SAW Gas Sensor

Introduction

A surface acoustic wave (SAW) is an acoustic wave propagating along the surface of a solid material. Its amplitude decays rapidly, often exponentially, with the depth of the material. SAWs are featured in many kinds of electronic components, including filters, oscillators, and sensors. SAW devices typically use electrodes on a piezoelectric material to convert an electric signal to a SAW, and back again.

In this model, you investigate the resonance frequencies of a SAW gas sensor. The sensor consists of an interdigitated transducer (IDT) etched onto a piezoelectric $LiNbO_3$ (lithium niobate) substrate and covered with a thin polyisobutylene (PIB) film. The mass of the PIB film increases as PIB selectively adsorbs CH_2Cl_2 (dichloromethane, DCM) in air. This causes a shift in resonance to a slightly lower frequency.

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Model Definition

Figure 1 shows a conceptual view of the gas sensor in this model.

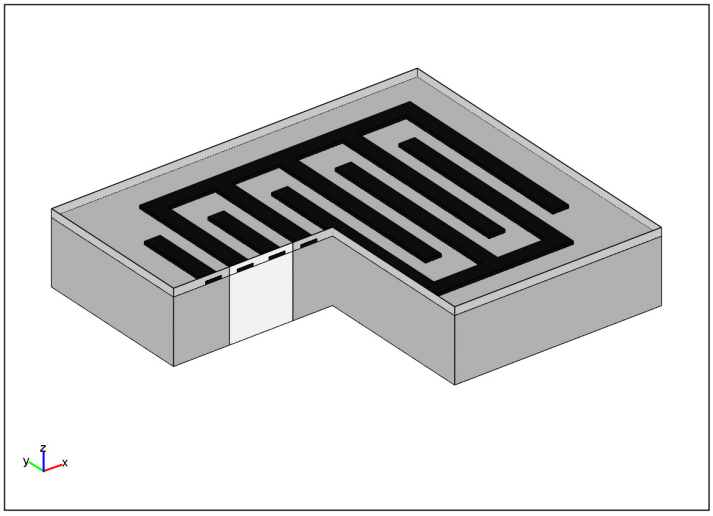

Figure 1: SAW gas sensor, showing the IDT electrodes (in black), the thin PIB film (light gray), and the $LiNbO_3$ substrate (dark gray). For the sake of clarity, the dimensions are not to scale and the IDT has fewer electrodes than in common devices. A slice of the geometry is removed to reveal the modeled unit cell (in white).

IDTs used in SAW devices may have hundreds of identical electrodes, and each electrode can be about 100 times longer than it is wide. You can therefore neglect the edge effects and reduce the model geometry to the periodic unit cell shown in Figure 2. The height of this cell does not have to extend all the way to the bottom of

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the substrate but only a few wavelengths down, so that the SAW has almost died out at the lower boundary. In the model, this boundary is fixed to a zero displacement.

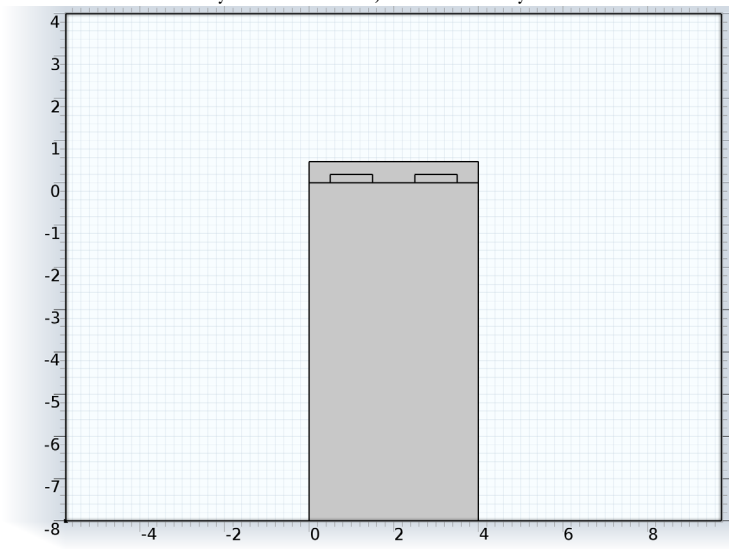

Figure 2: The modeled geometry of the model. A 500 nm PIB film covers two 1 μm-wide electrodes on top of the $LiNbO_3$ substrate. The substrate domain has a total height of 22 μm.

Set up the model using the predefined physics interface Piezoelectric Devices. Use the Plane Strain approximation so that the out-of-plane strain component is zero. This should be a valid assumption, considering that the SAW is generated in the model plane, and that the sensor is thick in the out-of-plane direction.

Use periodic boundary conditions to dictate that the electric potential and displacements be the same along both vertical boundaries of the geometry. This implies that the wavelength will be an integer fraction of the width of the geometry. The lowest SAW eigenmode has its wavelength equal to the width of the geometry, 4 μm. The eigenfrequency of this mode multiplied by 4 μm hence gives the velocity of the wave.

The substrate used in the simulation is YZ-cut $LiNbO_3$ with the following properties (cited in Ref. 2):

- *The Elasticity matrix:*

$$\begin{bmatrix} 2.424e11 & 0.752e11 & 0.752e11 & 0 & 0 & 0 \\ & 2.03e11 & 0.573e11 & 0 & 0.085e11 & 0 \\ & & 2.03e11 & 0 & -0.085e11 & 0 \\ & & & 0.752e11 & 0 & 0.085e11 \\ & & & & 0.595e11 & 0 \\ & & & & & 0.595e11 \end{bmatrix}$$

- *Coupling matrix:*

$$\begin{bmatrix} 1.33 & 0.23 & 0.23 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2.5 & 0 & 3.7 \\ 0 & -2.5 & 2.5 & 0 & 3.7 & 0 \end{bmatrix}$$

- *Relative permittivity:*

$$\begin{bmatrix} 28.7 & 0 & 0 \\ & 85.2 & 0 \\ & & 85.2 \end{bmatrix}$$

The density of the PIB film is from Ref. 1. The Poisson's ratio is taken to be 0.48, which corresponds to a rather rubbery material. The Young's modulus is set to 10 GPa. Even at the comparatively high frequencies considered in this model, this is likely an overestimation. However, a much lower value would result in a multitude of eigenmodes located inside the film. While those may be important to consider in designing a SAW sensor, the focus in this model is on the SAW modes.

The adsorption of DCM gas is represented as a slight increase of the density of the PIB film. In the third and final version of the model, the sensor is exposed to 100 ppm of DCM in air at atmospheric pressure and room temperature. The "partial density" of DCM in the PIB film is then calculated as

$$\rho_{\mathrm{DCM,PIB}} = KMc\,,$$

where $K = 10^{1.4821}$ (Ref. 1) is the air/PIB partition coefficient for DCM, M is its molar mass, and

$$c = 100 \cdot 10^{-6} \cdot p/(RT)$$

is its concentration in air. Any effects of the DCM adsorption on the material properties other than the density are neglected.

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Results and Discussion

The presence of the aluminum IDT electrodes and the PIB film cause the lowest SAW mode to split up in two eigensolutions, the lowest one representing a series resonance, where propagating waves interfere constructively and the other one a parallel ("anti-") resonance, where they interfere destructively. These two frequencies constitute the edges of the stopband, within which no waves can propagate through the IDT.

The resonance and anti-resonance frequencies evaluate to approximately 839 MHz and 849 MHz, respectively. Figure 3 and Figure 4 show the corresponding SAW modes. Figure 5 and Figure 6 show the electric potential distribution characteristics for these solutions.

Exposing the sensor to a 100 ppm concentration of DCM in air leads to a resonance frequency shift of approximately 200 Hz downwards. This is computed by evaluating the resonance frequency before and after increasing the density of adsorbed DCM to that of the PIB domain.

Note that the computational mesh is identical in both these solutions. This implies that the relative error of the frequency shift is similar to that of the resonance frequency itself. Thus the shift is accurately evaluated despite being a few magnitudes smaller than the absolute error of the resonance frequency.

In a real setup, the drift is often measured by mixing the signal from a sensor exposed to a gas with a reference signal from one protected from the gas. The beat frequency then gives the shift.

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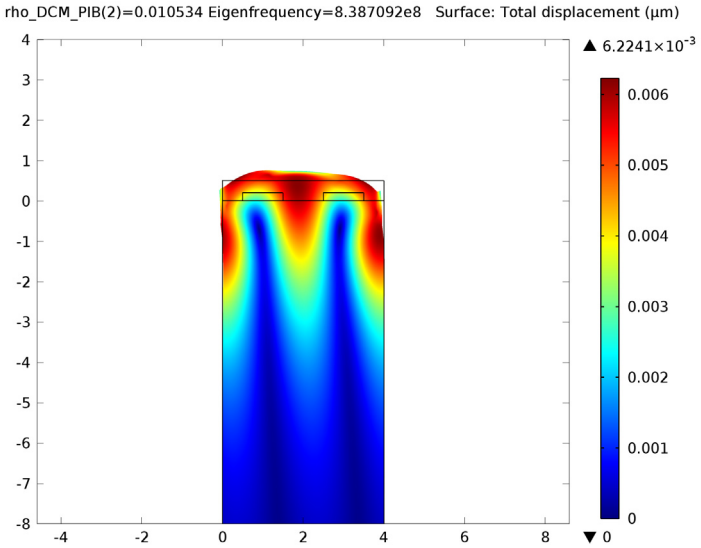

Figure 3: Deformed shape plot of the resonance SAW mode.

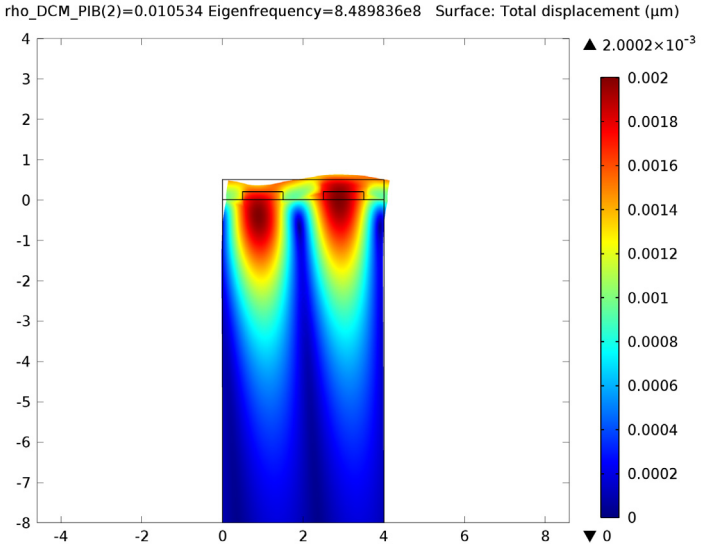

Figure 4: Deformed shape plot of the anti-resonance SAW mode.

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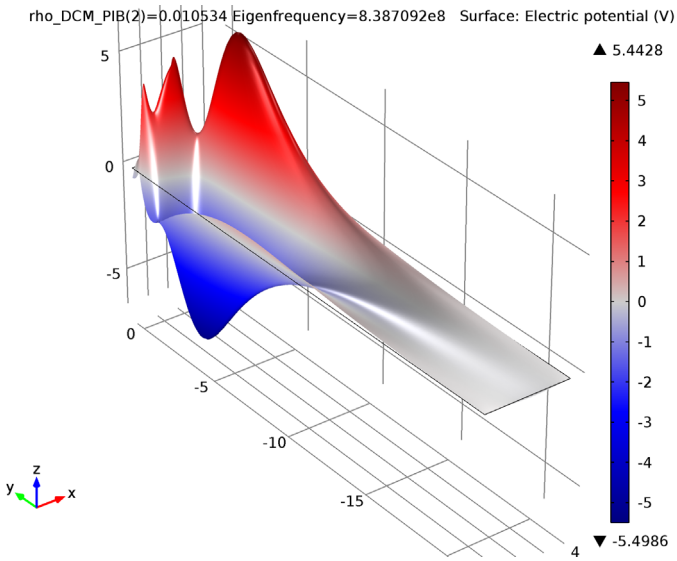

Figure 5: Electric potential distribution and deformations at resonance, symmetric with respect to the center of each electrode.

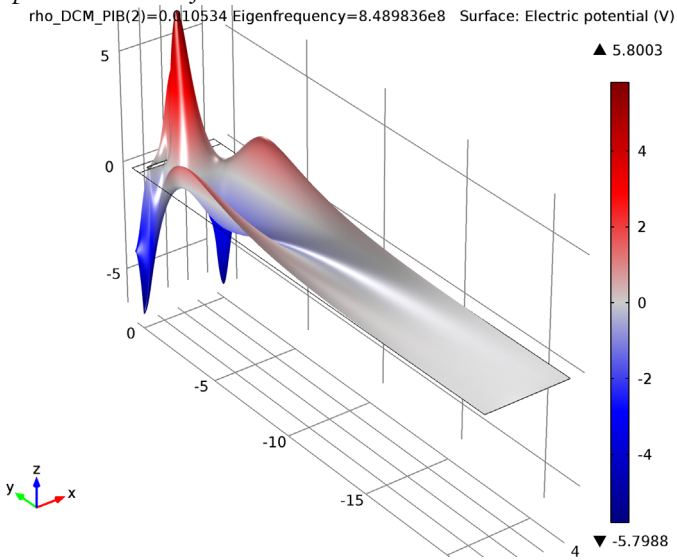

Figure 6: Electric potential distribution at anti-resonance, anti-symmetric with respect to the center of each electrode.

References

1. K. Ho and others, "Development of a Surface Acoustic Wave Sensor for In-Situ Monitoring of Volatile Organic Compounds", *Sensor*s vol. 3, pp. 236–247, 2003.

2. Ahmadi and others, "Characterization of Multi- and Single-layer Structure SAW Sensor", *Sensors 2004*, *Proceedings of IEEE*, vol. 3, pp. 1129–1132, 2004.

Model Library path: `MEMS_Module/Sensors/saw_gas_sensor`

Modeling Instructions

MODEL WIZARD

1 Go to the **Model Wizard** window.

2 Click the **2D** button.

3 Click **Next**.

4 In the **Add physics** tree, select **Structural Mechanics>Piezoelectric Devices (pzd)**.

5 Click **Next**.

6 Find the **Studies** subsection. In the tree, select **Preset Studies>Eigenfrequency**.

7 Click **Finish**.

GLOBAL DEFINITIONS

For quicker modeling, load the parameters from a file.

Parameters

1 In the **Model Builder** window, right-click **Global Definitions** and choose **Parameters**.

2 In the **Parameters** settings window, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Model Library folder and double-click the file `saw_gas_sensor_parameters.txt`.

GEOMETRY 1

1 In the **Model Builder** window, under **Model 1** click **Geometry 1**.

2 In the **Geometry** settings window, locate the **Units** section.

3 From the **Length unit** list, choose **μm**.

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Rectangle 1

1 Right-click **Model 1>Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

3 In the **Width** edit field, type `4`.

4 In the **Height** edit field, type `22.5`.

5 Locate the **Position** section. In the **y** edit field, type `-22`.

Rectangle 2

1 In the **Model Builder** window, right-click **Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

3 In the **Width** edit field, type `4`.

4 In the **Height** edit field, type `0.5`.

Rectangle 3

1 Right-click **Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

3 In the **Width** edit field, type `1.0`.

4 In the **Height** edit field, type `0.2`.

5 Locate the **Position** section. In the **x** edit field, type `0.5`.

Rectangle 4

1 Right-click **Geometry 1** and choose **Rectangle**.

2 In the **Rectangle** settings window, locate the **Size** section.

3 In the **Width** edit field, type `1`.

4 In the **Height** edit field, type `0.2`.

5 Locate the **Position** section. In the **x** edit field, type `2.5`.

6 Right-click **Geometry 1** and choose **Build All**.

DEFINITIONS

In the **Model Builder** window, expand the **Model 1>Definitions** node.

Axis

1 In the **Model Builder** window, expand the **Model 1>Definitions>View 1** node, then click **Axis**.

2 In the **Axis** settings window, locate the **Axis** section.

3 In the **x minimum** edit field, type `-4`.

4 In the **y minimum** edit field, type `-8`.

5 In the **x maximum** edit field, type `8`.

6 In the **y maximum** edit field, type `4`.

7 Click the **Apply** button.

PIEZOELECTRIC DEVICES

Linear Elastic Material 1

1 In the **Model Builder** window, under **Model 1** right-click **Piezoelectric Devices** and choose **Linear Elastic Material**.

2 Select Domains 2–4 only.

Electrical Material Model 1

1 In the **Model Builder** window, right-click **Piezoelectric Devices** and choose **Electrical Material Model**.

2 Select Domain 2 only.

MATERIALS

Material 1

1 In the **Model Builder** window, under **Model 1** right-click **Materials** and choose **Material**.

2 Right-click **Material 1** and choose **Rename**.

3 Go to the **Rename Material** dialog box and type `LiNbO3` in the **New name** edit field.

4 Click **OK**.

5 In the **Material** settings window, locate the **Geometric Entity Selection** section.

6 Click **Clear Selection**.

7 Select Domain 1 only.

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8 Locate the **Material Contents** section. In the table, enter the following settings:

Property	Name	Value
Elasticity matrix (Ordering: xx, yy, zz, yz, xz, xy)	cE	`{2.424e11, 0.752e11, 2.03e11, 0.752e11, 0.573e11, 2.03e11, 0[Pa], 0[Pa], 0[Pa], 0.752e11, 0[Pa], 0.085e11, -0.085e11, 0[Pa], 0.595e11, 0[Pa], 0[Pa], 0[Pa], 0.085e11, 0[Pa], 0.595e11}`
Coupling matrix (Ordering: xx, yy, zz, yz, xz, xy)	eES	`{1.33, 0, 0, 0.23, 0, -2.5, 0.23, 0, 2.5, 0, -2.5, 0, 0, 0, 3.7, 0, 3.7, 0}`
Relative permittivity	epsilonrS	`{28.7, 85.2, 85.2}`
Density	rho	`4647`

Note: Alternatively, you can click the **Edit** button below the **Output properties** table and use the matrix inputs to enter `cE`, `e`, and `epsilonrS` according to the material data shown under the **Model Definition** section.

Material 2

1 In the **Model Builder** window, right-click **Materials** and choose **Material**.

2 Right-click **Material 2** and choose **Rename**.

3 Go to the **Rename Material** dialog box and type `PIB` in the **New name** edit field.

4 Click **OK**.

5 Select Domain 2 only.

6 In the **Material** settings window, locate the **Material Contents** section.

7 In the table, enter the following settings:

Property	Name	Value
Young's modulus	E	`E_PIB`
Poisson's ratio	nu	`nu_PIB`
Density	rho	`rho_PIB+rho_DCM_PIB`
Relative permittivity	epsilonr	`eps_PIB`

Material Browser

1 From the **View** menu, choose **Material Browser**.

2 In the **Material Browser** settings window, In the tree, select **Built-In>Aluminum**.

3 Click **Add Material to Model**.

Aluminum

Select Domains 3 and 4 only.

PIEZOELECTRIC DEVICES

Fixed Constraint 1

1 In the **Model Builder** window, under **Model 1** right-click **Piezoelectric Devices** and choose the boundary condition **Structural>Fixed Constraint**.

2 Select Boundary 2 only.

The eigenfrequencies do not depend on the values of the potential, and therefore neither does the stop band. In fact, for linear eigenfrequency problems, the potential is automatically set to zero at the electrodes regardless of the applied values.

Ground 1

1 In the **Model Builder** window, right-click **Piezoelectric Devices** and choose the boundary condition **Electrical>Ground**.

2 Select Boundaries 6–9 and 12 only.

Periodic Condition 1

1 Right-click **Piezoelectric Devices** and choose **Periodic Condition**.

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2 Select Boundaries 1, 3, 16, and 17 only.

By default, the periodicity type is set to continuity for all dependent variables.

MESH 1

Size

1 In the **Model Builder** window, under **Model 1** right-click **Mesh 1** and choose **Free Quad**.

2 In the **Size** settings window, locate the **Element Size** section.

3 From the **Predefined** list, choose **Extremely fine**.

Size 1

1 In the **Model Builder** window, under **Model 1>Mesh 1** right-click **Free Quad 1** and choose **Size**.

2 In the **Size** settings window, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundaries 4, 7, 8, 10, 12, 13, and 15 only.

5 Locate the **Element Size** section. Click the **Custom** button.

6 Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.

7 In the associated edit field, type `0.05`.

8 Click the **Build All** button.

STUDY 1

Set up a parametric sweep with respect to the amount of adsorbed species on the sensor, and search for eigenfrequencies near 850 MHz.

Parametric Sweep

1 In the **Model Builder** window, right-click **Study 1** and choose **Parametric Sweep**.

2 In the **Parametric Sweep** settings window, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter names	Parameter value list
rho_DCM_PIB	`0 K*M_DCM*c_DCM_air`

Step 1: Eigenfrequency

1 In the **Model Builder** window, under **Study 1** click **Step 1: Eigenfrequency**.

2 In the **Eigenfrequency** settings window, locate the **Study Settings** section.

3 In the **Desired number of eigenfrequencies** edit field, type `2`.

4 In the **Search for eigenfrequencies around** edit field, type `8.5e8`.

5 In the **Model Builder** window, right-click **Study 1** and choose **Compute**.

RESULTS

Displacement (pzd)

The default plot shows the total displacement for an eigenmode near 837 MHz. Switch to the resonance SAW mode near 839 MHz:

1 In the **2D Plot Group** settings window, locate the **Data** section.

2 From the **Eigenfrequency** list, choose **8.387092e8**.

Adjust the deformed shape plot to see the effect of the wave localization near the surface.

3 In the **Model Builder** window, expand the **Results>Displacement (pzd)>Surface 1** node, then click **Deformation**.

4 In the **Deformation** settings window, locate the **Scale** section.

5 Select the **Scale factor** check box.

6 In the associated edit field, type `100`.

7 Click the **Plot** button.

Compare the resulting plot to that in Figure 3.

1 In the **Model Builder** window, click **Displacement (pzd)**.

2 In the **2D Plot Group** settings window, locate the **Data** section.

3 From the **Eigenfrequency** list, choose **8.489836e8**.

4 Click the **Plot** button.

This reproduces the plot shown in Figure 4.

To visualize the electric potential distribution for the eigenmodes, follow these steps:

Potential (pzd)

1 In the **Model Builder** window, under **Results** click **Potential (pzd)**.

2 In the **2D Plot Group** settings window, locate the **Data** section.

3 From the **Eigenfrequency** list, choose **8.387092e8**.

4 In the **Model Builder** window, under **Results>Potential (pzd)>Surface 1** click **Deformation**.

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5 In the **Deformation** settings window, locate the **Scale** section.

6 Select the **Scale factor** check box.

7 In the associated edit field, type 1.

8 In the **Model Builder** window, under **Results>Potential (pzd)** click **Surface 1**.

9 In the **Surface** settings window, locate the **Coloring and Style** section.

10 From the **Color table** list, choose **Wave**.

11 Right-click **Results>Potential (pzd)>Surface 1** and choose **Height Expression**.

12 In the **Model Builder** window, click **Potential (pzd)**.

13 In the **2D Plot Group** settings window, locate the **Data** section.

14 From the **Eigenfrequency** list, choose **8.489836e8**.

15 Click the **Plot** button.

Derived Values

To see all computed eigenfrequencies as a table, follow these steps:

1 In the **Model Builder** window, under **Results** right-click **Derived Values** and choose **Global Evaluation**.

2 In the **Global Evaluation** settings window, locate the **Data** section.

3 From the **Data set** list, choose **Solution 2**.

4 From the **Table columns** list, choose **Outer solutions**.

5 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Piezoelectric Devices>Frequency (pzd.freq)**.

6 Right-click **Results>Derived Values>Global Evaluation 1** and choose **Evaluate>New Table**.

7 In the **Table** window, click **Full Precision**.

The first 6 digits of the eigenfrequency are the same. Subtracting the new value from the previous value shows that the eigenfrequency with gas exposure is lower approximately 200 Hz.

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