Gas flow modeling in MEMS based microvalves for next generation CVD reactor designs

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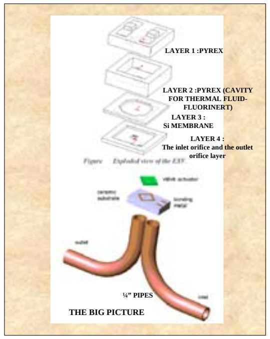
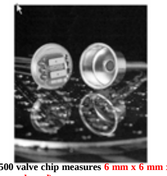
MEMS BASED MICROVALVES



THE 'SMALL' PICTURE



NC-1500 valve chip measures **6 mm x 6 mm x 2 mm (unpackaged).**

A dynamic flow rate range of 1,500sccm to 1slpm, the valve can be used for proportional control of gas flow.

Integrating the microvalve with a pressure sensor or a flow sensor and electronic feedback circuitry provides a closed-loop, programmable pressure regulator or flow regulator.

Source : Redwood Microsystems

THE CONSTRAINTS FOR THE MICROVAVLE

Mean Free Path Calculation / Continuum Assumption

$$\lambda = \frac{1}{\sqrt{2}\pi d^2 n}$$

(n: Molecular Density; d: Molecular Dia 2.5 A)

MFP at these conditions =1.1microns

So for continuum assumption to hold, the dimension of any Part of the microvalve (channel/orifice >10MFP)=11microns **@P=100torr, T=298K**

$$5sccm = 5*.4e{-7}\,moles/s * 2e{-3}\,kg/mole$$
$$= 7.4e{-9}\,kg/s = \dot{m}$$

Velocity calculation / Subsonic Flow Assumption

$$Vsonic = \sqrt{\frac{RT}{Mwt}} = 1113\,m/s \quad at \quad 298K$$
$$V\max = Vsonic = \frac{\dot m}{\rho A} = \frac{4\dot m}{\rho\pi D_{min}^2}$$
$$\rho \quad at \quad 100torr = 1.076e{-2}\,kg/m^3$$

Min Dia for below which sonic flow happens= 28 microns

So for subsonic flow assumption to hold, the dimension of any Part of the microvalve (channel/orifice >28microns)

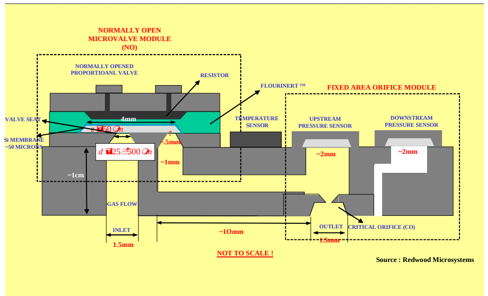
$$Re_{max} = \frac{\rho_{max} v_{max} D_{max}}{\mu}$$ **@P=100torr, T=298K**

Reynolds Number calculation / For Laminar Flow assumption

$$\rho_{max} = is\ at\ 300torr = 3.2268e{-2}\,kg/m^3$$
$$D_{max} = 300\,microns$$
$$\mu = .00884e{-3}\,kg/(m.s)$$
$$Re_{max} = 2100$$

So for laminar flow assumption to hold the the velocity in any part of the micromalve <1917m/s
<u>So subsonic flow imposes a tighter constraint</u>

SCHEMATIC OF A MEMS BASED MFC



THE FLUID FLOW EQUATIONS

For Channel 1
$$P_1 = P_0 - \frac{32V_1\mu L_1}{d_1^2} \Rightarrow P_1 - P_0 + \frac{32V_1\mu L_1}{d_1^2} = 0$$
→ Derived from Equation 6.1-4 Bird SL Hagen-Poisuille Law. Substituting for f=16/Re because flow is laminar and plugging in the exp for Re

For orifice 1
$$P_2 = P_1 - \frac{\rho_1 * V_1^2 * A_1^2[1-(A_{01}/A_1)^2]}{2C_{D1}^2A_{01}^2}$$
$$\Rightarrow P_2 - P_1 + \frac{\rho_1 * V_1^2 * A_1^2[1-(A_{01}/A_1)^2]}{2C_{D1}^2A_{01}^2} = 0$$
→ $Re = \rho V d_1/\mu$. Derived from Equation 7.5-34 Bird SL

For valve cavity with membrane
$$P_3 = P_2 + \frac{(P_{out}-P_2)}{z}s \Rightarrow P_3 - P_2 - \frac{(P_{out}-P_2)}{z}s = 0$$
→ A proportional flow valve

For Channel 2
$$P_4 = P_3 - \frac{32V_2\mu L_2}{d_2^2} - \xi V_2^2\rho \Rightarrow P_4 - P_3 + \frac{32V_2\mu L_2}{d_2^2} + \xi V_2^2\rho = 0$$
→ Contribution of bend to pressure drop

For orifice 2
$$P_5 - P_4 + \frac{\rho_2 * V_2^2 * A_2^2[1-(A_{02}/A_2)^2]}{2C_{D2}^2A_{02}^2} = 0$$

For Channel 3
$$P_{out} = P_5 - \frac{32V_3\mu L_3}{d_3^2} \Rightarrow P_{out} - P_5 + \frac{32V_3\mu L_3}{d_3^2} = 0$$

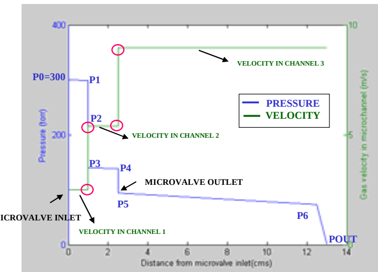
2 state equations
$$\frac{P_0+P_1}{2} = \frac{\rho_1 RT}{Mwt} \Rightarrow \frac{P_0+P_1}{2} - \frac{\rho_1 RT}{Mwt} = 0$$
$$\frac{P_3+P_4}{2} = \frac{\rho_2 RT}{Mwt} \Rightarrow \frac{P_3+P_4}{2} - \frac{\rho_2 RT}{Mwt} = 0$$
$$\frac{P_5+P_{out}}{2} = \frac{\rho_3 RT}{Mwt} \Rightarrow \frac{P_5+P_{out}}{2} - \frac{\rho_3 RT}{Mwt} = 0$$

2 Mass Balance Equations
$$\rho_1V_1A_1 = \rho_2V_2A_2 \Rightarrow \rho_1V_1A_1 - \rho_2V_2A_2 = 0$$
$$\rho_3V_3A_3 = \rho_2V_2A_2 \Rightarrow \rho_3V_3A_3 - \rho_2V_2A_2 = 0$$

11 equations(some non-linear) in 11 unknowns

Z(unknown):11 ROW VECTOR
g(z) comprises 11equations
6 fluid flow-pressure drop equations
3 equations of state
2 mass balance
Jacobian is a 11X11 matrix

SIMULATION RESULTS



SIMULATION GIVES THE PRESSURE DROP AND VELOCITY OF THE GAS AS IT MOVES THROUGH THE MICROVALVE. THE VELOCITY OF THE GAS IN THE ORIFICE IS NOT SHOWN IN THE FIGURE. IT IS IMPORTANT THAT THE GAS DOES NOT REACH SONIC VELOCITY.

MOTIVATION

<u>GAS DISTRIBUTION FACILITIES FOR NEW TECHNOLOGIES POSE THE FOLLOWING CHALLENGES:</u>

- **PARTICLES MUST BE REDUCED IN SIZE AND NUMBER: THIS REDUCTION REQUIRES**
  1. **INCREASED MATERIALS COMPATABILITY WITH PROCESS GASES (ESG COMPATIBLE)**
  2. **DECREASED DEAD SPACE VOLUMES, WELDS AND FACE SEALS**
- **COST**
- **RELIABILITY**
- **HIGHER RESOLUTION**

<u>MICROVALVES DISCUSSED HERE ARE SLATED TO ADDRESS ALL OF THE ABOVE CHALLENGES SUCESSFULLY</u>

- MATERIALS IN Si BASED MICROVALVES ARE COMPATIBLE WITH A WIDE RANGE OF ESG
- DEAD SPACE COLUMES, WETTED SURFACES AND FACE SEALS ARE REDUCED DRAMATICALLY
- GOOD RELIABILITY , AND HIGH RESOLUTION AND COMPARITIVELY LOWER COSTS OF THE DEVICES..
- THE APPROACH IS MODULAR WHERE MEMS BASED MODULES COMPRISING OF VALVES, PRESSURE SENSORS, MICROCHANNELS AND ORFICES ARE INTEGRATED TO BUILD MFC'S, PRESSURE REGULATORS AND SHUT OF VALVES FOR ESG GAS DISTRIBUTION.

THE OBJECTIVE : TO USE MEMS BASED MICROVAVLES FOR BULDING A GAS DISTRIBUTION SYSTEM FOR THE FUTURE PROGRAMMABLE REACTOR WHERE COMPACTNESS IS A KEY REQUIREMENT AMONGST OTHER THINGS .

SOLVING THE EQUATIONS:THE MATH INVOLVED

THE NEWTON RAPHSON METHOD:

<u>1 dimensional case:</u>

$$f(x) = 0; \quad (nonlinear)$$
$$initial\ guess\ x_0$$
$$compute\ new\ root\ x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

The new root is updated till $|x_{n+1} - x_n| < some\ defined\ tolerance$

<u>Multi dimensional case:</u> 11 equations(some non-linear) in 11 unknowns

$$g(z) = 0;$$
$$initial\ guess\ z_0$$

Compute new root vector $z_1 = z_0 - J^{-1}g(z_0)$

Compute new z vector z_1

$$Z = [P_1, P_2, P_3, P_4, P_5, V_1, V_2, V_3, \rho_1, \rho_2, \rho_3]^T$$

$$g = \begin{bmatrix} P_1 - P_0 + \frac{32V_1\mu L}{D^2} \\ P_L - P_2 + \frac{32V_2\mu L}{D^2} \\ P_2 - P_1 + \frac{\rho_1 * V_1^2 * A^2[1-(A_0/A)^2]}{2C_D^2A_0^2} \\ \frac{P_0+P_1}{2} - \frac{\rho_1 RT}{Mwt} \\ \frac{P_2+P_L}{2} - \frac{\rho_2 RT}{Mwt} \\ \rho_1V_1 - \rho_2V_2 \end{bmatrix}$$

Initial z vector z_0 → Compute g

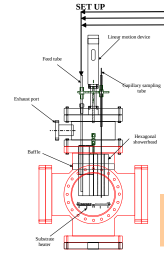
11 EQUATIONS IN THE EQUATION MATRIX

Compute J Jacobian Matrix

Stop iterations when the updated norm falls below some defined tolerance. Easily done in Matlab.

THE EXISTING GAS DISTRIBUTION SYSTEM

CURRENT GAS DISTRIBUTION SET UP

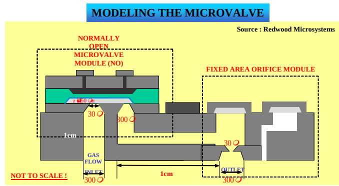


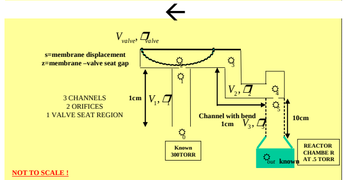
A 5 FT BY 3 FT CABINET

MEMS BASED MICROVALVES WOULD DRASTICALLY MINIMIZE THE SIZE OF THE GAS DISTRIBUTION SYSTEM, AND RENDER THE PROGRAMMABLE REACTOR A PLATFROM FOR PROGRAMMABILITY

PROGRAMMABLE REACTOR (MAIN CHAMBER DRAWING)

MODELING THE MICROVALVE





CONCLUSIONS AND FUTURE WORK

1)MEMS based micro valves-an idea about their working and their uses and their advantages.

2) Potential use of microvalves for future generations of the programmable reactor.

3) Modeling methodology and computation involved- fluid flow equations, Newton Raphson Method and Microvalve Design.

4)Future work: Compare simulations results with real data from literature if possible. Improve modeling by using more precise structures and dimensions and flow characteristics in our models. E.g. hexagonal channels(Hydraulic radius), compressible flow. Also incorporate materials of construction in our models and carry out simulations for Ar, WF_6 and H_2 flow.

fluid flow modeling: Start with assumptions to start out real simple, put down the equations, perform simulations and then add more to the model bit by bit and go with the flow. No pun intended.