Created in COMSOL Multiphysics 6.2

Thermal Stresses in a Monolithic Reactor

Introduction

The removal of pollutants from high-temperature gases is often required in combustion processes. In this example, the selective reduction of NOx by ammonia occurs as flue gas passes through the channels of a monolithic reactor. The chemical reactions take place on a V_2O_5/TiO_2 catalyst. The full reactor is a modular structure made up of blocks of reactive channels and supporting solid walls.

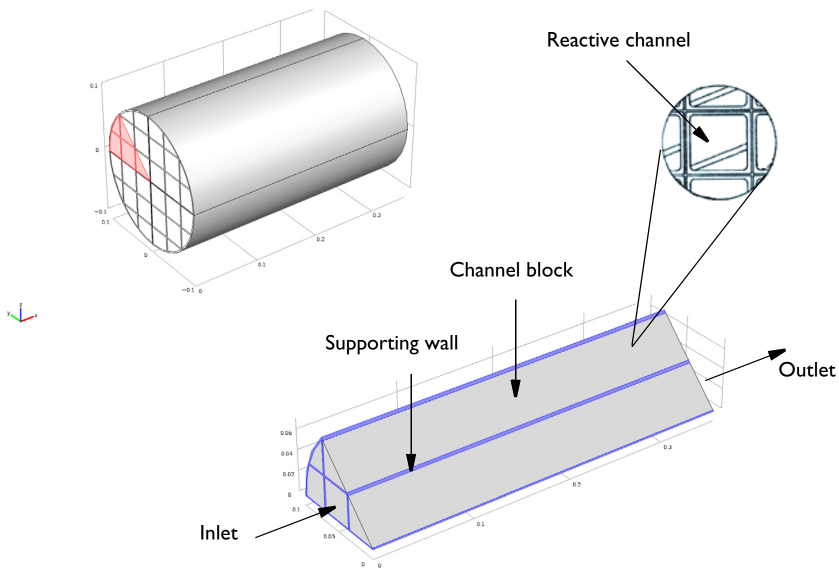

Figure 1: NOx reduction chemistry takes place in the channel blocks. Supporting walls hold together the full reactor geometry. Symmetry reduces the modeling domain to one eighth of the full reactor geometry.

Thermal gradients occur in the unit as heat is released by the chemical reactions while at the same time, heat is lost to the surroundings. This example investigates the thermal stresses in the reactor induced by the varying temperature field and the different material properties in the modular structure.

Note: This application requires the Chemical Reaction Engineering Module and the Structural Mechanics Module.

Model Definition

A separate model, NOx Reduction in a Monolithic Reactor, solves the coupled mass transport, heat transfer, and fluid flow equations representing the NO_x reduction process in the reactor. Load this example from the Chemical Reaction Engineering Module Application Library and extend it by coupling the temperature field to a structural mechanics analysis to evaluate the thermal stresses in the reactor. For a more detailed description of the reaction kinetics, see Analysis of NOx Reaction Kinetics.

The Solid Mechanics interface has the equations and features required for stress analysis and general linear and nonlinear solid mechanics, solving for the structural displacements. Thermal loads are introduced into the constitutive equations according to

$$\sigma = D\varepsilon_{el} + \sigma_0 = D(\varepsilon - \varepsilon_{th} - \varepsilon_0) + \sigma_0$$

where σ is the stress, D is the elasticity matrix, and ε represents the strain. The equation for the thermal strain is given by

$$\varepsilon_{th} = \alpha(T - T_{ref})$$

where α is the coefficient of thermal expansion, T is the temperature (K), and T_{ref} is the strain-free reference temperature (K).

Reactor Materials

As mentioned above, the reactor treated in this example has a modular structure and is made up of blocks of reactive channels and supporting solid walls. Both materials are treated as being linear elastic. The wall material is isotropic while the channel block material is orthotropic. Their properties are summarized in the tables below.

TABLE 1: WALL MATERIAL PROPERTIES.

	SUPPORTING WALLS
Young's modulus	1.5 GPa
Poisson's ratio	0.2
Coefficient of thermal expansion	2.7e-6 1/K

TABLE 2: CHANNEL BLOCK MATERIAL PROPERTIES.

	CHANNEL BLOCKS
Young's modulus	Ex = 85 GPa
	Ey =47 GPa
	Ez = 47 GPa
Poisson's ratio	νx = 0.19

TABLE 2: CHANNEL BLOCK MATERIAL PROPERTIES.

	CHANNEL BLOCKS
	vy = 0.021
	vz = 0.021
Shear modulus	Gxy = 35 GPa
	Gxz =35 GPa
	Gyz = 13 GPa
Coefficient of thermal expansion	4e-6 1/K

Results and Discussion

Figure 2 shows the x-component of the stress tensor plotted in a number of cross sections. The highest negative values are found in the channel blocks closest to the center, signaling compressive stresses in this part of the reactor. This is a direct result of the temperature field in the reactor as shown in NOx Reduction in a Monolithic Reactor; the material in regions with high temperatures expand more than material at lower temperatures. The opposite effect is observed in channel blocks located near the outer surface of the reactor. In this relatively cold region the monolith structure experiences tensile stresses. The maximum compressive stress is evaluated to approximately 7.0 MPa and the maximum tensile stress is approximately 9.0 MPa. This indicates moderate stress levels in the monolith working under the stationary conditions presented in this example. More pronounced stress levels are expected as thermal gradients increase, for instance, during system startup.

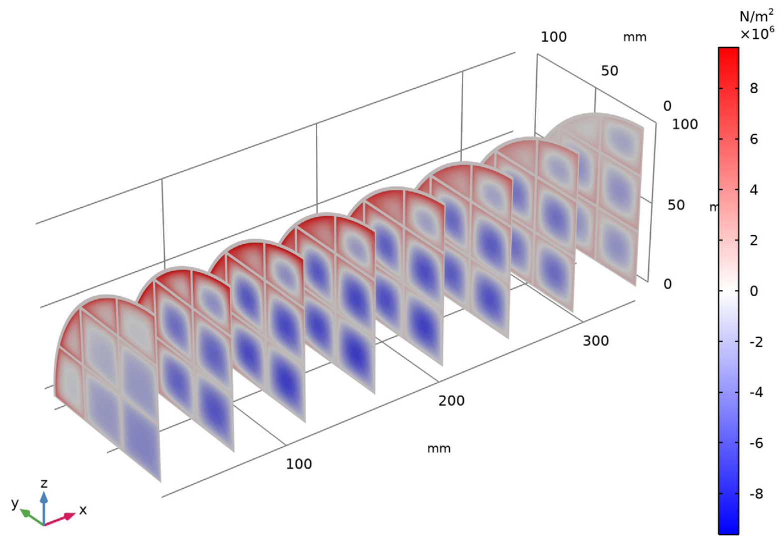

Figure 2: The stress tensor component in the x direction. Compressive stress is indicated by negative values, and tensile stress by positive values.

Reference

1. G. Schaub, D. Unruh, J. Wang, and T. Turek, "Kinetic analysis of selective catalytic NOx reduction (SCR) in a catalytic filter," *Chem. Eng. and Processing*, vol. 42, no. 5, pp. 365–371, 2003.

Application Library path: `Chemical_Reaction_Engineering_Module/Reactors_with_Porous_Catalysts/monolith_thermal_stress`

Modeling Instructions

APPLICATION LIBRARIES

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

2 In the **Application Libraries** window, select **Chemical Reaction Engineering Module>Tutorials>monolith_3d** in the tree.

3 Click **Open**.

3D MODEL (COMP2)

Add a **Solid Mechanics** interface to extend the model with an analysis of the thermal stresses in the reactor materials.

ADD PHYSICS

1 In the **Home** toolbar, click **Add Physics** to open the **Add Physics** window.

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

3 In the tree, select **Structural Mechanics>Solid Mechanics (solid)**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check boxes for **Study 1** and **Study 2**.

5 Click **Add to 3D Model** in the window toolbar.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

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

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Some Physics Interfaces>Stationary**.

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

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

STUDY 3

Step 1: Stationary

1 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

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

SOLID MECHANICS (SOLID)

Two **Linear Elastic Material** models are needed for the analysis, one for the supporting wall material and one for the channel blocks. Note that the wall material is isotropic while the block material is orthotropic.

Linear Elastic Material 2

1 In the **Model Builder** window, under **3D Model (comp2)** right-click **Solid Mechanics (solid)** and choose **Material Models>Linear Elastic Material**.

2 In the **Settings** window for **Linear Elastic Material**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Supporting walls**.

4 Locate the **Linear Elastic Material** section. From the E list, choose **User defined**. In the associated text field, type `1.5e9`.

5 From the ν list, choose **User defined**. In the associated text field, type `0.2`.

Add a **Thermal Expansion** feature to each **Linear Elastic** node. The features receive the temperature field solved by the **Heat Transfer in Fluids** interface as Model Input.

Thermal Expansion 1

1 In the **Physics** toolbar, click **Attributes** and choose **Thermal Expansion**.

2 In the **Settings** window for **Thermal Expansion**, locate the **Thermal Expansion Properties** section.

3 From the α list, choose **User defined**. In the associated text field, type `2.7e-6`.

Linear Elastic Material 1

1 In the **Model Builder** window, under **3D Model (comp2)>Solid Mechanics (solid)** click **Linear Elastic Material 1**.

2 In the **Settings** window for **Linear Elastic Material**, locate the **Linear Elastic Material** section.

3 From the **Material symmetry** list, choose **Orthotropic**.

4 From the **E** list, choose **User defined**. Specify the **associated** vector as

8.5e10	X
4.7e10	Y
4.7e10	Z

5 From the ν list, choose **User defined**. Specify the **associated** vector as

0.19	XY
0.021	YZ
0.021	XZ

6 From the **G** list, choose **User defined**. Specify the **associated** vector as

3.5E10	XY
1.3e10	YZ
3.5E10	X Z

Thermal Expansion 1

1 In the **Physics** toolbar, click **Attributes** and choose **Thermal Expansion**.

2 In the **Settings** window for **Thermal Expansion**, locate the **Thermal Expansion Properties** section.

3 From the α list, choose **User defined**. In the associated text field, type `4e-6`.

Complete the setup of the structural mechanics problem by defining the following boundary conditions.

Roller 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Roller**.

2 Select Boundaries 1, 4, 9, 13, 19, and 23 only.

You can use the **Selection List** from the **View** menu.

Symmetry 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Symmetry**.

2 In the **Settings** window for **Symmetry**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Symmetry**.

Follow the steps below to solve only the structural mechanics problem, using the temperature field from the solved reactor model as input to the calculations.

STUDY 3

1 In the **Model Builder** window, click **Study 3**.

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

3 Clear the **Generate default plots** check box.

This selection turns off the plots set up by default for each of the physics interfaces.

Step 1: Stationary

Clear all physics interfaces except **Solid Mechanics** to solve only for the displacement field.

1 In the **Model Builder** window, under **Study 3** click **Step 1: Stationary**.

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

3 In the table, clear the **Solve for** check boxes for **Reaction Engineering (re)**, **Chemistry 1 (chem)**, **Transport of Diluted Species in Porous Media (tds)**, **Heat Transfer in Porous Media 1 (ht)**, and **Darcy's Law 1 (dl)**.

Now, instruct the solver to use the results from the monolith 3D model for the variables not solved for.

4 Click to expand the **Values of Dependent Variables** section. Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

5 From the **Method** list, choose **Solution**.

6 From the **Study** list, choose **Study 2, Stationary**.

The monolith 3D model results are stored under **Study 2**.

7 In the **Home** toolbar, click **Compute**.

RESULTS

The **Datasets** node allows you great freedom to define tailored sets of plot data to be used by the plot nodes. Here, use the **Mirror 3D** feature to reflect the results in the symmetry planes of the model.

Mirror the data in the symmetry plane that is at a 45 degree angle to the *xy*-plane.

Mirror 3D 1

1 In the **Results** toolbar, click **More Datasets** and choose **Mirror 3D**.

2 In the **Settings** window for **Mirror 3D**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 3/Solution 37 (sol37)**.

4 Locate the **Plane Data** section. From the **Plane type** list, choose **General**.

5 In row **Point 2**, set **X** to `0.1`.

6 In row **Point 3**, set **Y** to `3.575e-3` and **Z** to `3.575e-3`.

Thermal Stress

1 In the **Results** toolbar, click **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Thermal Stress` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Mirror 3D 1**.

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

5 Locate the **Color Legend** section. Select the **Show units** check box.

Slice 1

1 Right-click **Thermal Stress** and choose **Slice**.
2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **3D Model (comp2)>Solid Mechanics>Stress>Stress tensor (spatial frame) - N/m²>solid.sGpxx - Stress tensor, xx-component**.
3 Locate the **Plane Data** section. In the **Planes** text field, type 8.
4 Locate the **Coloring and Style** section. Click **Change Color Table**.
5 In the **Color Table** dialog box, select **Wave>WaveLightClassic** in the tree.
6 Click **OK**.
7 In the **Settings** window for **Slice**, locate the **Coloring and Style** section.
8 From the **Scale** list, choose **Linear symmetric**.

Thermal Stress

1 In the **Model Builder** window, click **Thermal Stress**.
2 In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.
3 Clear the **Plot dataset edges** check box.
4 In the **Thermal Stress** toolbar, click **Plot**.
5 Click the **Zoom Extents** button in the **Graphics** toolbar.