This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-96SR18500 with the U.S. Department of Energy.

Electronics Upgrade of High Resolution Mass Spectrometers

Joe Cordaro
Advisory Engineer
Engineered Equipment and Systems
Savannah River National Laboratory
Washington Savannah River Co.
Aiken, SC 29808

John McIntosh
Principal Engineer
Engineered Equipment and Systems
Savannah River National Laboratory
Washington Savannah River Co.
Aiken, SC 29808

KEYWORDS

Spectrometer, Magnet, Resolution, Ion

ABSTRACT

High resolution mass spectrometers are specialized systems that allow researchers to determine the exact mass of samples to four significant digits by using magnetic and electronic sector mass analyzers. Many of the systems in use today at research laboratories and universities were designed and built more than two decades ago. The manufacturers of these systems have abandoned the support for some of the mass spectrometers and parts to power and control them have become scarce or obsolete. The Savannah River National Laboratory has been involved in the upgrade of the electronics and software for these legacy machines. The Electronics Upgrade of High Resolution Mass Spectrometers consists of assembling high-end commercial instrumentation from reputable manufacturers with a minimal amount of customization to replace the electronics for the older systems. By taking advantage of advances in instrumentation, precise magnet control can be achieved using high resolution current sources and continuous feedback from a high resolution hall-effect probe. The custom equipment include a precision voltage divider/summing amplifier chassis, high voltage power supply chassis and a chassis for controlling the voltage emission for the mass spectrometer source tube. The upgrade package is versatile enough to interface with valve control, vacuum and other instrumentation. Instrument communication is via a combination of Ethernet and traditional IEEE-488 GPIB protocols. The system software upgrades include precision control, feedback and spectral waveform analysis tools.

INTRODUCTION

The basic elements of a high resolution mass spectrometer are shown in Figure 1. Ionized gas molecules (positive charge) are accelerated using a combination of an electric and magnetic field in a high vacuum chamber. Depending on the mass spectrometer, the electric field or magnetic field will vary depending on the mass. For example, the electric field on a series of plates may stay fixed and the magnetic field is adjusted based on calibration with pure gases. To measure a gas peak, the magnetic field is then stepped by incrementing the current to the magnet in small micro-steps. A Faraday cup is typically used as the detector. This metal cup collects the positive ions generating a very small current, as low as 1e-14 Amps. This current is amplified by a Faraday Cup amplifier to a higher level (0 to 10V) signal that can be read by the data acquisition system. In some designs, the magnetic field is set to the center of the mass peak and the accelerating voltage is decreased in small steps to generate a Faraday cup signal vs. high voltage.

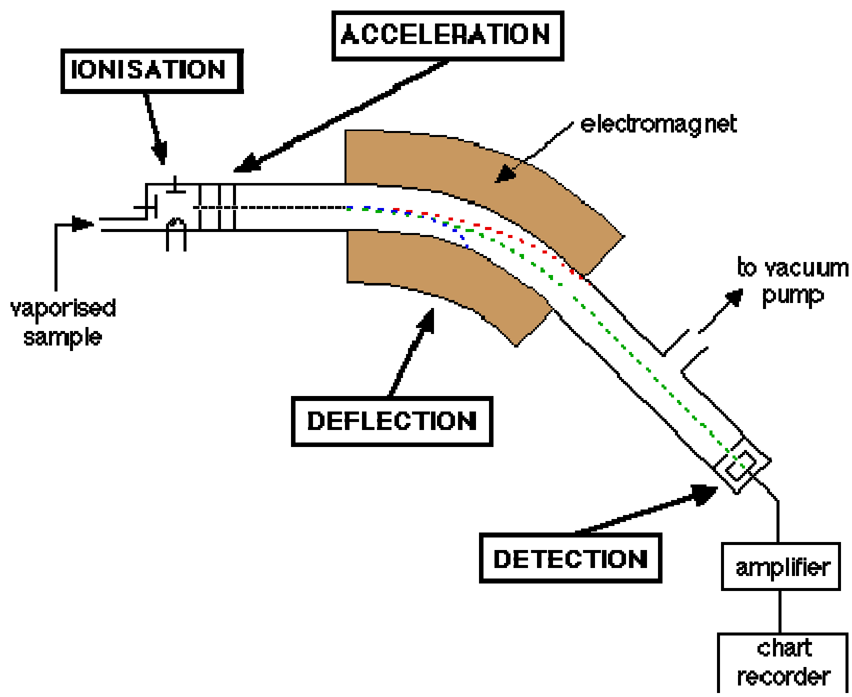

FIGURE 1 - MASS SPECTROMETER LAYOUT

The gas ionization occurs in the source housing as shown in Figure 2. The gas sample from the inlet system is ionized when exposed to a high amperage filament. Electrons are knocked loose generating positive gas ions. The filament current is based on a specific trap current, typically in the hundreds of micro-amps. The ion box floats at voltages up to 10,000 Volts. The electronics that control the filament current must also float at this voltage or arcing will occur.

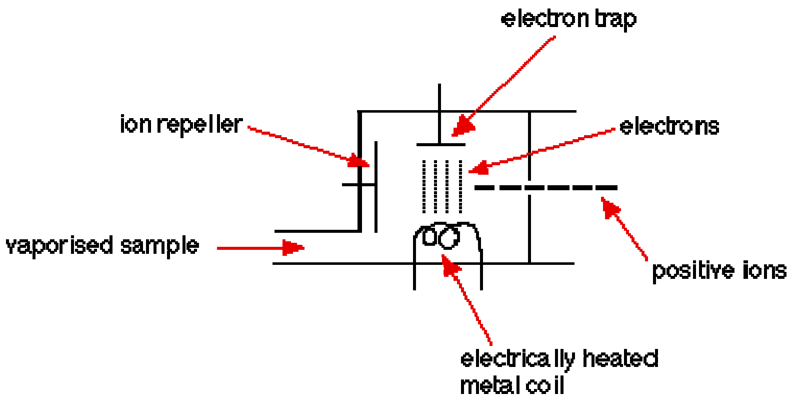

FIGURE 2 - GAS IONIZATION

MAJOR SYSTEM COMPONENTS

Faraday Cup Amplifiers

Figure 3 shows old and new models of Faraday Cup amplifiers. These amplifiers must amplify current in the low -14 amp range from the Faraday Cup. To amplify this very small current, a feedback resistor in the 100GΩ range is needed combined with a 1pF capacitor. The RC time constant of the feedback network dictates the time response. Typically a 100msec or faster response is needed. To measure current in the 1e-14 amp range, the printed circuit board must have ground planes and guarded traces. The input lead must be floated off the board with Teflon insulating posts or equivalent since the leakage current of the pc board itself will cause erroneous measurements. An amplifier that has the lowest possible offset current such as the Analog Devices AD549 must be used. A two stage amplifier provides for higher gain. To ensure low noise, the Faraday Cup amplifiers should be enclosed in a metal chamber that is under vacuum. A vacuum will provide low humidity and a stable temperature. High humidity will reduce the resistance of Giga-ohm resistors.

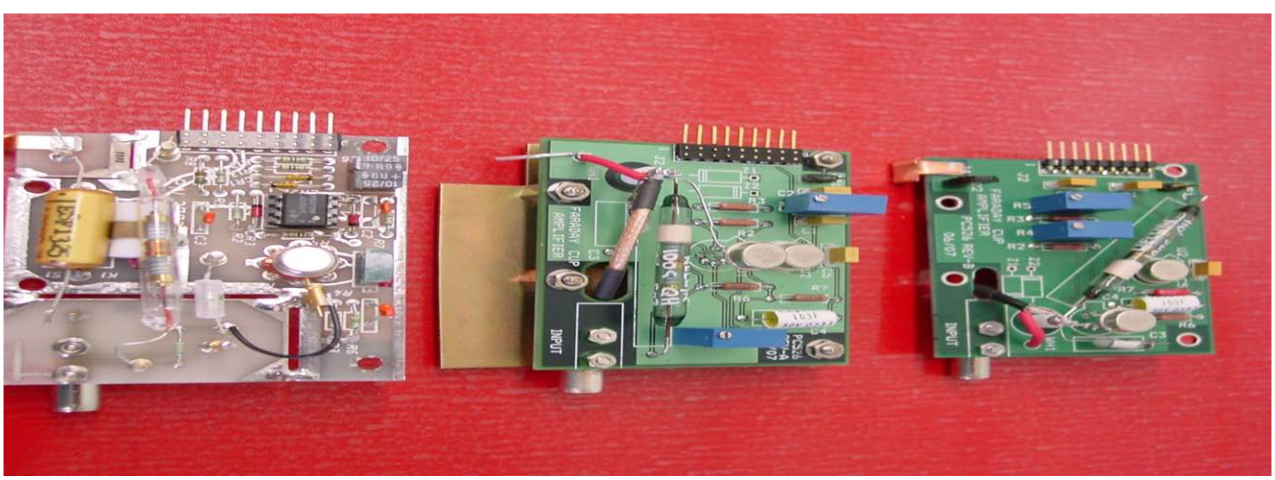

FIGURE 3 - FARADAY CUP AMPLIFIER

When an electron (negative charge) is accelerated through an electric field (see Reference 1), it gains kinetic energy. After acceleration through 70 Volts in a high vacuum, the electron has an energy of 70eV (electron volts). These energetic electrons can interact with uncharged, neutral molecules (M) by passing close to or even through the molecule, so as to eject an electron from the molecule (Equation1):

Equation 1 $$e^- + M \rightarrow M^{*+} + 2e^-$$

Thus two electrons exit the reaction zone leaving a positively charged molecule (M^{*+}) called an ion. Since the mass of the electron is very small compared to the mass of the molecule, the mass is essentially M^{*+}.

Emission Regulator

An Emission Regulator chassis is shown in Figure 4. This chassis supplies the electron energy and controls the filament current based on a desired emission current. The filament current will range from 2 to 5 Amps depending on the filament type.

FIGURE 4 - EMISSION REGULATOR CHASSIS

This chassis must be designed to float at the acceleration voltage of the mass spectrometer source which can be as high as 10,000 Volts. Figure 5 shows a top view of the chassis. The high voltage transformer in the back and the high voltage insulators on the front allow for safe manual control via the front panel trim pots. For computer control of the Emission Regulator Chassis, fiber optic communication is good option. The programmable intelligent computer (PIC) microchip on the emission regulator chassis can monitor and control signals at high voltage. A serial output from the PIC chip can be converted to a fiber optic signal and transmitted to the control computer.

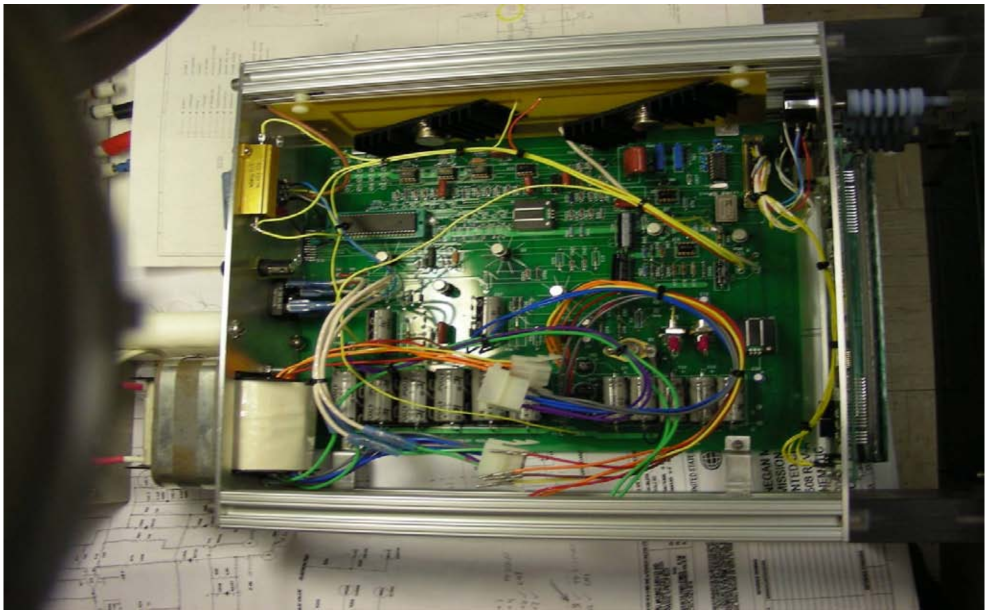

FIGURE 5 - EMISION REGULATOR CHASSIS TOP VIEW

Magnetic Field Detection

A Hall probe or magnetic field probe is used to the measure the magnetic field between the electromagnets. The field probe must have a low temperature coefficient and good linearity. Figure 6 shows the response of a commercial Lake Shore Hall probe. The current vs. field response is linear throughout a typical operating range of 0 to 4 KGauss.

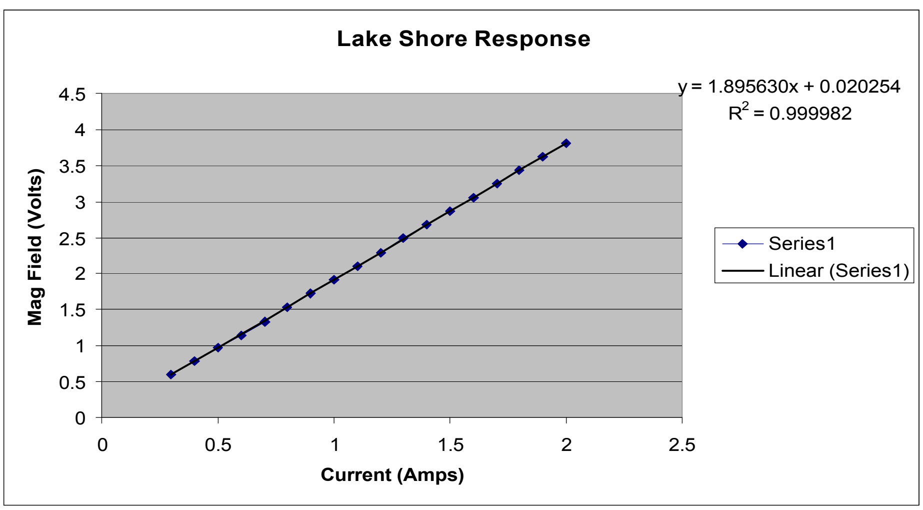

FIGURE 6 - MAGNETIC FIELD PROBE RESPONSE

High Voltage Power Supply

To control the electric field, stable DC high voltage supplies are needed. In addition, high resolution voltage control on the order of 22 bits is needed. This can be done with two 16 bit DACS. Both have an output of 0 to 10 Volts. The first is input directly into precision summing amplifier. The second is connected to a divider. With a 1:50 divider, the 10 volt signal is reduced to 0.2 Volts. This 0.2 volt signal is connected to the summing amplifier. The combined maximum voltage is 10.2 Volts and step changes of 3 micro volts (0.2/65536) can be made.

Precision Current Source

For small magnetic steps, precision current sources can be placed in parallel. One source can be on the amp range and one could be on the micro amp range. These current sources can be controlled via the front panel of each instrument or computer control. These constant current supplies can be set from the amp range to the nanoamp range providing the equivalent of greater than 20 bits of resolution from 0 to 6 Amps.

Small step size whether due to a changing current (i.e. magnetic field) or voltage (electric field) is essential to separating molecules with similar mass. For example, Figure 7 shows the separation of a 1% CO, 1% N2 mix with the balance Argon. The first peak is CO with a mass of 27.9949 and the second is N2 with a mass of 28.0062. The y-axis is the voltage from a Faraday Cup amplifier. The x-axis is the accelerating voltage in kV.

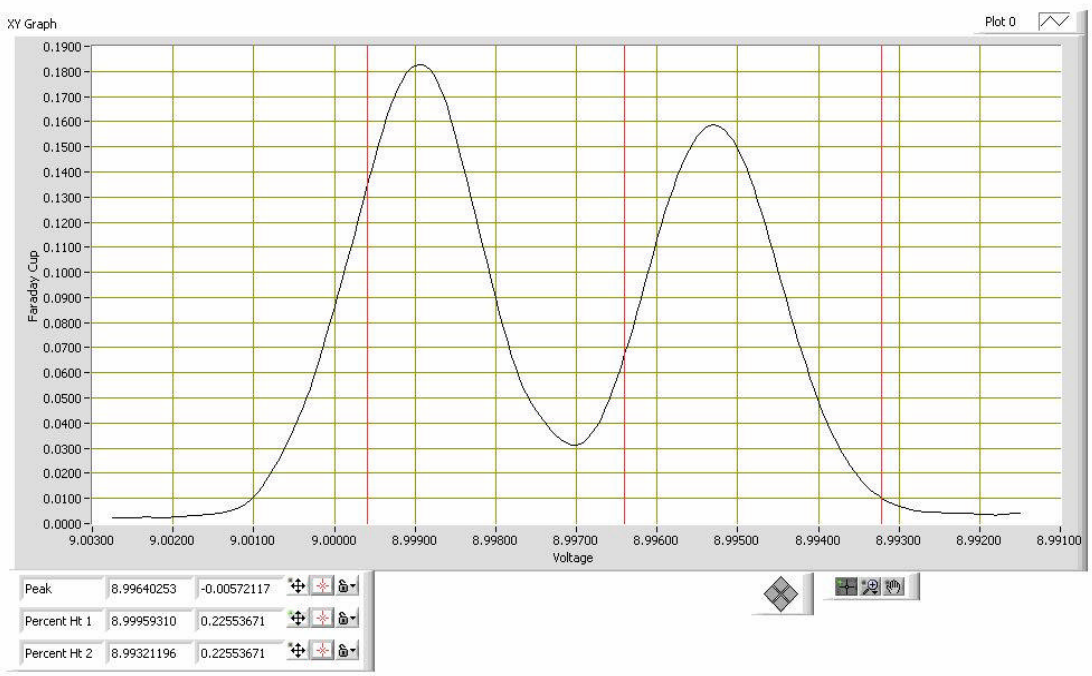

FIGURE 7 - CO/N2 SEPERATION

SOFTWARE AND DATA ACQUISTION

A National Instruments LabView executable program controls the electronics and the data acquisition. LabView has a high availability of drivers for the spectrometer instruments as well as powerful graphing capabilities. Figure 8 shows a typical control screen. From this screen, the electric or magnetic field can be controlled. Real time plots of the Faraday cup voltage or magnetic field can be shown.

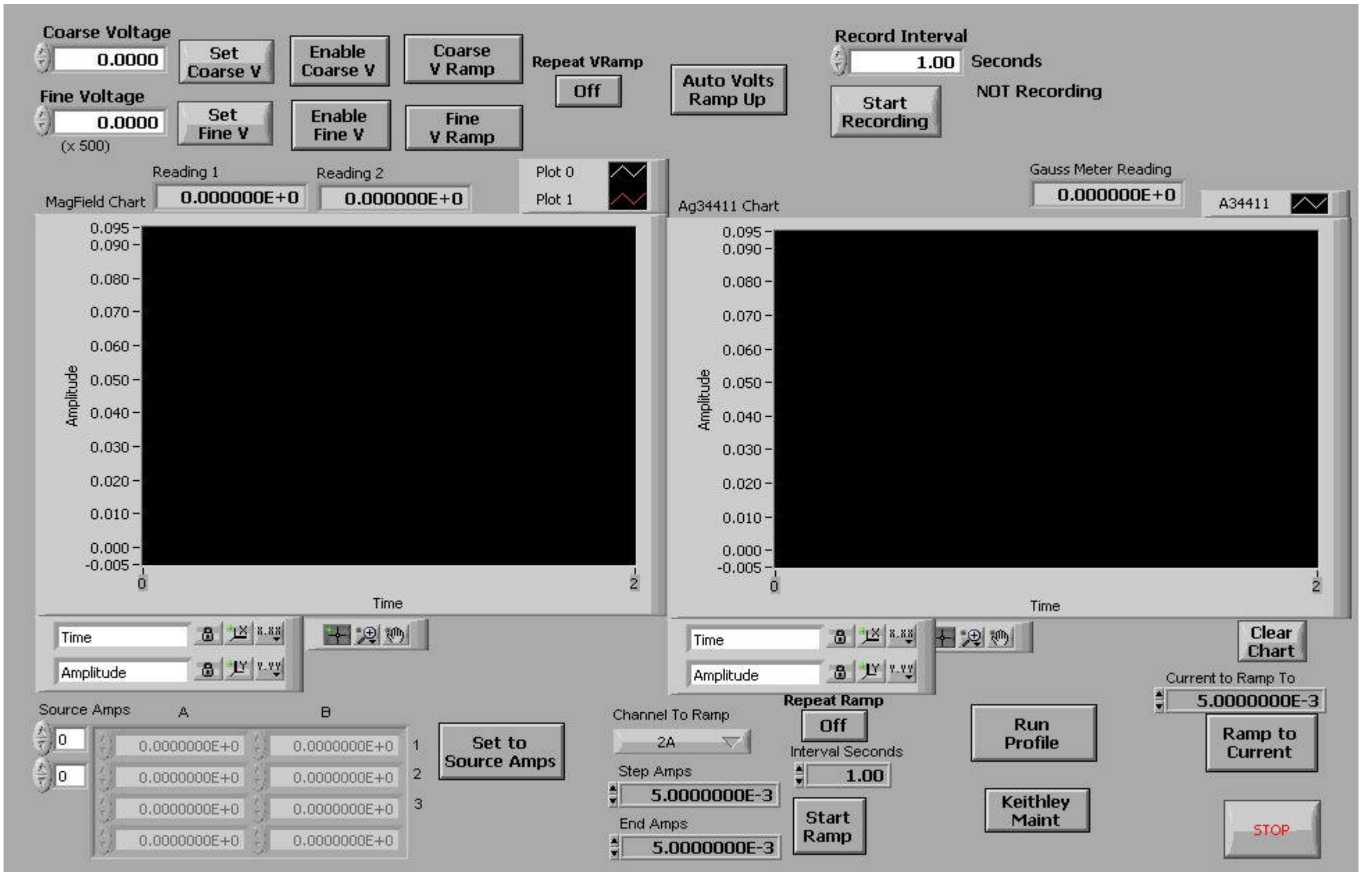

FIGURE 8 - LABVIEW SOFTWARE CONTROL

At the heart of the mass spectrometer system is a PC based data acquisition system. Communication to data acquisition equipment is achieved via Ethernet, IEEE-488 and RS-232 data transfer lines. Raw data sensor inputs are multiplexed to a high accuracy digital multimeter chassis. High resolution D/A converters and logic control cards are housed in separate data acquisition chassis. The software program has one main routine with several subroutines that perform calibrations, database maintenance and direct instrument interface. Figure 9 shows the block diagram of the electronics and interconnections with the data acquisition system.

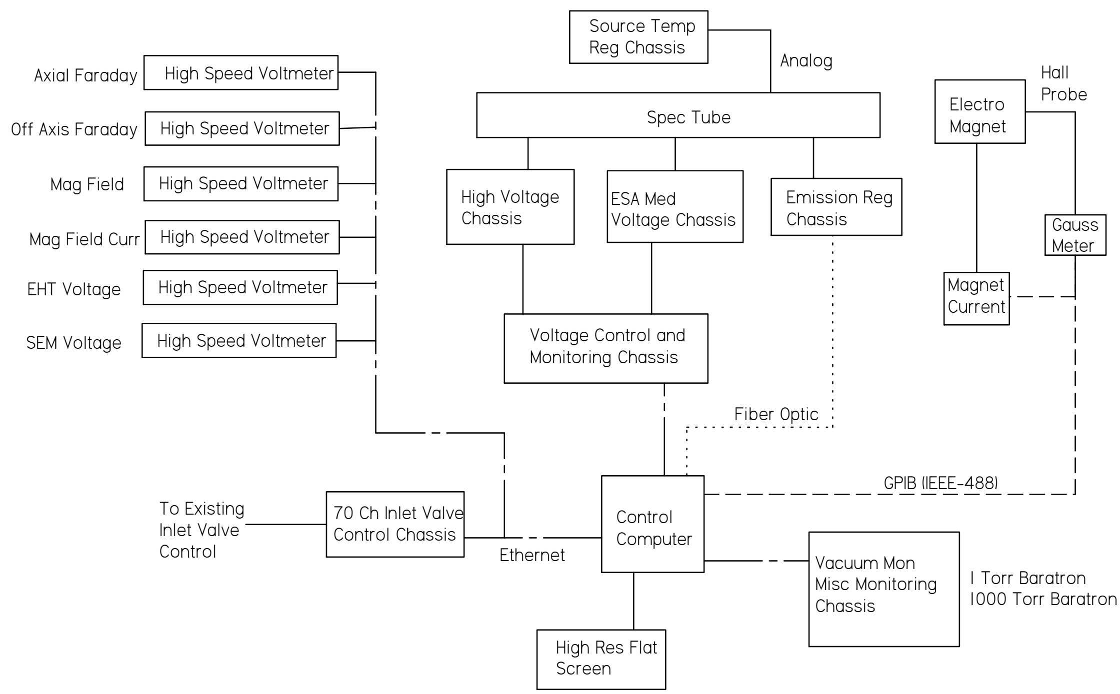

FIGURE 9 - MASS SPECTROMETER BLOCK DIAGRAM

The software program controls and monitors all aspects of the electronics upgrade package including:

- Precise magnet current control with dynamic feedback sense and adjustment
- High voltage power supply output control and sensing
- Real time display of Faraday voltages and magnetic field for peak detection
- Automated mass spectrometer tuning based on known samples
- Vacuum system pressure monitoring with software over-pressure interlocks
- Diagnostic routines to find and characterize system electrical noise
- Automated calibration of magnetic field probe response

GAS INLET SYSTEM

Figure 10 shows a virtual representation of a typical gas inlet system. The Labview screen allows the user to operate all valves via the front panel screen. Gas standards can be connected to the mass spectrometer to calibrate the system. A high vacuum pumping including a turbo with a backing pump is needed to evacuate the system prior to adding pure or unknown gas mixes.

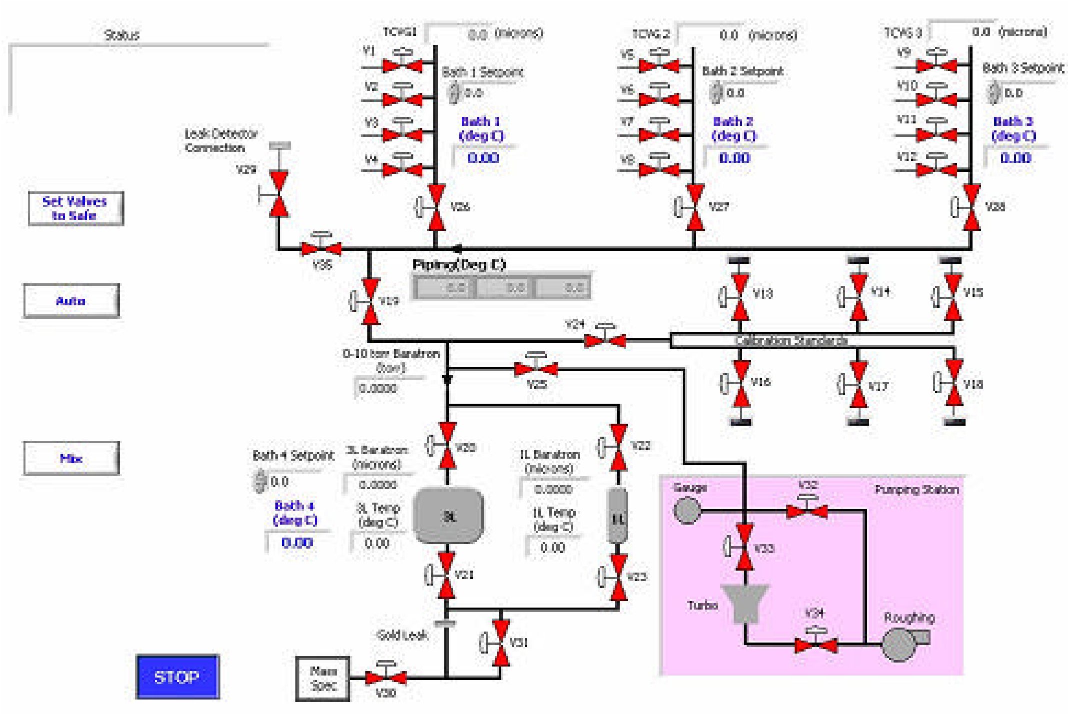

FIGURE 10 - MASS SPECTROMETER INLET

CONCLUSION

The Savannah River National Laboratory has designed a state-of-the-art data acquisition and control system for controlling high resolution Mass Spectrometers using a combination custom and commercial off the shelf components. This system is capable of extremely high resolution control of the magnetic and electric fields as well as high speed data acquisition.

REFERENCES

1. Herbert and Johnstone, "Mass Spectrometry Basics", CRC Press LLC 2000 N.W. Corporate Blvd., Boca Raton FL., (pages 13 and 16)