Homogenization in a Chemical Reactor

Introduction

This model illustrates how to simulate a periodic homogenization process in a space dependent chemical reactor model. This homogenization removes concentration gradients in the reactor at a set time interval.

The model demonstrates a technique by which you can implement the stopping of the time-dependent solver, then restarting it with an initial value obtained based on the solution.

Model Definition

The model studies the concentration of a diluted species in a reactor. The chemical reaction is defined by the reaction rate $k*c$. Only the diffusion transport is considered in the model, no convection term is included.

The initial species concentration in the reactor is 0 and a fixed concentration of 1 mol/m^3 is applied at the bottom boundary.

The homogenization takes place every 30 minutes, and it is assumed to be ideal. Thus, a homogeneous concentration is calculated as the average concentration in the reactor each time the solution is stopped. This concentration is then applied as the initial condition each time the solution is restarted.

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Results and Discussion

Figure 1 show the distribution of the concentration in the reactor after 30 minutes. The highest concentration appears close to the source boundary, while the lowest concentration is in the corner furthest away from it.

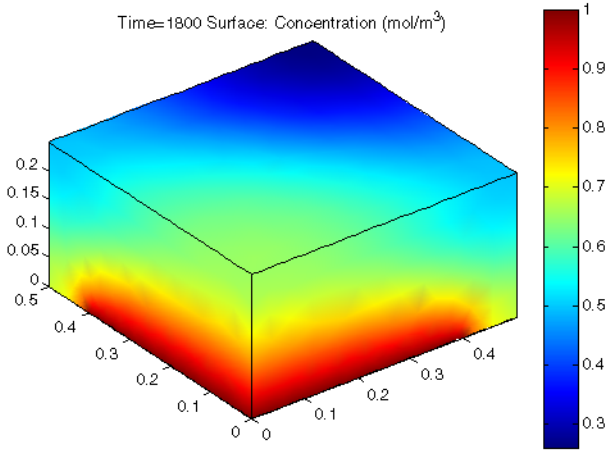

Figure 1: Concentration distribution after 30 minutes.

Figure 2 shows the concentration at the center of the top surface, defined by the coordinates (0.25m; 0.25m; 0.25m). The blue solid line denotes the concentration

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with the homogenization process. The dashed red line denotes the concentration when solving without homogenizing.

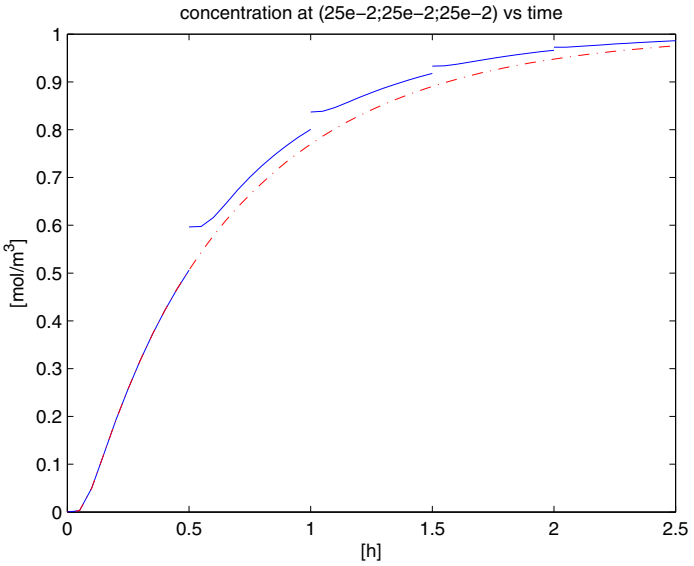

Figure 2: Evolution of the species concentration at (0.25m ,0.25m, 0.25m)

After 30 minutes the concentration in this point is much lower than the average value in the reactor. This can be seen by the jump in the concentration as the solver is restarted.

As evident from the figure the steady-state value for the concentration can be reached faster when applying the homogenization steps.

Notes About the COMSOL Implementation

The most efficient approach for this simulation is to start by setting up the diffusion problem in the graphical user interface of the COMSOL Desktop®. You can then save the model .mph file, which you can easily load into MATLAB®, where you continue to implement the script for solving the problem, including the homogenization steps.

Wrapper functions used by the script:

- **mphload** to load the model .mph file.
- **mphmean** to evaluate the average concentration in the reactor.
- **mphinterp** to evaluate the concentration at specific locations.

- **mphglobal** to evaluate global quantities in the model.
- **mphplot** to display plots.

Model Library path: `Model_library/LiveLink_for_MATLAB/Tutorial_Models/homogenization_llmatlab`

Modeling Instructions—COMSOL Desktop

Use the COMSOL Desktop to set-up the simulation of the chemical reactor. You can later load this model into MATLAB, using LiveLink™, to continue the model implementation.

MODEL WIZARD

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

2 Click **Next**.

3 In the **Add physics** tree, select **Chemical Species Transport>Transport of Diluted Species (chds)**.

4 Click **Next**.

5 Find the **Studies** subsection. In the tree, select **Preset Studies>Time Dependent**.

6 Click **Finish**.

GLOBAL DEFINITIONS

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 In the table, enter the following settings:

Name	Expression	Description
L	50[cm]	Geometry length
D	2e-5[m^2/s]	Diffusion coefficient
c0	1[mol/m^3]	Applied concentration
k	5e-11[1/s]	Reaction rate
t0	0	Initial time
dt	3[min]	Output time step

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Name	Expression	Description
T	30[min]	Period of homogenization
tf	t0+T	Final computational time

GEOMETRY 1

Block 1

1 In the **Model Builder** window, under **Model 1** right-click **Geometry 1** and choose **Block**.
2 In the **Block** settings window, locate the **Size and Shape** section.
3 In the **Width** edit field, type `L`.
4 In the **Depth** edit field, type `L`.
5 In the **Height** edit field, type `L/2`.
6 Click the **Build Selected** button.
7 In the **Model Builder** window, right-click **Geometry 1** and choose **Work Plane**.

Bézier Polygon 1

1 In the **Model Builder** window, under **Model 1>Geometry 1>Work Plane 1** right-click **Plane Geometry** and choose **Bézier Polygon**.
2 In the **Bézier Polygon** settings window, locate the **Polygon Segments** section.
3 Find the **Added segments** subsection. Click the **Add Linear** button.
4 Find the **Control points** subsection. In row **2**, set **xw** to `4/5*L`.
5 Find the **Added segments** subsection. Click the **Add Quadratic** button.
6 Find the **Control points** subsection. In row **2**, set **yw** to `4/5*L`.
7 In row **3**, set **xw** to `0`.
8 In row **3**, set **yw** to `4/5*L`.
9 Find the **Added segments** subsection. Click the **Add Linear** button.
10 Find the **Control points** subsection. Click the **Close Curve** button.
11 Click the **Build Selected** button.

TRANSPORT OF DILUTED SPECIES

Convection and Diffusion 1

1 In the **Model Builder** window, expand the **Transport of Diluted Species** node, then click **Convection and Diffusion 1**.
2 In the **Convection and Diffusion** settings window, locate the **Diffusion** section.
3 In the D_c edit field, type `D`.

Reactions 1

1 In the **Model Builder** window, right-click **Transport of Diluted Species** and choose **Reactions**.

2 Select Domain 1 only.

3 In the **Reactions** settings window, locate the **Reactions** section.

4 In the R_c edit field, type `k*c`.

Concentration 1

1 Right-click **Transport of Diluted Species** and choose **Concentration**.

2 Select Boundary 3 only.

3 In the **Concentration** settings window, locate the **Concentration** section.

4 Select the **Species c** check box.

5 In the $c_{0,c}$ edit field, type `c0`.

MESH 1

Free Tetrahedral 1

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

Size 1

1 In the **Model Builder** window, under **Model 1>Mesh 1** right-click **Free Tetrahedral 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 Boundary 3 only.

5 Locate the **Element Size** section. From the **Predefined** list, choose **Extra fine**.

6 Click the **Build All** button.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Time Dependent**.

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

3 In the **Times** edit field, type `range(t0,dt,tf)`.

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SAVE THE MODEL

1 You can now save the model in the COMSOL format, go to the **File** menu and select **Save**.

2 Browse to a directory which path is set in MATLAB and enter `homogenization_llmatlab` in the **File name** edit field.

Click **Save**.

Modeling Instructions—MATLAB®

In this section you find a detailed explanation of the commands you need to enter at the MATLAB command line in order to run the simulation.

1 Start **COMSOL with MATLAB**.

You now have two possibilities to continue:

- Enter each command, starting at step 2 below, at the MATLAB command line.
- Paste the full model script, included in the section Model M-File, into a text editor, then save the file with a ".m" extension, and finally run this file in MATLAB.

2 As a first step load the model containing the transient diffusion problem:

```
model = mphload('homogenization_llmatlab');
```

3 To define a for-loop that runs for five iterations type:

```
for i = 1:5
```

4 The first operation in the for-loop consists in computing the solution, do this with the command:

```
model.study('std1').run;
```

For the first iteration of the for loop the solver will stop after 30 minutes, according to the parameters, `t0` and `T`, specified in the model. For each subsequent iteration the solution will run for an additional 30 minutes, as you are changing the value of the start time `t0` in steps 7 and 8 below.

5 To obtain data for the plot shown in Figure 2 extract the concentration value at the specified location. Use the function **mphinterp** as shown below:

```
[t,c] = mphinterp(model,{'t','c'},...
    'coord',[25e-2;25e-2;25e-2],...
    'unit',{'h','mol/m^3'});
```

Now you can calculate the homogenized average concentration, which is the total amount of the substance, by integrating the concentration over the volume, and divide it by the reactor volume.

6 Evaluate the average concentration by typing the commands below:

```
c_av = mphmean(model,'c','volume','solnum','end');
```

7 To retrieve the current stop time from the solution, use the command **mphglobal** according to:

```
t0 = mphglobal(model,'t','solnum','end');
```

With the MATLAB variables `c_av` and `t0` define a new initial concentration and start time for the next re-start of the solver, in the next iteration of the for-loop.

8 Do this by typing:

```
model.physics('chds').feature('init1').set('c', 1, c_av);
model.param.set('t0',t0);
```

9 Type the sequence below to update the plot of the concentration versus time and display a message that indicates the iteration number:

```
plot(t,c)
hold on
disp(sprintf('End of iteration No.%d',i));
```

10 To close the for-loop type:

```
end
```

11 You can add plot settings, such as title and labels for the x-axis and the y-axis by typing the command below:

```
title('concentration at (25e-2;25e-2;25e-2) vs time')
xlabel('[h]');
ylabel('[mol/m^3]');
```

12 To compare the result to the simulation without the homogenization step, you can now modify the start and stop time, and the initial concentration for the simulation with the commands:

```
model.param.set('t0',0);
model.param.set('tf','2.5[h]');
model.physics('chds').feature('init1').set('c', 1, 0);
```

13 To solve again type:

```
model.study('std1').run;
```

14 Now evaluate the concentration and plot the result on the current figure:

```
[t,c] = mphinterp(model,{'t','c'},...
    'coord',[25e-2;25e-2;25e-2],...
    'unit',{'h','mol/m^3'});
plot(t,c,'r-.')
```

15 To reproduce the plot in Figure 1, you can also define a plot group in the model:

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```
model.result.create('pg1', 'PlotGroup3D');
model.result('pg1').feature.create('surf1', 'Surface');
model.result('pg1').set('solnum', '11');
```

16 Finally, display the plot in a new MATLAB figure:

```
figure
mphplot(model,'pg1','rangenum',1)
```

MODEL M-FILE

Below you find the full script of the model. You can copy it and paste it into a text editor and save it with the ".m" extension. To run the script in MATLAB make sure that the path to the folder containing the script is set in MATLAB, then type the file name without the ".m" extension at the MATLAB prompt.

```
model = mphload('homogenization_llmatlab');

for i = 1:5
    model.study('std1').run;
    [t,c] = mphinterp(model,{'t','c'},...
        'coord',[25e-2;25e-2;25e-2],...
        'unit',{'h','mol/m^3'});
    c_av = mphmean(model,'c','volume','solnum','end');
    t0 = mphglobal(model,'t','solnum','end');
    model.physics('chds').feature('init1').set('c', 1, c_av);
    model.param.set('t0',t0);
    plot(t,c)
    hold on
    disp(sprintf('End of iteration No.%d',i));
end

title('concentration at (25e-2;25e-2;25e-2) vs time')
xlabel('[h]');
ylabel('[mol/m^3]')

model.param.set('t0',0);
model.param.set('tf','2.5[h]');
model.physics('chds').feature('init1').set('c', 1, 0);
model.study('std1').run;

[t,c] = mphinterp(model,{'t','c'},...
    'coord',[25e-2;25e-2;25e-2],...
    'unit',{'h','mol/m^3'});
plot(t,c,'r-.')

model.result.create('pg1', 'PlotGroup3D');
model.result('pg1').feature.create('surf1', 'Surface');
model.result('pg1').set('solnum', '11');
```

```
figure
mphplot(model,'pg1','rangenum',1)
```

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