Setup of the Sample Cell Flow for Aerodyne's QCL Trace Gas Monitor

This document discusses the configuration of the sample flow in an Aerodyne QCL trace gas monitor. These instruments operate with the sample cell under vacuum. This vacuum is created by a downstream vacuum pump (typically a scroll pump). The desired sample cell flow and pressure are set using an upstream control valve and a downstream control valve under normal operation. This document describes the rationale and the standard procedure to set up the sample flow system.

Figure 1 shows the elements of the flow system. The sample flow enters the sample line at atmospheric pressure. Typically there is a sharp pressure drop at the control valve on the upstream side of the cell, CV_i. Inside the sample cell the pressure is held at a constant value usually somewhere between 5 Torr and 50 Torr. Often there is a second control valve at the outlet, CV_o. There may be a second pressure drop at this point. The sample flow proceeds through the pump line and on to the vacuum pump. A fundamental property of the cell is its volume, V_c. A typical value for V_c is 0.5 liters; Aerodyne's 76 meter cell has this volume. A fundamental property of the pump is its pumping speed, S_p (lpm). This is a volumetric flow rate and for most pumps it is not a strong function of pressure unless the pump is operated at very low pressure. Pumping speeds for scroll pumps vary from 30 lpm to 500 lpm.

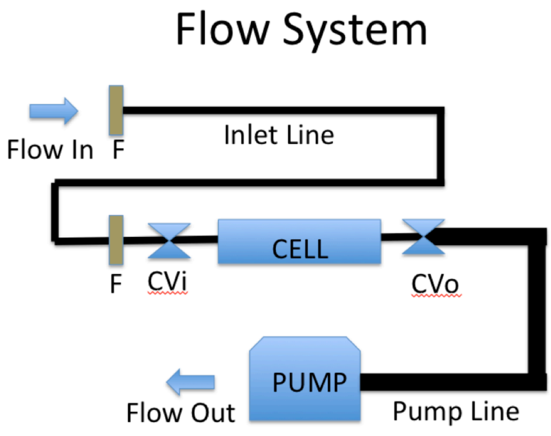

Figure 1. Diagram showing the components of the instrument flow system. Particle filters are indicated by F. The inlet and outlet control valves are labelled CV_i and CV_o.

The control valves can be adjusted to set three key variables: the total flow rate, Φ (slpm), the flow time response, τ(s), and the pressure in the sample cell, P_c (Torr). Two control valves allow you to choose two of these three variables. The third is constrained by Equation (1):

$$\tau\ (s) = [P_c(\text{Torr})/760] * [273/T_c(\text{K})] * Vc(l) * [60/\ \Phi(\text{slpm})]$$

$$\sim\ 0.072 * P_c(\text{Torr}) * V_c(l)\ /\ \Phi(\text{slpm}) \qquad (1)$$

Equation (1) is fundamental and does not depend on assumptions about conductance, pumping speed or critical flow. Note that the flow rate is expressed in units of standard liters per minute. It is therefore equivalent to a mass flow rate. This is not to be confused with the volumetric flow rate that characterizes the pump. Typical values of the mass flow rate range from 0.1 slpm to 20 slpm.

So, in principle, the user is free to set two of the three sample flow characteristics. For some applications the time response is critical (eddy covariance), for others the flow rate is critical (chamber measurements or leaf measurements). And in some cases the pressure in the sample cell is most important (to enhance signal to noise ratio or to reduce spectral congestion). In any case, only two of the three variables can be freely chosen. What is the practical procedure for setting the valves once the goals are set? There are two general cases that represent typical operation:

1) Low to moderate flow using two control valves
2) Moderate to high flow using one control valve

Low to moderate flow using two control valves

In this case, both CV_i and CV_o are used to control the flow. Often each valve will be operated in the critical flow regime. Critical flow is achieved when the pressure upstream of the valve is at least double the pressure downstream of the valve. In this case, the flow across the valve is proportional to the upstream pressure; the pressure downstream of the valve does not affect the flow across the valve. To achieve this, the pressure in the cell must be less than ½ of the inlet pressure and the outlet pressure must be less than ½ of the cell pressure. Typically, the inlet pressure will be near 760 Torr, the outlet pressure will be near zero Torr and the user can select a cell pressure between 5 Torr and 100 Torr.

When both valves are operated in the critical flow regime, they are each tied to specific adjustable variables. For example, the inlet valve selects Φ. Φ is independent of the adjustment of the outlet valve. Similarly, the outlet valve selects τ and τ is not affected by the inlet valve. P_c depends on both valves but can be calculated from Φ and τ by rearrangement of Equation (1):

$$P_c\,(\text{Torr}) = [\tau(\text{s}) * \Phi(\text{slpm})] / [0.072 * V_c(\text{l})] \qquad (1\text{a})$$

A practical scheme for setting the valve positions in this case would be:

1) Open CV_o completely.
2) Adjust CV_i to set the desired flow rate, Φ.
3) Adjust CV_o to set the cell pressure, P_c, to its desired value. This will also set τ but the cell pressure is easier to monitor.

Step (2) seems to require a flow meter. This is certainly the ideal way to set the valve position. However, it is possible to estimate the flow rate even without a flow meter if the outlet valve can be fully opened. When the outlet valve is fully opened, then the time response of the flow system is determined from the volume of the cell and the volumetric pumping speed:

$$\tau(s) = V_c(l)*[60/S_p(lpm)] \qquad (2)$$

If equation (2) is substituted into equation (1), then we find an equation for Φ as a function of P_c for the case of no flow restriction between the cell and the pump:

$$\Phi(slpm) = [P_c\,(Torr)/760] * [273/T_c(K)] * S_p(lpm)$$

$$\sim (0.00121) * P_c\,(Torr) * S_p(lpm) \qquad (1b)$$

This can be rearranged to give Pc as a function of Φ – again for the case of no flow restriction to the pump:

$$P_c\,(Torr) \sim 826 * \Phi(slpm) / S_p(lpm) \qquad (1c)$$

Hence, CV_i can be set by adjusting its position until P_c reaches the value that gives the desired flow rate. Details to note:

1) The desired flow rate is set (in the absence of a flow meter) by selecting the *appropriate* pressure in Step (2). This will not generally be the *operating* pressure. The cell is set to the operating pressure in Step (3) with the outlet valve.
2) S_p is the pumping speed of the pump unless the conductance of the inlet line and outlet valve are small enough to limit the pumping speed. If the pumping speed is limited by the conductance of the tubing between the cell and the

pump, then S_p should be replaced by the effective pumping speed at the cell, S_e.

3) If two control valves are used but critical flow is not achieved, then the procedure above can still be used but it will be more iterative in nature. You will need to simultaneously measure Φ and P_c and set them to the desired values using the two valves.

A special case arises in some instruments, where the inlet control valve is electronically controlled and its position is set by the instrument software (TDLWintel) in order to maintain a constant pressure in the sample cell. This is called "Pressure Lock". With the pressure fixed, the outlet valve can be adjusted to set Φ and τ simultaneously. If a flow meter is used, then the desired flow rate can be set by adjusting the outlet control valve. Even though the flow rate is actually controlled by the inlet valve (at least in the critical flow case), adjustment of the outlet valve will vary the flow rate because the inlet valve is adjusted by the TDLWintel software to hold the pressure constant. Operation of the electronic control valve is discussed in more detail in the appendix.

Moderate to high flow using one control valve

In this case, CV_i is used to control the flow rate and CV_o is absent. This configuration is typically used in high flow rate situations where a very fast time response is desired. This configuration is often used for eddy covariance measurements where fast time response is a primary consideration. With the outlet valve absent or fully opened, the time response of the flow system is as fast as possible and can be calculated from equation (2) above. With the outlet valve wide open or absent, the pressure in the sample cell will generally be too low unless the flow rate is very large. Hence, guided by equation (1c), the user generally opens CV_i in order to provide sufficient flow to reach an adequate cell pressure. Under these high flow conditions it is quite possible to encounter conductance limitations on both the inlet side and the outlet side. Some practical guidelines for increasing the conductance follow.

On the outlet side, the conductance is often limited by the pump line unless care is taken to select a large diameter pump line. The length of the line is less important. This follows from the equation for conductance of a tube (for viscous air flow):

$$C(\text{lpm}) = 10{,}800 \times D^4(\text{cm}) / L(\text{cm}) \times P(\text{Torr}) \qquad (3)$$

where D is the tube *inner* diameter, L is its length and P is the average pressure in the tube. It is important that the conductance be larger than the pumping speed of the pump – otherwise it will limit the pumping speed. A practical example may be helpful. A large scroll pump might have a pumping speed of 500 lpm. Consider two different pump lines:

1) A ¼" OD tube that is 1 meter long. This tube has an outer diameter, OD, of about 6 mm, but its inner diameter, ID, is typically 4 mm. Equation (3) implies a conductance of only 83 lpm at 30 Torr. So this would reduce the effective size of the pump by a factor of 6.
2) A 5/4" OD tube that is 20 meters long. This tube has an OD of 33 mm. Its ID will vary but might be 25 mm. Equation (3) implies a conductance of 6300 lpm at 30 Torr. So even though the tube is 20x longer than in the first example, its conductance is still much larger than the pumping speed and will not hinder it.

How much will the finite conductance of the pump line limit the pumping speed? This is shown in equation (4) which expresses the overall or effective pumping speed, S_e, as a function of the pump tube conductance, C, and the pumping speed of the pump, S_p:

$$1/S_e = 1/C + 1/S_p \qquad (4)$$

So for the second example discussed above, the effective pumping speed would be 463 lpm, only slightly reduced from the 500 lpm speed of the pump.

When high flow rates are used it is equally common to encounter flow restrictions on the inlet side of the flow system. Elements that can restrict flow on the inlet side include:

1) the inlet tubing
2) the particle filter
3) the inlet flow control valve, CV_i

Fortunately, the inlet flow occurs at much higher pressure so the conductance limitations on the inlet tubing are not as strict as on the outlet tubing. For example, 1" ID sample lines are not required. For flow rates up to 20 slpm, ½" OD sample lines generally suffice. The particle filter can become a significant flow restriction; especially as filters become dirty. One technique for avoiding this problem is to use a large area filter or multiple filters in parallel. Finally, the control valve itself can restrict flow. A potential solution to this is to create a large bypass flow in parallel with the flow controller. If 80% of the flow bypasses the flow controller, the flow controller can still modify the 20% that passes through it to maintain a constant pressure.

Appendix: Adjustment and Use of the Electronic Control Valve

The electronic flow control valve is controlled by the TDLWintel software. The software sends a 0 – 5 V control signal to the upstream control valve in order to change its diameter. Zero volts corresponds to valve fully closed, meanwhile five volts corresponds to valve fully open. The settings for the flow controller, such as the pressure set point, range, correction, response time and the control parameter dV/dP, can be adjusted in the software through the "Control Inlet Valve(s)" window under the "Command" option. dV/dP is the linear response of the cell pressure to the controller voltage signal. The flow controller can be activated by the "PL" (pressure lock) button in the toggle control panel at the lower left corner on the TDLwintel window.

To configure the sample flow system with an electronic control valve:

1. Connect and check the sample flow line. Along the flow direction, it should have a sample inlet, a control valve (electronically connected to the flow control port on the back panel of the instrument), a sample cell, a pump valve and a vacuum pump.
2. Connect a flow meter upstream in front of the inlet. Turn on the pump and fully open the pump valve.
3. Adjust the flow controller voltage until the desired flow rate is reached. The adjustment is done by manually putting in values in the blank space below "Adjust valve" in the "Control Inlet Valve(s)" window and hit "change set point" button below the blank space.
4. Adjust outlet control valve to reach the desired cell pressure.
5. Determine the dV/dP value around the pressure set point and enter it in the software menu. This value is determined by changing the flow controller voltage in small steps and observing the response of the cell pressure.
6. Set parameters in the "Control Inlet Valve(s)" window. Then activate the "PL" toggle button on the lower left corner of the TDLwintel window.

Things to note:

1. If the inlet pressure changes (such as in the case of switching samples from ambient air to a compressed tank), then the flow rate changes momentarily. The flow controller will adjust the control valve in order to keep the same cell pressure and hence the same mass flow rate.
2. The tube diameter between the cell and the pump should be carefully chosen in order to not limit the pump speed. This is discussed above.
3. Leak rate measurements should include the sample inlet line, not just the region between the control valve and the pump valve. The leak rate in standard liters/minute can be derived from the pressure rise rate in Torr/min multiplied by the total test volume in liters and divided by the ambient pressure in Torr.
4. The voltage signal of the flow controller that is sent to the control valve and also indicated in the "Control Inlet Valve(s)" window is not linearly related to the control valve orifice size or to the flow rate.