COMSOL Multiphysics Simulations for a liquid metal surface on a curved geometry.

**Abstract**

COMSOL Multiphysics software enables combining computational fluid dynamics with electrostatics. The simulation shows the surface form of liquid mercury evolve under a gravity load environment using a basic electrowetting model for acurved surface. The mercury surface profile is separated from the Mechanical and Controls simulation to assess the residual surface form error created by only the liquid metal surface itself. The original theme was to model a continuous film of mercury under electrostatic forces on a curved surface. Due to non-convergence issues the single continuous mercury film was separated into segmented containers or baffles to overcome the inertial forces and obtain a surface form that is segmented. The mercury surface form can be simulated for long time intervals using an electrowetting model and slewing conditions for a near parabolic surface. The residual surface form error of +/- 50 are observed for a multi tub configuration over a 45 mm radius and can be expanded out to 0.5 m with varying slewing conditions.

1. **Introduction**

The Physics modules used for the simulation are the following.

* CFD Laminar flow
* Mercury and Air interface.
* Electrowetting
* Electrostatics

**Note:** Electrostatics module is integrated in the .mph file with a multiple container configuration. But due to the computational expense of integrating electrostatic surface forces a factor of two increase in computational time was observed. The .mph file has the electrostatics module deactivated or electric potential undefined for the multi tub configuration. The electrostatics module is integrated later for a single tub at 0 and 10 degrees away from the vertical axis.

**Setting-up the COMSOL simulation for a multi container configuration**

The multi tub configuration will be discussed first with electrowetting and then a single tub with electrowetting and electrostatics physics.

**Comment:** If sudden events such as ‘expulsion’ events occur in the moving mesh configuration or level set configuration, the simulation has a probability of having non-convergence. Such effects are created by amplified electric fields due to edge effects which create a surface distortion beyond the surface tension threshold of mercury. Or in the case of a voltage controlled contact angle determined by the Young Lipmann equation, if the change in the initial contact angle and equilibrium contact angle are beyond tens of degrees non convergence of the simulation occurs. When the steady state configuration and initial state configuration are similar to each other this enables convergence of the simulation.

**Multi Tub Configuration**

**File: 2D Flat x 11 2mm Hg and Air w ACDC Pulse FULLY ON tilted at 10 deg NO Fes Z\_ OSCILLA 2sec w SLEWING \_PARAB ALIGNED Center tub 0 deg OFF 4\_01\_24.mph**

The simulation that provided a steady state evaluation of a curved mercury surface in real time will be discussed first. The geometry uses eleven containers or tubs with a 2 mm width and a separation distance of 1 mm between adjacent tubs with an increasing inclination angle. A f-number of 1.5 for a 0.5 m diameter optic creates a focal length of 0.75 m with the edge tub set at approximately 10 degrees. The simulation uses 11 tubs to simulate the surface form for an equivalent curvature of an f-number of 1.5.

The simulation uses the ‘Electrowetting Lens’ template from COMSOL which utilizes a 2D axisymmetric model and leverages the settings from the .mph template to start from a known and computational efficient model. For explicit detailed steps the reader should defer to the COMSOL’s white paper [Electrowetting Lens, COMSOL]. The file is converted to 2D and uses a mercury and air interface and a contact angle that is voltage controlled from both sides of the tub. The surface form is extracted in 2D and revolved manually in Matlab. The total computational time in COMSOL is about 1hr and 30 minutes.

**Settings:**

1. In the model Wizard click on 2D.
2. Physics: Laminar Two- Phase Flow, Moving Mesh
3. General Studies: Time Dependent.

**Geometry:**

1. Select the Geometry and chosen length units of mm.
2. Select Rectangle: Width is 3mm and height of 2mm.
3. Expand the Layers section and added 1.5mm thickness for Mercury.

Graphical user interface, application

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1. The general course alignment steps for placing each tub in COMSOL is to select a rectangle and activate ‘Sketch’ and place each tub in a ‘course position’. Then adjust adjacent tubs until the fluid surface level is set at the same height. The angles and positions used for the simulation are shown in the Table 1. They were chosen to: 1) create a parabolic surface, 2) to recreate a inclination angle of 10 degrees tilt for a f-number=1.5 for a primary mirror telescope of 0.5 m diameter at the edges. 3) To guide the surface level height for adjacent tubs for a parabolic surfaced. The simulations that scale to 40 mm shows what surface deviations would be anticipated at the outer edges while being able to reach a stable equilibrium and fast computational times.

**Note:** If a user wanted to change the tub configuration to expand out to 0.5 m in a spreadsheet with column x and column y, the radial values in column x can be listed from 0 mm to 250 mm. The y-column uses the expression: 1.76mm + C \* x^2. The 1.76mm is the offset height and the C =1/4\*focal length where f=122 mm. In the case of f=1500 mm then C can be calculated and the user can adjust the number of tubs and width of each tub and calculate the local inclination angle of each tub.

|  |  |  |  |
| --- | --- | --- | --- |
|  | x (mm) | Y (mm) | Rotation Angle(deg) |
| 1 | -0.109 | 0.260 | 0 |
| 2 | 4 | 0.260 | 1 |
| 3 | 8.25 | 0.3 | 2 |
| 4 | 12.4 | 0.45 | 3 |
| 5 | 16.6 | 0.65 | 4 |
| 6 | 20.7 | 1 | 5 |
| 7 | 24.8 | 1.4 | 6 |
| 8 | 28.9 | 1.9 | 7 |
| 9 | 33 | 2.4 | 8 |
| 10 | 37.2 | 3 | 9 |
| 11 | 41.4 | 3.65 | 10 |

Table 1. The coordinates for each container of mercury placed along a curved surface.

Using the .m file the fitted coefficients can be obtained using Matlab’s Fitting Application and Table 2 shows the high resolution position and angle of each tub. The surface fitting analysis steps are provided later on.

5.Open the file: High Resolution positioning 03\_31\_24.xlsx. Located the height of tub 1 and adjust the local inclination angle and confirm the x-position of tub 1. Then scroll to tub 2 in the excel sheet and locate the liquid surface position in COMSOL. Rotate the tub 2 to the corresponding angle. Check that adjacent surface heights are parallel using a straight edge.

|  |  |  |  |
| --- | --- | --- | --- |
|  | x (mm) | Y (mm) | Rotation Angle(deg) |
| 1 | -0.109 | 0.260 | 0.25 |
| 2 | 4 | 0.260 | 1.32 |
| 3 | 8.25 | 0.340 | 2.35 |
| 4 | 12.4 | 0.49 | 3.29 |
| 5 | 16.6 | 0.72 | 4.288 |
| 6 | 20.7 | 1.025 | 5.265 |
| 7 | 24.8 | 1.395 | 6.139 |
| 8 | 28.9 | 1.840 | 7.12 |
| 9 | 33 | 2.345 | 8.04 |
| 10 | 37.2 | 2.95 | 8.96 |
| 11 | 41.4 | 3.61 | 9.98 |

Table 2. The higher resolution coordinates for each container of mercury placed along a curved surface.

**Note:** The evaluation out to 250 mm radii uses 66 tubs or six times more containers.

**Parameters**

1. Click parameters 1. [COMSOL, “Electrowetting lens”]
2. In setting window for the Parameters tab input the settings leveraged from COMSOL for a mercury and a dielectric side walls with permittivity of 2.65:

Table

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**Definitions**

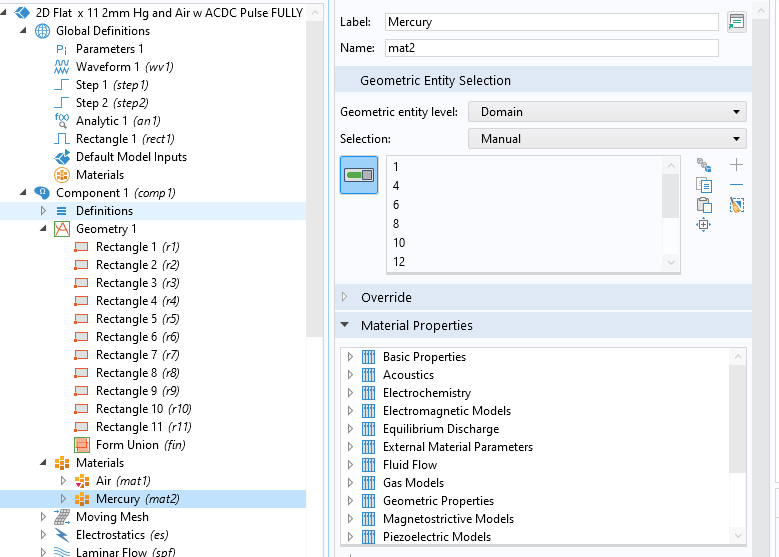
1. Right click on Global Definitions and chose Local Variables.
2. In the Variables Table enter the Young Lipman Equation:

Graphical user interface, text, application, email

Description automatically generated

**Materials**

1. Right click on materials and “Add Materials from Library” and select: Air and Mercury. Use the default parameters for each material. For long computational times it is efficient for the user to perform a ‘sensitivity’ test to tune parameters in order assess or ‘bound the problem’, for example: adjusting the viscosity by a factor of x2 or more.
2. Select in settings each domain that is specified as mercury and air.

Graphical user interface, application, table, Excel

Description automatically generated

**Contact Angle:**

1. Laminar Flow-> Fluid to fluid interface I-> Contact angle: type in theta ( determined from the Young-Lippman equation)
2. For the point selection in the Graphics display, click on each point along the mercury and air interface.

Graphical user interface, application

Description automatically generated

**Mesh:**

1. Select the mesh element size to be ‘Normal’ for Fluid Dynamics.

**Note:** For the .mph file, if an error window of appears during a simulation, increasing the mesh density can enable a converging solution but increase the computational time by 20-50%.

1. Right click the Mesh 1-> Scale. For Scale 1 select the contact angle for each tub and set the element size to 0.2. This will enable a higher mesh density at the contact angle point as most of the longitudinal motion of the liquid will occur at the contact line due to electrowetting. The voltage is set to provide a near 90 degree contact angle.
2. Free triangular mesh is chosen, since ‘surface forces’ can be introduced by adding a ‘boundary layer’ to the mercury surface at the liquid to air interface.

Graphical user interface

Description automatically generated

**Pressure Initial Conditions:**

1. Select the right upper corner of each tub to have a zero pressure [COMSOL], else the simulation will not converge.

Graphical user interface, application

Description automatically generated

**Navier Slip conditions**

1. Right click Laminar flow and select: Wall
2. Select the boundaries corresponding to the viscous frictional forces assumed from Navier Slip conditions in Wall 2. Set fh to nominal factor 0.5.

Graphical user interface, application

Description automatically generated

**Slewing**

1. Slewing can be enabled by introducing an existing defined variable: t
2. Laminar Flow-> Gravity-> Input for gravity the syntax for x and y as :

X: -g\_const\*sin(t/180 [s] \*pi)

Y: -g\_const\*cos(t/180 [s] \*pi)

**Note:** This will enable slewing at a rate of 1 degree/sec which is contained in the arguments for each sinusoidal expressions. If a slew rat of 2 deg/s is used, multiply by a factor of 2. The unit defined as [s] in the expression is needed in order to provide a unitless ‘argument’ in the sinusoidal functions.

**Note:** The slewing rate and evaluation time can be expanded beyond 1 second.

**Export of 2D lineout [COMSOL, S. Dossa]:**

1. The lineout is exported by right clicking the Results and manually selecting the surfaces of each mercury container. Select the y-axis Data and x-axis Data to be y and x shown below. Click ‘Plot’. Then export by right clicking: Line Graph 1 and selecting: ‘Add Plot Data to Export’. The process will allow one to export the surface profile in a spreadsheet in a .txt file for all time frames.

Graphical user interface, application

Description automatically generated

1. Remove the headers in notepad and save as a .csv file.
2. The data can transfer to Matlab and be revolved for a given number of rotations and appended. The rotational angles are defined in line 9, which corresponds to 12 angles. The array of x,y, and z coordinates are appended using multiple instances of code line 20 thru 25.

Text

Description automatically generated

1. To generate an interpolated plot with the data the following code is needed and figure for the interpolated plot is generated:

Text

Description automatically generated

Chart, surface chart

Description automatically generated

1. The dataset is then analyzed using Matlab’s Curve Fitting App. Select x,y, and z as shown in the figure as xtest, ytest, and ztest. With the offset of 1.709 and coefficient of 0.001988 obtained from the analysis below. These values are close to optimal but may change slightly.

Graphical user interface, chart

Description automatically generated

1. Transfer the fitting coefficients into the .m file as shown in Figure below on line 161. The code lines 153-186 takes the interpolated data and subtracts the parabolic expression ( theoretical expression with fitted coefficients) from the interpolated data.

**Note:** The preliminary interpretation of the residual surface form shows that the center and edges should be actuated downward.

Text

Description automatically generated with medium confidence

The following residual error plot is generated. Note that the slew angle of 1deg/s is integrated into the figure at t=1 second. The evaluation of the residual surface error is exported at time t=1 second, which corresponds to a steady state, based on the y height probe domain evaluation of mercury as shown in Figure 1.

Chart, surface chart

Description automatically generatedGraphical user interface

Description automatically generated with low confidence

Figure 1. Residual surface form error for a 2mm tub with the applied voltage set to 563 V. The slewing rate is 1 deg/sec and the surface form is evaluated at time t=1 second which corresponds to the gravity angle shifted to 1 deg and a (right figure) steady state configuration.

**Instructions and Future code evaluation:**

1. Select ‘Compute’ the simulation should run for 1hr and 30 minutes.

2. The ability to tune the Vapp or voltage controlled contact angle has not be studied. This can be adjusted in the parameters section for the file. The Figure 1. shows voltage set to 563V.

3. The dimensions of each tub can be adjusted manually in the simulation file to explore different separation distances and tub widths and explore an f-number larger than one to simulate slower f-numbers or angles of inclination smaller than 10 degrees. A separate excel sheet is needed and can be evaluated based on the instructions above to place each tub and angle needed for the specific f-number.

4.The slew rate can be controlled as mentioned in the section for slewing.

By extrapolating the residual surface form one can perform a ray trace to observe the direction of each ray reflected off the surface of the parabola using a paraxial ray approximation for a curved reflecting surface to predict the spot size at the focal plane in Matlab or Zemax.

**CONCLUSION**

The simulations provided by COMSOL to obtain the surface form over time was created using Mercury and air interface with a basic electrowetting model. The COMSOL simulation allows one to observe how the surface from evolves over time under a gravity load environment for a specific geometric configuration under slewing conditions. The exporting process for the surface form is in 2D and assumes a 2D axisymmetry solution but the surface form over time is evaluated over 40 mm and future radius of 0.5 m and larger is in progress. The surface data was subtracted from a parabolic surface to obtain the residual surface form at a 1deg/s slewing rate. Additional frames can be evaluated to further predict the performance of a liquid mercury surface required for correction.

**COMSOL Single Container Simulation for Liquid Hg and Air with dielectric added to the walls and electrostatic forces.**

**(File:** **2D Flat 20mm Hg e is 80 and Air AND DIELECTRIC w ACDC Pulse FULLY ON \_ NEW BC ON RHS \_ ADDED ON Fes RHS BOT TOP 4\_01\_24 CORRECTED Left Side and FORCE\_WORKS 200ms.mph)**

The mercury surface under electrostatic conditions with side walls and electrostatic forces between the fluid and solid interface was modeled. The continuous film of mercury was applied a voltage across the surface to simulate a surface charge distribution and expected voltage distribution with respect to ground. The voltage across the fluid metal surface and volume and a separate surface analysis enabled the field to be determined by the voltage per distance value to calculate the surface electrostatic forces on mercury and attraction to the sidewalls. The initial settings were carried over from the multi tub configuration to the single tub configuration. The electrostatics and forces are added to the model and will be discussed.

**Electrostatics**

The electrostatics module is added in the simulation.

Graphical user interface

Description automatically generated

1. The voltage boundary conditions are as follows:

Graphical user interface, application

Description automatically generated

Graphical user interface, application

Description automatically generated

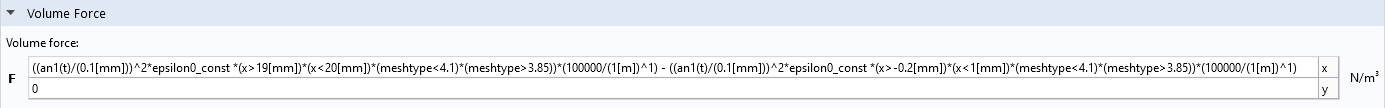
1. Ground is activated at the outer edges of the dielectric which is assumed to be quartz with approximately a 100um thickness. 100um was chosen in order to evaluate the electric field within the dielectric using a taper mesh density and five points across the dielectric. Note: The Young Lippman equation assumes a 10um thick dielectric.

Graphical user interface, application

Description automatically generated

1. Volume force is activated in Mercury and the code for electrostatic surface forces is: ((an1(t)/(0.1[mm]))^2\*epsilon0\_const\*(x>19[mm])\*(x<20[mm])\*(meshtype<4.1)\*(meshtype>3.85))\*(100000/(1[m])^1) - ((an1(t)/(0.1[mm]))^2\*epsilon0\_const \*(x>0.2[mm])\*(x<1[mm])\*(meshtype<4.1)\*(meshtype>3.85))\*(100000/(1[m])^1).

**Note:** Meshtype specified in the equation in step 3) above activates a surface force at the fluid and solid interface. There are two terms defined by the equation coming from the 1st order Coulomb Force equation between a charged metal liquid surface and the ground plane on each side.



**Note:** The ‘Boundary Layer Mesh’ is activated at the liquid to surface (highlighted in blue) interface. The Moving Mesh CFD allows the user to integrate a 1st order surface force that in the mercury domain and the surface can be used along the fluid-air interface as well as the fluid to solid interface.

Graphical user interface, application

Description automatically generated

**Materials:**

Graphical user interface, application

Description automatically generated

**Deactivate the Quartz Region [COMSOL, V. Gurusamy]:**

1. To enable a 2nd solid to be introduced in the mercury and air geometry, add a 2nd solid in the Materials Section, in this case it is Quartz. Deactivate the Quartz domain in the geometry along the edges by deselecting the domain in the *Laminar Flow* as highlighted below. Note that domains 2 and 3 are selected that correspond to air and mercury, else COMSOL will consider quartz as a fluid versus a solid domain. More solid materials can be added to the liquid Mercury in the Moving Mesh CFD module.

Graphical user interface, application

Description automatically generated

**Instructions and Future code evaluation**

1.Select ‘Compute’ the simulation should run for 1hr.

2. The ability to tune the Vapp or voltage controlled contact angle has not be studied. This can be adjusted in the parameters section for the file.

3. The dimension of each tub can be adjusted manually in the simulation file to explore different tub widths.

4.The slew rate can be controlled as mentioned in the section for slewing or evaluated at a fixed angle by removing the variable ‘t’ and [s] unit and setting the angle to 0 or 10 degrees or other.