Model created in COMSOL Multiphysics 6.4

Optimization of Chemical Etching

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Introduction

This model is based on the model *Chemical Etching* in the Chemical Engineering folder of the COMSOL Multiphysics Application Library, which models wet etching under laminar flow using the Deformed Geometry interface.

In the model at hand, the symmetry of the etching is optimized by allowing the concentration and convection to change over time, while constraining the average etching depth.

Model Definition

The objective is to minimize the squared deviation between the two sides:

$$\varphi = \int_{\partial\Omega} (y_{\text{spatial}} - y_{\text{spatial,mirror}})^2 ds ,$$

where $y_{\text{spatial,mirror}}$ is constructed using a **General Extrusion** operator. The minimization is achieved by allowing the concentration at the boundaries and the wall movement to be controlled by two separate **Control Function** features. The geometry is symmetric before etching, so a design without etching exists as a trivial solution to this optimization. This solution can be made infeasible by imposing a minimum value on the average etching depth

$$\psi = \int_{\partial\Omega} (y_{\text{spatial}} / y_{\text{spatial,init}}) ds > 1, \quad \text{where} \quad y_{\text{spatial,init}} = \int_{\partial\Omega} y_{\text{spatial}} ds / \int_{\partial\Omega} ds$$

Note that the constraint is scaled so that a bound equal to 1 can be used. Similarly, the objective is scaled based on the initial value. A solution to the optimization problem is found with the MMA method using move limits equal to 0.1. The optimization is limited to 25 iterations to avoid a long computational time.

Results and Discussion

Figure 1 displays the optimized control functions. The convection causes the asymmetry, so it makes sense that this decreases when the concentration is increased. However, such changes tend to violate the constraint. Therefore, those trends are reversed toward the end of the simulation, where the convection introduces less anisotropy, because the cavity is larger than early on.

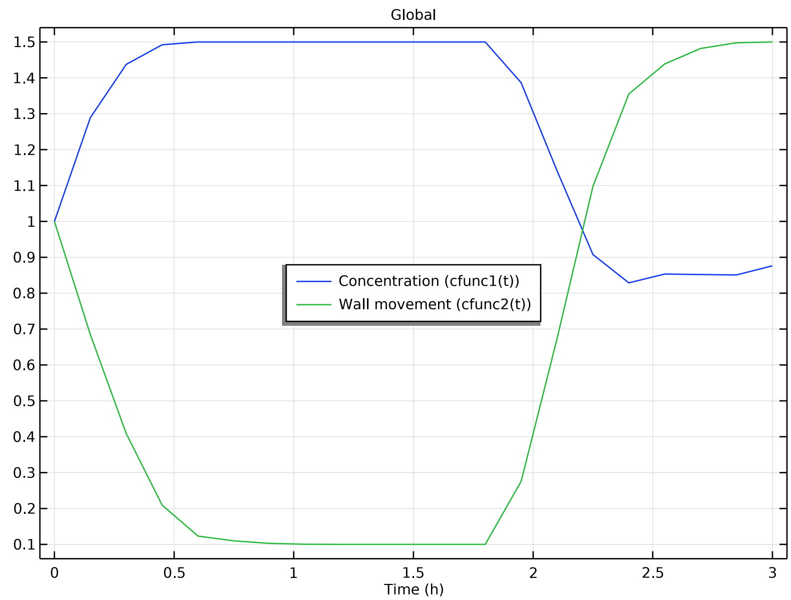

Figure 1: The plot shows that the concentration is doubled throughout the first half of the simulation and then drops sharply to half the initial value toward the end. In contrast, the wall movement behaves in the opposite way, dropping to the minimum value throughout the first half and then increasing to the maximum value toward the end.

The final shape of the cavity before and after optimization is shown in Figure 2. Some of the asymmetry remains, but most of it has been removed by the optimization.

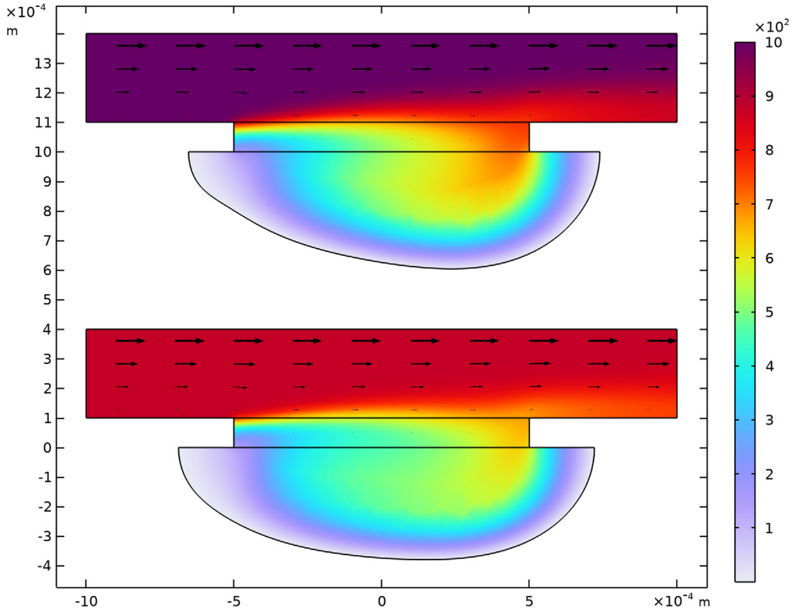

Figure 2: The plot shows the concentration and velocity field at the end of the process before (top) and after optimization (bottom). The optimization increases the symmetry significantly without reducing the etching depth.

Notes About the COMSOL Implementation

The time-dependent part of the problem is initialized with the result of a stationary problem. However, there is no support for gradient-based optimization over the combination of a **Stationary** solver followed by a **Time Dependent** solver. Therefore, the **Control Function** features are set up with a Dirichlet boundary condition for the initial time, so that the optimization can be restricted to the **Time Dependent** study step.

Application Library path: `Optimization_Module/Optimal_Control/chemical_etching_optimization`

Modeling Instructions

This example starts from an existing model from the COMSOL Multiphysics Application Library.

APPLICATION LIBRARIES

1. From the **File** menu, choose **Application Libraries**.
2. In the **Application Libraries** window, select **COMSOL Multiphysics** > **Chemical Engineering** > **chemical_etching** in the tree.
3. Click **Open**.

STUDY 1: INITIAL

1. In the **Model Builder** window, click **Study 1**.
2. In the **Settings** window for **Study**, type `Study 1: Initial` in the **Label** text field.

RESULTS

Evaluation Group 1

1. In the **Results** toolbar, click **Evaluation Group**.
2. In the **Settings** window for **Evaluation Group**, locate the **Data** section.
3. From the **Time selection** list, choose **Last**.

Line Average 1

1. Right-click **Evaluation Group 1** and choose **Average** > **Line Average**.
2. In the **Settings** window for **Line Average**, locate the **Selection** section.
3. From the **Selection** list, choose **Bottom**.
4. Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
y	m	y-coordinate

5. In the **Evaluation Group 1** toolbar, click **Evaluate**.

Add the initial etching depth as a parameter together with the parameter for the time to allow the use of **Control Function** features with this argument in stationary solvers. Note that the value of the parameter will be overwritten by time dependent solvers.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
yavg	-319[um]	-3.19E-4 m	Initial etching depth
t	0[s]	0 s	Time

COMPONENT 1 (COMP1)

The initial profile is symmetric, so it is easy to achieve a symmetric profile by avoiding etching. This trivial solution can be avoided by imposing a constraint on the etching depth using a **Boundary Probe**.

DEFINITIONS

Boundary Probe 1 (bnd1)

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

2 Right-click **Component 1 (comp1)** > **Definitions** and choose **Probes** > **Boundary Probe**.

3 In the **Settings** window for **Boundary Probe**, type `constr` in the **Variable name** text field.

4 Locate the **Source Selection** section. Click **Clear Selection**.

5 From the **Selection** list, choose **Bottom**.

6 Locate the **Expression** section. In the **Expression** text field, type `y/yavg`.

Control Function 1 (cfunc1)

1 In the **Definitions** toolbar, click **Control Variables** and choose **Control Function**.

2 In the **Settings** window for **Control Function**, locate the **Input** section.

3 In the x_{end} text field, type `tmax`.

4 Locate the **Output** section. In the f_{min} text field, type `0.1`.

5 In the f_{max} text field, type `1.5`.

6 From the **Start boundary condition** list, choose **Dirichlet**.

7 In the $f(x_{start})$ text field, type `1` to avoid setting unphysical initial conditions for the **Time Dependent** solver.

8 In the c_0 text field, type `1`.

9 Locate the **Control Variable Discretization** section. From the **Control type** list, choose **Piecewise Bernstein polynomial**.

10 In the **Order** text field, type 3 to increase the design freedom a bit.

Control Function 2 (cfunc2)

Right-click **Control Function 1 (cfunc1)** and choose **Duplicate**.

Use the control function to scale the concentration and wall movement.

TRANSPORT OF DILUTED SPECIES (TDS)

In the **Model Builder** window, expand the **Component 1 (comp1)** > **Transport of Diluted Species (tds)** node.

TRANSPORT OF DILUTED SPECIES (TDS)

Concentration 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Laminar Flow (spf)** node, then click **Component 1 (comp1)** > **Transport of Diluted Species (tds)** > **Concentration 1**.
2 In the **Settings** window for **Concentration**, locate the **Concentration** section.
3 In the $c_{0,\mathrm{cCuCl2}}$ text field, type `cCuCl2_bulk*cfunc1(t)`.

LAMINAR FLOW (SPF)

Wall 2

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Laminar Flow (spf)** click **Wall 2**.
2 In the **Settings** window for **Wall**, click to expand the **Wall Movement** section.
3 Specify the $\mathbf{u}_{\mathrm{tr}}$ vector as

1[mm/s]*cfunc2(t)	x

Add a **General Extrusion** operator so that this can be used to construct an objective function that quantifies the asymmetry.

DEFINITIONS (COMP1)

General Extrusion 1 (genext1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **General Extrusion**.
2 In the **Settings** window for **General Extrusion**, locate the **Source Selection** section.

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

4 From the **Selection** list, choose **Bottom**.

5 Locate the **Destination Map** section. In the **x-expression** text field, type `-x`.

6 In the **y-expression** text field, type `Yg`.

7 Locate the **Source** section. Select the **Use source map** checkbox.

8 In the **y^{i}-expression** text field, type `Yg`.

Boundary Probe 2 (bnd2)

1 In the **Definitions** toolbar, click **Probes** and choose **Boundary Probe**.

2 In the **Settings** window for **Boundary Probe**, type `obj` in the **Variable name** text field.

3 Locate the **Source Selection** section. Click **Clear Selection**.

4 From the **Selection** list, choose **Bottom**.

5 Locate the **Expression** section. In the **Expression** text field, type `if(isnan(genext1(y)),0, (y-genext1(y))^2)` to avoid contributions where the asymmetry prevents retrieval of a y coordinate for the comparison.

ADD STUDY

1 In the **Home** toolbar, click **Windows** and choose **Add Study**.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies** > **Stationary**.

4 Click the **Add Study** button in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 1: INITIAL

Step 2: Time Dependent

1 In the **Model Builder** window, expand the **Study 1: Initial** node.

2 Right-click **Study 1: Initial** > **Step 2: Time Dependent** and choose **Copy**.

STUDY 2

In the **Model Builder** window, right-click **Study 2** and choose **Paste Time Dependent**.

Step 1: Stationary

1 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

2 In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Deformed Geometry**.

Shape Optimization

1 In the **Study** toolbar, click **Optimization** and choose **Shape Optimization**.

2 In the **Settings** window for **Shape Optimization**, locate the **Optimization Solver** section.

3 From the **Study step** list, choose **Time Dependent**.

4 In the **Move limits** text field, type `0.2`.

5 In the **Maximum number of iterations** text field, type `25`.

6 Click **Add Expression** in the upper-right corner of the **Objective Function** section. From the menu, choose **Component 1 (comp1) > Definitions > comp1.obj - Boundary Probe 2 - m²**.

7 Locate the **Objective Function** section. Find the **Objective settings** subsection. From the **Objective scaling** list, choose **Initial solution based**.

8 Click **Add Expression** in the upper-right corner of the **Constraints** section. From the menu, choose **Component 1 (comp1) > Definitions > comp1.constr - Boundary Probe 1 - 1**.

9 Locate the **Constraints** section. In the table, enter the following settings:

Expression	Lower bound	Upper bound
`comp1.constr`	1	

10 Click to expand the **Output** section. From the **Probes** list, choose **None**.

11 In the **Model Builder** window, click **Study 2**.

12 In the **Settings** window for **Study**, type `Study 2: Optimization` in the **Label** text field.

13 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

14 In the **Study** toolbar, click **Get Initial Value**.

RESULTS

Concentration (tds), Deformed Geometry, Evaluation Group 1, Mesh, Pressure (spf), Velocity (spf)

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Concentration (tds)**, **Velocity (spf)**, **Pressure (spf)**, **Deformed Geometry**, **Mesh**, and **Evaluation Group 1**.

2 Right-click and choose **Group**.

Initial

In the **Settings** window for **Group**, type `Initial` in the **Label** text field.

Concentration (tds) 1

1 In the **Model Builder** window, right-click **Concentration (tds)** and choose **Duplicate**.
2 Expand the **Results** > **Datasets** node.
3 Right-click **Concentration (tds) 1** and choose **Move Out**.
4 In the **Model Builder** window, click **Concentration (tds) 1**.
5 In the **Settings** window for **2D Plot Group**, locate the **Data** section.
6 From the **Dataset** list, choose **Study 2: Optimization/Solution 3 (sol3)**.

STUDY 2: OPTIMIZATION

Shape Optimization

1 In the **Model Builder** window, under **Study 2: Optimization** click **Shape Optimization**.
2 In the **Settings** window for **Shape Optimization**, locate the **Output** section.
3 Select the **Plot** checkbox.
4 From the **Plot group** list, choose **Concentration (tds) 1**.

Solver Configurations

In the **Model Builder** window, expand the **Study 2: Optimization** > **Solver Configurations** node.

Solution 3 (sol3)

1 In the **Model Builder** window, expand the **Study 2: Optimization** > **Solver Configurations** > **Solution 3 (sol3)** node, then click **Optimization Solver 1**.
2 In the **Settings** window for **Optimization Solver**, locate the **Optimization Solver** section.
3 Clear the **Globally Convergent MMA** checkbox.
4 Click to expand the **Advanced** section. From the **Compensate for nojac terms** list, choose **Off** to avoid warnings in the log.
5 In the **Model Builder** window, expand the **Study 2: Optimization** > **Solver Configurations** > **Solution 3 (sol3)** > **Optimization Solver 1** > **Time-Dependent Solver 1** node, then click **Advanced**.
6 In the **Settings** window for **Advanced**, click to expand the **Assembly Settings** section.
7 Clear the **Reuse sparsity pattern** checkbox to avoid warnings in the log.
8 In the **Study** toolbar, click = **Compute**.

RESULTS

Add a plot to visualize the concentration and wall movement as a function of time.

Control Functions

1 In the **Results** toolbar, click **1D Plot Group**.
2 In the **Settings** window for **1D Plot Group**, type `Control Functions` in the **Label** text field.
3 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Optimization/Solution 3 (sol3)**.
4 Locate the **Legend** section. From the **Position** list, choose **Center**.

Global 1

1 Right-click **Control Functions** and choose **Global**.
2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.
3 In the table, enter the following settings:

Expression	Unit	Description
`cfunc1(t)`	1	`Concentration`
`cfunc2(t)`	1	`Wall movement`

4 Locate the **x-Axis Data** section. From the **Unit** list, choose **h**.
5 Click to expand the **Legends** section. Find the **Include** subsection. Clear the **Solution** checkbox.
6 Select the **Expression** checkbox.
7 In the **Control Functions** toolbar, click **Plot**.

Use a **Transformation** dataset to simplify the construction of a thumbnail plot showing the initial and optimized profile together.

Transformation 2D 1

1 In the **Results** toolbar, click **More Datasets** and choose **Transformation 2D**.
2 In the **Settings** window for **Transformation 2D**, locate the **Transformation** section.
3 Select the **Move** checkbox.
4 In the **y** text field, type `10*h_mask`.

Concentration (tds) 1

In the **Model Builder** window, expand the **Results** > **Concentration (tds) 1** node.

Arrow Surface 1, Surface 1

1 In the **Model Builder** window, under **Results** > **Concentration (tds) 1**, Ctrl-click to select **Surface 1** and **Arrow Surface 1**.

2 Right-click and choose **Duplicate**.

Surface 2

1 In the **Settings** window for **Surface**, locate the **Data** section.

2 From the **Dataset** list, choose **Transformation 2D 1**.

3 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Surface 1**.

Arrow Surface 2

1 In the **Model Builder** window, click **Arrow Surface 2**.

2 In the **Settings** window for **Arrow Surface**, locate the **Data** section.

3 From the **Dataset** list, choose **Transformation 2D 1**.

4 In the **Concentration (tds) 1** toolbar, click **Plot**.

Surface 2

1 In the **Model Builder** window, click **Surface 2**.

2 Click **Plot**.

Thumbnail

1 In the **Model Builder** window, under **Results** click **Concentration (tds) 1**.

2 In the **Settings** window for **2D Plot Group**, type `Thumbnail` in the **Label** text field.

3 Click to expand the **Title** section. From the **Title type** list, choose **None**.

Line 1

1 Right-click **Thumbnail** and choose **Line**.

2 In the **Settings** window for **Line**, locate the **Data** section.

3 From the **Dataset** list, choose **Transformation 2D 1**.

4 Locate the **Expression** section. In the **Expression** text field, type `1`.

5 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

6 From the **Color** list, choose **Black**.

7 In the **Thumbnail** toolbar, click **Plot**.

Concentration (tds)

1 In the **Model Builder** window, under **Results** > **Initial** click **Concentration (tds)**.

2 In the **Concentration (tds)** toolbar, click **Plot**.