MEMS based Heavy Metal: Mercury and Cadmium Ion Detection in Laminar flow of water

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Abstract. Innumerable Nations are enduring biohazard complications because of potable Water contamination. Water contamination is due to the presence of heavy metals like Nickel, Lead, Mercury, copper, iron, manganese, Cadmium, and Zinc in ppb (parts per billion) level. The most effective MEMS-based cantilever design capable of detecting Mercury and Cadmium ionic pressures with better geometry is highly demanded. Heavy metal ion detection in the vapor phase at a particular temperature is highly recommended. The project primly proposes a comparative study of divergent MEMS-based micro-cantilever beam structures with an active layer coating for heavy-metal Mercury and Cadmium ion detection and the structures were appraised based on the mechanical displacement under the pressure influence of target ions. The project proposes a concernment study of the laminar flow of water (liquid) through divergent structural designs. The laminar flow characteristics of water are engaged to find the maximal and minimal velocity and pressure positions. On altering the Inlet flow rates; the outlet flow rate, maximal and minimal velocity and pressure positions vary. Laminar structures were appraised based on the variation of outlet flow rate and pressure with respect to inlet flow velocity. The MEMS-based micro-cantilever structure with superior mechanical displacement is lodged at a maximal pressure locus of laminar flow structures. The pressure quantification at the locus of the micro-cantilever structure is calibrated for Heavy metal: Mercury and Cadmium ions pressure concentration. The finite element analysis of heavy metal Mercury and Cadmium Ion detection is executed using COMSOL Multiphysics 5.4

1. Introduction
Environmental issues are major causes for the disruption of human health across the globe, among those water adulteration is considered the most perilous as claimed by reputed Health Syndicates and compels swift remedies [1]. As stated by experts, millions of infants perish beneath 5 years by virtue of illness engendered by potable water [2]. Heavy metals are technically analogous to that of Metallic components of groundwater which possesses their corresponding metal density above 5g/cm$^3$ and their corresponding atomic- weights alter from 63.5gmol$^{-1}$to 200.6gmol$^{-1}$[3][4]. Among myriad Metal Ions, cadmium, lead, copper, cadmium, and mercury are contemplated to be supremely noxious and pernicious and even mentioned in the regulations for National Potable Water [5].

Predominantly Cadmium harms Kidneys resulting in renal failure and resides inside the human system possessing a life expectancy of about 10 years. Infants absorb much larger lead than grownups and digesting components of Lead can evolve into Nervous disorders and Anaemia.
Owing to rapid growth in Urban and Industrial developments, Heavy Metals are conveyed into Water bodies by modes of Water runoff, giving rise to water adulteration. Since all the polluted ingredients are emitted into the water resources and subsequently consumed by aquatic plants, fish and animals and ultimately get accumulated in the human system and cause diversified diseases.

Heavy Metals impact human health in a colossal manner. Nonthoughtful exhaustion of the metals can occur by way of simple non-treated water from incognito supplies [6]. Supplied water may have been stockpiled by metals from sources like Agriculture, disregarded water and mine wastes. The potentiality to probe the metal deposits in water is predominant to minimize the health endangerment [7]. The finite element analysis of a sensor with different pressure percentage variations effectuated in COMSOL could evince Heavy metal lead ion detection.

The heavy metals analysis for the groundwater samples is during the span of monsoon, pre-monsoon, post-monsoon. The heavy metals mercury, cadmium, Copper, Iron, Manganese, Chromium, and Lead were analyzed. The areas chosen for the survey are in and around Karaikal. The Karaikal areas were selected because at this location the waste water flows into the ocean. In different monsoon periods, water samples were collected at various stations such as Ambakarathur, Nagore, Kollapuram, Kottucherry, Poraivar, Varichikkudi, Malavangiyur, and T.R.Pattinam. The sanctioned limit of Mercury and cadmium stipulated by W.H.O is 0.01mg/l. The survey results imply that the mercury and cadmium concentrations are above the permissible limit [8].

The paper intends to explicate the mechanical characteristics of MEMS-based micro-cantilever structural displacement with disparate geometries under the influence of Heavy metal Mercury and Cadmium ionic pressures. The project perpetrates the perusal of laminar flow attributes such as velocity and pressure of multiple structures for disparate flow velocities and geometries. The results emanate the superlative structure with prime geometrical parameters.

2. Simulation & Materials
2.1. Simulation of Heavy Metal Ion Detection
The Mercury and Cadmium ion detection functions on the fundamentals of Cantilever Beam. On subjecting the micro-cantilever beam plane to mass or pressure, the plane beam gets swerved from its equilibrium position. This infers that the alterations of the mechanical displacement are subjected to the pressure of Mercury and cadmium ion. Micro-cantilever structure functions as a Transducer that metamorphoses Mechanical Energy into Mechanical displacement. The Micro-cantilever structure is built with Silicon Nitride or PolySilicon. An active layer built with gold is employed to acquire the particular bending of the active layer. In the Micro-fluidic framework, the metal ions that need to be detected are called analyte [9]. Analyte utilizes minimal energy and delivers results at the micro-level. This project employs Heavy Metal Ions Hg$^{2+}$ and Cd$^{2+}$ as analytes.

In Solid Mechanics analysis, the parameter altered to study the mechanical displacement characteristics of the micro-cantilever beam is vapour pressure. Disparate pressure percentages of Mercury are varied by maintaining the operating temperature at 449K. The maximum vapour pressure of the Heavy Metal Ion Mercury is 1000 Pa at 449K. Disparate pressure percentages of Cadmium are varied by maintaining the operating temperature at 745K. The maximum vapour pressure of the Heavy Metal Ion Cadmium is 1000 Pa at 745K. In Solid Mechanics analysis, the active layer height is also varied to study the displacement characteristics of the micro-cantilever beam. Different heights of the sensing layer are analyzed by applying congruent vapour pressure at operating temperatures of 449K and 745K.
The thickness is varied from 0.1µm-1.0µm with an applied pressure of 1000Pa for mercury and cadmium detection. The anatomization of Mercury and Cadmium heavy metal ion is effectuated with Silicon Nitride and PolySilicon as an active layer for sensing heavy metal ion pressures.

In Laminar Flow analysis, the channel inlet flow is altered for disparate structures with divergent geometries to study the flow attributes like outlet flow velocity and pressure. The anatomization also infers the velocity positions (max and min) and pressure positions (max and min). The flow velocity is varied from 1m/s-50m/s. The specification of materials used in the anatomization of the micro-cantilever beam is specified in the following table.1.

| Table 1. Material attributes of COMSOL Simulation design. |
|----------------------------------------------------------|
| **Materials**                | **Young’s Modulus** | **Density** | **Poisons Ratio** |
|--------------------------------|---------------------|-------------|-------------------|
| Gold (Active layer)            | E(T[1/k])           | rho(T[1/k])| nu(T[1/k])        |
| Silicon Nitride (Substrate Layer) | 250e9              | 3100        | 0.23              |
| PolySilicon (Substrate Layer)  | 169e9               | 2320        | 0.22              |

The attributes altered for COMSOL Simulation of Solid Mechanics and Laminar flow analysis are specified in the following table.2.

| Table 2. Attributes altered for COMSOL Simulation. |
|---------------------------------------------------|
| **Attributes Varied**                 | **Solid Mechanics** | **Laminar Flow** |
|---------------------------------------|---------------------|------------------|
| The thickness of the Active Layer     | 0.1 µm – 1.0µm      | -                |
| Pressure % of Lead                    | 10%-100%            | -                |
| Inlet Velocity                        | -                   | 5m/s-50m/s       |

MEMS based Micro-cantilever beam structures signified in Figure.1 are destined to undergo a mechanical displacement under the pressure influence of Mercury and Cadmium ions at their respective operating conditions i.e., 449K for Mercury and 745K for Cadmium ions. The papers constitute shapes like Meander, Fin, and Spiral [10]. The Structural designs employed in my project are inspired by the designs of micro heater. The substrate coat is carried out with Silicon Nitride and PolySilicon and sensing layer coat is carried out with Gold. Pressure has impinged on the surface of the micro-cantilever beam that is anchored at one periphery. The structural pattern is contrived with a geometric width of 100µm and a depth of 30µm for the substrate and sensing layer. The thickness of the active layer is altered from 0.1µm-1.0µm. The micro-cantilever beam structures signified in Figure.1 are designated in the sequence of Upend “G” Shape, Step Shape, Key shape, Spanner shape. The geometrical specifications of respective Micro-cantilever structures are tabulated as follows in Table.3.

| Table 3. Geometrical specifications of micro-cantilever Structures. |
|------------------------------------------------------------------|
| **Structure** | **Surface Area (µm²)** | **Volume (µm³)** |
|----------------|------------------------|-----------------|
| Upend G Shape   | 5540 µm²               | 3637.5 µm³     |
| Steps Shape     | 8312 µm²               | 2200 µm³      |
| Key Shape       | 1338.8 µm²             | 7513 µm³      |
| Spanner Shape   | 1324.7 µm²             | 794.86 µm³   |
2.2. Simulation of Laminar Flow Analysis of Water

Laminar Flow design renders functionality for modelling a static course of fluid in a structure. In Laminar flow, fluid advances smoothly in methodical paths, in contradistinction to turbulent flow. In turbulent flow, the fluid endures aberrant undulations. The velocity and pressure attributes of fluid diverge with the contours and geometry of the structure. To detect Heavy metal: Mercury and Cadmium ions concentration in water, laminar flow analysis is employed. In laminar flow analysis, water is used as a cladding material to perceive the maximal and minimal flow velocity and flow pressure placements. By placing the cantilever beams at maximal pressure placements, the heavy metal: Mercury and Cadmium ions concentration in water (fluid) is quantified. Laminar flow structures signified in Figure.2 are destined to evince the maximal and minimal flow velocity and pressure specifics. The Laminar flow structures signified in Figure.2 are designated in the sequence of Meander, Fin, Spiral, Window, Track, Hollow Two Inlet Structure. The geometrical specifications of respective Laminar flow structures are tabulated as follows in Table.4.

Table 4. Geometrical specifications of Laminar flow structures.

| Structure          | Area (µm²) | Perimeter (µm) |
|--------------------|------------|----------------|
| Meander            | 78200      | 6094           |
| Fin                | 114800     | 9890.9         |
| Spiral             | 300810     | 20927          |
| Window             | 205810     | 15934          |
| Track              | 122630     | 10932          |
| Hollow Two Inlet   | 17266      | 2962.7         |

Figure 1. MEMS based Micro-cantilever structures.
3. Results and Discussion

3.1. Displacement results of MEMS-based micro-cantilever beams

The vapour pressure of Mercury and Cadmium is altered from 10%-100% to quantify the displacement of disparate MEMS-based micro-cantilever beams. In this perusal, the operating temperature is retained constant at 449K for Mercury and 745K for Cadmium and the height of the sensing layer is 1µm. The following table signifies the displacement of disparate MEMS-based micro-cantilever beams for % Pressure variation of Mercury and Cadmium respectively.

The following figure signifies the displacement of micro-Cantilever beams. The following figure and figure signifies the displacement plot of micro-Cantilever beams for % Pressure variation of Mercury and Cadmium respectively. On variation the better structure is found to be “Upend G” and “Step”.

Figure 2. Laminar Flow Structures.
Table 5. Displacement of MEMS-based micro-cantilever beams for % Pressure variation of Mercury at 449K and Cadmium at 745K.

| Pressure percentage of heavy metal ion | Displacement (µm) |
|---------------------------------------|-------------------|
|                                       | Hg2+    | Cd2+    | Hg2+    | Cd2+    | Hg2+    | Cd2+    |
| 10%                                   | 0.0395  | 0.0413  | 3.82E-04| 4.09E-04| 5.52E-05| 5.84E-05|
| 20%                                   | 0.07907 | 0.0827  | 7.64E-04| 8.19E-04| 1.10E-04| 1.17E-04|
| 30%                                   | 0.11861 | 0.1240  | 1.15E-03| 1.23E-03| 1.65E-04| 1.75E-04|
| 40%                                   | 0.15815 | 0.1654  | 1.53E-03| 1.64E-03| 2.21E-04| 2.33E-04|
| 50%                                   | 0.19769 | 0.2067  | 1.91E-03| 2.05E-03| 2.76E-04| 2.92E-04|
| 60%                                   | 0.23723 | 0.2481  | 2.29E-03| 2.46E-03| 3.31E-04| 3.50E-04|
| 70%                                   | 0.27677 | 0.2895  | 2.68E-03| 2.87E-03| 3.86E-04| 4.09E-04|
| 80%                                   | 0.31630 | 0.3308  | 3.06E-03| 3.28E-03| 4.41E-04| 4.67E-04|
| 90%                                   | 0.3558  | 0.3722  | 3.44E-03| 3.69E-03| 4.96E-04| 5.25E-04|
| 100%                                  | 0.3953  | 0.4135  | 3.82E-03| 4.10E-03| 6.52E-04| 5.84E-04|

Figure 3. Displacement of micro-cantilever structures.
Figure 4. Displacement plot of micro-Cantilever beams for % Pressure variation of Mercury at 449K.

Figure 5. Displacement plot of micro-Cantilever beams for % Pressure variation of Cadmium at 745K.
The height of the sensing layer is altered from 0.1µm-1.0µm to quantify the displacement of disparate MEMS-based micro-cantilever beams. In this perusal, the operating temperature is retained constant at 449K for Mercury and 745K for Cadmium and vapour pressure of Mercury and Cadmium is 1000Pa. The following table 6 signifies the displacement of disparate MEMS-based micro-cantilever beams for height variation of the active layer. The following figure 6 and figure 7 signifies the Displacement plot of micro-Cantilever Beams for the height variation of the active layer. On variation the better structure is found to be “Upend G” and “Step shape”.

| Height of Sensing layer (µm) | Displacement (µm) | Upend G | Step | Key | Spanner |
|------------------------------|-------------------|---------|------|-----|---------|
|                              | Hg²⁺ Cd²⁺         | Hg²⁺ Cd²⁺ | Hg²⁺ Cd²⁺ | Hg²⁺ Cd²⁺ | Hg²⁺ Cd²⁺ |
| 0.1 µm                       | 0.7842 0.7940     | 0.0048 0.0049 | 7.30E-04 7.41E-04 | 3.15E-04 3.20E-04 |
| 0.3 µm                       | 0.5608 0.5791     | 0.0045 0.0047 | 6.57E-04 6.84E-04 | 2.86E-04 2.97E-04 |
| 0.5 µm                       | 0.3953 0.4135     | 0.0038 0.0040 | 6.52E-04 5.84E-04 | 2.45E-04 2.59E-04 |
| 0.7 µm                       | 0.2819 0.2971     | 0.0031 0.0038 | 4.55E-04 4.86E-04 | 2.06E-04 2.20E-04 |
| 0.9 µm                       | 0.2054 0.2173     | 0.0025 0.0027 | 3.75E-04 4.03E-04 | 1.73E-04 1.86E-04 |
| 1.0 µm                       | 0.1768 0.1873     | 0.0023 0.0025 | 3.41E-04 3.87E-04 | 1.60E-04 1.72E-04 |

**Figure 6.** Displacement plot of micro-Cantilever beams for height variation of active layer (Mercury at 449K).
3.2. Flow velocity results of Laminar flow structures

The channel inlet flow is varied from 5m/s - 50m/s to quantify the Outlet Flow Velocity and outlet pressure of channel flow of liquid in Laminar flow structures. In this perusal, the operating temperature is retained constant. The following figure 8 signifies the Outlet Flow Velocity of channel flow of liquid in Laminar flow structures designated in the sequence of Meander, Fin, Spiral, Window, Track, Hollow Two Inlet structures.
iii. Spiral  iv. Window

v. Track  vi. Two Inlet Hollow

**Figure 8.** Outlet Flow Velocity of channel flow of liquid in Laminar flow structures.

The following table 7 signifies the channel Outlet Flow Velocity of laminar flow structures for the alteration of channel inlet velocity respectively. The following figure 9 signifies the velocity plot Laminar Flow Structures in variance to channel inlet Velocity. On variation the better structure is found to be “Fin Structure”.
Table 7. Channel Outlet Flow Velocity for the alteration of Channel Inlet Velocity.

| Channel Inlet Velocity (m/s) | Channel Outlet Flow Velocity (m/s) |
|------------------------------|-----------------------------------|
| Meander                      | Fin                               |
| Spiral                       | Window                            |
| Track                        | Hollow Two Inlet                  |
| 5 m/s                        | 26.434                           |
|                              | 41.952                           |
|                              | 15.853                           |
|                              | 6.9934                           |
|                              | 9.4842                           |
|                              | 63.817                           |
| 7 m/s                        | 37.271                           |
|                              | 58.762                           |
|                              | 22.243                           |
|                              | 10.119                           |
|                              | 13.271                           |
|                              | 100.89                           |
| 10 m/s                       | 53.389                           |
|                              | 86.361                           |
|                              | 32.183                           |
|                              | 14.735                           |
|                              | 18.836                           |
|                              | 150.91                           |
| 12 m/s                       | 64.175                           |
|                              | 105.13                           |
|                              | 38.778                           |
|                              | 18.07                            |
|                              | 22.438                           |
|                              | 188.86                           |
| 16 m/s                       | 85.749                           |
|                              | 142.32                           |
|                              | 52.008                           |
|                              | 24.762                           |
|                              | 29.391                           |
|                              | 201.44                           |
| 20 m/s                       | 107.2                            |
|                              | 180.16                           |
|                              | 65.27                            |
|                              | 31.997                           |
|                              | 36.376                           |
|                              | 251.9                            |
| 25 m/s                       | 134.05                           |
|                              | 227.79                           |
|                              | 82.158                           |
|                              | 41.271                           |
|                              | 45.419                           |
|                              | 314.78                           |
| 35 m/s                       | 187.46                           |
|                              | 322.14                           |
|                              | 116.58                           |
|                              | 59.908                           |
|                              | 63.603                           |
|                              | 440.42                           |
| 40 m/s                       | 214.232                          |
|                              | 369.248                          |
|                              | 133.927                          |
|                              | 69.349                           |
|                              | 73.144                           |
|                              | 503.62                           |
| 50 m/s                       | 267.88                           |
|                              | 463.82                           |
|                              | 168.67                           |
|                              | 88.455                           |
|                              | 92.084                           |
|                              | 630.64                           |

Figure 9. Velocity plot of Laminar Flow Structures in variance to channel inlet Velocity.
3.3. Flow pressure results of Laminar flow structures
The following figure 10 signifies the Outlet pressure of channel flow of liquid in Laminar flow structures designated in the sequence of Meander, Fin, Spiral, Window, Track, Hollow Two Inlet structures.

Figure 10. Outlet Pressure of channel flow of liquid in Laminar flow structures.
The following table 8 signifies the channel outlet Pressure of laminar flow structures. The following figure 11 signifies the pressure plot of Laminar Flow Structures in variance to channel inlet Velocity. On variation the better structure is found to be “Fin Structure”.

Table 8. Channel Outlet Flow Velocity for the alteration of Channel Inlet Velocity.

| Channel Inlet Velocity (m/s) | Meander | Fin   | Spiral | Window | Track | Hollow Two Inlet |
|------------------------------|---------|-------|--------|--------|-------|------------------|
| 5 m/s                        | 2.65E+06 | 8.84E+06 | 1.89E+06 | 5.20E+05 | 6.34E+05 | 6.13E+06 |
| 7 m/s                        | 4.41E+06 | 1.59E+07 | 2.94E+06 | 8.21E+05 | 9.82E+05 | 1.39E+07 |
| 10 m/s                       | 7.87E+06 | 3.08E+07 | 4.78E+06 | 1.35E+06 | 1.61E+06 | 2.93E+07 |
| 12 m/s                       | 1.07E+07 | 4.37E+07 | 6.20E+06 | 1.76E+06 | 2.09E+06 | 4.46E+07 |
| 16 m/s                       | 1.78E+07 | 7.63E+07 | 9.54E+06 | 2.71E+06 | 3.21E+06 | 5.04E+07 |
| 20 m/s                       | 2.66E+07 | 1.17E+08 | 1.35E+07 | 3.81E+06 | 4.52E+06 | 7.70E+07 |
| 25 m/s                       | 4.00E+07 | 1.79E+08 | 1.97E+07 | 5.41E+06 | 6.43E+06 | 1.18E+08 |
| 35 m/s                       | 7.48E+07 | 3.42E+08 | 3.57E+07 | 9.38E+06 | 1.12E+07 | 2.26E+08 |
| 40 m/s                       | 9.62E+07 | 4.43E+08 | 4.56E+07 | 1.17E+07 | 1.41E+07 | 2.93E+08 |
| 50 m/s                       | 1.47E+08 | 6.88E+08 | 6.09E+07 | 1.72E+07 | 2.11E+07 | 4.55E+08 |

Figure 11. Pressure plot of Laminar Flow Structures in variance to channel inlet Velocity.

The MEMS-based micro-cantilever structure with superior mechanical displacement is lodged at a maximal pressure locus of laminar flow structures. The pressure quantification at the locus of the micro-cantilever structure is calibrated for Heavy metal: Mercury and Cadmium ions pressure concentration. The channel inlet flow is altered from 5m/s-50m/s to quantify the outlet pressure of
channel flow of liquid. The pressure encountered by the micro-cantilever structure is metamorphosed into pressure percentage of Heavy metal: Mercury and Cadmium ions in water. The following table 9 signifies the pressure percentage of Heavy metal: Mercury and Cadmium ions measured by Upend “G” micro-cantilever beam lodged at maximal pressure locus of Fin Laminar structure.

**Table 9.** Pressure % plot of Mercury and Cadmium ions by Upend “G” micro-cantilever beam lodged at maximal pressure locus of Fin Laminar structure.

| Channel Inlet Velocity (m/s) | Pressure % measured by Upend “G” and Fin Laminar Structure |
|------------------------------|-------------------------------------------------------------|
| 5 m/s                        | Mercury 2.24E+09 % Cadmium 2.14E+09 %                     |
| 7 m/s                        | Mercury 4.03E+09 % Cadmium 3.85E+09 %                     |
| 10 m/s                       | Mercury 7.80E+09 % Cadmium 7.46E+09 %                     |
| 12 m/s                       | Mercury 1.11E+10 % Cadmium 1.06E+10 %                     |
| 16 m/s                       | Mercury 1.93E+10 % Cadmium 1.85E+10 %                     |
| 20 m/s                       | Mercury 2.96E+10 % Cadmium 2.83E+10 %                     |
| 25 m/s                       | Mercury 4.53E+10 % Cadmium 4.33E+10 %                     |
| 35 m/s                       | Mercury 8.66E+10 % Cadmium 8.28E+10 %                     |
| 40 m/s                       | Mercury 1.12E+11 % Cadmium 1.07E+11 %                     |
| 50 m/s                       | Mercury 1.74E+11 % Cadmium 1.67E+11 %                     |

The following graph 7 signifies the Pressure % plot of Mercury and Cadmium ions by Upend “G” micro-cantilever beam lodged at maximal pressure locus of Fin Laminar structure.

**Figure 12.** Pressure % plot of Mercury and Cadmium ions by Upend “G” micro-cantilever beam lodged at maximal pressure locus of Fin Laminar structure.
4. Conclusion
MEMS-based micro-cantilever beam structures were devised and the mechanical displacement for disparate percentage pressures of heavy metal: Mercury and Cadmium ions is analyzed. The displacement plots of disparate micro-Cantilever Beams for % Pressure variation of Mercury at 449K and % Pressure variation of Cadmium at 745K were evaluated and the structure with superior mechanical displacement is found to be Upend “G” for Mercury ion pressure and Cadmium ion pressure. Multiple Laminar flow structures were designed for Laminar flow analysis with divergent channel inlet flow. On altering the channel inlet flow, Outlet Flow and pressure attributes of laminar flow structures is analyzed. The velocity and pressure plots of disparate Laminar flow structures for channel flow variation of water were evaluated and the structure that renders the superior pressure is figured out to be “Fin Structure”. The MEMS-based micro-cantilever structure with superior mechanical displacement is lodged at a maximal pressure locus of laminar flow structures. The pressure encountered by the micro-cantilever structure is metamorphosed into pressure percentage of Heavy metal: Mercury and Cadmium ions in water.

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