Created in COMSOL Multiphysics 6.3

Solidly Mounted Resonator 2D with Uncertainty Quantification

Introduction

This tutorial demonstrates how to use the Uncertainty Quantification Module by running a series of uncertainty quantification studies for a solidly mounted resonator (SMR). The SMR is a piezoelectric MEMS resonator formed on top of an acoustic mirror with a thick substrate underneath. The acoustic mirror comprises alternating layers of materials with high and low acoustic impedances and their thicknesses influence the resonance frequency. This tutorial studies how manufacturing variation introduces variation in the resonance frequency of the device. The design objective is that the resonance frequency should not be less than 865 MHz.

Model Definition

The geometry of the SMR model and its key components are shown in Figure 1. Note that for clarity, the vertical scale is magnified to show the layers. All dimensions are parameterized in the model, including the thickness of each layer. Various selection features are used for the construction of the geometry and the setup of physics and mesh. The fabrication of the device is discussed in Ref. 1. A more detailed description of the final structure and an explanation of its principle of operation can be found in the documentation for the model Solidly Mounted Resonator 2D.

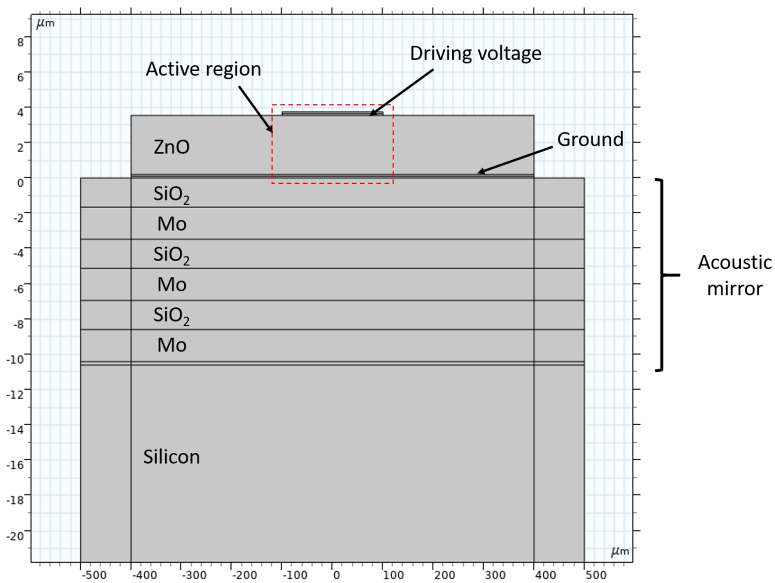


Figure 1: Model geometry showing the key components of the solidly mounted resonator.

The ideal structure has a resonance frequency of 870 MHz but we assume some uncertainty in the thickness of each layer as a result of manufacturing variations. In this context, the thickness of the low impedance layer `t_lil`, for example, is an input parameter. Other input parameters are `t_e`, `t_hil`, and `t_pe`. The Modeling Instructions show how to specify the distribution function associated with each input parameter. The subsequent Uncertainty Quantification (UQ) studies compute the resulting probability distributions for the resonance frequency `f0` as the quantity of interest (QoI). In practice, the input parameters `t_e`, `t_hil`, and `t_pe` are correlated since different parts of the resonator are processed with similar manufacturing procedures. Here, to demonstrate the effect of correlated input parameters, we considered both cases where the input parameters are correlated and uncorrelated. For the correlated case, we assume the correlation between `t_e` and `t_hil` to be 0.15, the correlation between `t_e` and `t_pe` to be 0.4, and the correlation between `t_pe` and `t_hil` to be 0.7.

This tutorial begins with the setup of the Eigenfrequency study for computing `f0` for the subsequent UQ studies. Nominally, `f0` is 870 MHz but to compute its deviation from the nominal value we need to search over a range of frequencies. However, there are many spurious solutions around the mode of interest that are not usable in the UQ studies so these must be excluded using the Combine Solutions step. The Modeling Instructions describe how this is done.

To save time and reduce file size, a relatively coarse mesh is used, in particular in the horizontal direction (Figure 2). Thus only the main lower modes will be resolved in this model. The same approach was taken in the reference paper.

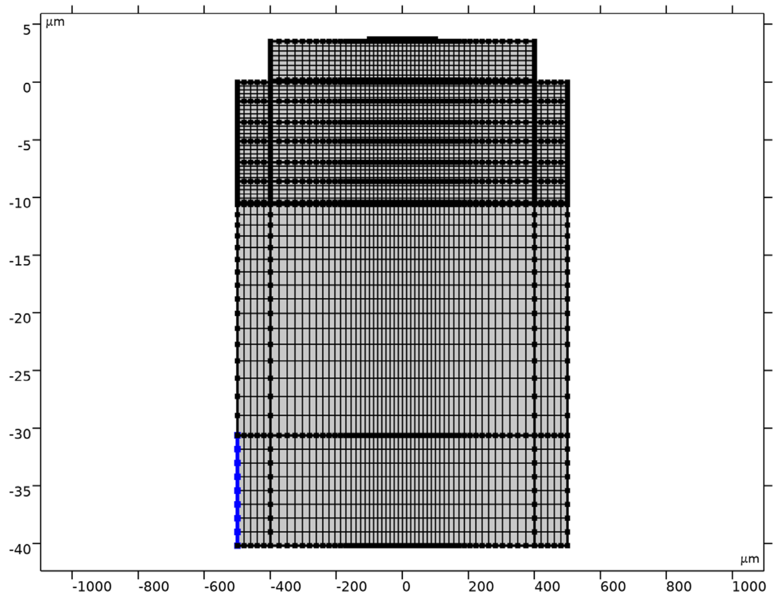


Figure 2: The mesh used in the model.

THE UNCERTAINTY QUANTIFICATION STUDIES

The Uncertainty Quantification Module provides four different study types:

- Screening, MOAT
  - Identifies the most influential inputs, for each QoI
  - Is based on the Morris One-At-a-Time (MOAT) method
  - Outputs MOAT mean and MOAT standard deviation values
- Sensitivity Analysis
  - Computes the fraction of impact for the inputs, for each QoI
  - Outputs first-order and total Sobol indices
- Uncertainty Propagation
  - Computes the statistical variation of the QoI
  - Outputs a kernel density estimation (KDE) plot representing an estimate of the probability distribution of the QoI

- Reliability Analysis
  - Computes the probability for the fulfillment of a condition based on the QoI
  - For example, what is the probability `f0` < 865 MHz.

For more information, see the *Uncertainty Quantification Module User's Guide*.

SURROGATE MODELS

To get statistical data based on a physics model you need to run a lot of simulations, varying the parameters of the inputs according to their probability distributions. For a 3D model, this might be computationally unfeasible. To get around this problem, the Uncertainty Quantification Module first builds up a so-called surrogate model that is used for sensitivity analysis, uncertainty propagation, and reliability analysis (but not for screening).

This process is typically adaptive and the surrogate model can approximate the original model to a high degree of accuracy (which can be modified by the user). The Uncertainty Quantification Module uses two different types of surrogate models:

- Sparse Polynomial Chaos Expansion (SPCE)
  - This surrogate model improves its accuracy by adaptively solving the full model and thereby adding new QoI data by using sequential Latin hypercube sampling.
- Gaussian Process (GP)
  - This surrogate model improves its accuracy by, using information from the current Gaussian Process surrogate model, adaptively solve the full model for new carefully selected sets of parameter values.

First, a set of UQ studies are done with the assumption that the input parameters are not correlated. Then the Uncertainty Propagation and the Reliability Analysis were repeated with the assumptions that the input parameters are correlated.

Results and Discussion

Figure 3 shows the mode shape of the fundamental mode of the resonator at 870 MHz as intended by the design described in Ref. 1.

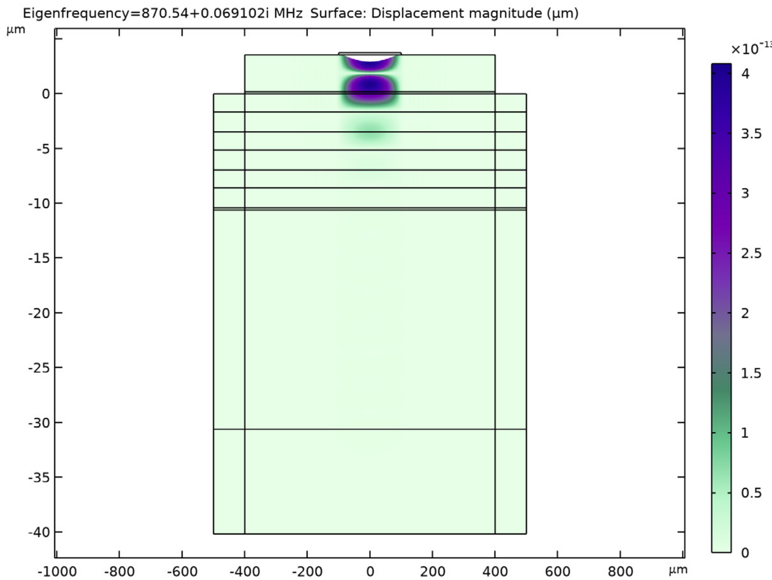


Figure 3: Surface plot of displacement indicating mode shape of the resonator's fundamental mode.

In the case where input parameters are not correlated, the UQ study gives the kernel density estimation plot shown in Figure 4.

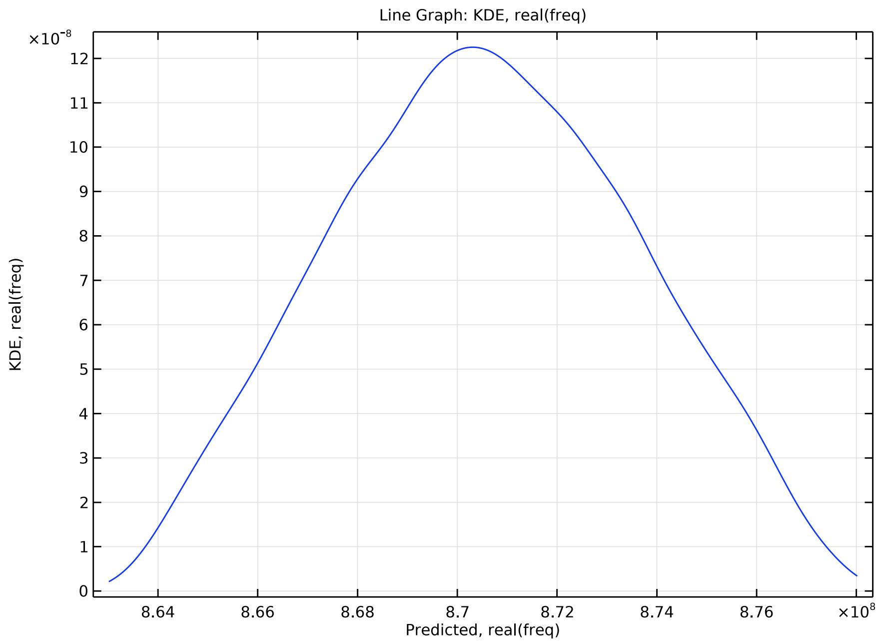


Figure 4: Kernel density estimation for when input parameters are not correlated.

The associated confidence interval information can be seen in the table for QoI Confidence Interval under the Uncertainty Propagation node group.

The Reliability Analysis study shows that the probability for the resonance frequency to be lower than 865 MHz is about 0.0305 or 3.0% when the input parameters are not correlated. This result is made available in the table Probability for Conditions under the Reliability Analysis node group.

For the case where input parameters are correlated, the UQ study gives the kernel density estimation plot shown in Figure 5. The associated confidence interval information is in the table for QoI Confidence Interval 1under the Uncertainty Propagation 1node group.

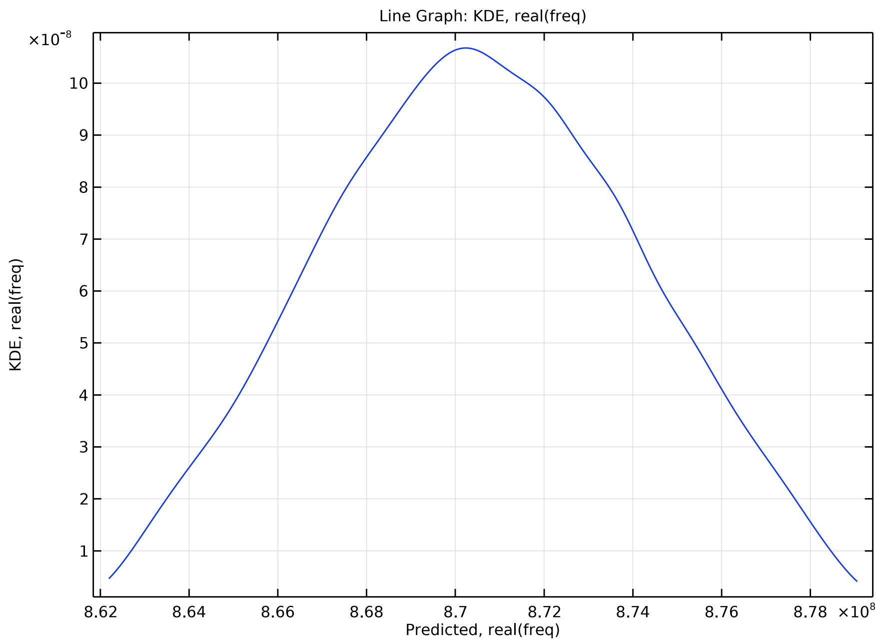


Figure 5: Kernel density estimation for when input parameters are correlated.

When the input parameters are correlated, the probability for the resonance frequency to be lower than 865 MHz is about 0.0588 or 5.9%. This result is made available in the table Probability for Conditions 1 in the node group Reliability Analysis 1.

Reference

1. F.H. Villa-López and others, "Design and Modelling of Solidly Mounted Resonators for Low-Cost Particle Sensing," *Meas. Sci. Technol.*, vol. 27, no. 2, 025101, 2016.

Application Library path: `MEMS_Module/Piezoelectric_Devices/solidly_mounted_resonator_2d_uncertainty_quantification`

ROOT

Start from the existing stationary model.

APPLICATION LIBRARIES

1 From the **File** menu, choose **Application Libraries**.

2 In the **Application Libraries** window, select **MEMS Module** > **Piezoelectric Devices** > **solidly_mounted_resonator_2d** in the tree.

3 Click **Open**.

COMPONENT 1 (COMP1)

In the **Model Builder** window, expand the **Component 1 (comp1)** node.

DEFINITIONS

Define an Integration nonlocal coupling over the boundary between top electrode and piezoelectric layer to measure y-displacement as a criteria for the Combine Solutions step.

Integration 1 (intop1)

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Definitions** node.

2 Right-click **Definitions** and choose **Nonlocal Couplings** > **Integration**.

3 In the **Settings** window for **Integration**, locate the **Source Selection** section.

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

5 Click **Paste Selection**.

6 In the **Paste Selection** dialog, type 44 in the **Selection** text field.

7 Click **OK**.

Add a Combine Solutions step to Study 1 to exclude spurious solutions. Study 1 (Eigenfrequency) is the basis for subsequent uncertainty quantification studies where the operational eigenfrequency will be computed as the input parameters are varied. Nominally, the eigenfrequency is 870 MHz but to compute its deviation from the nominal value we need to search over a range of frequencies. However, around the mode of interest there are many spurious solutions that must be excluded from the uncertainty quantification study and this is done through the Combine Solutions step. Then re-compute the Eigenfrequency study to compute 30 solutions around 855 MHz.

STUDY 1 - MODES

Step 1: Eigenfrequency

1 In the **Model Builder** window, expand the **Study 1 - Modes** node, then click **Step 1: Eigenfrequency**.

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

3 In the **Desired number of eigenfrequencies** text field, type `30`.

4 In the **Search for eigenfrequencies around shift** text field, type `855`.

Step 2: Combine Solutions

1 In the **Study** toolbar, click **Combine Solutions**.

2 In the **Settings** window for **Combine Solutions**, locate the **Combine Solutions Settings** section.

3 From the **Solution operation** list, choose **Remove solutions**.

4 From the **Exclude method** list, choose **Implicit**.

5 In the **Excluded if** text field, type `abs(comp1.intop1(comp1.v))/comp1.intop1(abs(comp1.v))<0.99`.

6 In the **Study** toolbar, click **Compute**.

Next, add a screening analysis to see which input parameters are most significantly impacting the resonance frequency (QoI). The screening study is added as a study reference which means it refers back to the already defined eigenfrequency study. The parameters that participate in the uncertainty quantification are all assumed to be normally distributed around their nominal values, according to the instructions below. The mean and standard deviation, as well as the max and min limits are all defined in terms of their nominal parameters (from **Global Definitions** > **Parameters**).

7 In the **Model Builder** window, right-click **Study 1 - Modes** and choose **Uncertainty Quantification** > **Add Uncertainty Quantification Study Using Study Reference**.

STUDY 3 - SCREENING

In the **Settings** window for **Study**, type `Study 3 - Screening` in the **Label** text field.

Uncertainty Quantification

1 In the **Model Builder** window, under **Study 3 - Screening** click **Uncertainty Quantification**.

2 In the **Settings** window for **Uncertainty Quantification**, locate the **Quantities of Interest** section.

3 Click **Add**.

4 In the table, enter the following settings:

Expression	Individual solution selection
`real(freq)`	From "Solution selection"

5 Locate the **Input Parameters** section. Click + **Add**.

6 In the table, enter the following settings:

Parameter	Source type	Parameter description
t_pe (Piezoelectric layer thickness)	Analytic	Normal

7 From the **Distribution** list, choose **Normal(μ,σ)**.

8 In the **Mean** text field, type `t_pe`.

9 In the **Standard deviation** text field, type `0.005*t_pe`.

10 From the **CDF-Lower** list, choose **Manual**.

11 In the **Lower bound** text field, type `t_pe-2*0.005*t_pe`.

12 From the **CDF-Upper** list, choose **Manual**.

13 In the **Upper bound** text field, type `t_pe+2*0.005*t_pe`.

14 Click + **Add**.

15 In the table, enter the following settings:

Parameter	Source type	Parameter description
t_lil (Low impedance layer thickness)	Analytic	Normal

16 From the **Distribution** list, choose **Normal(μ,σ)**.

17 In the **Mean** text field, type `t_lil`.

18 In the **Standard deviation** text field, type `0.005*t_lil`.

19 From the **CDF-Lower** list, choose **Manual**.

20 From the **CDF-Upper** list, choose **Manual**.

21 In the **Lower bound** text field, type `t_lil-2*0.005*t_lil`.

22 In the **Upper bound** text field, type `t_lil+2*0.005*t_lil`.

23 Click + **Add**.

24 In the table, enter the following settings:

Parameter	Source type	Parameter description
t_hil (High impedance layer thickness)	Analytic	Normal

25 From the **Distribution** list, choose **Normal(μ,σ)**.

26 In the **Mean** text field, type `t_hil`.

27 In the **Standard deviation** text field, type `0.005*t_hil`.

28 From the **CDF-Lower** list, choose **Manual**.

29 From the **CDF-Upper** list, choose **Manual**.

30 In the **Lower bound** text field, type `t_hil-2*0.005*t_hil`.

31 In the **Upper bound** text field, type `t_hil+2*0.005*t_hil`.

32 Click **Add**.

33 In the table, enter the following settings:

Parameter	Source type	Parameter description
t_e (Electrode thickness)	Analytic	Normal

34 From the **Distribution** list, choose **Normal(μ,σ)**.

35 In the **Mean** text field, type `t_e`.

36 In the **Standard deviation** text field, type `0.005*t_e`.

37 From the **CDF-Lower** list, choose **Manual**.

38 From the **CDF-Upper** list, choose **Manual**.

39 In the **Lower bound** text field, type `t_e-2*0.005*t_e`.

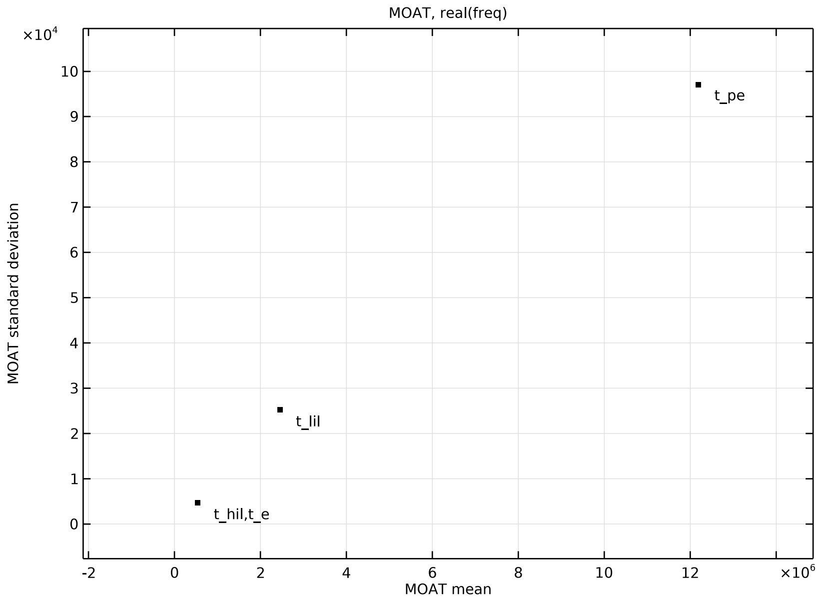
40 In the **Upper bound** text field, type `t_e+2*0.005*t_e`.

41 Locate the **Advanced Settings** section. From the **Error handling** list, choose **Skip problematic parameters**.

42 In the **Study** toolbar, click **Compute**.

RESULTS

MOAT, real(freq)



The screening results indicate that the thicknesses of the piezoelectric layer (t_pe), the electrode, and the low impedance layer (t_lil) are influential on the quantity of interest. The high impedance layer thickness (t_hil) appears to be insignificant. A high value of the MOAT mean means that the parameter is significantly influencing the quantity of interest. A high value of the MOAT standard deviation means that the parameter is influential and that it is either interacting with other parameters and/or that it has a nonlinear influence.

The next step is a sensitivity analysis. Use the results from the screening to decide which parameters to include in the sensitivity analysis. Sensitivity is more computationally demanding than screening and for this reason we would prefer to pick a subset of the parameters used for the screening study. In this example, we exclude the high impedance layer thickness (t_hil). We do not need to type all of the uncertainty quantification parameters again but we can define the new Uncertainty Quantification study for the sensitivity analysis by reusing the information in the screening study.

STUDY 3 - SCREENING

Uncertainty Quantification

Right-click **Uncertainty Quantification** and choose **Add New Uncertainty Quantification Study For** > **Sensitivity Analysis**.

STUDY 4 - SENSITIVITY ANALYSIS

1 In the **Model Builder** window, click **Study 4**.

2 In the **Settings** window for **Study**, type `Study 4 - Sensitivity Analysis` in the **Label** text field.

1 In the **Model Builder** window, under **Study 4 - Sensitivity Analysis** click **Uncertainty Quantification**.

2 In the **Settings** window for **Uncertainty Quantification**, locate the **Input Parameters** section.

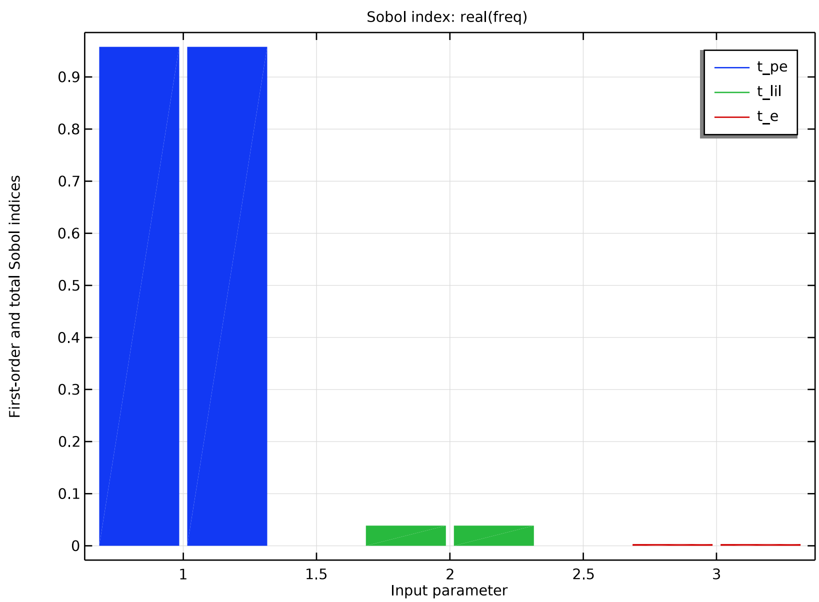
3 In the table, click to select the cell at row number 3 and column number 1.

4 Click **Delete**.

5 In the **Study** toolbar, click **Compute**.

RESULTS

Sobol Index, real(freq)



The sensitivity analysis is based on the Sobol method, also known as variance-based sensitivity analysis. The result of the sensitivity analysis is a set of Sobol indices and an associated Sobol table and Sobol plot. There are two different types of Sobol indices: first order-index and total index. The first-order index of a parameter shows the sensitivity by varying this parameter alone. The total index shows how much a parameter contributes to the overall sensitivity. In this case, the first and total indices are equal, up to the computed accuracy, for all parameters which indicates very little or no interaction between the parameters. The Sobol plot indicates that piezoelectric layer thickness is most sensitive. This is consistent with the screening results.

For the final two studies, Uncertainty Propagation and Reliability Analysis, we will keep all the parameters to get an accurate estimate of the uncertainties.

STUDY 4 - SENSITIVITY ANALYSIS

Uncertainty Quantification

Right-click **Uncertainty Quantification** and choose

Add New Uncertainty Quantification Study For > **Uncertainty Propagation**.

STUDY 5 - UNCERTAINTY PROPAGATION

1. In the **Model Builder** window, click **Study 5**.
2. In the **Settings** window for **Study**, type `Study 5 - Uncertainty Propagation` in the **Label** text field.

1. In the **Model Builder** window, under **Study 5 - Uncertainty Propagation** click **Uncertainty Quantification**.
2. In the **Settings** window for **Uncertainty Quantification**, locate the **Uncertainty Quantification Settings** section.
3. From the **Compute action** list, choose **Analyze only**.

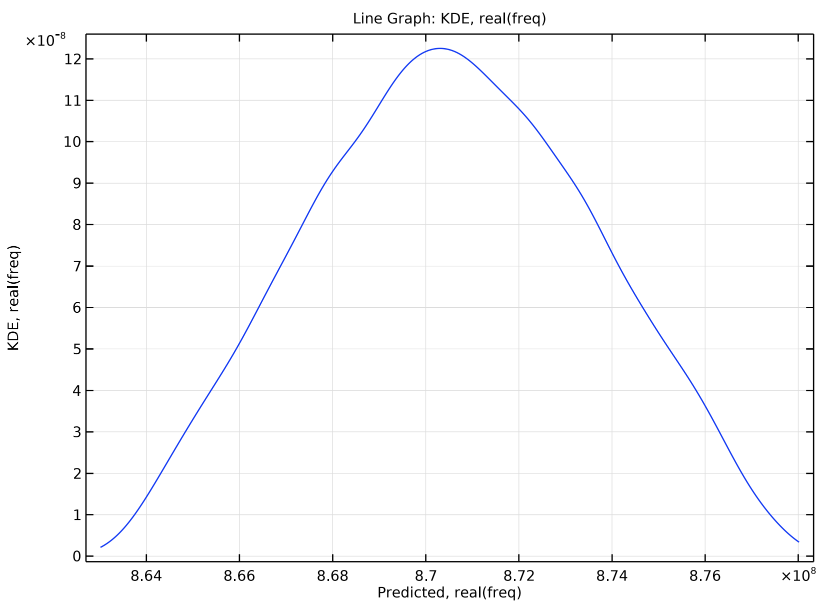
Uncertainty Quantification 3

In the **Study** toolbar, click **Compute**.

RESULTS

Kernel Density Estimation, real(freq)

1. In the **Model Builder** window, under **Results** > **Uncertainty Quantification Graph 2** click **Kernel Density Estimation, real(freq)**.



The uncertainty propagation study computes a so-called kernel density estimation or KDE. You can think of the KDE as a smooth form of a histogram showing an estimate of the probability density function of the quantity of interest, given the input parameters and their distributions. We can see from the QoI confidence interval table, shown earlier in the Results and Discussion section, that the mean is about 870 MHz with a standard deviation of 3 MHz. The KDE plot gives us this information graphically. From the values in the table we can also see that there appears to be some risk that the angle falls below 865 MHz.

To get a more accurate estimate of the risk for falling below 865 MHz, we will next run a reliability analysis.

STUDY 5 - UNCERTAINTY PROPAGATION

Uncertainty Quantification

In the **Model Builder** window, under **Study 5 - Uncertainty Propagation** right-click **Uncertainty Quantification** and choose **Add New Uncertainty Quantification Study For** > **Reliability Analysis**.

STUDY 6 - RELIABILITY ANALYSIS

1 In the **Model Builder** window, click **Study 6**.

2 In the **Settings** window for **Study**, type `Study 6 - Reliability Analysis` in the **Label** text field.

1 In the **Model Builder** window, under **Study 6 - Reliability Analysis** click **Uncertainty Quantification**.

2 In the **Settings** window for **Uncertainty Quantification**, locate the **Uncertainty Quantification Settings** section.

3 Find the **Surrogate model settings** subsection. In the **Relative tolerance** text field, type `0.01`.

4 Locate the **Quantities of Interest** section. In the table, enter the following settings:

Function name	Expression	Individual solution selection	True if	Threshold
	`real(freq)`	From "Solution selection"	Smaller than threshold	`8.65e8[Hz]`

5 In the **Study** toolbar, click **Compute**.

The reliability analysis performs a so-called importance sampling that refines the full model results near the threshold that we give for our quantity of interest. Recall that we are here asking for the probability that this frequency is lower than 865 MHz. The reliability analysis study gives us a table named Probability for condition having the value ~0.0305. This means that with the given conditions, there is a ~3% risk of the frequency to fall below 865 MHz.

As a final step, we can also produce a response surface of pairs of input parameters, in this case t_pe and t_lil.

6 In the **Model Builder** window, click **Uncertainty Quantification**.

7 Locate the **Surrogate-Based Response Surface** section. Click **Response Surface** in the upper-right corner of the section.

RESULTS

Response surface

Click the **Zoom Extents** button in the **Graphics** toolbar.

Now repeat the Uncertainty Propagation and Reliability Study with correlated input parameters. In MEMS device fabrications, deposition processes may interact when processing equipment is shared, for example. The degree of correlation between thickness of various films would be known or quantified through routine protocols of Statistical Process Control, or SPC.

STUDY 4 - SENSITIVITY ANALYSIS

Uncertainty Quantification

In the **Model Builder** window, under **Study 4 - Sensitivity Analysis** right-click **Uncertainty Quantification** and choose **Add New Uncertainty Quantification Study For** > **Uncertainty Propagation**.

STUDY 7 - UNCERTAINTY PROPAGATION, CORRELATED

1 In the **Model Builder** window, click **Study 7**.

2 In the **Settings** window for **Study**, type `Study 7 - Uncertainty Propagation, Correlated` in the **Label** text field.

1 In the **Model Builder** window, under **Study 7 - Uncertainty Propagation, Correlated** click **Uncertainty Quantification**.

2 In the **Settings** window for **Uncertainty Quantification**, locate the **Uncertainty Quantification Settings** section.

3 Find the **Surrogate model settings** subsection. From the **Surrogate model** list, choose **Adaptive Gaussian process**.

4 In the **Relative tolerance** text field, type `0.005`.

5 Locate the **Input Parameters** section. Select the **Correlated input parameters** checkbox.

6 Click **Add**.

7 Under **Group**, click **Add**.

8 In the **Add** dialog, in the **Group** list, choose **t_pe**, **t_lil**, and **t_e**.

9 Click **OK**.

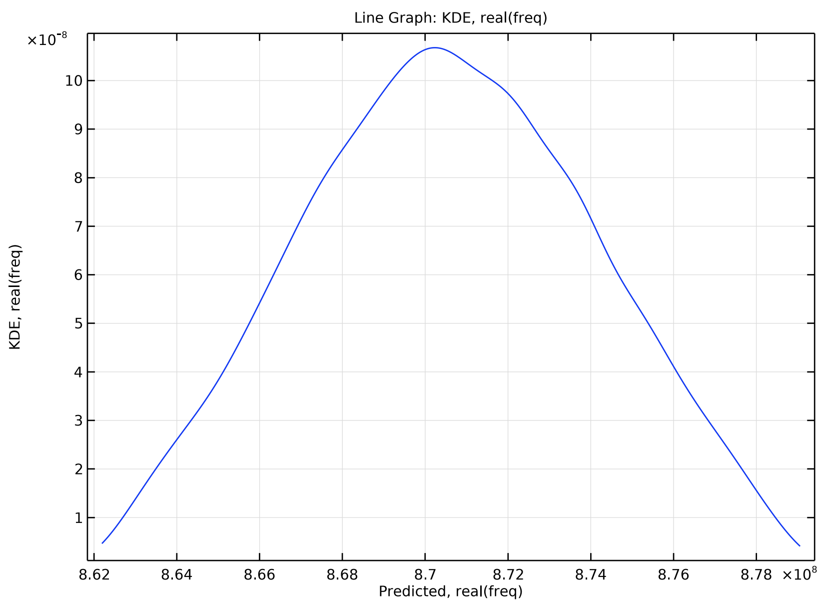
10 In the **Settings** window for **Uncertainty Quantification**, locate the **Input Parameters** section.

11 In the **Correlation groups** table, enter the following settings:

Correlation groups	Correlation matrix	Active
t_pe,t_lil,t_e	{1, 0.7, 1, 0.4, 0.15, 1}	√

Uncertainty Quantification 5

In the **Study** toolbar, click **Compute**.



Uncertainty Quantification

1 In the **Model Builder** window, expand the **Study 7 - Uncertainty Propagation, Correlated** > **Job Configurations** > **Design of Experiments 5** node.

2 Right-click **Study 7 - Uncertainty Propagation, Correlated** > **Uncertainty Quantification** and choose **Add New Uncertainty Quantification Study For** > **Reliability Analysis**.

STUDY 8 - RELIABILITY ANALYSIS, CORRELATED

1 In the **Model Builder** window, click **Study 8**.

2 In the **Settings** window for **Study**, type `Study 8 - Reliability Analysis, Correlated` in the **Label** text field.

1 In the **Model Builder** window, under **Study 8 - Reliability Analysis, Correlated** click **Uncertainty Quantification**.

2 In the **Settings** window for **Uncertainty Quantification**, locate the **Quantities of Interest** section.

3 In the table, enter the following settings:

Function name	Expression	Individual solution selection	True if	Threshold
	`real(freq)`	From "Solution selection"	Smaller than threshold	`8.65e8[Hz]`

4 In the **Study** toolbar, click **Compute**.

5 In the **Model Builder** window, click **Uncertainty Quantification**.

6 Locate the **Surrogate-Based Response Surface** section. Click **Response Surface** in the upper-right corner of the section.

RESULTS

Response surface 1

Click the **Zoom Extents** button in the **Graphics** toolbar.