

# **Assignment 3 - Process Simulation**

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## **Introduction**

This report aims to address the key tasks involved in computational simulations and modelling of processes in microelectronic fabrication. The tasks include:

1. Generating random numbers that follow a Lorentzian distribution using both transformation and Monte Carlo methods
2. Simulating the hole etching using ViennaPS with different oxygen flux values
3. Modelling the deposition process for Tetraethyl orthosilicate (TEOS) in chemical vapor deposition (CVD) using both single and multi-particle approaches.

The simulation tools used in this assignment, particularly ViennaPS, are essential for understanding and optimizing fabrication processes at the microscopic level. These tools provide assistance in exploring various parameters and their impact on processes such as etching and deposition. Accurate modelling of these processes is vital for improving the efficiency and reliability of modern semiconductor manufacturing techniques.

## **Task Overview**

### **Task 1: Random Number Generation (Lorentzian Distribution)**

In this task, the objective is to generate random numbers following a Lorentzian distribution using two methods, the transformation method, which follows the one-dimensional Lorentzian distribution and the Accept/Reject Monte Carlo method. The Lorentzian distribution is known for its characteristic heavy tails.

The two methods were compared in terms of how efficiently they generated values that conformed to the theoretical distribution.

### **Task 2: ViennaPS - Hole Etching Simulation**

In this task, the goal was to simulate a hole etching process using the ViennaPS simulation framework. ViennaPS models the physical and chemical processes involved in semiconductor fabrication. The focus of this simulation is to study the impact of varying the oxygen flux (increasing and decreasing by a factor of 10) on the etch depth and surface quality.

Etching is a critical process in microelectronics fabrication, as it creates features such as holes and trenches on semiconductor wafers. The oxygen flux parameter plays a vital role in controlling the etching process by influencing the balance between etching and surface passivation.

### **Task 3: Simple TEOS CVD Process Simulation**

The third task focuses on simulating the Chemical Vapor Deposition (CVD) of Tetraethyl orthosilicate (TEOS) using ViennaPS. CVD is a crucial process for depositing thin films of materials such as silicon dioxide ( $\text{SiO}_2$ ) on semiconductor wafers. The goal is to model the deposition process, adjust key parameters, and compare the simulation results to experimental data. TEOS decomposes in the CVD process to form  $\text{SiO}_2$ .

### **Task 4: Multi-Particle TEOS CVD Model**

In this task, the single-particle TEOS model was extended to a multi-particle model by introducing an intermediate precursor molecule that contributes to the deposition process. The goal is to improve the accuracy of the deposition profile by considering additional chemical species involved in the reaction.

## **Results**

### **Task 1.1:**

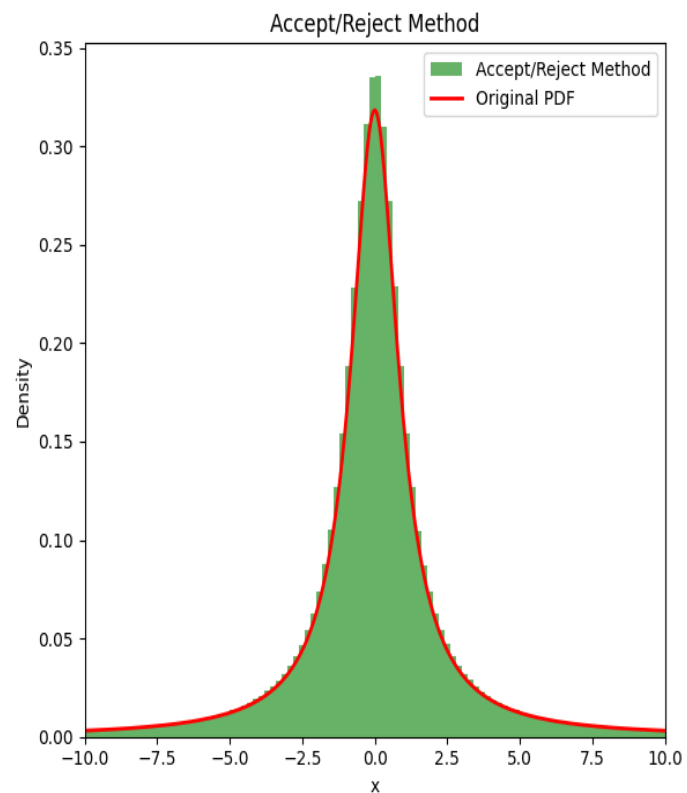
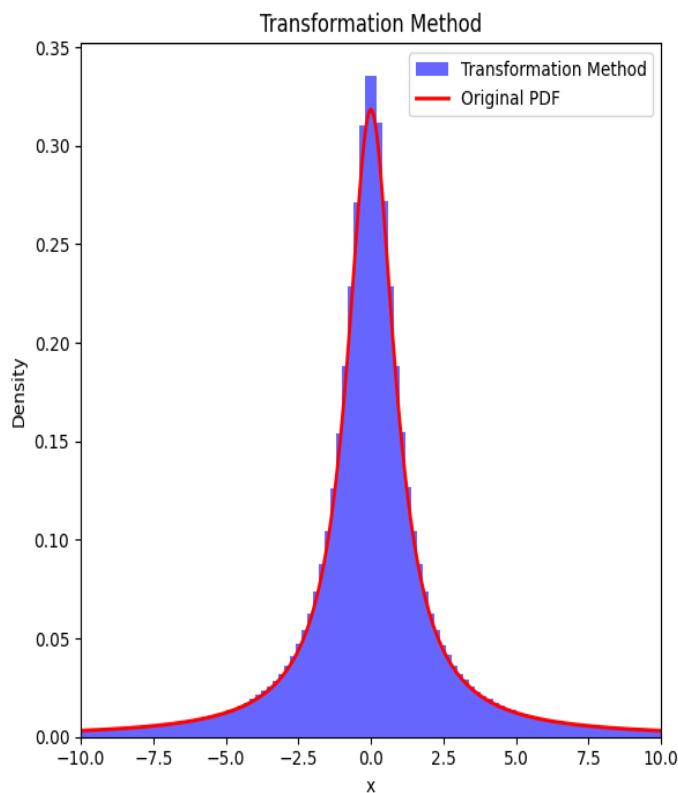
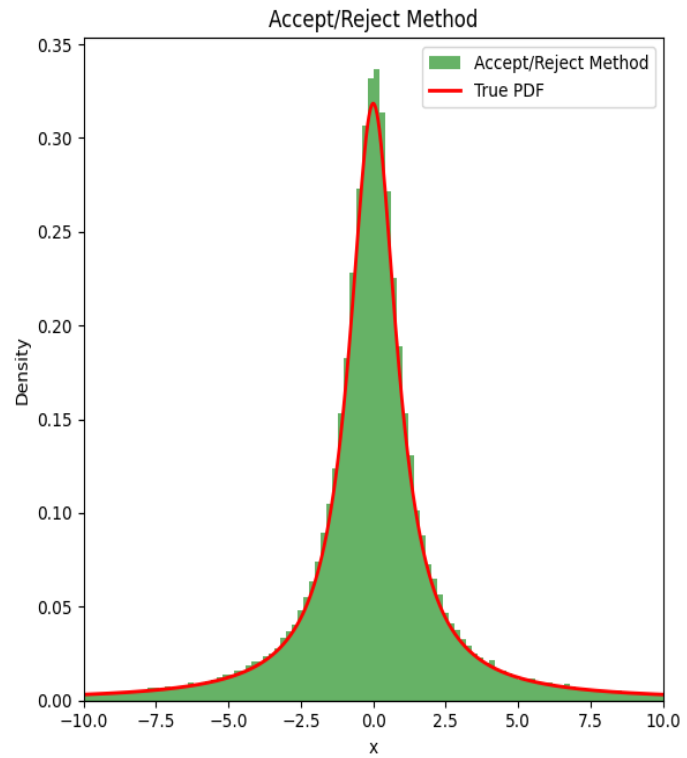
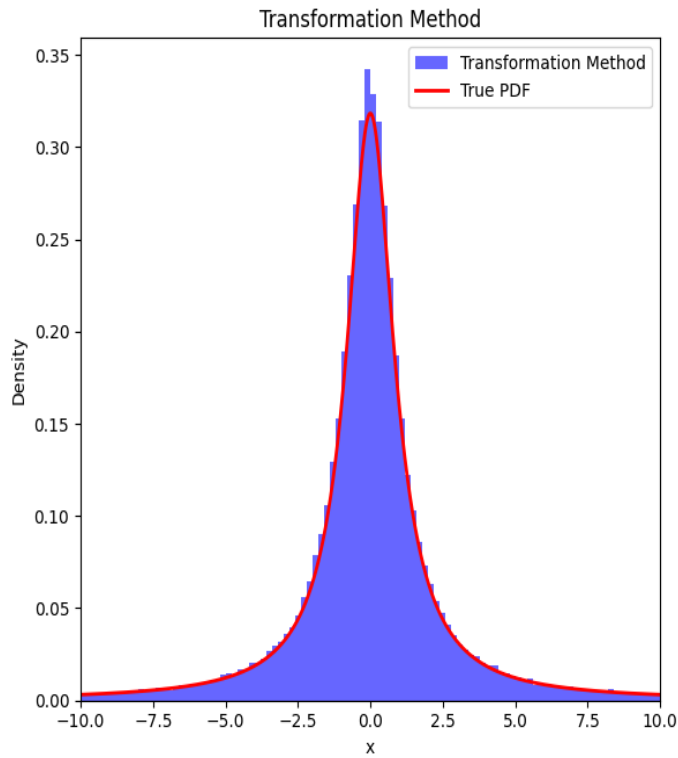
Transformation Method: Uniform random numbers were generated. These numbers were transformed using the inverse cumulative distribution function (CDF) of the Lorentzian distribution. This method is efficient because it involves direct transformation without rejection of generated numbers.

Accept/Reject Monte Carlo Method: Random numbers were first generated from a simpler distribution. A set of criteria based on the Lorentzian PDF was used to accept or reject the generated numbers.

Now, in the visual comparison, the generated data from each method is compared to the original PDF. The Transformation Method produced a distribution that closely matched the theoretical Lorentzian PDF, with a significant speed advantage due to the absence of rejection.

The Accept/Reject Method also generated a correct Lorentzian distribution, but at a higher computational cost. This method required the rejection of numbers, leading to a slower process.

The task is run through cmd by the command, `python Task1.1.py`. Here are the distributions I got for 100,000 and 10,000,000 samples respectively. The first distribution is for 100,000 samples and the second is for 10,000,000 samples:



It can be observed from the above distributions that both the methods were successful in generating Lorentzian-distributed random numbers and show the similar distribution for 100,000 samples. However, the transformation method was more computationally efficient and faster, making it the preferable choice for this distribution. Also, with larger sample size, the distributions become more smoother and more closely match the original PDF.

### Task 2.1:

The hole etching process was first simulated with the default parameter of oxygenFlux set to 30, as in the original example. Then, I modified the flux to explore different etching conditions:

Increased OxygenFlux (300, multiplied by factor of 10): A ten-fold increase was applied to study the effect of enhanced passivation.

Decreased OxygenFlux (3, divided by factor of 10): A tenfold decrease was used to explore the effect of reduced passivation.

The simulation domain was set up with an appropriate grid resolution and material properties and using the config.txt file. This task is run through cmd by the command: `python Task2.1.py config.txt` It gave the following output for Oxygen flux = 30:

1) Process SF6O2Etching took: 3.286026 s

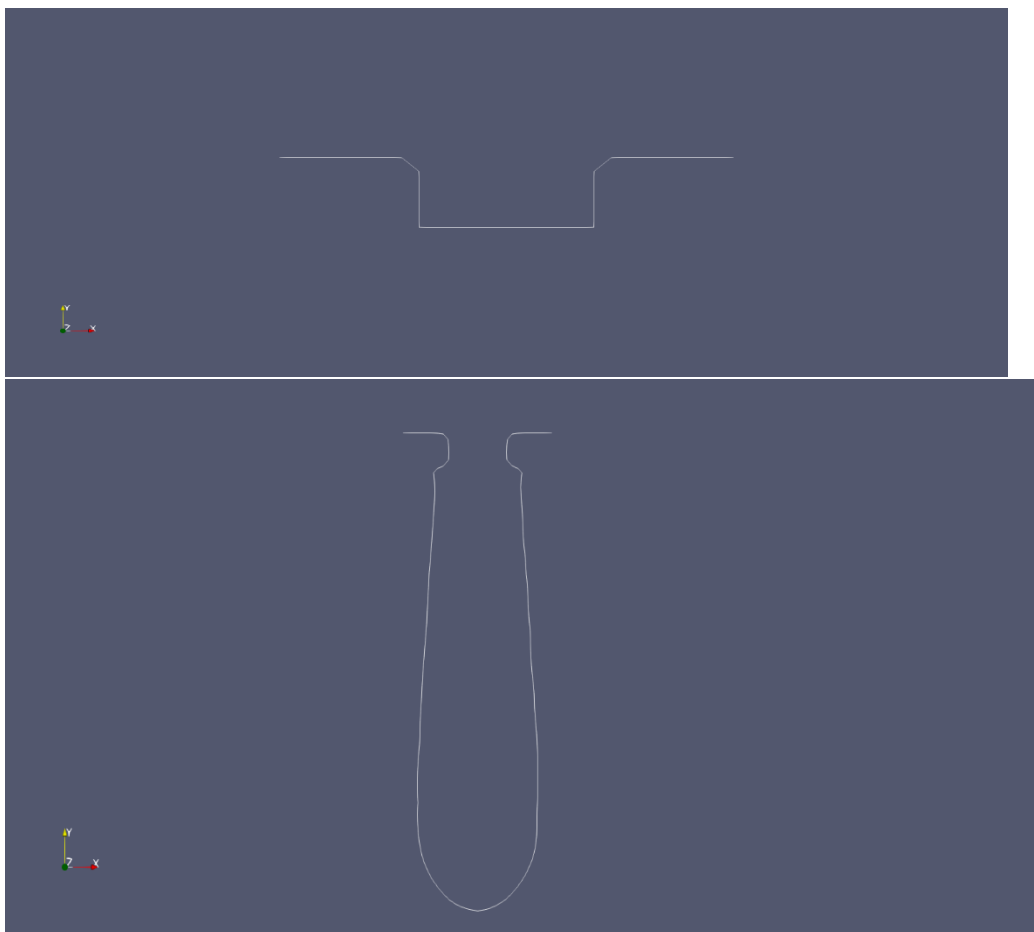
Surface advection total time: 0.541765 s

Percent of total time: 16.486941

Top-down flux calculation total time: 1.649753 s

Percent of total time: 50.205116

Here is how the visualizations look like in ParaView of initial and final surface:



It can be seen that at flux = 30, the etched hole is deeper and the etch rate is moderate.

2) Now, for the increased OxygenFlux = 300, it gave the following output:

Process SF6O2Etching took: 0.761834 s

Surface advection total time: 0.128984 s

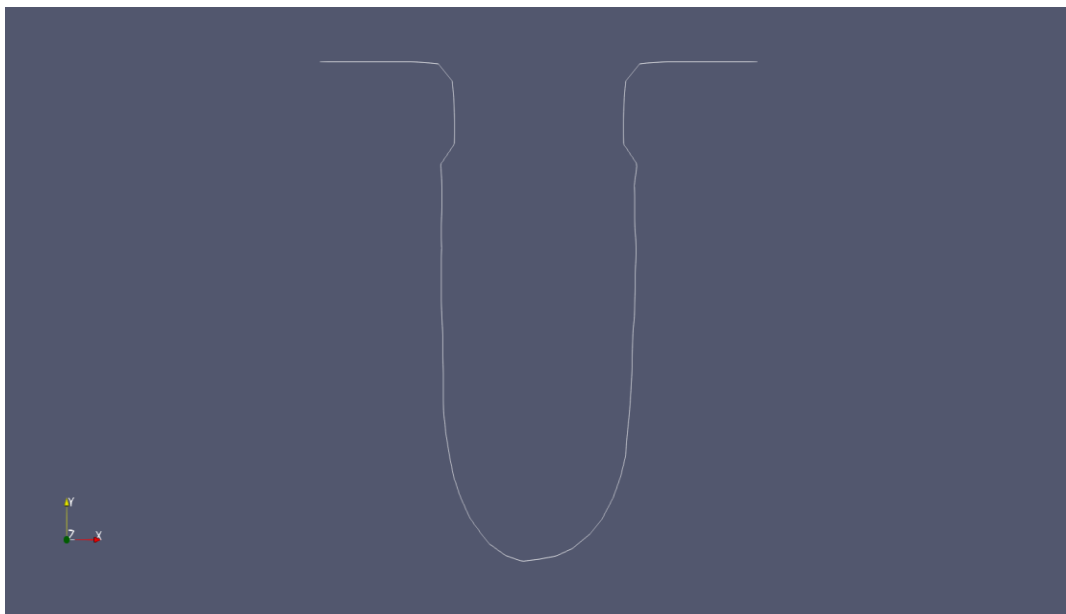
Percent of total time: 16.930779

Top-down flux calculation total time: 0.286922 s

Percent of total time: 37.662060

It can be seen from above that increasing the flux 10-fold reduces the time for the process of etching and advection.

Here is how the visualizations look like:



It can be seen from the above that the etching for flux = 300 increased flux generated more uniform etch as compared to flux = 30 and the etched hole is comparatively shallow and smaller as the etch rate is slower.

3) For the decreased OxygenFlux = 3, it gave the following output:

Process SF6O2Etching took: 3.703379 s

Surface advection total time: 0.722527 s

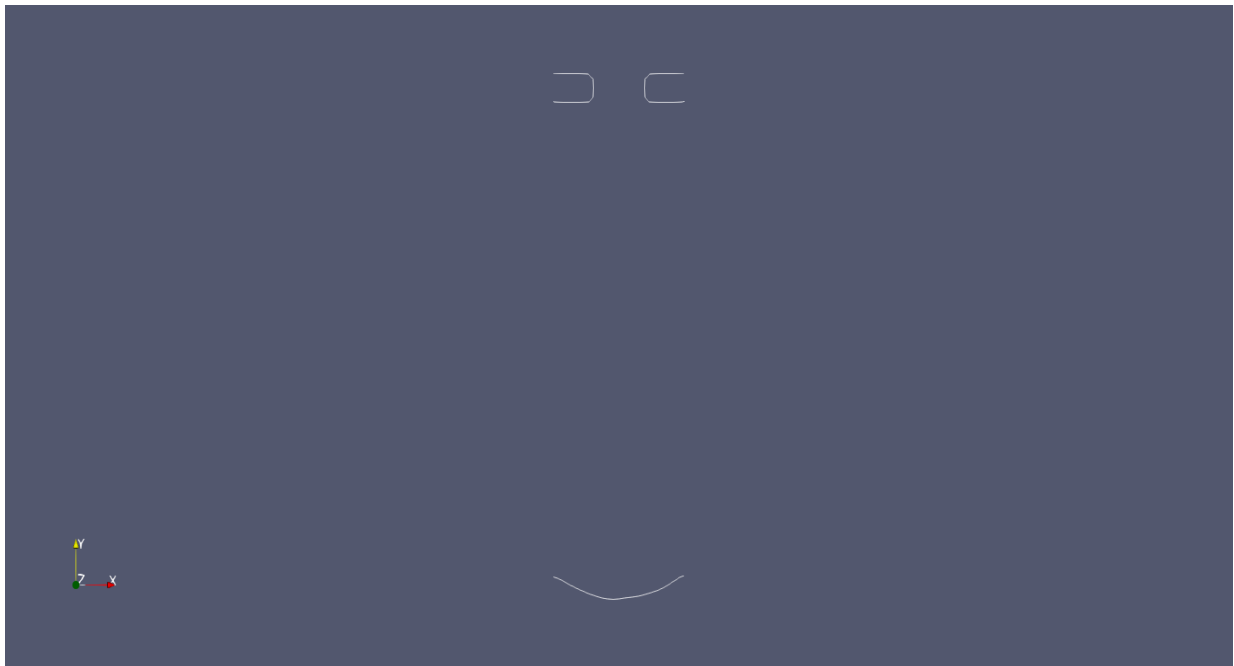
Percent of total time: 19.509927

Top-down flux calculation total time: 1.690310 s

Percent of total time: 45.642353

So, it can be noticed from this output that if the Oxygen flux is decreased 10 times, then the time for etching and surface advection is more compared to that of flux of both 30 and 300.

The visualization of the surface at flux = 3 is as under:



It can be observed from the above that reduced oxygen flux increased the etch rate which led to very deep etch as the surface is broken apart. Also, the surface is rougher and non-uniform.

### Task 3.1:

1) Theoretical calculation of the deposition rate

The flux is given by, Flux,  $F = (P \cdot v) / (4 \cdot k \cdot T) = (n \cdot v) / 4$

Where, P is the partial pressure of TEOS in the reactor,

$P = 66 \text{ Pa}$

$v$  = mean velocity

$k = 1.38 \times 10^{-23} \text{ J/K}$  is Boltzmann's constant.

$n$  = number density

$T = 730 + 273.15 = 1003.15 \text{ K}$  is the temperature in Kelvin.

So, to find the flux F the mean velocity of the TEOS molecules needs to be calculated. By Maxwell-Boltzmann distribution, mean velocity is,  $v = [(8 \cdot k \cdot T) / (\pi \cdot m_{\text{TEOS}})]^{1/2}$

mass of TEOS  $M_{\text{TEOS}} = 208.33 \text{ g/mol} = 208.33 \times 10^{-3} \text{ kg/mol} = 3.46 \times 10^{-25} \text{ kg/molecule}$

So,  $v = 319.193 \text{ m/s}$

Now compute the flux  $F = 66 \times 319.193 / 4 \times 1.38 \times 10^{-23} \times 1003.15$

$F = 3.80445 \times 10^{23} \text{ molecules/m}^2 \cdot \text{s}$

The deposition rate is then given by,  $R = (F \cdot S) / \rho$

$S = \text{Sticking probability} = 0.1$

$\rho$  is the number of  $\text{SiO}_2$  molecules per unit volume

So, deposition rate is,

$$R = 0.102 \text{ } \mu\text{m} / \text{min}$$

Now, comparing this theoretical value with the shown in Figure 2 (taking the trench geometry as  $70 \times 70 \text{ nm}$ ):

After 150 minutes (a): The deposition has only started to fill the trench.

After 250 minutes (b): A significant amount of the trench has been deposited, but the trench is not completely full.

After 350 minutes (c): The trench is almost fully filled, but some tapering at the top remains.

Now, comparing how much deposition happens theoretically at each time with the experimental measurements:

**1. Theoretical Thickness After 150 minutes:**

$$\text{Thickness} = 0.102 \text{ } \mu\text{m}/\text{min} \times 150 \text{ min} = 15.3 \text{ } \mu\text{m}$$

**2. Theoretical Thickness After 250 minutes:**

$$\text{Thickness} = 0.102 \text{ } \mu\text{m}/\text{min} \times 250 \text{ min} = 25.5 \text{ } \mu\text{m}$$

**3. Theoretical Thickness After 350 minutes:**

$$4. \text{ Thickness} = 0.102 \text{ } \mu\text{m}/\text{min} \times 350 \text{ min} = 35.7 \text{ } \mu\text{m}$$

If we compare this with the trench geometry (which is  $70 \text{ } \mu\text{m}$  wide and  $70 \text{ } \mu\text{m}$  deep), it appears that the theoretical deposition rate is much faster than the experimental results would suggest. This may indicate that the model needs adjustments, either in terms of deposition rate, sticking probability, or reaction order.

**2) Simulating the Process in ViennaPS:**

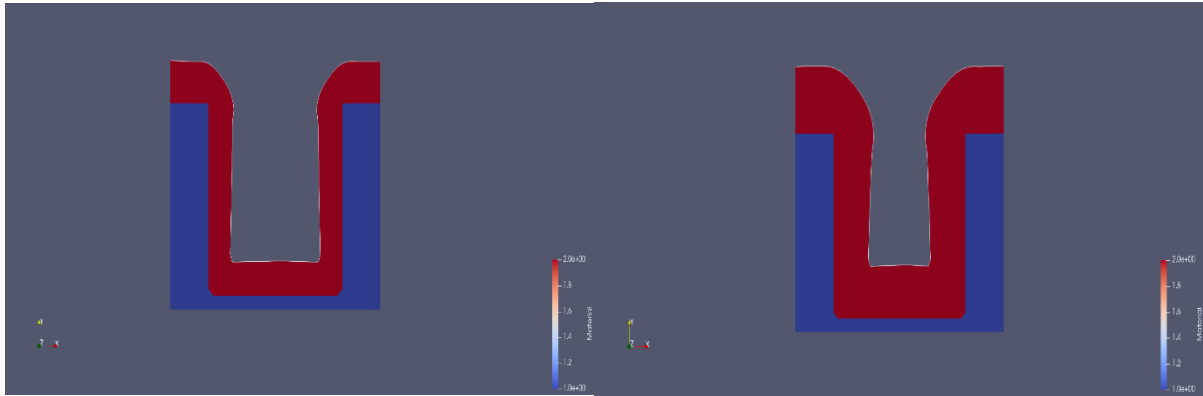
Now that we have a theoretical estimate, we can simulate the process using ViennaPS and try to match the experimental profiles. The code is run through cmd by: `python Task3.1.py singleTEOS_config.txt`

**Initial Configuration:**

Set the sticking probability to 0.1, as given.

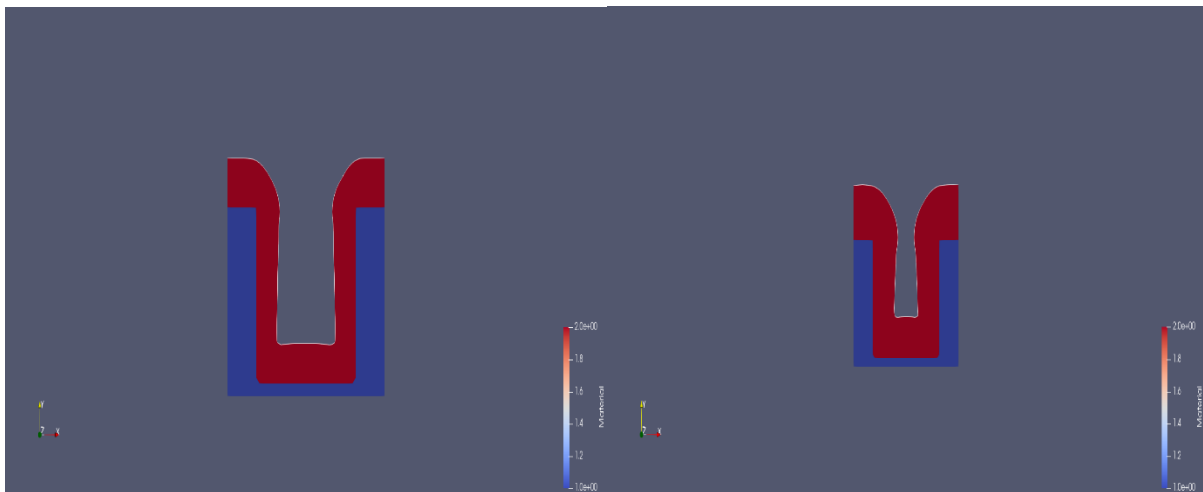
Set the deposition rate to the calculated theoretical rate  $R = 0.102 \text{ } \mu\text{m}/\text{min}$

So, at 150 min, 250 min and 350 min respectively, the visualizations look like:



So, it seems these do not match the figure 2 of Experimental measurements. So, there should be some changes made in sticking coefficient and the deposition rate.

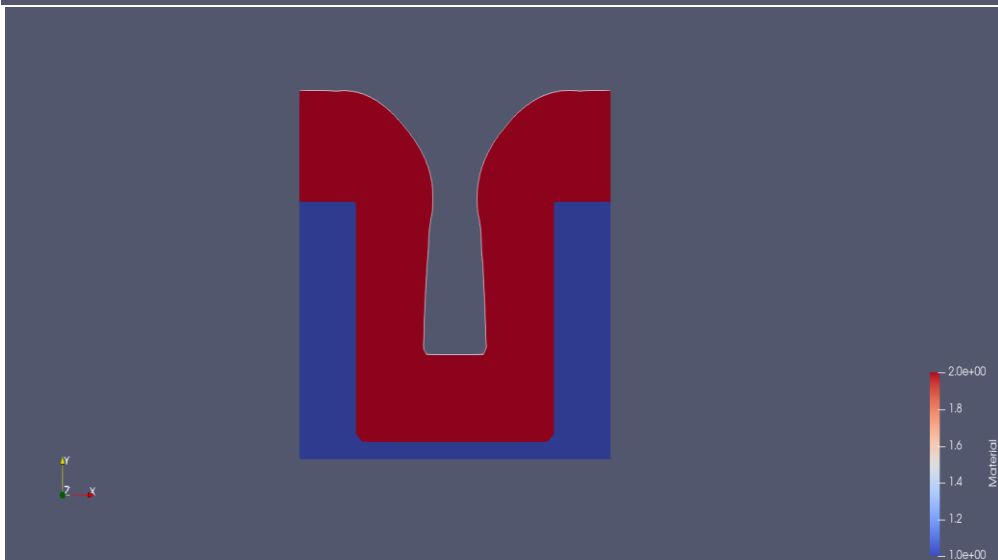
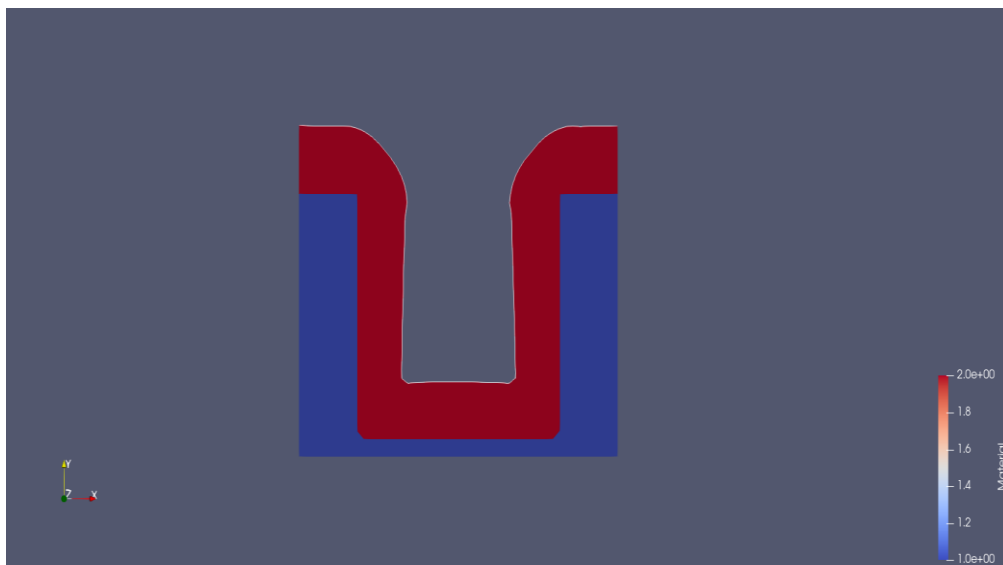
Taking deposition rate as  $0.13 \mu\text{m}/\text{min}$ , and sticking coefficient the same as 0.1, these are the results for 150, 250 and 350 mins:







Now, finally after this I changed the sticking probability = 0.08 and kept the deposition rate same = 0.13, so I get satisfactory results, for  $t = 150, 250$  and  $350$  mins respectively:





So, observing at the above images, the image with  $t = 150$  mins quite well matches with the experiment figure (a) After 150 minutes. Also, for  $t = 250$  mins, the above figure matches with the experimental figure, but for  $t = 350$  mins, it still doesn't match fully with the experimental figure, and I tried different deposition rates and sticking coefficients and they match the first 2 figures but not with the  $t = 350$  mins fully. This can be due to the linear model that is being used and also because of non-linear reactions, mass transport limitations, or surface saturation.

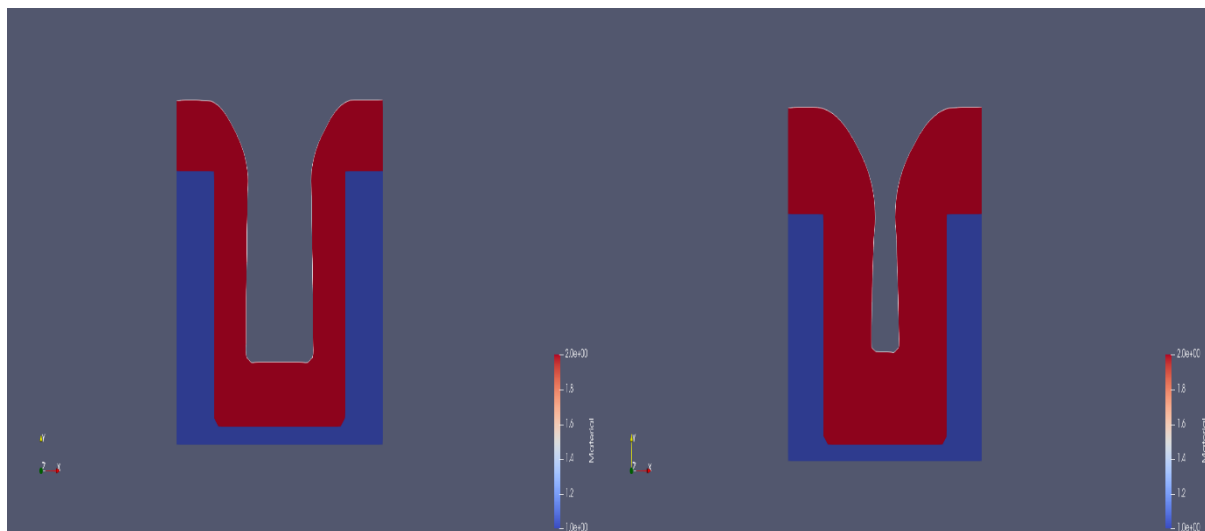
So, the values that best fit the experiment are,

**Deposition Rate =  $0.13 \text{ } \mu\text{m} / \text{min}$**

**Sticking Probability = 0.08**

3) Now, the reaction order is to be fixed at 0.5, while changing the deposition rate and the sticking probability.

Now, first without changing the previous deposition rate = 0.13 and the sticking probability = 0.08, I got the following figures for  $t = 150, 250$  and  $350$  mins:





These figures do not look too similar to the experimental ones, so the deposition rate and sticking coefficient needs to be altered.

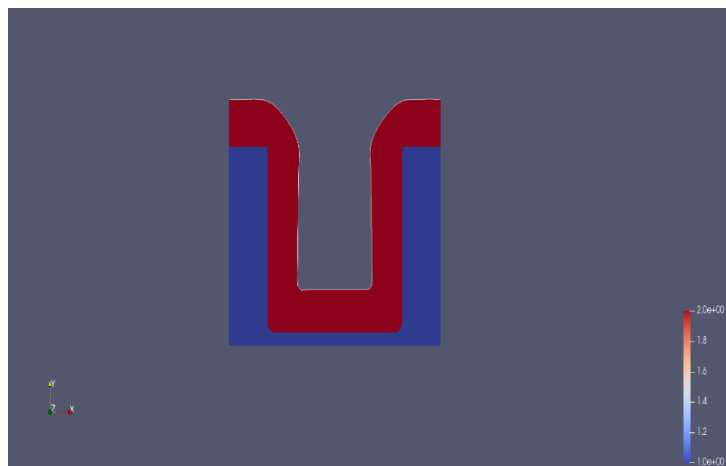
So, at these settings and values I get satisfactory results:

Deposition Rate = 0.12  $\mu\text{m} / \text{min}$

Sticking Probability = 0.09

Reaction Order = 0.5

The results at  $t = 150, 250$  and  $350$  are:





So, assuming a lower reaction order = 0.5 and using Deposition Rate = 0.12  $\mu\text{m} / \text{min}$  and Sticking Probability = 0.09, the result after  $t = 350 \text{ min}$  gives a better fit to the measured topography but still does not fully resemble it as a lower reaction order slows down the process but does not give good results for  $t = 350 \text{ mins}$ .

#### Task 4.1:

##### 1) Theoretical Calculation of Deposition Rates

We have two components contributing to the deposition:

1. TEOS Molecule: Has a low sticking coefficient, contributing weakly to deposition.
2. Intermediate Precursor: Has a high sticking coefficient, contributing significantly to deposition.

For calculation, the values are:

TEOS sticking coefficient:  $S_{\text{TEOS}} = 10^{-4}$

Precursor sticking coefficient:  $S_{\text{precursor}} = 1$

TEOS partial pressure:  $P_{\text{TEOS}} = 66 \text{ Pa}$

Precursor partial pressure:  $P_{\text{precursor}} = 10^{-4} \times P$

Mean velocity and density of both gases are assumed to be the same.

Flux,  $F = (P \cdot v) / (4 \cdot k \cdot T) = (n \cdot v) / 4$

TEOS flux,

$$F_{\text{TEOS}} = (66 \times 319.193) / (4 \times 1.38 \times 10^{-23} \times 1003.15) = 3.8045 \times 10^{23}$$

Precursor flux,  $P_{\text{precursor}} = 10^{-4} \times P_{\text{TEOS}} = 6.6 \times 10^{-3} \text{ Pa}$

$$F_{\text{Precursor}} = (6.6 \times 10^{-3} \times 319.193) / (4 \times 1.38 \times 10^{-23} \times 1003.15) = 3.8045 \times 10^{19}$$

So, the deposition rate,

For TEOS,

Sticking probability:  $S_{\text{TEOS}}=10^{-4}$

$\rho=2.2 \times 10^{28}$  molecules/m<sup>3</sup>

$R_{\text{TEOS}}= 0.104 \text{ } \mu\text{m/min}$

For Precursor,

Sticking probability,  $S_{\text{precursor}}=1$

$R_{\text{Precursor}} = 0.1038 \text{ } \mu\text{m/min} = 0.104 \text{ } \mu\text{m/min}$  (approx.)

A low sticking probability means that most TEOS molecules do not immediately stick to the surface upon contact. Instead, they tend to continue diffusing or moving in the reactor. This has several effect:

TEOS molecules have more chances to diffuse to different parts of the trench (including the sidewalls and bottom) before reacting with the surface. As a result, TEOS contributes more uniformly to the deposition across the trench (top, sidewalls, and bottom).

A low sticking coefficient naturally means slower deposition because fewer TEOS molecules get incorporated into the film with each pass.

TEOS molecules can reach deeper into the trench, leading to relatively better deposition at the bottom of the trench compared to a scenario where TEOS has a higher sticking probability. This improves the step coverage of the deposition.

A high sticking probability means that almost every precursor molecule that contacts the surface sticks to it, leading to very rapid deposition at the point of contact.

Due to the high sticking probability, the precursor molecules will deposit heavily at the top of the trench where they first encounter the surface. This creates less uniformity in the deposition across the trench, with a much higher rate at the top and slower deposition at the bottom.

With a high sticking coefficient, fewer precursor molecules will reach the bottom of the trench, as they are more likely to deposit at the top. This results in poor deposition at the bottom and a less uniform film thickness and uneven deposition profile.

#### Deposition Rate: Bottom vs Top of the Trench

- TEOS: Since TEOS has a low sticking probability, it diffuses more uniformly into the trench, allowing for a relatively even deposition rate between the top and bottom.
- Precursor: The precursor, with its high sticking probability, will deposit faster at the top than the bottom of the trench. The rate at the bottom will be lower because most of the precursor will stick to the top surface, leading to less precursor available for deposition further down into the trench.

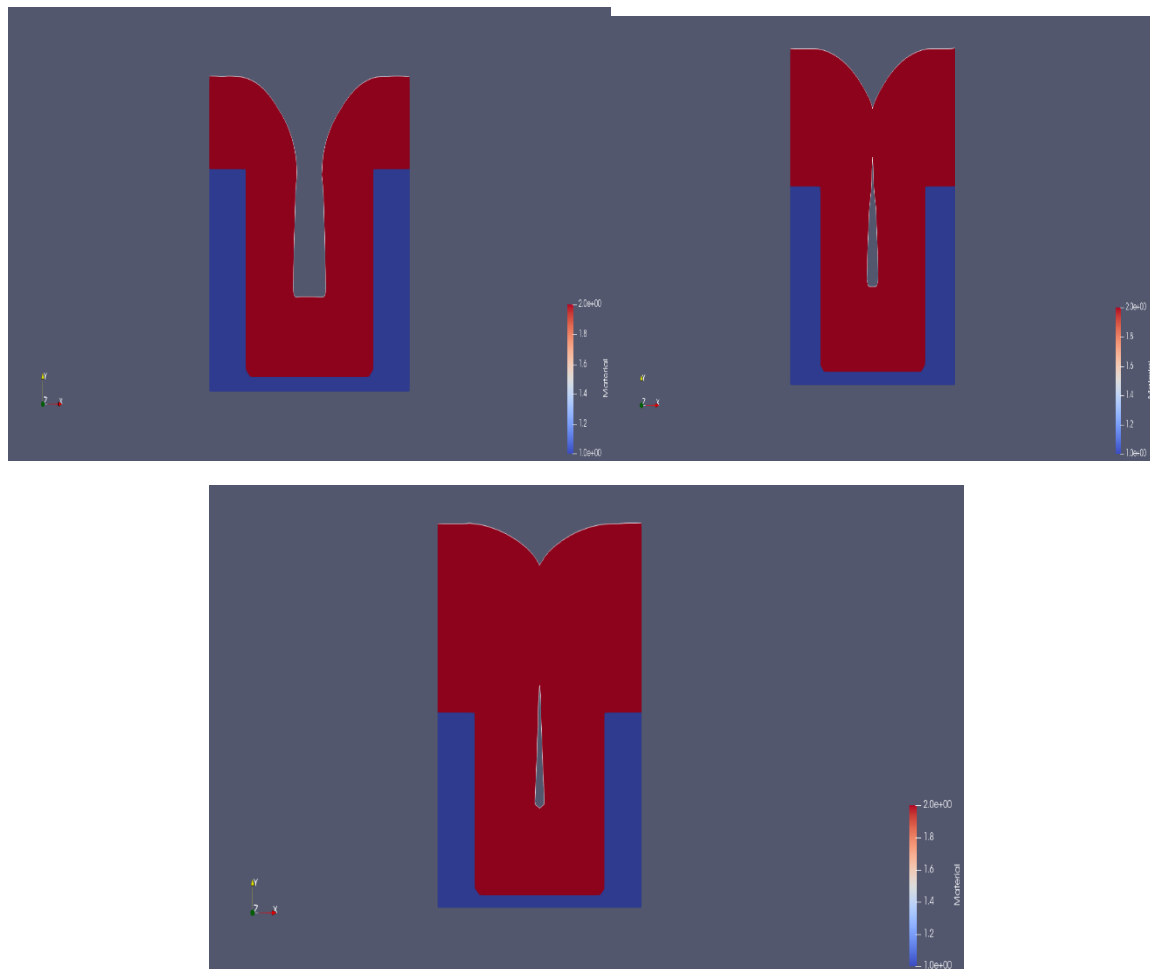
As for the model, yes, it is a better model because:

- The single-particle model only accounted for TEOS deposition, which could not fully replicate the experimental observations, especially at later times (beyond 250 minutes).
- By introducing a second particle (the precursor), the model now accounts for additional deposition behaviour, potentially improving the accuracy and match to experimental data.
- The multi-particle model better reflects the complex chemical behaviour in the reactor, where TEOS dissociates into reactive intermediates, which may deposit differently than the parent TEOS molecule.

2) Now, using the theoretical obtained deposition rates for simulation,

$$R_{\text{Precursor}} = 0.104 \mu\text{m}/\text{min} = R_{\text{TEOS}}$$

Keeping the other values the same in configuration file, the results obtained for  $t = 150$ , 250 and 350 mins are:



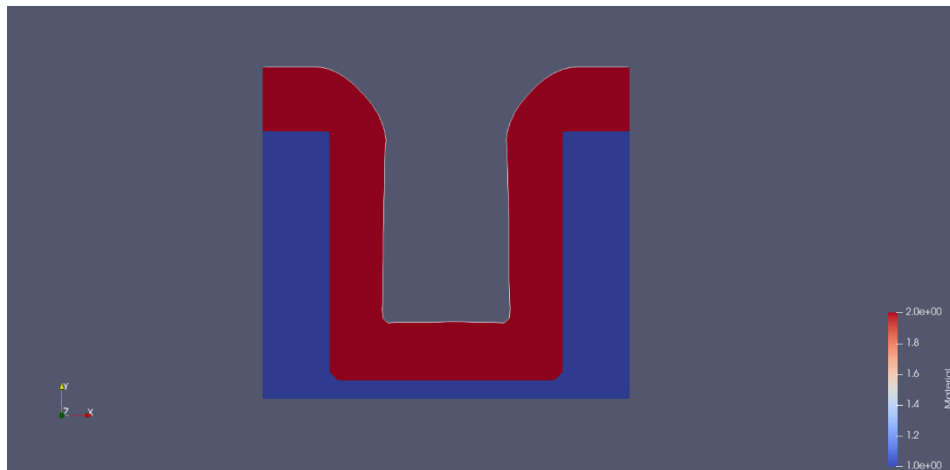
So, from the above figures, it can be seen that using theoretical deposition rates, the good fit is seen in the figure for  $t = 350$  mins which closely resembles the experimental figure. The other two do not resemble their respective experimental figures.

So, now adjusting the deposition rates to get the best fit, I get these values of deposition rates which give the best fit for all the figures:

**Deposition Rate P1 = 0.05**

**Deposition Rate P2 = 0.07**

This setting gives the best results and fit for all the three figures and they very nearly resemble their experimental figures respectively. Here are the visualizations of the figures at  $t = 150, 250$  and  $350$  mins respectively:



### Assumptions That Led to Initial inaccurate parameters:

- **Uniform Properties:** Assuming that both TEOS and the precursor have identical properties except for the sticking probability was likely too simple. For example, molecular size, energy, or temperature sensitivity could vary between the two particles.
- **Precursor Proportion:** The assumption that 1 in 10,000 TEOS molecules dissociates into the precursor might not hold exactly true in the experimental setup, especially under real reactor conditions. This could affect the precursor's actual contribution to deposition.
- **TEOS Diffusion:** The initial TEOS diffusion might have been underestimated, leading to the necessity of increasing its deposition rate.
- **Process Uniformity:** The assumption that the gas phase is homogeneous throughout the reactor could be too normal and it may be non - uniform. Real reactors might have gradients in temperature, pressure, and gas concentration, affecting the deposition rates differently.

3) Now, if it is assumed that the error in the TEOS deposition rate of the theoretical two-particle model only stems from a wrong assumption of the sticking coefficient, then using the simulation for finding the best value of sticking coefficient for the TEOS keeping every other parameter as constant, so the deposition rates are:

$$R_{\text{Precursor}} = 0.104 \mu\text{m}/\text{min} = R_{\text{TEOS}}$$

And Precursor sticking coefficient:  $S_{\text{precursor}} = 1$

Now, the best fit sticking coefficient is to be found out from the simulation.

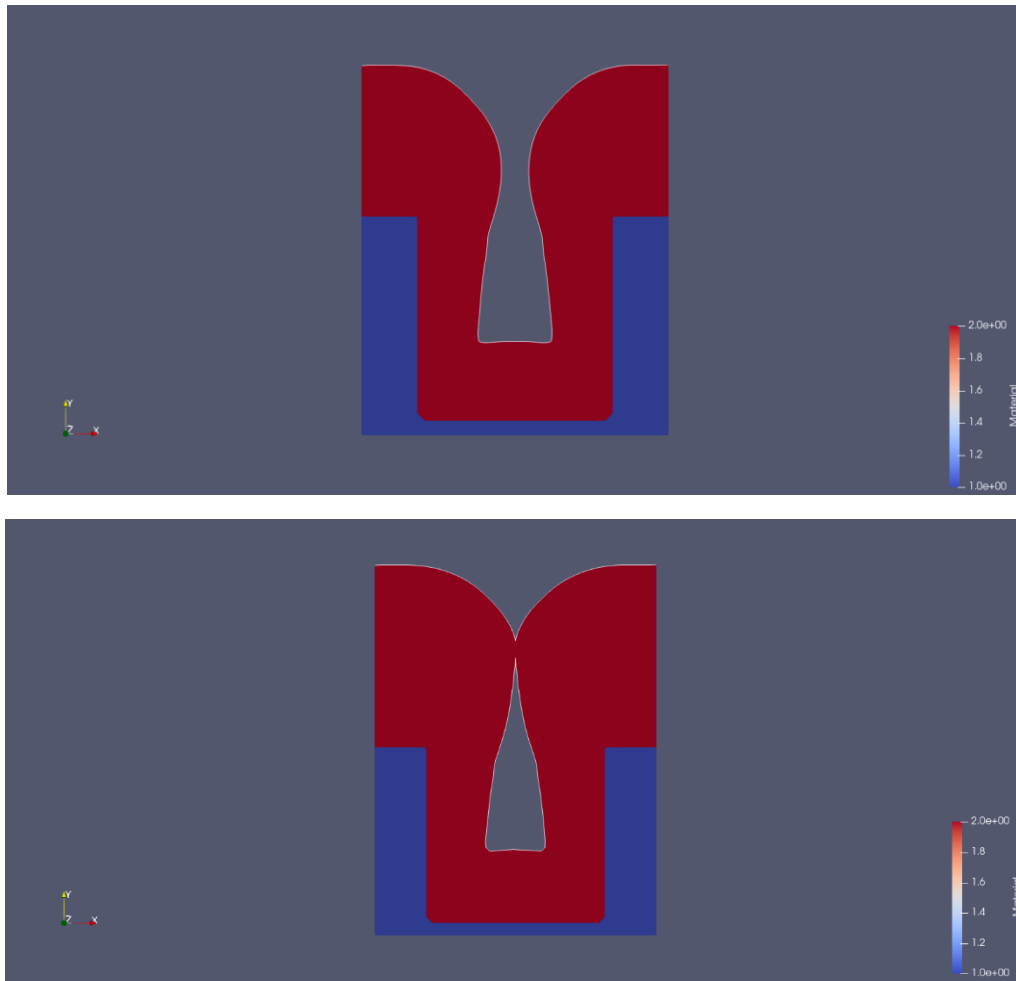
So, after the simulation after calibrating the model on various sticking coefficients, I found the best fit for the TEOS sticking coefficient as,

$$S_{\text{TEOS}} = 0.06$$

The results obtained are as under in the images for  $t = 150, 250$  and  $350$  mins respectively. For this sticking coefficient, all the three images show resemblance quite near to their respective experimental figures:







So, the correct sticking coefficient according to simulations which creates similar images to the experimental ones is,

$$S_{\text{TEOS}} = 0.06$$

