# Analytical Modelling of Microfluidic Cantilever Sensor with Evaporating Ethanol

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## ABSTRACT

Resonating microcantilevers are increasingly used for a broad range of ultra-sensitive biochemical sensing applications wherein a shift in the resonant frequency is used to detect minute changes in the cantilever mass. An extension of this technique has been realized using integrated microfluidic cantilevers wherein the resnonace shift is due to changes in fluid mass within an internal microchannel. In this paper, we develop computational models for predicting the behavior of microfluidic microcantilever sensors and validate the models using experimental data based on the evaporation of ethanol. Two computational models are presented, a one-dimensional structural beam element model and a three-dimensional finite-element structural dynamic model. The numerically predicted increase in the resonant frequencies due to a decrease in ethanol mass correlates well with experimental data. The models enable proof-of-concept studies and the rational design of novel microfluidic microcantilever biochemical sensing systems.

***Keywords***: microfluidic cantilever, biosensing, modal analysis, finite element method

## 1 INTRODUCTION

In many industries such as petrochemical, pharmaceutical, and biomedical, there is a need to accurately determine the evaporation rate of volatile liquids. Of particular interest is the evaproation rate of ethanol, one of the most important and widely used cleaning reagents in day-to-day applications. While various techniques to measure evaporation rates of minute liquid samples have been reported [1], [2], [3], resonant microstructures enable relatively low-cost, reliable and ultra-sensitive solutions for such applications.

A vibrating microstructure can be designed with a sharp narrow-band resonace that is ultra-sensitive to changes in mass. Specifically, in resonating microcantilevers, a shift in the frequency can be used to measure changes in mass down to the level of a single virus. Understanding the dependence of the resonant mode frequencies on the changing mass is essential for improving sensitivity and selectivity of the device. We have developed two distinct numerical models to predict the resonant behavior of microfluidic microcantilevers that contain an internal flow-through microchannel: a one-dimensional structural beam element model and a three-dimensional finite-element structural dynamic model. The models are based on finite-element analysis (FEA) and are validated using data from experiments that are designed to meassure the evaportation of ethanol from within the channel. To simplify the analysis, ethanol is modeled as an elastic material with a very low Young's modulus, relative to that of the cantilever. To determine the sensitivity of the resonant frequency to the contained ethanol mass, ethanol is removed from the microchannel and the resnonant frequency is recalculated. Although the models do not calculate the evaporation rate of ethanol, they provides a frequency vs. unloaded mass dataset, which can be used to tune the sensitivity of the microcantilever. We show that the predicted data are within 5% of the corresponding measured values. Both models are useful for rational design of microfluidic micromechanical sensors and will be discussed in the following sections.

## 2 EXPERIMENTAL MEASUREMENT

We have employed a resonating microfluidic cantilever (MC516, Fourien Inc. Canada) system to measure the sensitivity of the resonant frequency to an evaporating ethanol with volume as small as *4.8 pL*. The cantilever consists of an enclosed microfluidic channel structure (with a U-shaped turn around for flow) bonded to an ultrathin rounded microbeam on top of cantilever base (**Figs. 1 and 2**). Both the cantilever channel walls and the cantilever base are made of low stress silicon-rich silicon nitride Unlike other techniques, where a sample is exposed to the ambient environment, the ethanol sample is confined by the microchannel, and exposed only at the inlet to allow for evaporation. The presence of an enclosed channel facilitates consistent measurements by reducing the effects of ambient conditions such as temperature and pressure. Silicon nitride is hydrophobic, therefore the ethanol sample can be conveniently loaded into the channel just through capillary forces. The relevant mechanical properties of silicon-rich silicon nitride are as follows: modulus of elasticity $E = 224$ $GPa$ and Poisson ratio $v = 0.25$. **Figure 1** shows a diagram of a single clamped microcantilever used for the experiment. The length and width of the cantilever are $500\ \mu m$ and $44$ $\mu m$, respectively. The width and height of the microchannel

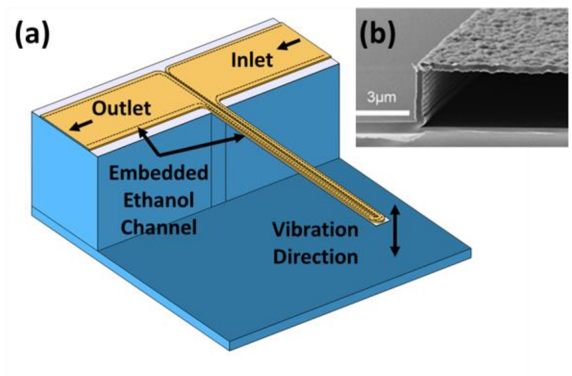


**Figure 1**: (a) 3D illustration of a microfluidic cantilever with an embedded microfluidic channel, (b) scanning electron microscope image of part of the cross section of the microchannel.

are *17 μm* and *3 μm*, respectively. The thickness of the channel walls is 0.5 *μm*.

Measurements were taken with the microfluidic cantilever operating in a vacuum level of $5.2\times10^{-5}$ *mbar*. The resonant frequency of the cantilever is measured through a laser Doppler vibrometer (LDV, Polytec, Germany). The LDV facilitates a continuous measurement of the resonance frequency while the sample evaporates through the microchannel. In order to improve signal to noise ratio, the cantilever is mechanically excited by a piezoelectric actuator.

The resonant frequency of the cantilever is at first continuously sampled by the LDV when the channel is empty and open to ambient air. The objective here is to identify its first four vibrational modes, i.e. the lowest frequency harmonics. Thus, during the experiment, the cantilever is separately excited at each of these modes, as demonstrated in **Fig. 2**. The nodal points of each modal shape are sequentially marked from *N1* to *N14*, along the length of the channel.

The microchannel is then filled with ethanol in order to investigate the sensitivity of the resonant frequency to the fluid mass inside. The additional mass of the ethanol causes a decrease in the resonance frequency. For example, in the first vibrational mode, the corresponding frequency $f_1$ decreases from a maximum of *31.62 kHz* for an empty channel to *25.76 kHz* for an ethanol filled channel. When the inlet of the channel is opened to the ambient air while the outlet is sealed, the ethanol gradually evaporates. The resonant frequency is continuously measured during evaporation and is observed to increase as the fluid mass decreases. This procedure is repeated for each of the four vibrational modes. An analogous trend is observed for all four frequecies $f_1$ to $f_4$. As the meniscus retracts from the inlet into the microchannel, it encounters the vibrational nodal regions shown in **Fig. 2**, where changes in the fluid mass cannot affect the resonant frequency. The effect of ethanol mass on the mode shapes is so small that the position of nodal points remains practically unchanged during evaporation.

# 3 MODAL ANALYSIS

We used our computational models to predict the eigenfrequencies and eigenmodes of the microfluidic microcantilever. In these models, the domain is discretized into a collection of elements. The governing equations along with boundary conditions are transformed and solved as a system of algebraic equations. As noted, we employ we employ two distinct models: a one-dimensional (1D) Euler-Bernoulli structural beam model using MATLAB, and a three-dimensional (3D) solid element numerical model in the COMSOL multiphysics program (www.comsol.com). The former is convenient and computationally inexpensive, while the latter provides more accurate results, at the expense of longer computational time. For simplicity, we neglect the effect of ethanol removal on the lateral movement of the cantilever. For this purpose, in the three-dimensional COMSOL model, we constrain the out-of-plane movements of the vertical mid-plane of microfluidic cantilever. This enables modeling only half of the system by imposing a symmetry boundary condition at the center of the microflidic cantilever along its lengh. This is crucial to reduce the computational cost.

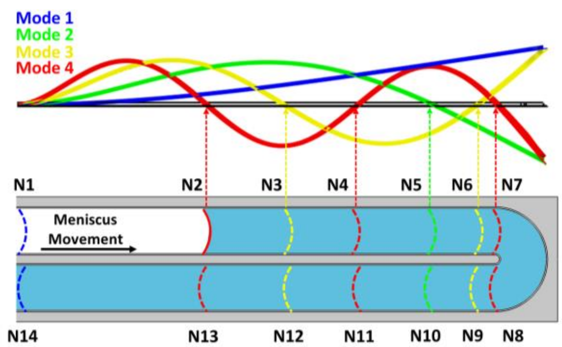


**Figure 2**: Top down view of the microfluidic cantilever channel and an illustration of different resonance modes, with their corresponding nodal points along the length of the cantilever.

## 3.1 Euler-Bernoulli Beam Element Model

A 1D finite element beam model based on Euler-Bernouli classical beam theory is used to analyze the free vibration of the cantilever beam. This approach simplifies the elasticity approach for a 1D beam with small deformations in the vertical direction [4].

For isotropic materials, the independent elastic constants are the bulk Young's modulus *E*, and Poisson's ratio ν. Using Hamilton's principle, the finite element formulation for the free vibration of the beam is obtained as

$$\mathbf{M}\frac{d^2\mathbf{U}}{dt^2}+\mathbf{KU}=0 \tag{1}$$

where **K**, **M**, and **U** denote the global stiffness matrix, the mass matrix, and the displacement vector, respectively. In order to account for the effect of ethanol in the model, it


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should be included in the beam element wherever it exists inside the channel. Since ethanol is not an elastic material, it does not affect the stiffness matrix of the element. However, the mass matrix of every element in the regions filled with ethanol would change due to the additional mass.

A custom MATLAB code was implemented to solve the eigenvalue problem defined by Equation (1). We found that *400* beam elements were needed to achieve sufficient accuracy using the beam element method.

## 3.2 Three-Dimensional Finite Element Model

The 3D numerical model was implemented using the COMSOL Multiphysics 5.3a program (www.comsol.com). Specifically, the Solid Mechanics module was used to solve the governing elastodynamic partial differential equations. For this analysis, the computational domain is discretized using three-dimensional hexahedral elements for the straight section and prism elements around the rounded portion of the channel. Note that each node has three translational degrees of freedom. As previously discussed, in order to simplify the analysis, any out-of-plane modes are avoided by restricting the lateral motion of the cantilever. Thus, to reduce memory and solution time, the model represents only half of the microfluidic cantilever in the lateral direction to take advantage of the cantilever symmetry. Since the flowing effect of ethanol in the channel is negligible, it is modeled as an elastic solid material with a Young's modulus several orders of magnitude lower relative to the silicon nitride cantilever material. This simplification is justifiable because the resonance frequencies of the cantilever are most sensitive to the mass of the ethanol inside the channel, rather than to the viscous effects of the fluid interacting with the silicon nitride channel. The model assumes a constant evaporation rate, i.e. a constant decrease of the ethanol mass.

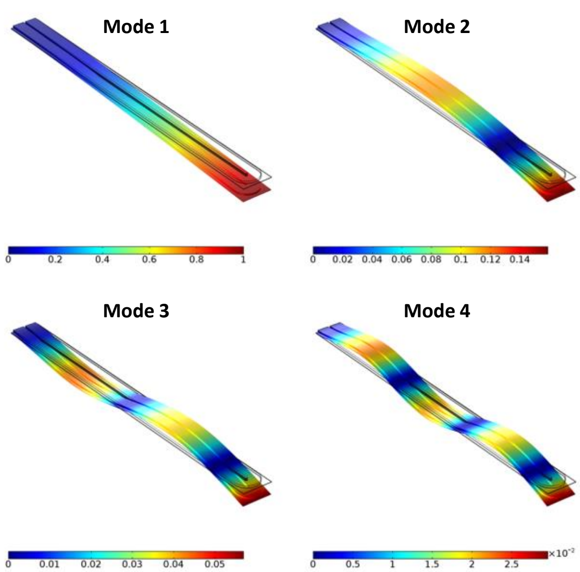


**Figure 3**: Deformation of each resonant mode, relative to the largest deformation in Mode 1 as calculated by COMSOL.

## 4 RESULTS AND DISCUSSION

As mentioned above, we analyzed the first four modes of vibration corresponding to the lowest eignfrequencies. The corresponding modal shapes produced by COMSOL are shown in **Fig. 3**. The cantilever experiences its lowest resonant frequency for each mode when it is fully filled because of the additional mass of ethanol present in the microchannel. As the ethanol mass is removed, the resonant frequencies increase, but there is a negligible change in the modal shapes which are shown in **Fig. 3**.

The frequencies of these first four modes are presented in **Table 1**. The first set of data corresponds to the fully filled cantilever before the evaporation starts, and the second set represents the frequencies of the empty cantilever, after the evaporation has ended. The simulation results are in excellent agreement with experimental data, especially for the 3D COMSOL model. The highest error corresponds to the results from the one-dimensional analysis for the fully filled case. This is likely because there is no shear deformation in the simplified model and the mass distribution of ethanol is non-symmetric with respect to the neutral axis of the beam.

| | **Experiment** ($kHz$) | **1D FEM** ($kHz$) | **3D COMSOL** ($kHz$) |
|---|---|---|---|
| **Fully Filled Channel** | | | |
| $f_1$ | 25.7 | 26.9 | 25.2 |
| $f_2$ | 160.7 | 168.7 | 157.5 |
| $f_3$ | 446.4 | 472.4 | 437.6 |
| $f_4$ | 865.0 | 925.4 | 847.6 |
| **Empty Channel** | | | |
| $f_1$ | 31.6 | 30.7 | 30.6 |
| $f_2$ | 160.7 | 192.3 | 190.6 |
| $f_3$ | 446.4 | 538.2 | 529.5 |
| $f_4$ | 865.0 | 1,054.4 | 1025.7 |

**Table 1**: Resonant frequencies for fully filled vs empty microfluidic cantilever.

**Figure 4** illustrates the change in the modal frequencies with respect to the percentage of the removed mass of ethanol during the evaporation process. The three sets of data in each plot correspond to the experimental evaporation, and two numerical simulations, respeciively. As expected, the COMSOL simulation produces the most accurate results. It is noteworthy that the error in the results from the 1D model decreases as the ethanol evaporates. This is because the non-symmetric distribution of the ethanol mass with respect to the neutral axis of the beam model becomes less significant.

Since the ethanol evaporates from the inlet of the channel, its meniscus travels from the inlet to the outlet (**Fig. 2**). The labels *N1* to *N14* on the evaporating profiles in Fig. 4 shows the points at which the meniscus reaches each

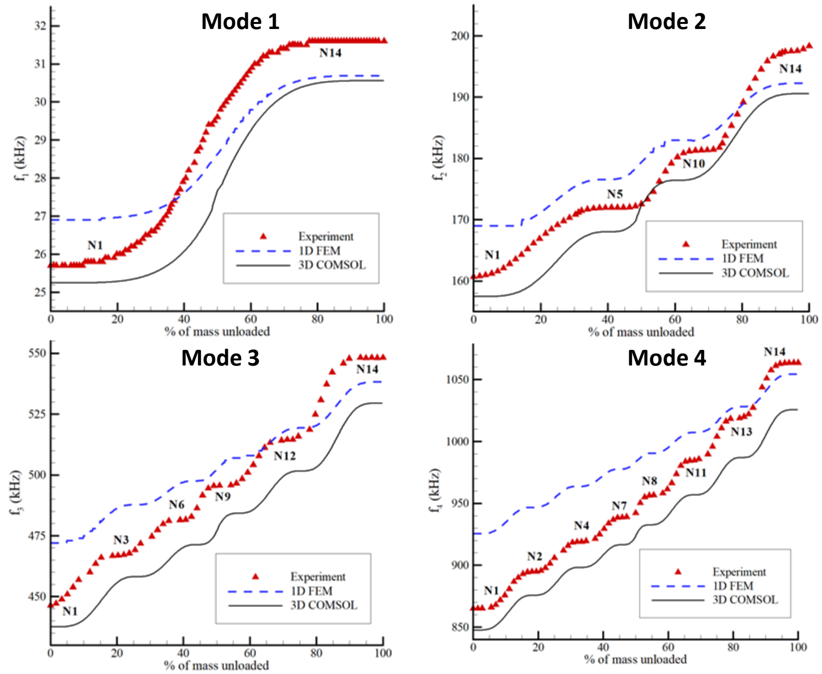


**Figure 4**: Changes in the resonant modal frequencies of the cantilever as ethanol evaporates in the channel.

node.The rate of change in the frequencies are analogous for all modes as the slopes of the profiles are very similar for each set of data. However, each subsequent mode contains additional nodal points where the meniscus is not able to affect the resonant frequency (**Fig. 3**); this is reflected by the additional flat regions in **Fig. 4**.

When the cantilever is vibrating at its first mode, only one slope is shown in its evaporating profile (**Fig. 4**)**,** while for the second mode, three sloped regions are created by the evaporation frequencies. The first region from *N1* to *N5*, the second between *N5* and *N10* and the third region from *N10* to *N14*. One can recognize five regions for $f_3$ and the number of regions increase to seven for $f_4$. Each of these regions are directly related to the distances between the nodal points for every vibrating mode. This can be explained by the ethanol meniscus moving along the microchannel. As the meniscus reaches each node, the cantilever does not feel mass unloading. This is because the vibrational amplitude of the cantilever is almost zero and any mass present at that point does not affect the resonance frequency of the cantilever. Although, as meniscus of the evaporating liquid moves inward into the channnel, the change in mass starts to affect the resonance frequency again, which is marked as the start of the next region. Note that for each node, although the amplitude of the cantilever deflection is ideally zero along a 2D plane (marked by flat lines in **Fig. 4**), in reality, the resonance frequency is insensitive for a finite region (colroed dark blue in **Fig. 3**). In the nodal regions along the microchannel, the vibrational amplitude is so small that cannot affect the resonant frequency. It should be noticed that for higher frequencies with more number of nodes, the nodal regions are smaller.

As previously mentiond, the model is based on a constant decrease rate of ethannol mass during the evaporation time. The good correlation with the experimental data shows that the model is capable of predicting the evaporation rate quite accurately.

## 5 CONCLUSION

The natural frequencies of a microfluidic microcantilever containing evaporating ethanol are predicted using a simplified 1D Euler-Bernoulli beam model and a 3D COMSOL model. The simulation results are validated using experimental data. These models can be used for the rational design of novel ultrasensitive hybrid microfluidic micromechanical resonance-based sensors for a broad range of applications.

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