A Compact, Pressure- and Structure-Based
Gas Flow Model for Microvalves

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ABSTRACT

The advent of microfluidic systems demands compact models for the description of flow in the constituent system components. The situation is analogous to the evolution of compact models for electron flow in MOSFETs, which were essential for the development of integrated microelectronic systems. We develop here a compact gas flow model for microvalves, which relates valve flow to a limited but meaningful set of parameters. Specifically, these are the gas type; inlet and outlet pressures; ambient temperature; valve inlet diameter; the gap between the membrane and the valve inlet; and the coefficient of discharge of the valve inlet. The result is a simple, accurate model, appropriate for the design and analysis of microfluidic systems. We also demonstrate a characterization methodology for extracting the required model parameters from measurements of flow versus pressure and gap. This characterization has produced values for the coefficient of discharge, which match expectations based on previous theory and measurement. It has also produced a single parameter describing the effect of the gap in controlling flow, across broad ranges of valve inlet diameter, membrane-to-inlet gap, and pressure.

Keywords: MEMS, microvalve, microfluidics, mass flow control, compact gas flow model, flow characterization procedure

LIST OF VARIABLES

	Mass flow (usually in sccm, normalized to 273 K and 1 atm)
P_{in}	Inlet pressure
P_{out}	Outlet pressure
g	Ratio of specific heats, c_p/c_v
a	$= \sqrt{g\left(\frac{2}{1+g}\right)^{\frac{g+1}{g-1}}}$
d	$= \sqrt{\frac{4g}{(g+1)(g-1)}}$
R	Gas constant in $p = rRT$ (8314 m^2/K-sec^2 divided by molecular weight)
D	Microvalve inlet diameter
z	Microvalve membrane-to-inlet gap
A	Microvalve effective flow area
C_d	Microvalve inlet coefficient of discharge

1.0 INTRODUCTION

Microvalves for a wide variety of applications have been studied for some time.[1,2] Microfluidic systems, using microvalves and other flow-controlling or flow-generating actuators, have also been the subject of study for several decades. Of particular interest to us has been a relatively simple system, the mass flow controller, wherein a microvalve is coupled in series with a flow sensor.[3-5] Recently, the level of integration of fluidic systems has increased. The practical realization of microfluidic systems for DNA analysis has commanded attention.[6,7] Arrays of microfluidic structures,[8] mixers,[9] check valves,[10] and microreactors,[11] have all been presented. Interconnections between array components have been devised,[12] which themselves will create system pressure drops.[13] Arrays of pneumatic valves have also been developed.[14]

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The control and distribution of flow in all these systems is essential to their utility. Quantitative descriptions of the effects of individual components in these systems are required in order to design and evaluate their behavior and performance. As systems increase in complexity, with more components, describing the complete flow using finite element tools[15] becomes too cumbersome to serve this purpose. This increase in component integration demands the development of compact models for the description of flow in the constituent components. The situation is analogous to the evolution of compact models for electron flow in MOSFETs, which were essential for the development of integrated microelectronic systems.

Microvalves have been studied extensively. However, studies of flow in microvalves have been limited. In our early valve work, we described the relationship between the valve membrane-to-inlet gap, and the inlet diameter, in terms of a loss coefficient model.[5] This model required extensive measurements for calibration, followed by the generation of four fitting parameters to describe the relationship between valve structural parameters, and a loss coefficient used to modify a simple definition of mass flow. The resulting model worked only for a single valve inlet diameter, so that each version of a microvalve required an extensive characterization procedure. Furthermore, the comparison of the model itself to the data was unsatisfactory.

Two recent attempts have been made to model flow in microvalves. One elegant example is unfortunately related to a device which does not rely on the motion of a mechanical membrane to adjust flow, and so is not adequate for our purposes.[16] The other relies on a simple description of flow, wherein the gas flow is proportional to the pressure drop across the valve, the speed of sound under STP conditions for the gas of interest, and the flow area, defined by the membrane-to-valve seat gap multiplied by the valve inlet periphery.[17] While such a simple model is attractive, in our experience it cannot explain the fullest range of flow in a microvalve. In particular, it does a poor job when the valve is near full closure. Since we are often concerned with vacuum leak rates in our microvalves,[5] a better description is required.

As a result, we develop here a compact gas flow model for microvalves, which relates valve flow to a limited but meaningful (from the standpoint of analysis and design) set of parameters. We will also demonstrate a characterization methodology for extracting the required model parameters from measurements of flow versus pressure and gap. This characterization has produced values for the coefficient of discharge, which match expectations based on previous theory and measurement. It has also produced a single parameter describing the effect of the gap in controlling flow, across broad ranges of valve inlet diameter, membrane-to-inlet gap, and pressure.

2.0 MICROVALVE GAS FLOW MODEL DETAILS

Regardless of the actuation method, flow in a microvalve is governed by the structural parameters shown in Figure 1. The valve inlet diameter D is of great importance, as is the distance z between the valve membrane and valve seat. A true compact model must accurately describe the flow as a function of these two parameters, over the widest range possible of z and D.

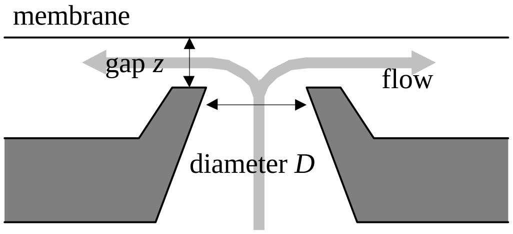

Figure 1: Important structural parameters in a microvalve.

To relate the flow to the ambient temperature, and to the pressure boundary conditions at the valve inlet and outlet, adiabatic, compressible flow equations are used.[5,18] These equations break the flow into sonic and subsonic regions, depending upon the ratio of the inlet and outlet pressures, and the ratio of the specific heats at constant pressure and constant volume for the gas under consideration. Note that the gas is assumed to be ideal. The equations which so describe sonic and subsonic flow in terms of gas type, T, P_{in} and P_{out}, coefficient of discharge C_d (which is related to the shape of the microvalve inlet structure), and effective area A are shown in Figure 2. The microvalve is thus treated as an orifice, where its effective area A varies as a function of D and z, but independently of the other structural attributes captured by C_d.

$$\dot{m}_{sonic} = C_d A \frac{P_{in}}{\sqrt{RT}} \sqrt{g\left(\frac{2}{1+g}\right)^{\frac{g+1}{g-1}}}$$

$$\dot{m}_{subsonic} = C_d A \frac{P_{in}}{\sqrt{RT}} \left(\frac{2g}{g-1}\right)^{1/2} \left(\frac{P_{out}}{P_{in}}\right)^{\frac{g+1}{2g}} \sqrt{\left(\frac{P_{in}}{P_{out}}\right)^{\frac{g-1}{g}} - 1}$$

$$\sqrt{A} = D\left\{1-\exp\left[-\frac{z/D}{(z/D)_0}\right]\right\}$$

Figure 2: Model flow equations. R is the universal gas constant divided by the gas molecular weight. g is the specific heat ratio c_p/c_v.

4.0 CHARACTERIZATION PROCEDURE

The key to the model here is the simultaneous establishment of C_d and A as functions of D and z. The characterization process begins by measuring flow as a function of z, P_{in} and P_{out}. An example of such a set of measurements is shown in Figure 3. The measurements were taken using one of our micromachined valve orifices,[5] with a micrometer used to vary the gap between the 'membrane' (cylinder of the micrometer) and the valve seat in a controlled fashion.

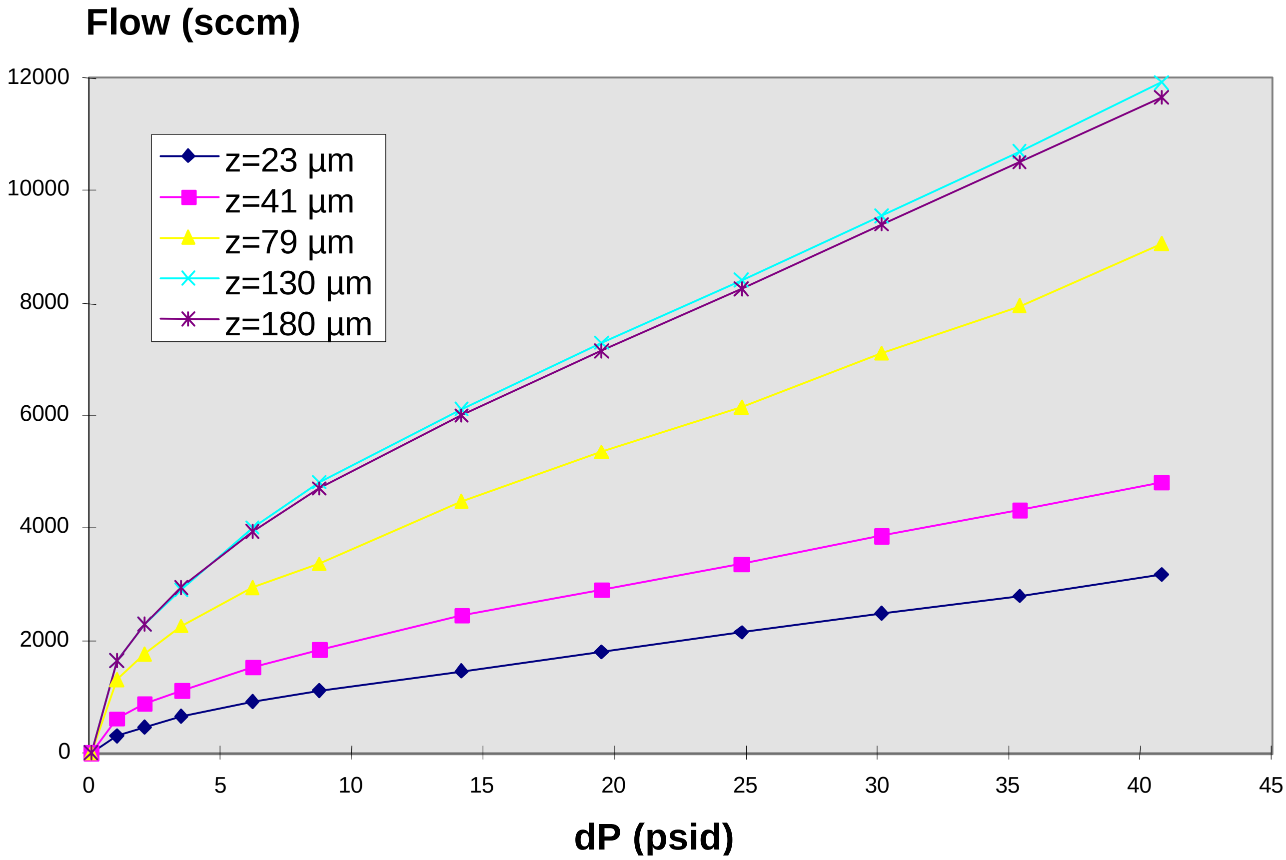

Figure 3: Measured N_2 flow (impingement mode) vs. pressure and gap for a silicon microvalve inlet, and a micrometer used as a membrane. The inlet is a square, with an edge of 570 µm. P_{out}=14.7 psia, and dP=P_{in}- P_{out}.

The adiabatic flow equations from Figure 2 are then used to fit the flow versus pressure data at each value of *z*, by setting the coefficient of discharge equal to unity, and adjusting *A* in the equations (see Figure 4). In so doing, the values of *A* which are found, contain information on both the effective area and the coefficient of discharge.

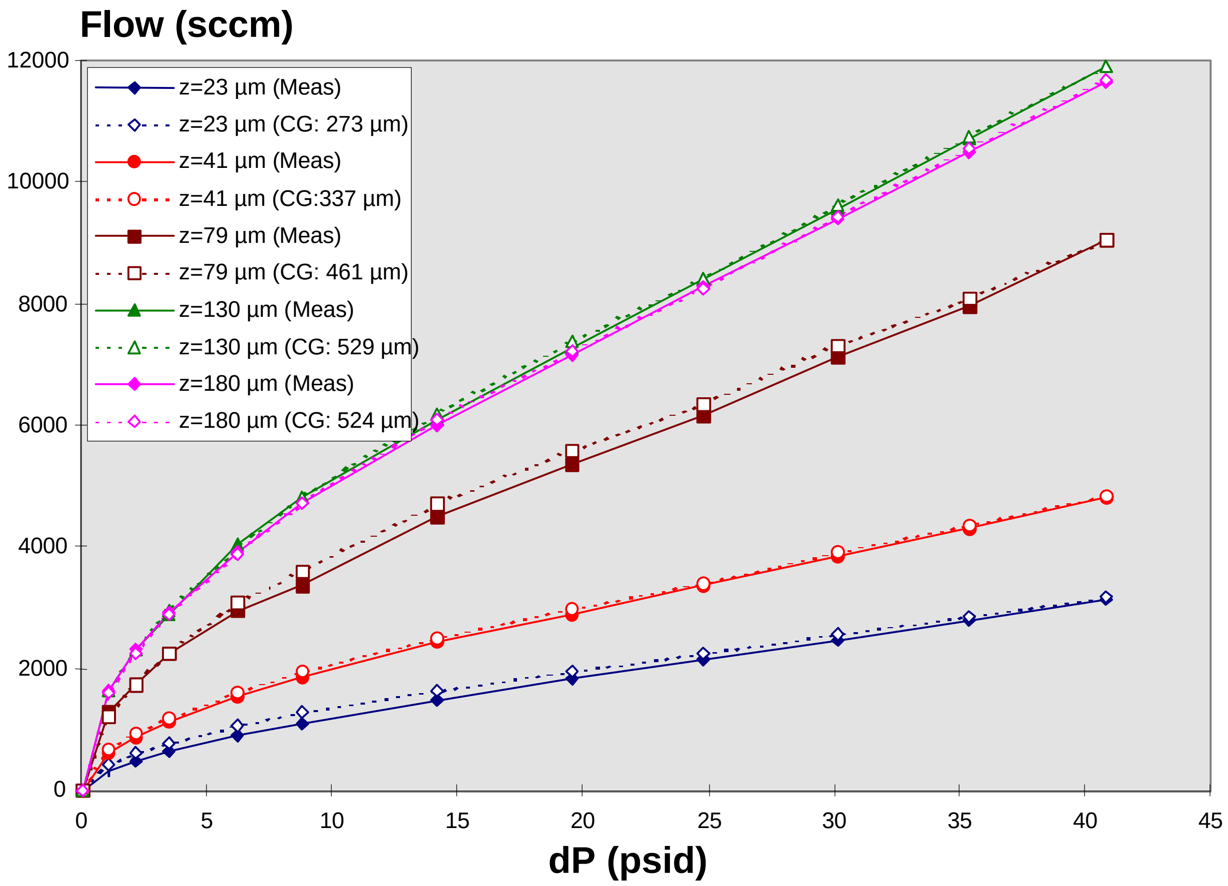

Figure 4: Measured N_2 flow vs. pressure and gap of Figure 3, plotted alongside results from the compressible gas equations of Figure 2. C_d has been set equal to unity, and the flow area adjusted arbitrarily until the best fit is achieved. Values of the square root of this flow area are shown in the legend as ‘CG:’.

In order to detach or separate the effect of the coefficient of discharge from the effective area once more, the square root of these fitted flow areas is then plotted versus the ratio *z/D* (see Figure 5). In performing this procedure, we discovered the resulting curve exhibits exponential behavior, where the coefficient of the exponential is 0.068, leading to the last expression in the complete flow model (Figure 2) for *A*.

Given that gas flow, even through a small, microvalve inlet orifice, exhibits the type of continuum behavior which includes a boundary layer, it is perhaps not surprising that the observed behavior is exponential: as the membrane comes close to the valve seat, the membrane and its boundary layer will penetrate the boundary layer associated with the inlet, causing a departure from a cross-sectional or effective flow area determined solely by the gap and the perimeter around the inlet diameter. We have observed this model coefficient to work for gases ranging from light (helium) to heavy (SF_6). However, we would expect the value to vary if more viscous fluids were employed, or if the valve inlet were comprised of a material other that silicon, with a significantly different interaction between the molecules of the solid wall, and the fluid molecules.

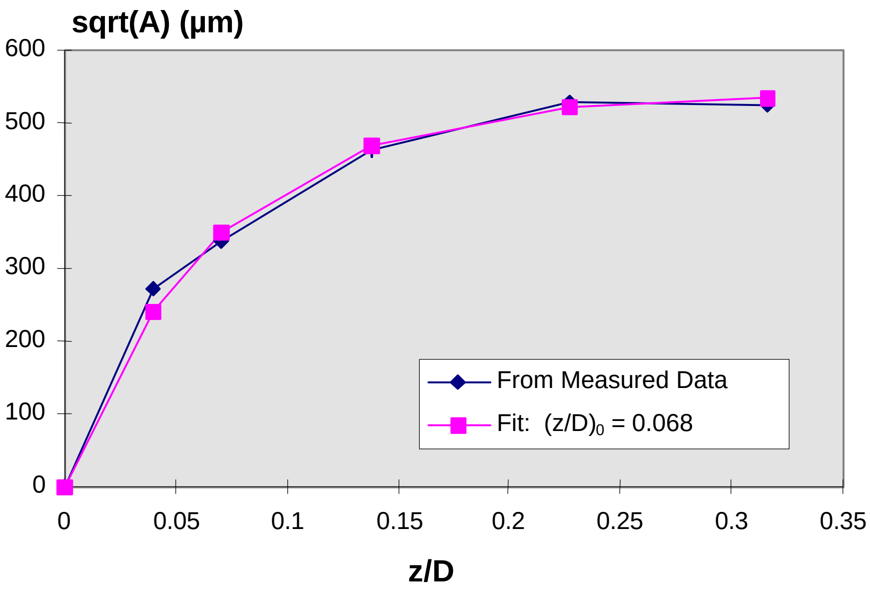

Figure 5: The values of the square root of the effective flow areas found in Figure 4 are plotted, allowing extraction of the value of $(z/D)_0$.

Finally, C_d is adjusted globally, and the entire data set (measured, and fitted with the final model) is plotted in Figure 6, using the full equations in Figure 2 (Figure 6). For the type of inlet shape studied in Figures 3-6, direct measurements of C_d (measuring the flow through the microvalve inlet orifice, with no membrane attached to the microvalve) established a value of 0.86. Our valve inlet orifices tend to be knife-edge in nature. The theoretical[19] and independently verified[20] value for such an orifice has been established as 0.898, which matches well with our measurements.

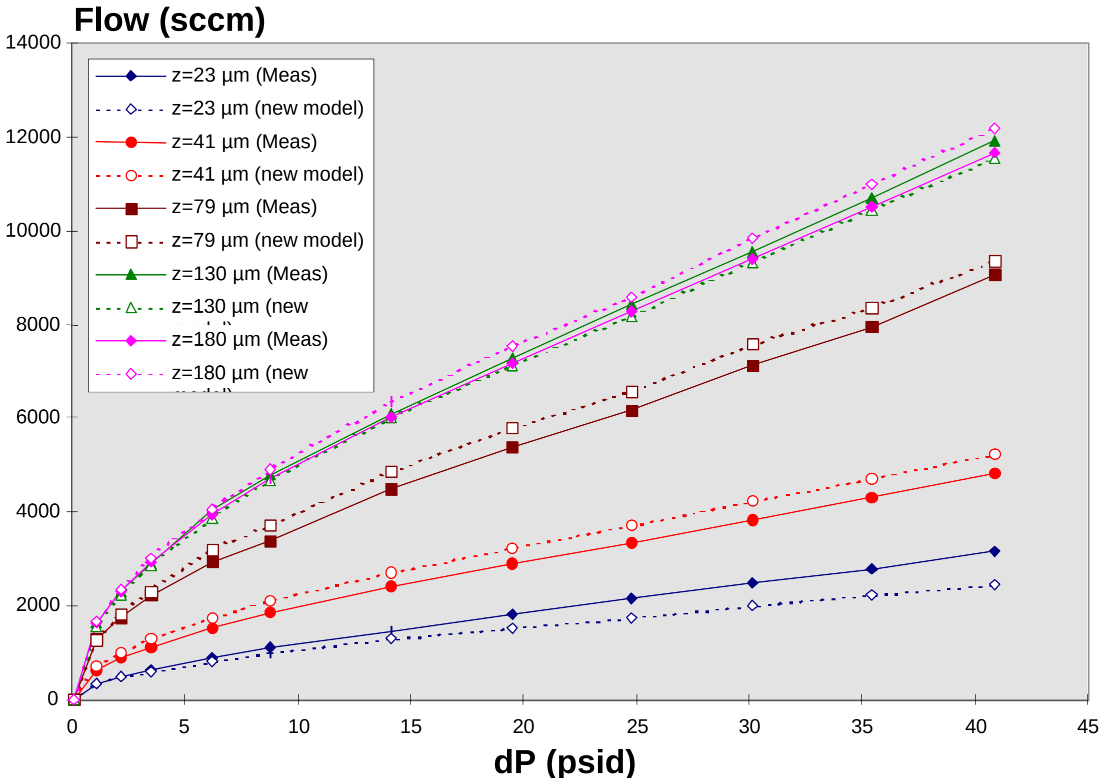

Figure 6: Plot of the measurements, as well as the full model results. The model value of C_d is 0.86.

4.0 OTHER RESULTS

We replicated the micrometer-based procedure using an all-silicon microvalve. The results are shown in Figure 7. The physical gap was determined using a laser-based measurement system. The procedure has been applied to silicon microvalves with valve inlet diameters ranging from 10 to 2000 µm, and with full-open gaps ranging from 2 to 100 µm, with good results. The results are uniform, whether the membrane is smooth over its entire area (usually 4 mm); or whether it has a boss, smaller than the full membrane area, located directly over the valve inlet. The model has been observed, however, to break down under conditions of rarefied flow, where the transition to molecular flow has begun (Knudsen regime).

C_d variations can occur by design in our microvalves. Figure 8 shows the result for another orifice design, whose intrinsic coefficient of discharge is 0.75. The same exponential parameter for $(z/D)_0$ of 0.068 holds in all cases, however.

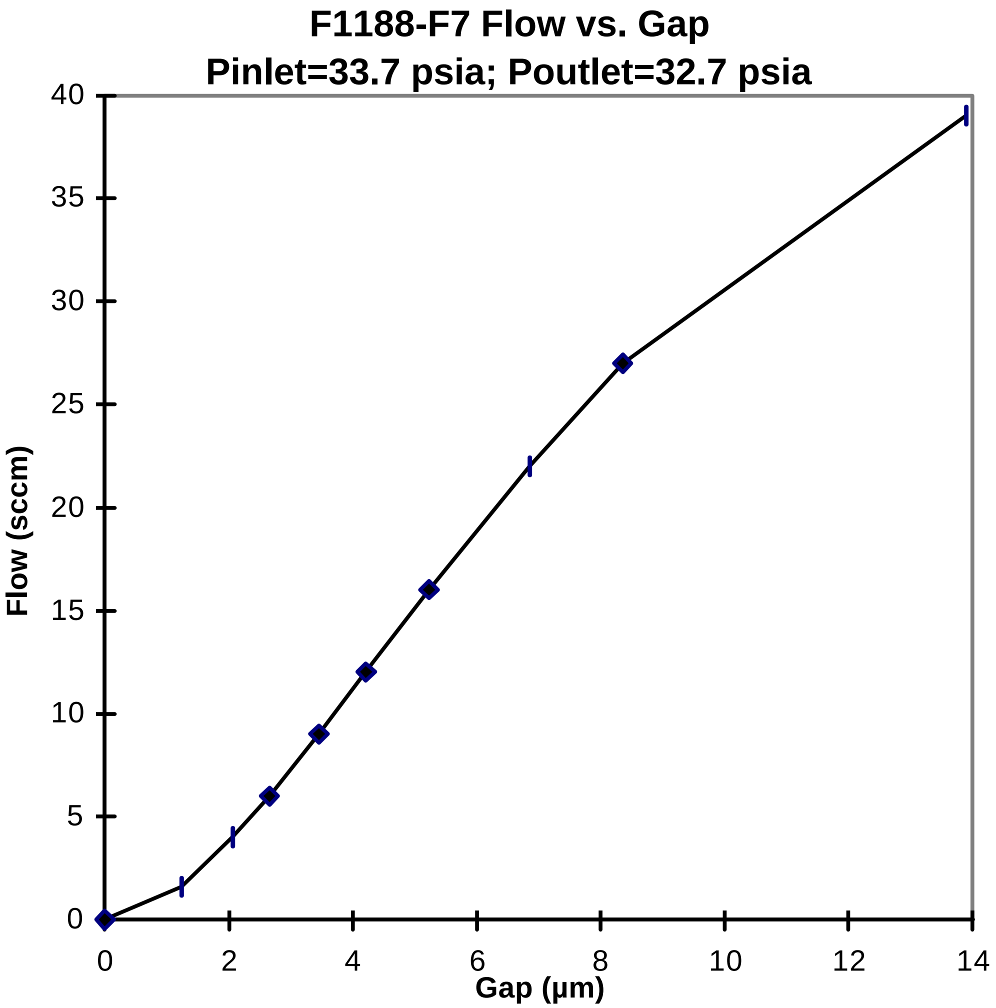

Figure 7: Measured flow versus for a normally-open microvalve. The predicted curve differs by less than 2% of reading, over the range of the gap *z*.

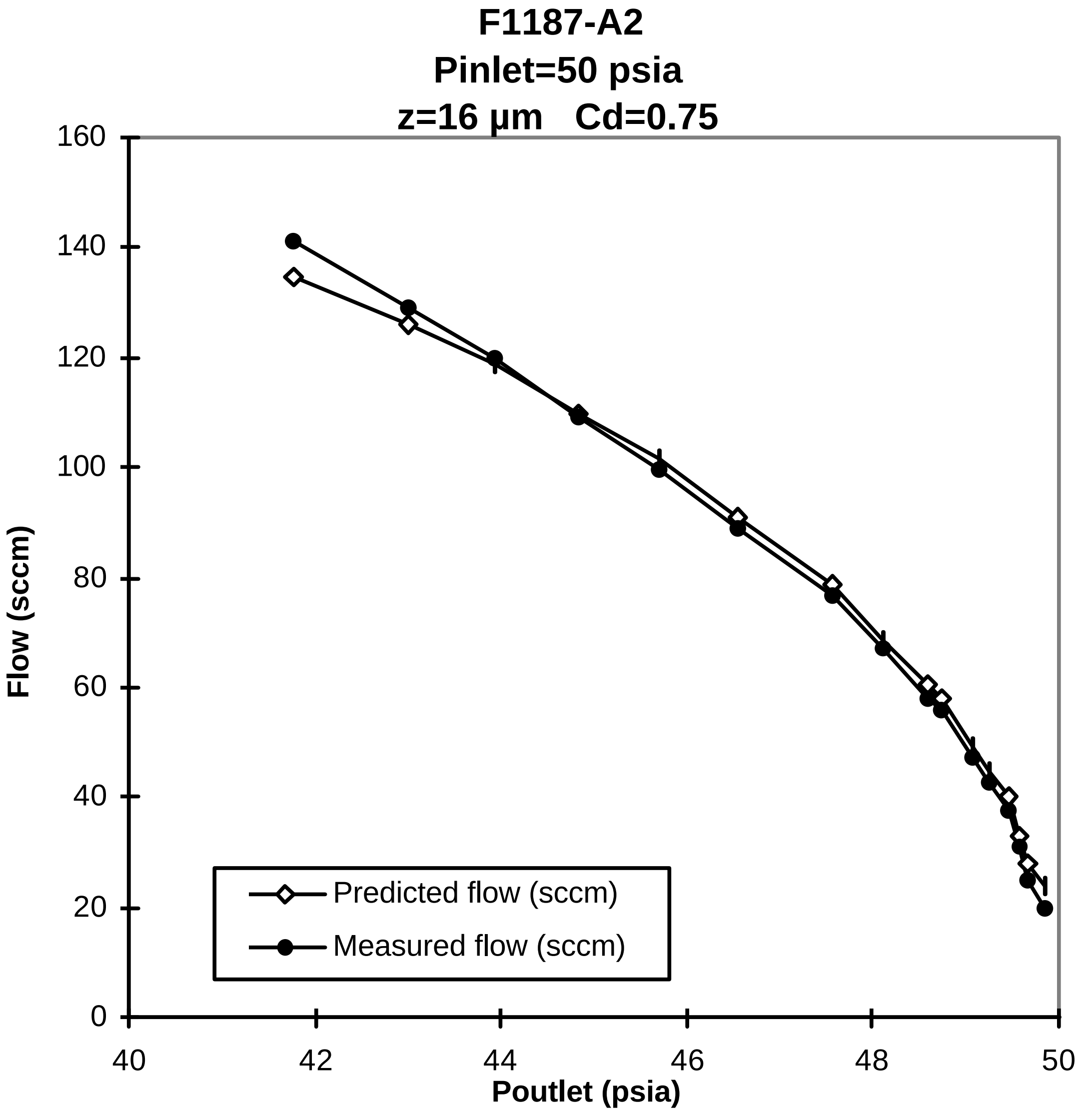

Figure 8: Comparison of modeling and measurements of open (unpowered) flow for a normally-open thermopneumatic microvalve.

4.0 CONCLUSIONS

We have developed a compact gas flow model for microvalves, which relates valve flow to a limited but meaningful set of parameters, which are useful in the analysis and design of these valves. Since the model is compact, it lends itself particularly well to the design of large-scale systems which incorporate microvalves. We have also demonstrated the characterization methodology for extracting the required model parameters from measurements of flow versus pressure and gap. Applying this characterization to our own microvalves, we have produced values for the valve coefficient of discharge, which match expectations based on previous theory and measurement. The characterization procedure has also produced a single parameter which describes the effect of the membrane-to-valve-seat gap, in controlling flow across broad ranges of valve inlet diameter, membrane-to-inlet gap, and pressure. Based on the success of this characterization, we expect it to be extended readily to other flow models, especially those involving incompressible (liquid) flow in microvalves.

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