frac{4.5\,x10^{-5}\,kmol}{1.850\,x10^{-7}\,kmol}$$

$$Relative\ Losses = 243.24$$

This means that over 200 times more CO_2 can dissolve into the humidifier than is in it at any time suggesting that the water would take a long time to reach a saturated steady state of dissolved CO_2

Figure showing quantities for gas volume calculation:



G. Equilibrium Calculation Setup

Note: script was not giving viable results when work was stopped

```
%%Equalibrium Calculations
% 10/21/12

clear all; close all; format compact; clc
%Air is mixed at a ratio of .017:1 with BAR 97 Blend 32 Calibration Gas
%BAR 97 Specifications:             %Air Specifications
%    200ppm    C3H8                    78.67%       N2
%    0.50%     CO                      20.94%       02
%    6%        CO2                      0.39%       CO2
%    300ppm    NO                      note: other components assumed to be
%    Balance   N2 (93.45%)                   N2

%Determine concentrations of of components in a mole of gas to test chamber
%ASSUMPTION: All gases ideal --> volume fraction = mole fraction
AirRatio = .017;
GasRatio = 1;
Total = AirRatio + GasRatio;

%        C3H8    CO    C02    NO      N2    02
Bar97 = [200/1E6 0.005 0.06   300/1E6 .9345 0 ];
sum(Bar97)  %check

%      C3H8    CO    C02    NO      N2    02
Air = [0       0     .0039  0       .7867 .2094 ];
sum(Air) %check

Blend = AirRatio.*Air + Bar97.*GasRatio;
Blend = Blend./Total;
sum(Blend) %check

%Set up equalibrium calculations
%ASSUMPTION: Reactions in the tank can be described by the following
%reactions:
%   C3H8 + O2 --> H20 + CO2
%   2CO + O2 --> CO2
%   2NO --> N2 + O2
%Since the tank is a closed system, amounts of H, C, O, and N must remain
%the same- calculate molar quantities of each element
H = 8*Blend(1)+2
C = 3*Blend(1)+Blend(2)+Blend(3)
N = Blend(4)+2*Blend(5)
O = Blend(2)+ 2*Blend(3)+Blend(4)+2*Blend(6)
H+C+N+O %Check

X0 = [0 0 0 0 Blend 0 0 0 0 0];
options.MaxFunEvals = 10000;
options.MaxIter = 10000;
[Equalibrium, fval] = fsolve(@equations2, X0, options);
sum(Equalibrium) %check
Equalibrium = Equalibrium/sum(Equalibrium); %Change to % Concentrations
sum(Equalibrium) %check

titles = ['H           C           N           O  C3H8         CO           C02       NO
N2        02                  H20         C2H6        CH4         NO2         H2'];

disp(titles)
disp(num2str(X0))
disp(num2str(Equalibrium))
```

Additionally the equation matrix used in the script:

```
%Set up equalibrium equations
% X = [H C N O] [C3H8 CO C02 NO N2 02] [H20 C2H6 CH4 NO2 H2]
%      1 2 3 4   5    6  7   8  9  10   11  12   13  14  15
function F = equations2(X)
     %Product     H        C        N        O         (K)
  F =[ X(5)   /   (X(1)^8 * X(2)^3                  ) - exp(4.1432);  %C3H8
       X(6)   /   (         X(2)            * X(4)  ) - exp(23.9125); %CO
       X(7)   /   (         X(2)            * X(4)^2) - exp(68.661);  %CO2
       X(8)   /   (                  X(3)   * X(4)  ) - exp(-15.3439);%NO
       X(9)   /   (                  X(3)^2         ) - exp(0);       %N2
       X(10)  /   (                           X(4)^2) - exp(0);       %O2
       X(11)  /   (X(1)^2                   * X(4)^2) - exp(39.784);  %H20
       X(12)  /   (X(1)^6 * X(2)^2                  ) - exp(5.4957);  %C2H6
       X(13)  /   (X(1)^4 * X(2)                    ) - exp(8.8135);  %CH4
       X(14)  /   (                  X(3)   * X(4)^2) - exp(-9.1283); %NO2
       X(15)  /   (X(1)^2                           ) - exp(0);       %H2
       X(1) + 8*X(5) + 2*X(11)+ 6*X(12)+ 4*X(13) + 2*X(15)           - 2.0016;
       X(2) + 3*X(5) +   X(6) +   X(7) + 2*X(12) +   X(13)           - 0.0646;
       X(3) +   X(8) + 2*X(9) +   X(14)                              - 1.8644;
       X(4) +   X(6) + 2*X(7) +   X(8) + 2*X(10) +   X(11) + 2*X(14) - 0.1303 ];
```

H. Flow Rate and Slug Length Calculation and Figures

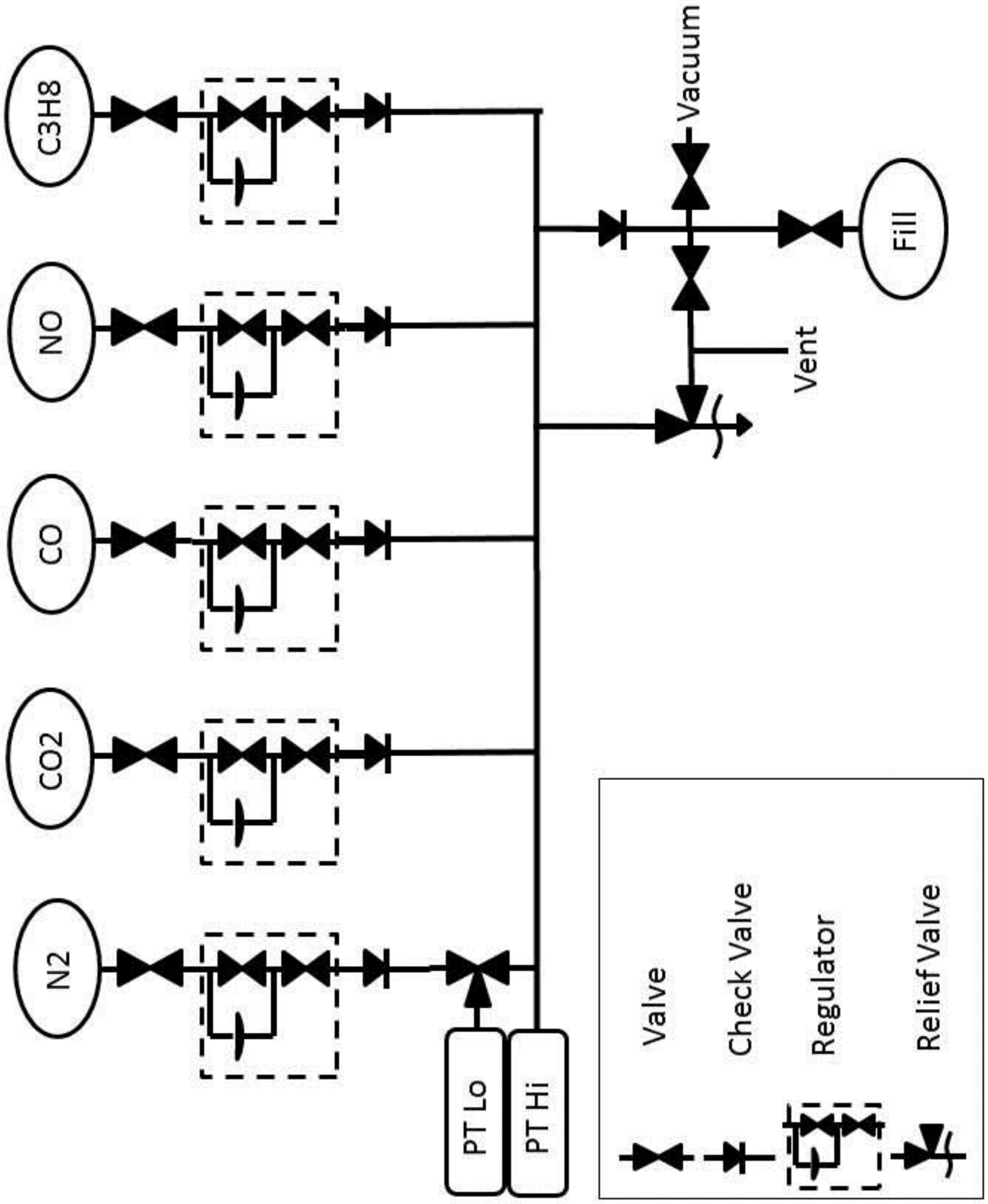
```
%% Mass Flow Rate and Slug Length Calculations
clear all; close all; clc

%Define Constants
    h_t = 0.04115;  %(m) height of the test chamber
    d_t = 0.02159; %(m) diameter of the test chamber
    T_l = 300;  %(K) temperature of the line
    P_l = 100;  %(kPa) presure in of the line
    f = 1;      %(1/s) switching frequency

    R = .287;   %(kJ/kg K) universal gas constant

%Define Inputs
    T_c = 100:50:1000;  %temperature of test chamber (deg C)
    s = 0:5:50;         %space velocity

    d_l = .002:.0005:.006;  %(m) diameter of the line
    m_dot = 0:5E-5:.0005;

%Mass Flow Rate Calculation and Plot
    figure
    V_t = pi*(d_t/2)^2*h_t;         %(m3) volume of test chamber
    [S, T] = meshgrid(s, T_c);
    Z = S.*V_t.*P_l./R./(T+273.15);
    C = Z;
    surf(S, T, Z, C)
    xlabel('Space Velocity (1/s)')
    ylabel('Temperature (C)')
    zlabel('Mass Flow (kg/s)')

%Slug Length Calculation and Plot
    figure
    A_l = pi.*(d_l./2).^2;   %(m2) area of line cross section
    [D, M] = meshgrid(d_l, m_dot);
    Z2 = M.*R.*T_l./P_l./(pi.*(D./2).^2)./f;
    C2 = Z2;
    surf(D, M, Z2, C2)
    xlabel('Line Diameter (m)')
    ylabel('Mass Flow Rate (kg/s)')
    zlabel('slug length (m)')
```

I. Humidification Calculation

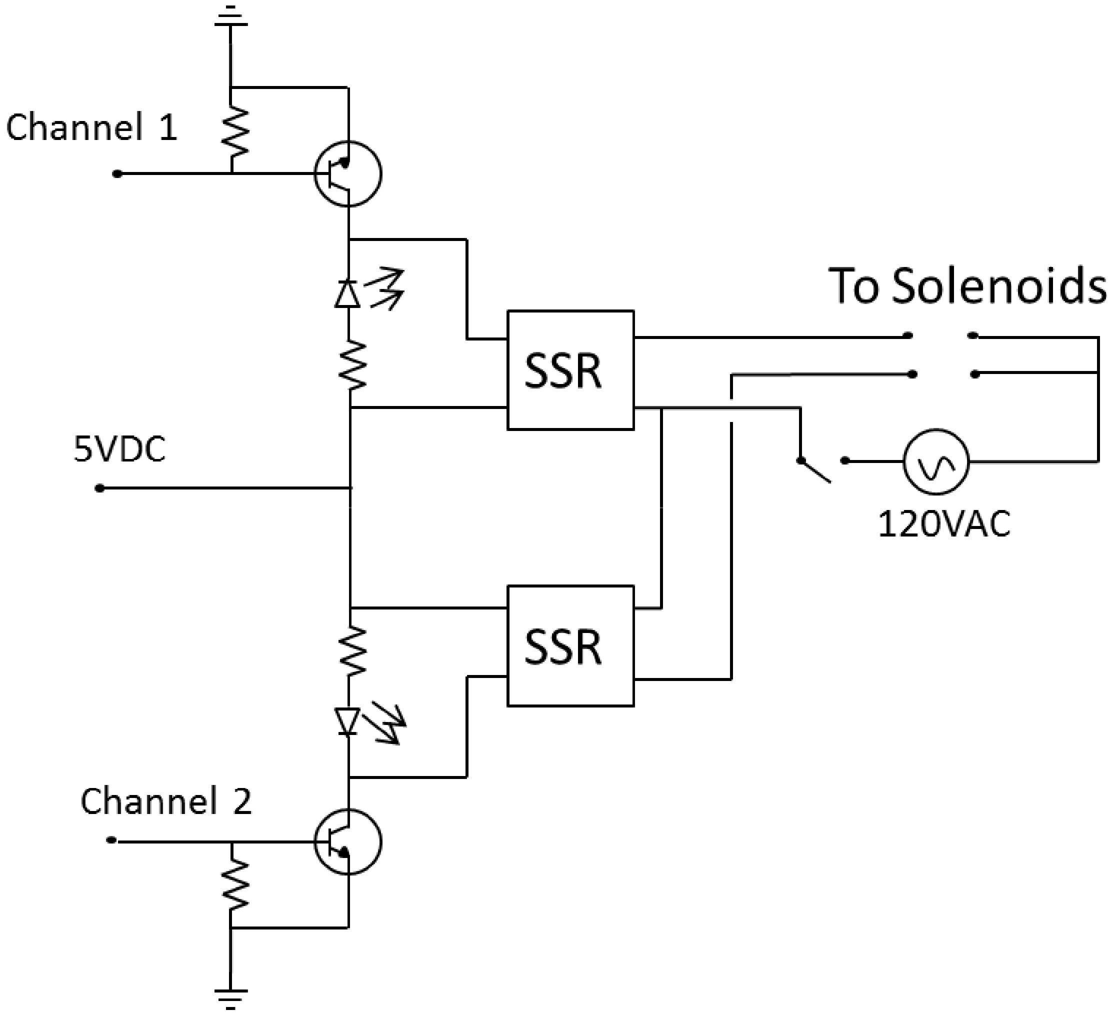
```
%Humidification Requirements Calculations - 10/29/12
%ASSUME a Stoicheometric Burn
%Determine concentrations of of components in a mole of charge to engine
%ASSUMPTION: All gases ideal --> volume fraction = mole fraction
%clear; clc; format compact

AirRatio = 14.7 /28.97; % molecular mass of air = 28.97kg/kmol (engineering
toolbox)
FuelRatio = 1 /114.22; % molecular mass of fuel = 114.22 kg/mol (engineering
toolbox)

%        C8H18    N2     O2     CO2      H20
Fuel =  [1       0     0     0       0  ];

%        C8H18    N2     O2     CO2      H20
Air  =  [0       .79   .21   0       0  ];

Mix = AirRatio.*Air + Fuel.*FuelRatio;
Mix = Mix./sum(Mix);
%sum(Mix) %check
disp('Mix')
disp('    C8H18     N2        O2             CO2       H20')
disp(Mix)

%Determine resulting exhuast components at stoicheometric burn
%  The concentration of water in 'Exhaust' represents the required molar
%  concentration of water in the humidified exhaust
%  Coeffficients for CO2 and H20 come from balanced chemical equation

Consumed = Mix(1)+Mix(3); %check
Mix(1)=0; Mix(3)=0;
%           C8H18    N2     O2     CO2            H20
Products = [0       0     0     8/17*Consumed  9/17*Consumed];
%sum(Products) %check

Exhaust = Mix + Products;
%sum(Exhaust) %check
disp('Exhaust')
disp('     C8H18        N2        O2       CO2       H20')
disp(Exhaust)

%Add Water Concentration to BAR97 + Air Blend
    %Air is mixed at a ratio of .017:1 with BAR 97 Blend 32 Calibration Gas
    %BAR 97 Specifications:             %Air Specifications
    %    200ppm    C3H8                    78.67%       N2
    %    0.50%     CO                      20.94%       02
    %    6%        CO2                      0.39%       CO2
    %    300ppm    NO                      note: other components assumed to be
    %    Balance   N2 (93.45%)                   N2

    %Determine concentrations of of components in a mole of gas to test chamber
    %ASSUMPTION: All gases ideal --> volume fraction = mole fraction
    AirRatio = .017;
    GasRatio = 1;
    Total = AirRatio + GasRatio;

    %        C3H8    CO    C02    NO      N2    02
    Bar97 = [200/1E6 0.005 0.06   300/1E6 .9345 0 ];
    %sum(Bar97)  %check

    %      C3H8    CO    C02    NO      N2    02
```

```
    Air = [0       0     .0039  0       .7867 .2094 ];
    %sum(Air) %check

    Blend = AirRatio.*Air + Bar97.*GasRatio;
    Blend = Blend./Total;
    %sum(Blend) %check
Humidified_Blend = [Blend./(sum(Blend)+ Exhaust(5)) Exhaust(5)]
```

J. GMS Final Schematic

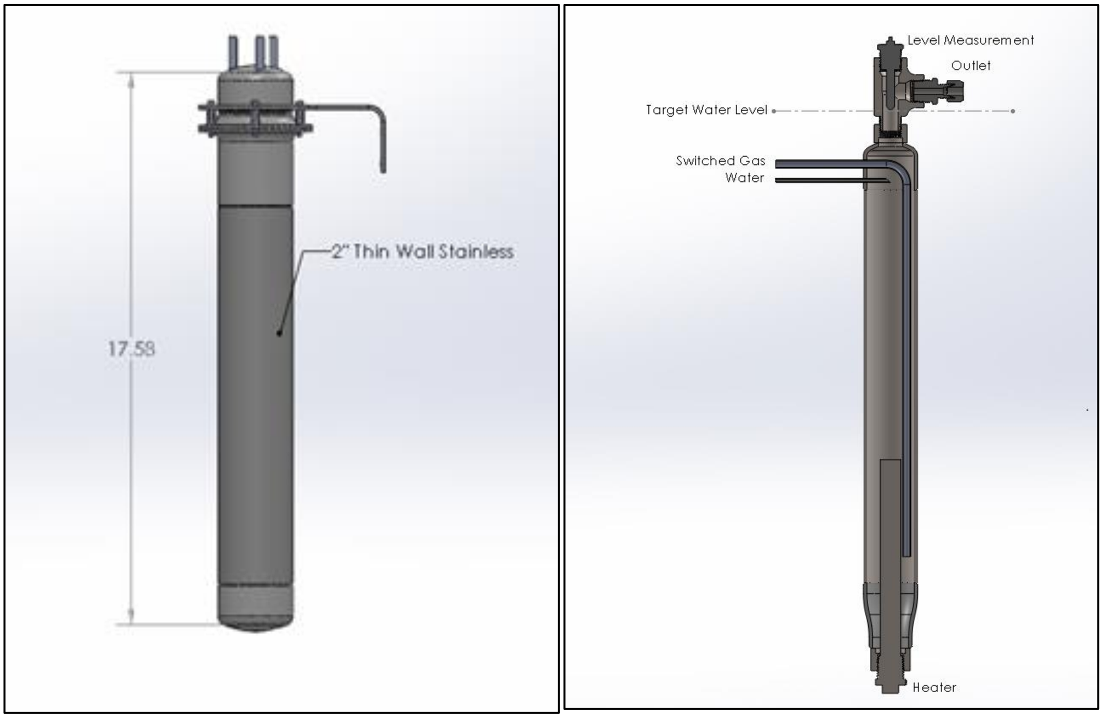


K. Control Circuit for Switching



L. Designs for Bubbler Humidifier

Two iterations of a potential design for a bubbler humidifier using thin walled stainless steel pipe. All of the pipe sections and fittings are welded together. One of the advantages of using standard pipe as a vessel material is that it can be insulated using pipe insulation. The first iteration is designed to use a rope heater as its primary heater and is flanged to allow disassembly for cleaning. The mounting bracket is separated from the flanges by nylon spacers to minimize heat transfer.

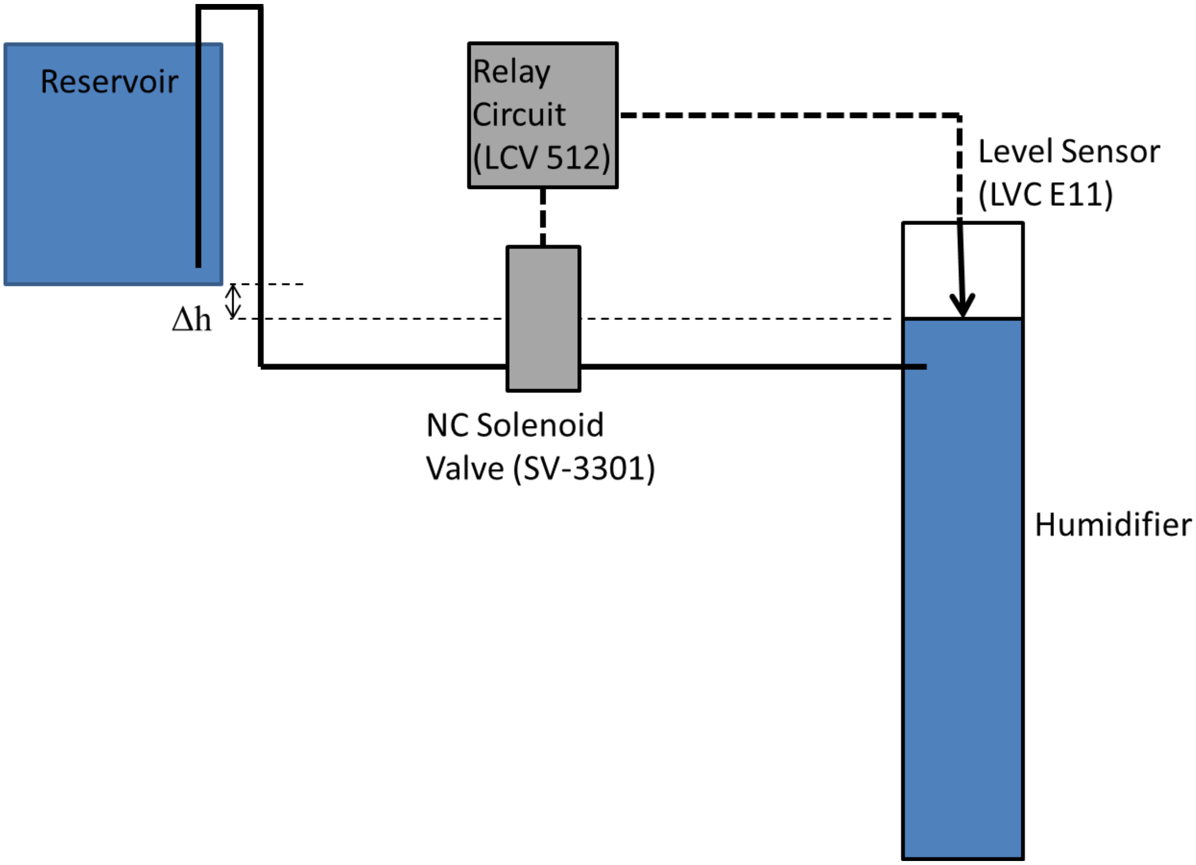


Right: first iteration of bubbler humidifier design, Left: second iteration

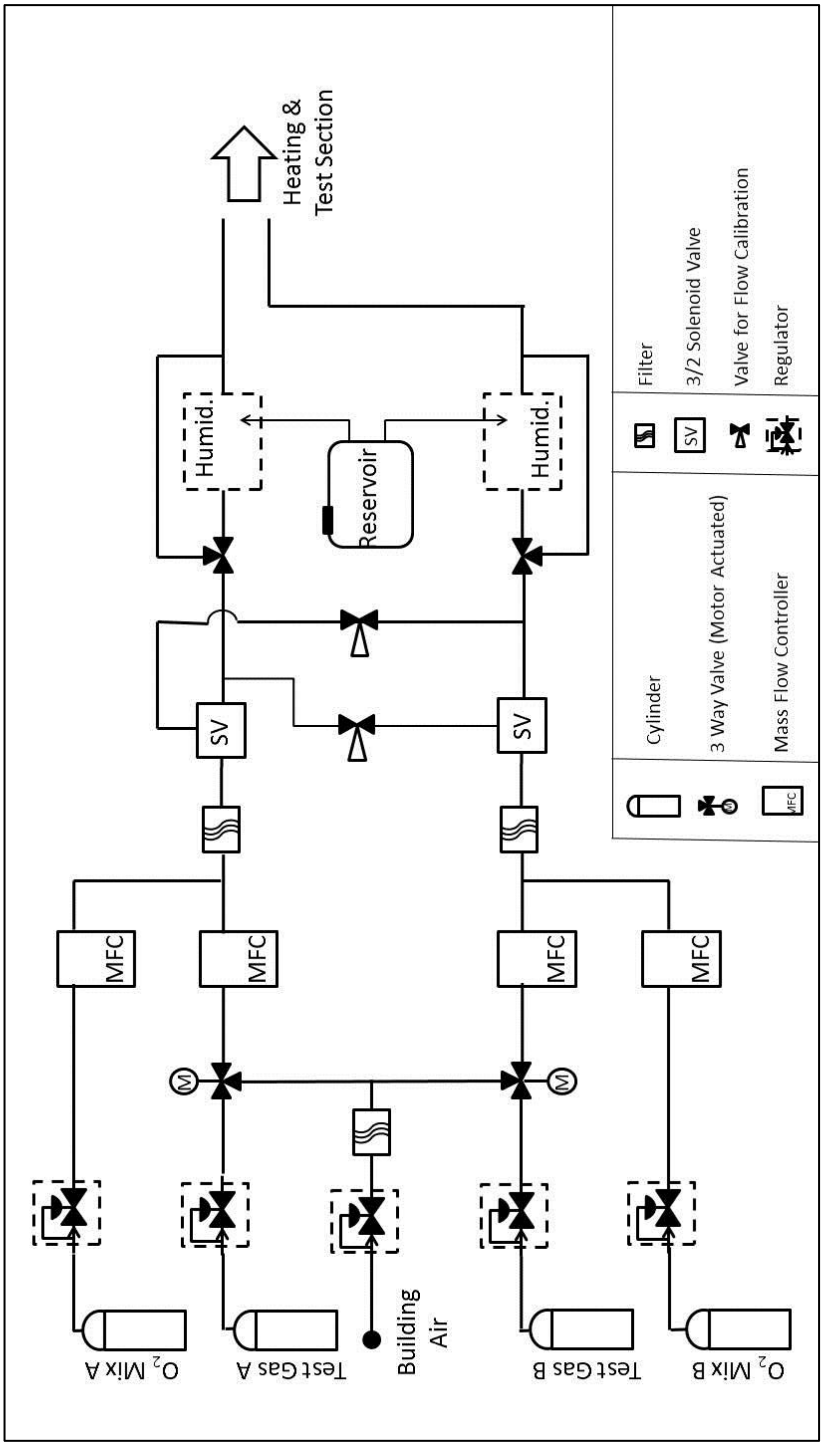
The second iteration works to address several issues. The first is to reduce the diameter at the top to minimize the unwetted volume and thereby minimize some slug mixing. The second is to use a more efficient immersion heater in the place of the rope heater. This heater threads into the bottom of the vessel. Finally a conductive level control sensor is included in the top. The conductive level control system is discussed in the next attachment. Since there are large threaded openings to access the inside of the vessel the flanged section was removed.

M. Leveling System For Bubbler Humidifier

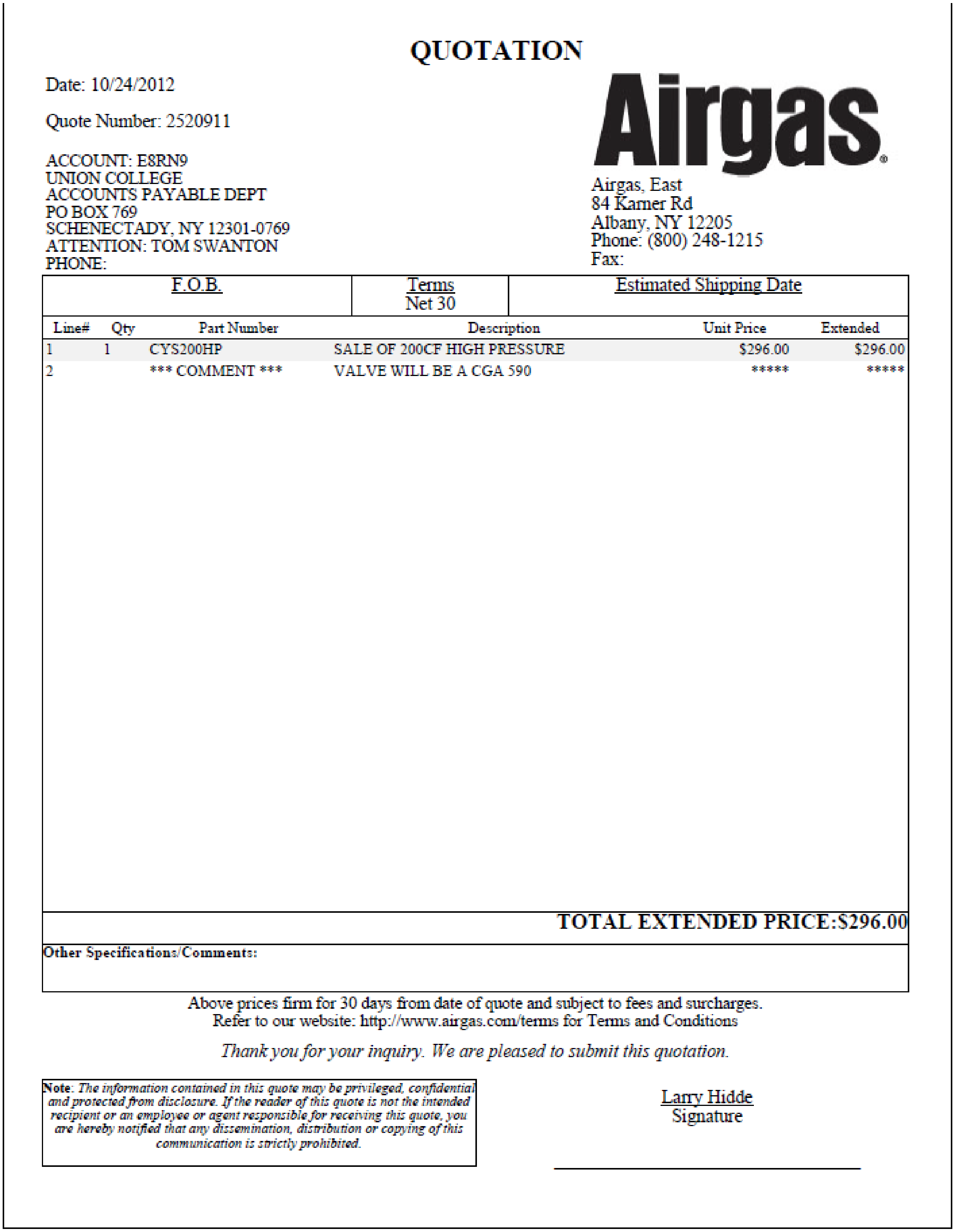
The standard method for maintaining the water level in a tank is to use what is called a conductive leveling system which uses the water to create a circuit. When the water level drops the circuit is opened and more water is added until the water level reaches the sensor again. The conductive method proves difficult in this application because deionized water has a very high resistance. Therefore specialized components must be used. A sample of one of these systems using components from Omega® Engineering is shown below. The conductive circuit is monitored by a relay which powers a solenoid valve on the water line. When the valve opens gravity moves water into the humidifier.



N. Global Schematic



O. GMS Tank Quote (Airgas)



QUOTATION

Date: 10/24/2012

Quote Number: 2520911

ACCOUNT: E8RN9
UNION COLLEGE
ACCOUNTS PAYABLE DEPT
PO BOX 769
SCHENECTADY, NY 12301-0769
ATTENTION: TOM SWANTON
PHONE:

Airgas
Airgas, East
84 Karner Rd
Albany, NY 12205
Phone: (800) 248-1215
Fax:

F.O.B.	Terms	Estimated Shipping Date
	Net 30	

Line#	Qty	Part Number	Description	Unit Price	Extended
1	1	CYS200HP	SALE OF 200CF HIGH PRESSURE	$296.00	$296.00
2		*** COMMENT ***	VALVE WILL BE A CGA 590	*****	*****

TOTAL EXTENDED PRICE:$296.00

Other Specifications/Comments:

Above prices firm for 30 days from date of quote and subject to fees and surcharges.
Refer to our website: http://www.airgas.com/terms for Terms and Conditions

Thank you for your inquiry. We are pleased to submit this quotation.

Note: *The information contained in this quote may be privileged, confidential and protected from disclosure. If the reader of this quote is not the intended recipient or an employee or agent responsible for receiving this quote, you are hereby notified that any dissemination, distribution or copying of this communication is strictly prohibited.*

Larry Hidde
Signature

P. Alarm Recommendations

Gas Mixing System: Recommended Alarms **October 23, 2012**

Air Aware Fixed Gas Detector- Oldham Gas List Price: $911.50

- For detecting Nitric Oxide(NO)
- Wall mounted for w/ AC adaptor
- Audible Alarm

Product Configuration:
68100056-21011

Link: *http://www.oldhamgas.com/en/gas-detector-transmitter-airaware*

Wall Mount Combustible Gas Detector- McMaster Carr List Price: $288.89

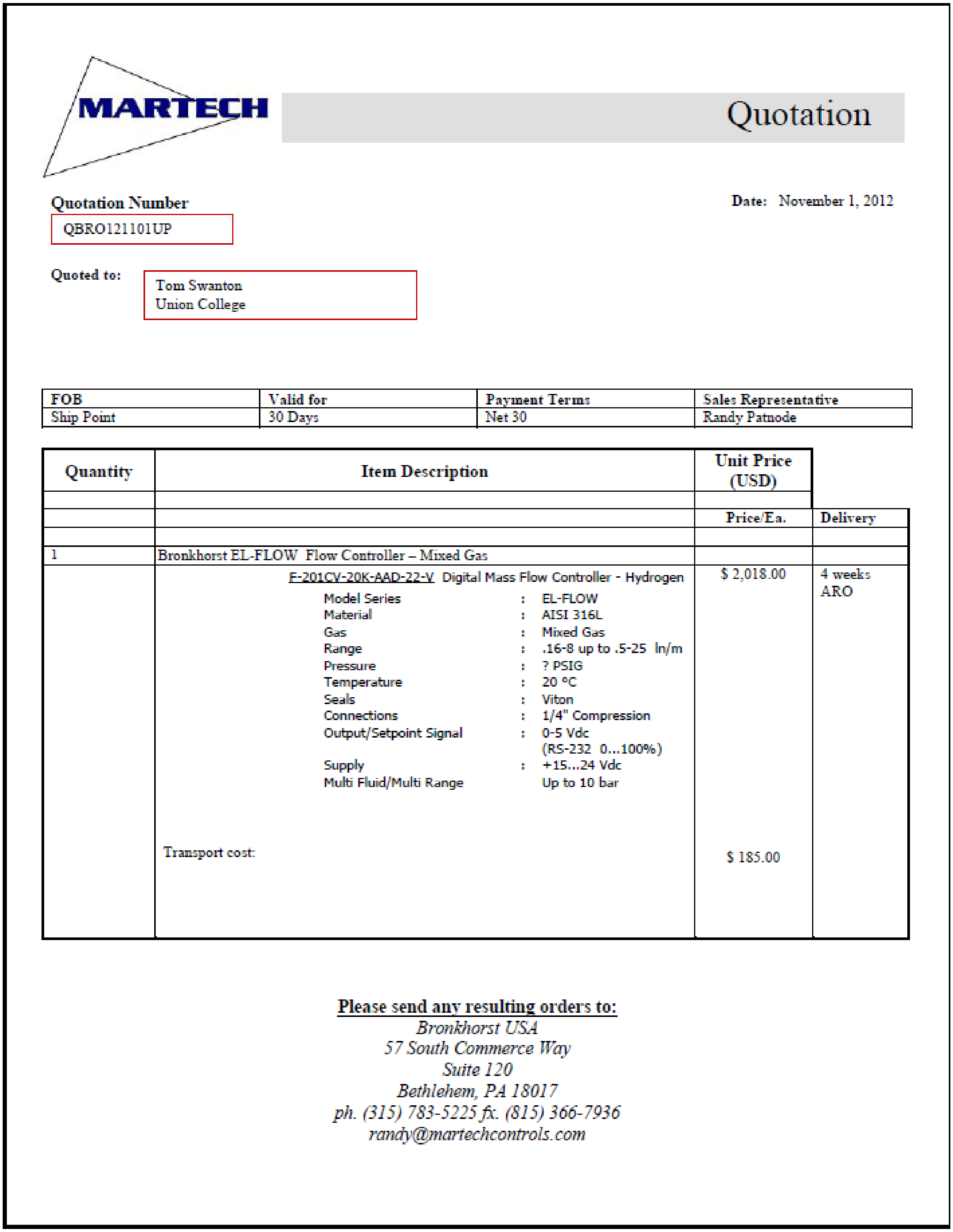
- For detecting propane(C_3H_8) and carbon monoxide(CO)
- Wall mounted
- Audible Alarm

Product Number:
6631T18

Link: *www.mcmaster.com/#carbon-monoxide-(co)-alarms/*

Total Price: $1201.49

Q. Bronkhorst MFC Quote (Martech)



MARTECH

Quotation

Quotation Number

QBRO121101UP

Date: November 1, 2012

Quoted to:

Tom Swanton
Union College

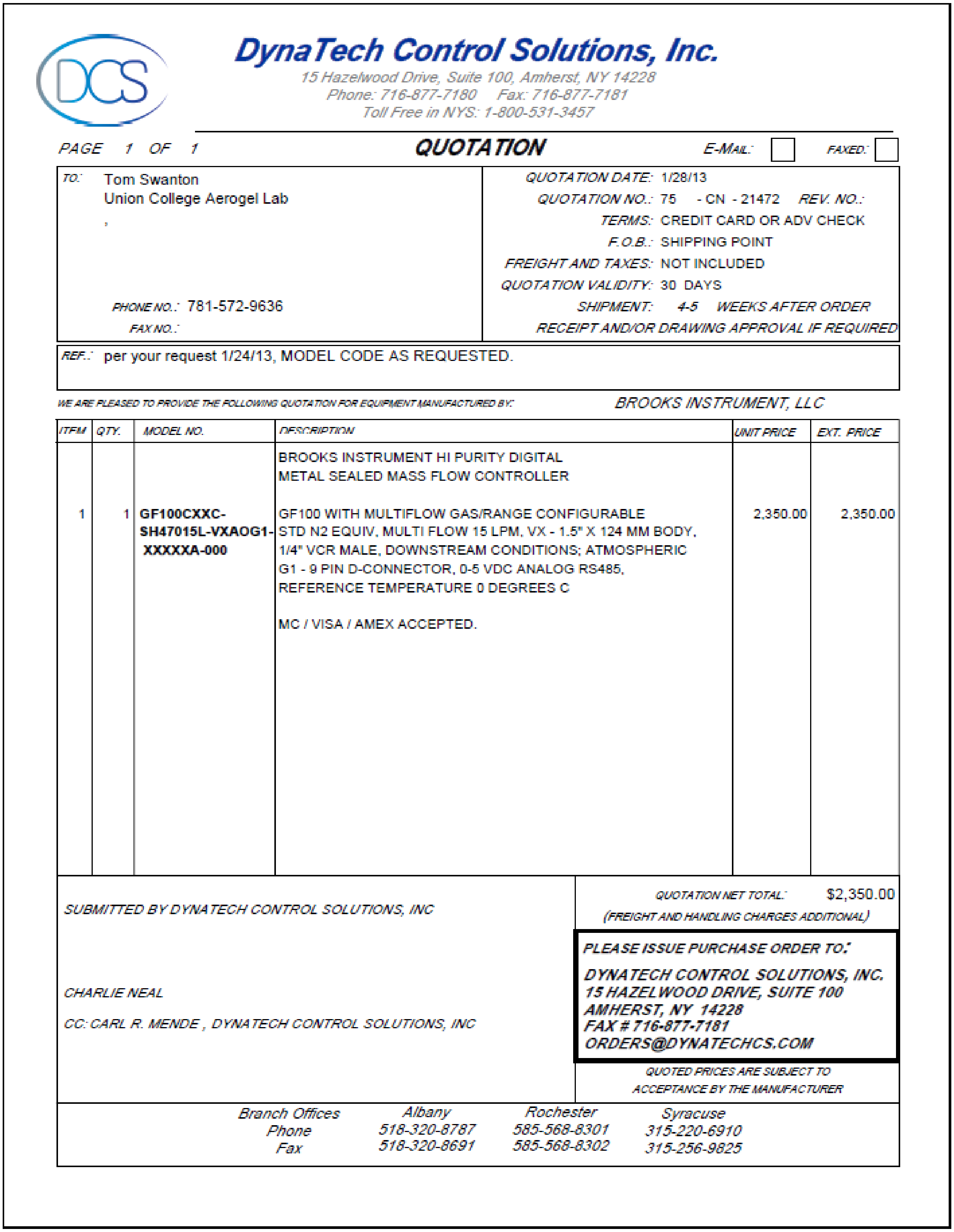
FOB	**Valid for**	**Payment Terms**	**Sales Representative**
Ship Point	30 Days	Net 30	Randy Patnode

Quantity	**Item Description**	**Unit Price (USD)** **Price/Ea.**	**Delivery**
1	Bronkhorst EL-FLOW Flow Controller – Mixed Gas		
	F-201CV-20K-AAD-22-V Digital Mass Flow Controller - Hydrogen Model Series : EL-FLOW Material : AISI 316L Gas : Mixed Gas Range : .16-8 up to .5-25 ln/m Pressure : ? PSIG Temperature : 20 °C Seals : Viton Connections : 1/4" Compression Output/Setpoint Signal : 0-5 Vdc (RS-232 0…100%) Supply : +15…24 Vdc Multi Fluid/Multi Range Up to 10 bar	$ 2,018.00	4 weeks ARO
	Transport cost:	$ 185.00	

Please send any resulting orders to:

Bronkhorst USA
57 South Commerce Way
Suite 120
Bethlehem, PA 18017
ph. (315) 783-5225 fx. (815) 366-7936
randy@martechcontrols.com

R. Brooks MFC Quote



DynaTech Control Solutions, Inc.

15 Hazelwood Drive, Suite 100, Amherst, NY 14228
Phone: 716-877-7180 Fax: 716-877-7181
Toll Free in NYS: 1-800-531-3457

PAGE 1 OF 1

QUOTATION

E-MAIL: ☐ *FAXED:* ☐

TO: Tom Swanton
Union College Aerogel Lab
,

PHONE NO.: 781-572-9636
FAX NO.:

QUOTATION DATE: 1/28/13
QUOTATION NO.: 75 - CN - 21472 *REV. NO.:*
TERMS: CREDIT CARD OR ADV CHECK
F.O.B.: SHIPPING POINT
FREIGHT AND TAXES: NOT INCLUDED
QUOTATION VALIDITY: 30 DAYS
SHIPMENT: *4-5 WEEKS AFTER ORDER RECEIPT AND/OR DRAWING APPROVAL IF REQUIRED*

REF.: per your request 1/24/13, MODEL CODE AS REQUESTED.

WE ARE PLEASED TO PROVIDE THE FOLLOWING QUOTATION FOR EQUIPMENT MANUFACTURED BY: *BROOKS INSTRUMENT, LLC*

ITEM	*QTY.*	*MODEL NO.*	*DESCRIPTION*	*UNIT PRICE*	*EXT. PRICE*
			BROOKS INSTRUMENT HI PURITY DIGITAL METAL SEALED MASS FLOW CONTROLLER		
1	1	**GF100CXXC-SH47015L-VXAOG1-XXXXXA-000**	GF100 WITH MULTIFLOW GAS/RANGE CONFIGURABLE STD N2 EQUIV, MULTI FLOW 15 LPM, VX - 1.5" X 124 MM BODY, 1/4" VCR MALE, DOWNSTREAM CONDITIONS; ATMOSPHERIC G1 - 9 PIN D-CONNECTOR, 0-5 VDC ANALOG RS485, REFERENCE TEMPERATURE 0 DEGREES C	2,350.00	2,350.00
			MC / VISA / AMEX ACCEPTED.		

SUBMITTED BY DYNATECH CONTROL SOLUTIONS, INC

CHARLIE NEAL

CC: CARL R. MENDE , DYNATECH CONTROL SOLUTIONS, INC

QUOTATION NET TOTAL: $2,350.00
(FREIGHT AND HANDLING CHARGES ADDITIONAL)

PLEASE ISSUE PURCHASE ORDER TO:

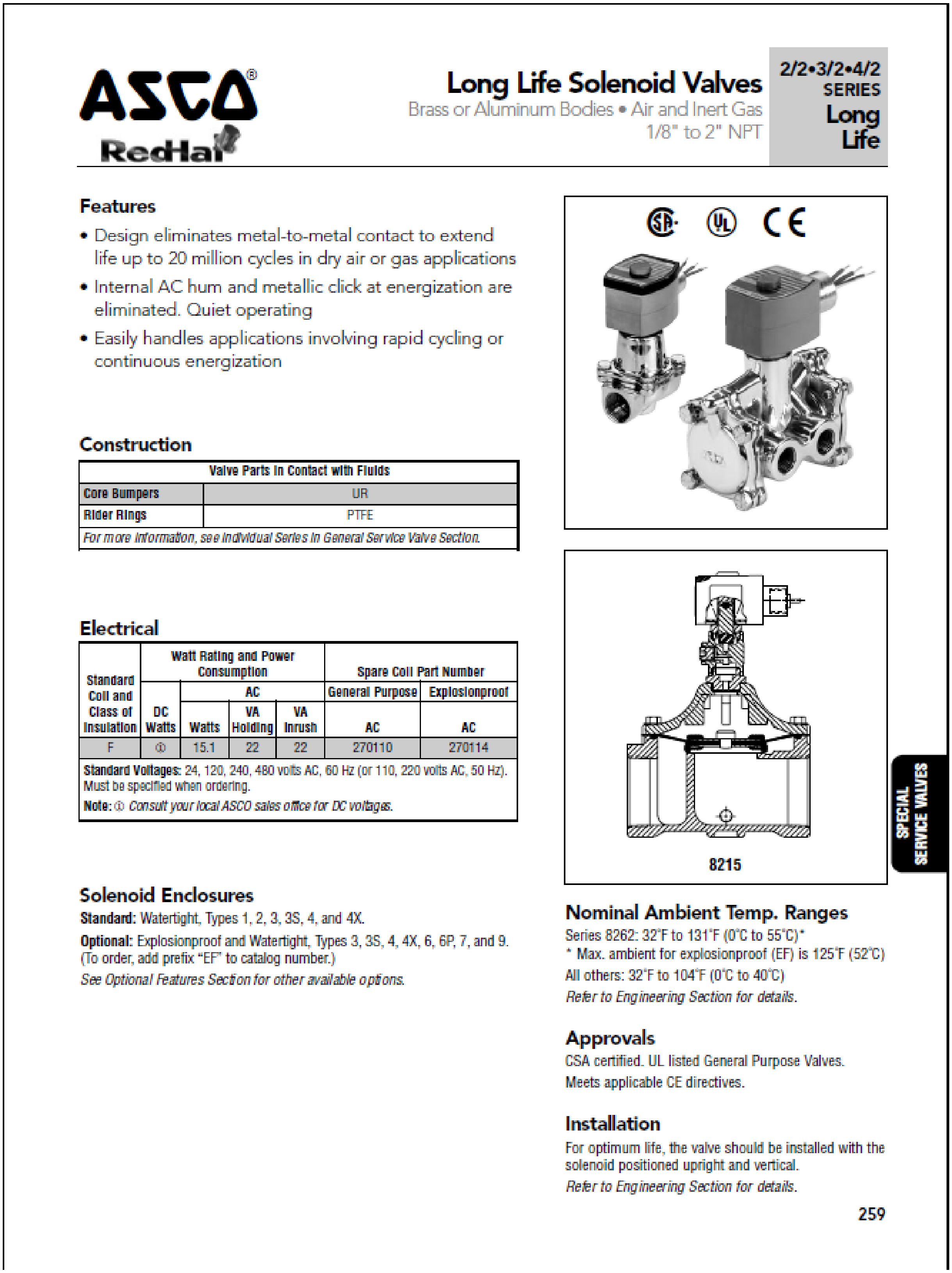
DYNATECH CONTROL SOLUTIONS, INC.
15 HAZELWOOD DRIVE, SUITE 100
AMHERST, NY 14228
FAX # 716-877-7181
ORDERS@DYNATECHCS.COM

QUOTED PRICES ARE SUBJECT TO ACCEPTANCE BY THE MANUFACTURER

Branch Offices	*Albany*	*Rochester*	*Syracuse*
Phone	*518-320-8787*	*585-568-8301*	*315-220-6910*
Fax	*518-320-8691*	*585-568-8302*	*315-256-9825*

S. Solenoid Valve Specifications

(http://www.ascovalve.com/Common/PDFFiles/Product/LongLifeR2.pdf)



ASCO® RedHat

Long Life Solenoid Valves

Brass or Aluminum Bodies • Air and Inert Gas
1/8" to 2" NPT

2/2•3/2•4/2
SERIES
Long
Life

Features

- Design eliminates metal-to-metal contact to extend life up to 20 million cycles in dry air or gas applications
- Internal AC hum and metallic click at energization are eliminated. Quiet operating
- Easily handles applications involving rapid cycling or continuous energization

Construction

Valve Parts in Contact with Fluids	
Core Bumpers	UR
Rider Rings	PTFE

For more information, see individual Series in General Service Valve Section.

Electrical

Standard Coil and Class of Insulation	Watt Rating and Power Consumption				Spare Coil Part Number	
		AC			General Purpose	Explosionproof
	DC Watts	Watts	VA Holding	VA Inrush	AC	AC
F	①	15.1	22	22	270110	270114

Standard Voltages: 24, 120, 240, 480 volts AC, 60 Hz (or 110, 220 volts AC, 50 Hz). Must be specified when ordering.

Note: ① *Consult your local ASCO sales office for DC voltages.*

Solenoid Enclosures

Standard: Watertight, Types 1, 2, 3, 3S, 4, and 4X.

Optional: Explosionproof and Watertight, Types 3, 3S, 4, 4X, 6, 6P, 7, and 9. (To order, add prefix "EF" to catalog number.)

See Optional Features Section for other available options.

8215

SPECIAL SERVICE VALVES

Nominal Ambient Temp. Ranges

Series 8262: 32°F to 131°F (0°C to 55°C)*
* Max. ambient for explosionproof (EF) is 125°F (52°C)
All others: 32°F to 104°F (0°C to 40°C)
Refer to Engineering Section for details.

Approvals

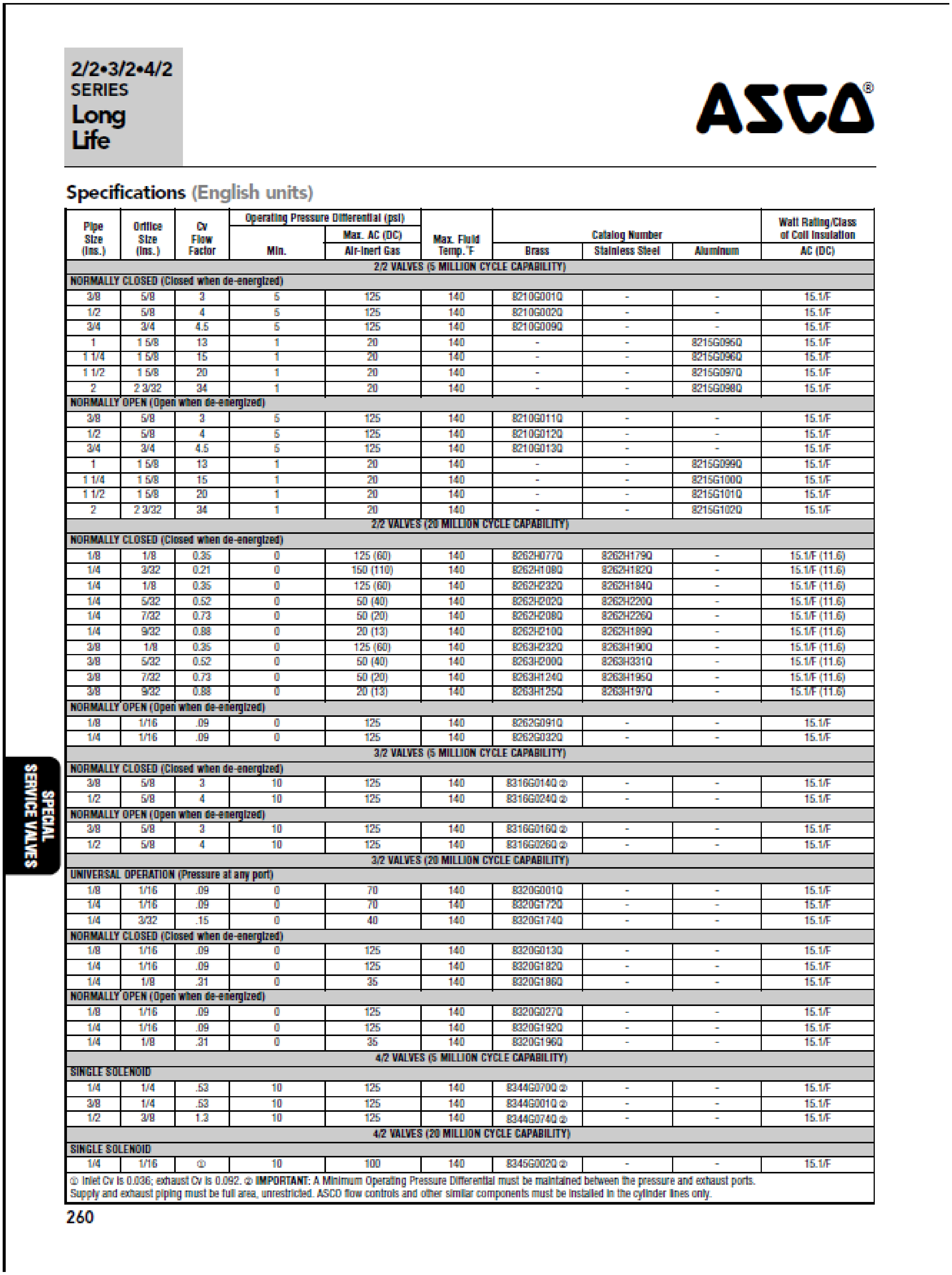
CSA certified. UL listed General Purpose Valves.
Meets applicable CE directives.

Installation

For optimum life, the valve should be installed with the solenoid positioned upright and vertical.

Refer to Engineering Section for details.

259



2/2•3/2•4/2
SERIES
Long Life

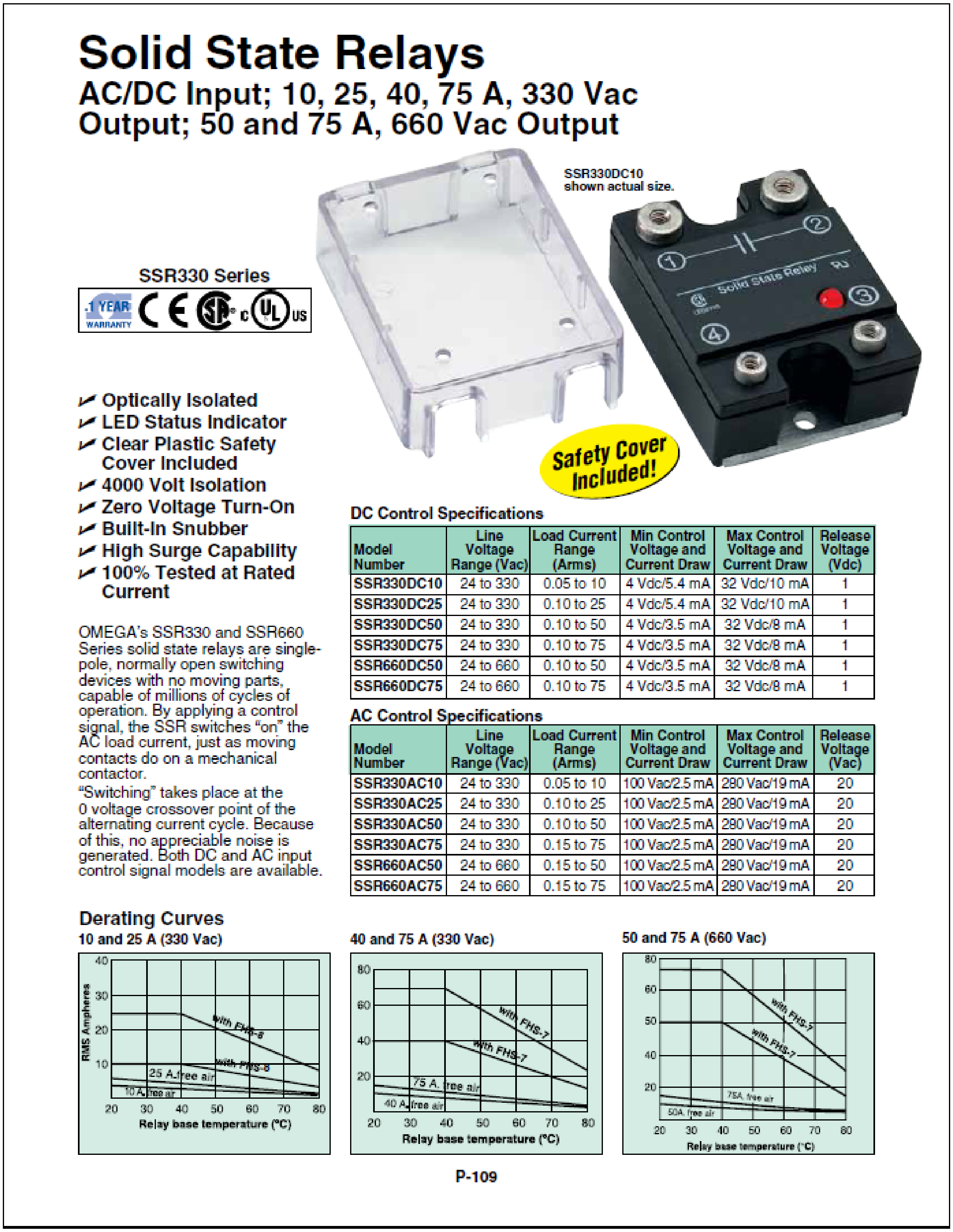
Specifications (English units)

Pipe Size (Ins.)	Orifice Size (Ins.)	Cv Flow Factor	Operating Pressure Differential (psi)		Max. Fluid Temp. °F	Catalog Number			Watt Rating/Class of Coil Insulation
			Min.	Max. AC (DC) Air-Inert Gas		Brass	Stainless Steel	Aluminum	AC (DC)
2/2 VALVES (5 MILLION CYCLE CAPABILITY)									
NORMALLY CLOSED (Closed when de-energized)									
3/8	5/8	3	5	125	140	8210G001Q	-	-	15.1/F
1/2	5/8	4	5	125	140	8210G002Q	-	-	15.1/F
3/4	3/4	4.5	5	125	140	8210G009Q	-	-	15.1/F
1	1 5/8	13	1	20	140	-	-	8215G096Q	15.1/F
1 1/4	1 5/8	15	1	20	140	-	-	8215G096Q	15.1/F
1 1/2	1 5/8	20	1	20	140	-	-	8215G097Q	15.1/F
2	2 3/32	34	1	20	140	-	-	8215G098Q	15.1/F
NORMALLY OPEN (Open when de-energized)									
3/8	5/8	3	5	125	140	8210G011Q	-	-	15.1/F
1/2	5/8	4	5	125	140	8210G012Q	-	-	15.1/F
3/4	3/4	4.5	5	125	140	8210G013Q	-	-	15.1/F
1	1 5/8	13	1	20	140	-	-	8215G099Q	15.1/F
1 1/4	1 5/8	15	1	20	140	-	-	8215G100Q	15.1/F
1 1/2	1 5/8	20	1	20	140	-	-	8215G101Q	15.1/F
2	2 3/32	34	1	20	140	-	-	8215G102Q	15.1/F
2/2 VALVES (20 MILLION CYCLE CAPABILITY)									
NORMALLY CLOSED (Closed when de-energized)									
1/8	1/8	0.35	0	125 (60)	140	8262H077Q	8262H179Q	-	15.1/F (11.6)
1/4	3/32	0.21	0	150 (110)	140	8262H108Q	8262H182Q	-	15.1/F (11.6)
1/4	1/8	0.35	0	125 (60)	140	8262H232Q	8262H184Q	-	15.1/F (11.6)
1/4	5/32	0.52	0	50 (40)	140	8262H202Q	8262H220Q	-	15.1/F (11.6)
1/4	7/32	0.73	0	50 (20)	140	8262H208Q	8262H226Q	-	15.1/F (11.6)
1/4	9/32	0.88	0	20 (13)	140	8262H210Q	8262H189Q	-	15.1/F (11.6)
3/8	1/8	0.35	0	125 (60)	140	8263H232Q	8263H190Q	-	15.1/F (11.6)
3/8	5/32	0.52	0	50 (40)	140	8263H200Q	8263H331Q	-	15.1/F (11.6)
3/8	7/32	0.73	0	50 (20)	140	8263H124Q	8263H195Q	-	15.1/F (11.6)
3/8	9/32	0.88	0	20 (13)	140	8263H125Q	8263H197Q	-	15.1/F (11.6)
NORMALLY OPEN (Open when de-energized)									
1/8	1/16	.09	0	125	140	8262G091Q	-	-	15.1/F
1/4	1/16	.09	0	125	140	8262G032Q	-	-	15.1/F
3/2 VALVES (5 MILLION CYCLE CAPABILITY)									
NORMALLY CLOSED (Closed when de-energized)									
3/8	5/8	3	10	125	140	8316G014Q ②	-	-	15.1/F
1/2	5/8	4	10	125	140	8316G024Q ②	-	-	15.1/F
NORMALLY OPEN (Open when de-energized)									
3/8	5/8	3	10	125	140	8316G016Q ②	-	-	15.1/F
1/2	5/8	4	10	125	140	8316G026Q ②	-	-	15.1/F
3/2 VALVES (20 MILLION CYCLE CAPABILITY)									
UNIVERSAL OPERATION (Pressure at any port)									
1/8	1/16	.09	0	70	140	8320G001Q	-	-	15.1/F
1/4	1/16	.09	0	70	140	8320G172Q	-	-	15.1/F
1/4	3/32	.15	0	40	140	8320G174Q	-	-	15.1/F
NORMALLY CLOSED (Closed when de-energized)									
1/8	1/16	.09	0	125	140	8320G013Q	-	-	15.1/F
1/4	1/16	.09	0	125	140	8320G182Q	-	-	15.1/F
1/4	1/8	.31	0	35	140	8320G186Q	-	-	15.1/F
NORMALLY OPEN (Open when de-energized)									
1/8	1/16	.09	0	125	140	8320G027Q	-	-	15.1/F
1/4	1/16	.09	0	125	140	8320G192Q	-	-	15.1/F
1/4	1/8	.31	0	35	140	8320G196Q	-	-	15.1/F
4/2 VALVES (5 MILLION CYCLE CAPABILITY)									
SINGLE SOLENOID									
1/4	1/4	.53	10	125	140	8344G070Q ②	-	-	15.1/F
3/8	1/4	.53	10	125	140	8344G001Q ②	-	-	15.1/F
1/2	3/8	1.3	10	125	140	8344G074Q ②	-	-	15.1/F
4/2 VALVES (20 MILLION CYCLE CAPABILITY)									
SINGLE SOLENOID									
1/4	1/16	①	10	100	140	8345G002Q ②	-	-	15.1/F

① Inlet Cv is 0.036; exhaust Cv is 0.092. ② **IMPORTANT:** A Minimum Operating Pressure Differential must be maintained between the pressure and exhaust ports. Supply and exhaust piping must be full area, unrestricted. ASCO flow controls and other similar components must be installed in the cylinder lines only.

T. Solid State Relay Specifications

(http://www.omega.com/Temperature/pdf/SSR330_660.pdf)



Solid State Relays

AC/DC Input; 10, 25, 40, 75 A, 330 Vac Output; 50 and 75 A, 660 Vac Output

SSR330DC10 shown actual size.

SSR330 Series

- ✓ Optically Isolated
- ✓ LED Status Indicator
- ✓ Clear Plastic Safety Cover Included
- ✓ 4000 Volt Isolation
- ✓ Zero Voltage Turn-On
- ✓ Built-In Snubber
- ✓ High Surge Capability
- ✓ 100% Tested at Rated Current

OMEGA's SSR330 and SSR660 Series solid state relays are single-pole, normally open switching devices with no moving parts, capable of millions of cycles of operation. By applying a control signal, the SSR switches "on" the AC load current, just as moving contacts do on a mechanical contactor.

"Switching" takes place at the 0 voltage crossover point of the alternating current cycle. Because of this, no appreciable noise is generated. Both DC and AC input control signal models are available.

DC Control Specifications

Model Number	Line Voltage Range (Vac)	Load Current Range (Arms)	Min Control Voltage and Current Draw	Max Control Voltage and Current Draw	Release Voltage (Vdc)
SSR330DC10	24 to 330	0.05 to 10	4 Vdc/5.4 mA	32 Vdc/10 mA	1
SSR330DC25	24 to 330	0.10 to 25	4 Vdc/5.4 mA	32 Vdc/10 mA	1
SSR330DC50	24 to 330	0.10 to 50	4 Vdc/3.5 mA	32 Vdc/8 mA	1
SSR330DC75	24 to 330	0.10 to 75	4 Vdc/3.5 mA	32 Vdc/8 mA	1
SSR660DC50	24 to 660	0.10 to 50	4 Vdc/3.5 mA	32 Vdc/8 mA	1
SSR660DC75	24 to 660	0.10 to 75	4 Vdc/3.5 mA	32 Vdc/8 mA	1

AC Control Specifications

Model Number	Line Voltage Range (Vac)	Load Current Range (Arms)	Min Control Voltage and Current Draw	Max Control Voltage and Current Draw	Release Voltage (Vac)
SSR330AC10	24 to 330	0.05 to 10	100 Vac/2.5 mA	280 Vac/19 mA	20
SSR330AC25	24 to 330	0.10 to 25	100 Vac/2.5 mA	280 Vac/19 mA	20
SSR330AC50	24 to 330	0.10 to 50	100 Vac/2.5 mA	280 Vac/19 mA	20
SSR330AC75	24 to 330	0.15 to 75	100 Vac/2.5 mA	280 Vac/19 mA	20
SSR660AC50	24 to 660	0.15 to 50	100 Vac/2.5 mA	280 Vac/19 mA	20
SSR660AC75	24 to 660	0.15 to 75	100 Vac/2.5 mA	280 Vac/19 mA	20

Derating Curves

10 and 25 A (330 Vac)

40 and 75 A (330 Vac)

50 and 75 A (660 Vac)

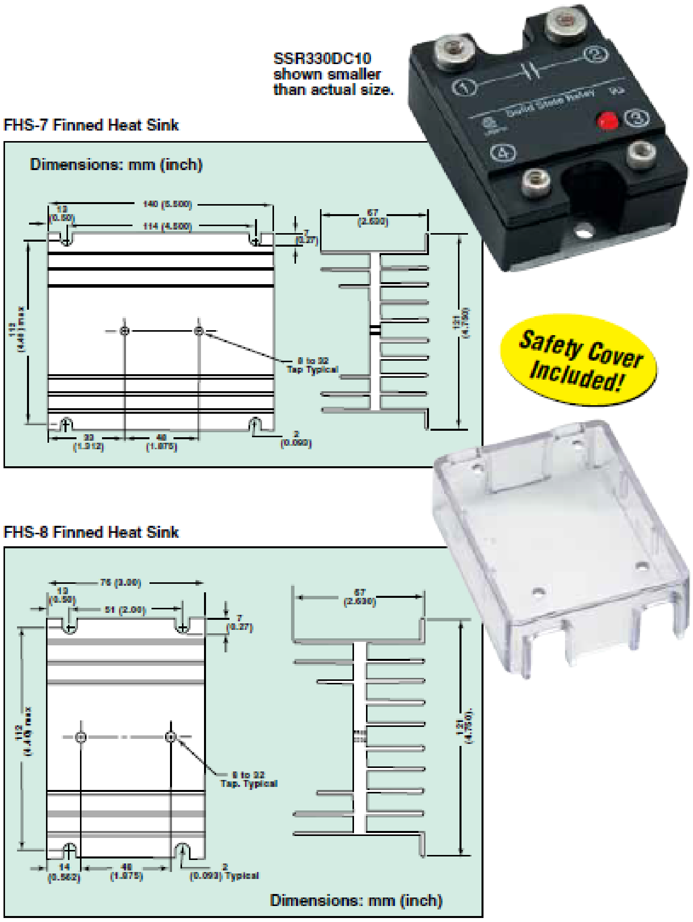
Heat is developed in a solid state relay due to the nominal voltage drop across the switching device. To dissipate the heat, an SSR must be mounted vertically on a finned heat sink or an aluminum plate. An SSR should be located where the ambient temperature is relatively low, since the current switching rating is lowered as temperature increases. Refer to the thermal derating curves shown on the previous page to determine the proper heat sink required.

Solid state relay cycle life is many times that of an equivalently priced mechanical contactor. OMEGA® recommends solid state relays for use with proportional temperature controllers and other applications where long life and solid state reliability are needed.

In contrasting solid state relays with mechanical contactors, it should be noted that a solid state relay is more prone to failure due to overload and improper initial wiring. Solid state relays can fail, contact closed, on overloaded circuits.

OMEGA® finned heat sinks (FHS) are aluminum fabrications and come complete with tapped mounting holes and screws. Refer to thermal derating curves for heat sink selection.

SSR baseplate to heat sink thermal resistance is affected by use of a thermally conducting compound. OMEGATHERM® OT-201 placed between the heat sink and SSR baseplate will significantly improve the thermal conductivity. It is also suggested that 10"/lb of torque be used on the SSR mounting screws.


SSR330DC10 shown smaller than actual size.

FHS-7 Finned Heat Sink

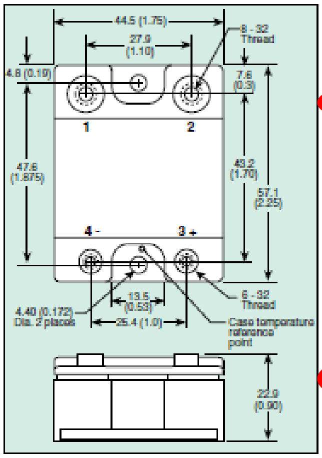
Dimensions: mm (inch)

Safety Cover Included!

FHS-8 Finned Heat Sink

Dimensions: mm (inch)

SSR330 Series



To Order *Visit omega.com/ssr330_660 for Pricing and Details*

Model No.	Price	Description	Nominal Rating
SSR330DC10	$21	DC control signal (330 Vac line)	10 A
SSR330DC25	26		25 A
SSR330DC50	37		50 A
SSR330DC75	61		75 A
SSR660DC50	45	DC control signal (660 Vac line)	50 A
SSR660DC75	65		75 A
SSR330AC10	25	AC control signal (330 Vac line)	10 A
SSR330AC25	30		25 A
SSR330AC50	40		50 A
SSR330AC75	65		75 A
SSR660AC50	48	AC control signal (660 Vac line)	50 A
SSR660AC75	69		75 A
FHS-7	30	Finned heat sink	1.0°C/W
FHS-8	20		1.5°C/W

Comes complete with operator's manual and safety cover.

***Ordering Example:** **SSR330DC25,** DC control signal, 25 A solid-state relay.*