

Mineral Physics 101: Multi-Anvil Cell Assembly Problem Set

Goals of this problem set:

To appreciate the effect of sample assembly design and the role of the thermal conductivity of sample assembly parts on the thermal regimes inside multi-anvil cells and the accuracy of temperature measurements.

Reference:

Hernlund, J.; Leinenweber, K.; Locke, D.; Tyburczy, J.A. (2006) A numerical model for steady-state temperature distributions in solid-medium high-pressure cell assemblies. *American Mineralogist* 91, 295-305.

Project:

1. Download the files from the “Cell Assembly” folder at this site:
<http://multianvil.asu.edu/Kurt%27s%20Thermal%20modelling/ThermalModeling.htm>
2. You will need to copy and save the text in the .prp file in a new .txt file.
3. Run the “CellAssembly” application
4. Open the “G2.cas” CAS file
5. Open the new .txt file you created
6. The program will open in a new window

The program is now in Design mode, so we can design our multi-anvil cell assembly and examine the effect of using materials with different thermal conductivities in different locations of the assembly. The program window should look like this:

Drop down menus ↓ screen shows ¼ of the assembly

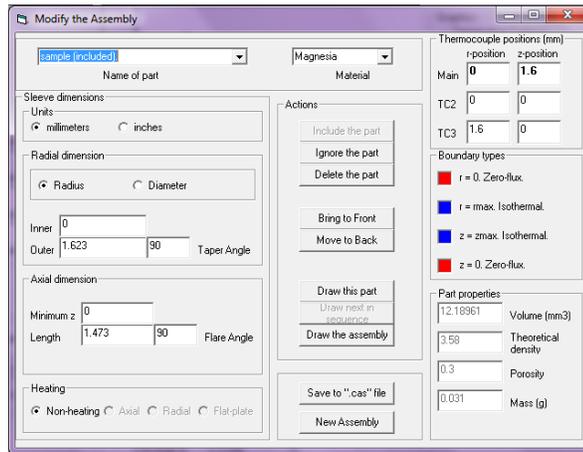
The screenshot displays the CellAssembly software interface. At the top, a menu bar includes File, Picture, Model, Properties, Results, and Help. The main window is divided into several panels:

- Thermal model:** Contains input fields for Current in Amps (100), Radial grid size (64), and Boundaries (25). It also has checkboxes for "Include the press in the calculation" and "Multi-grid".
- Grid settings and iterations:** Includes settings for single grid (1.8 w, 10 NCond, 10 NInner) and multi-grid (checked, 10 NInner).
- Run:** Features a "Run" button, "Run cycles" (2), "Converge to residual" (0.008), "Converge to Temperature" (1200), and "Target residual" (1).
- Graphics:** Includes "Temperature Contours" with "Auto", "Add Contour", "Plot All", and "Clear" buttons. It also has "Plot Labels" and "Separate plot window" options.
- Results:** Displays "Thermocouple Temperatures (deg C)" and "Integrated power (Watts)".

Red arrows and text annotations highlight specific features:

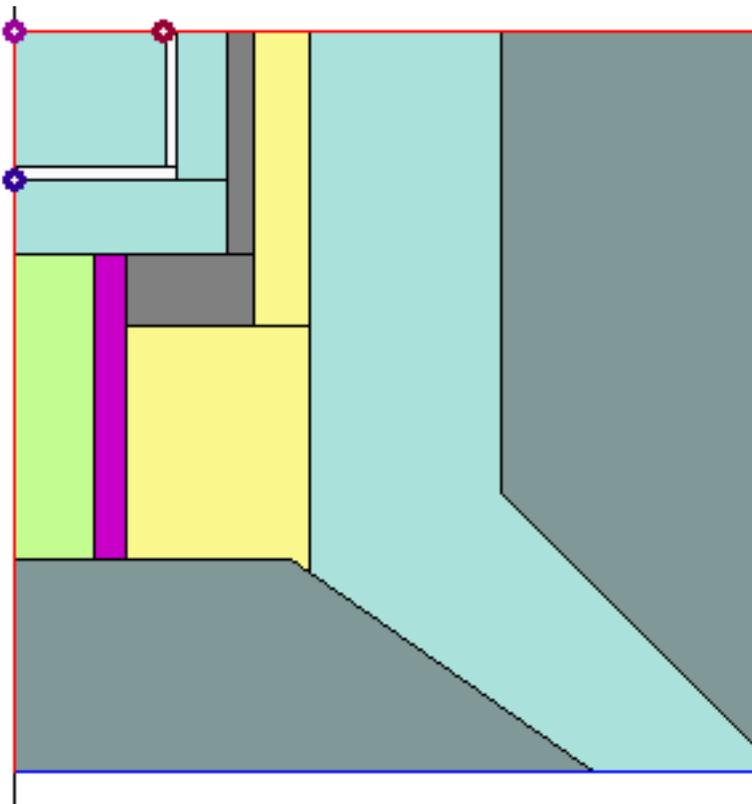
- "Drop down menus" points to the Model and Properties menus.
- "screen shows ¼ of the assembly" points to the central assembly diagram.
- "Initialize Button" points to the "Initialize" button in the bottom left.
- "Converge to Temperature" points to the "Converge to Temperature" input field in the Run panel.

7. Let's start by leaving the assembly as is in order to examine the components of the assembly. Click on the "model" drop down menu then "modify assembly". A new window will open:



This window allows you to change the properties of any of the materials/components of the assembly, but for now let's just use it to examine the pre-made assembly. Move this new window to the side so that you can see the picture of the assembly. Click on the different components in the image and notice that they "part name" and properties change in the "modify assembly" window. Label the image below with the appropriate part names:

- a. sample
- b. Carbide top
- c. Carbide side
- d. Capsule wall
- e. Capsule lid
- f. Inner Sleeve
- g. Inner Cap
- h. Furnace Cap
- i. Furnace Sleeve
- j. TZM ring
- k. TZM stuffing
- l. Insulating end sleeve
- m. Insulating sleeve
- n. Octahedron

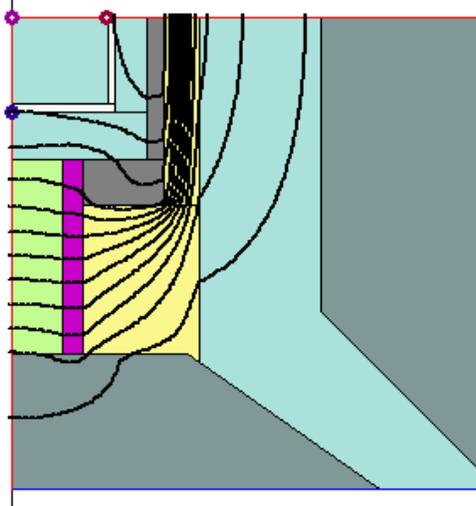


8. List the material and thermal conductivity coefficients of the following parts, the thermal conductivities are found in the “materials properties” window under the “Properties” drop down menu:

- a. Carbide top
- b. Carbide side
- c. Capsule wall
- d. Capsule lid
- e. Inner sleeve
- f. Inner cap
- g. Furnace Cap
- h. Furnace sleeve
- i. TZM ring
- j. TZM stuffing
- k. Insulating end sleeve
- l. Insulating sleeve
- m. Octahedron

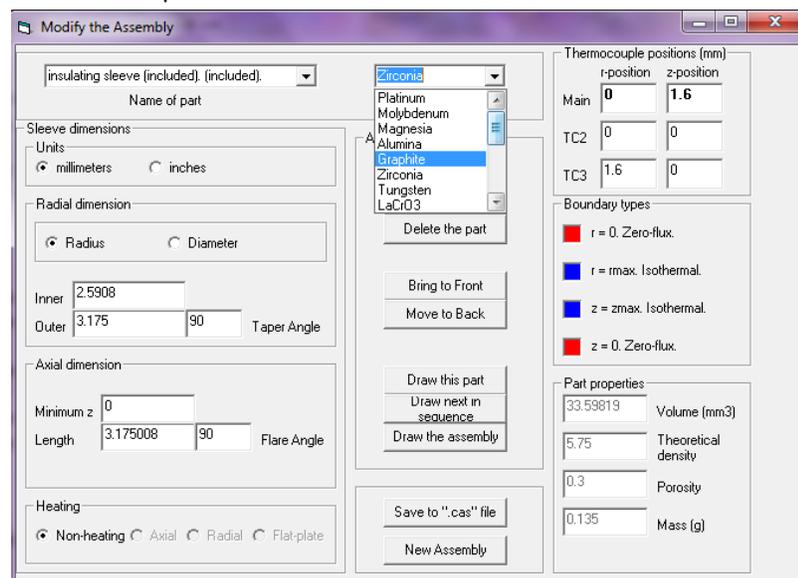
9. Now that you know where the Furnace is, where do you think the hottest part of the assembly is? Draw a star on the assembly image above to indicate your answer.

Now that we know a bit more about the assembly and its materials we can use this program to model the effects of different materials and configurations of the assembly. Press “Initialize” in the bottom left. The conversation box should now say, “The Assembly is ready to run” in blue letters. We want the model to heat the sample to 1200°C. To do this, make sure the target temperature box reads “1200” then press “Converge to Temperature”. The black lines that have appeared on the assembly are isotherms that depict the geothermal gradient. You can read the temperature modeled by this program anywhere in the cell simply by clicking on the cell assembly picture.



10. Where is the hottest part of the cell after you run the model? Where is the coldest? What temperature is the coldest?
11. Judging by the thermal gradients, do you think the sample is uniformly heated?
12. Typical locations for thermocouple beads are represented by the small blue and maroon circles. How well do you think the thermocouples reflect the temperature at the center of the sample (marked by the violet circle)?
13. Let's examine how the materials used for assembly parts change effect the thermal gradient in the assembly. . .

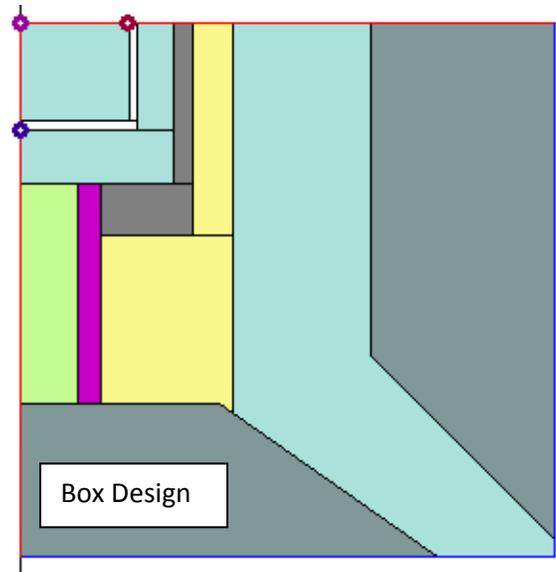
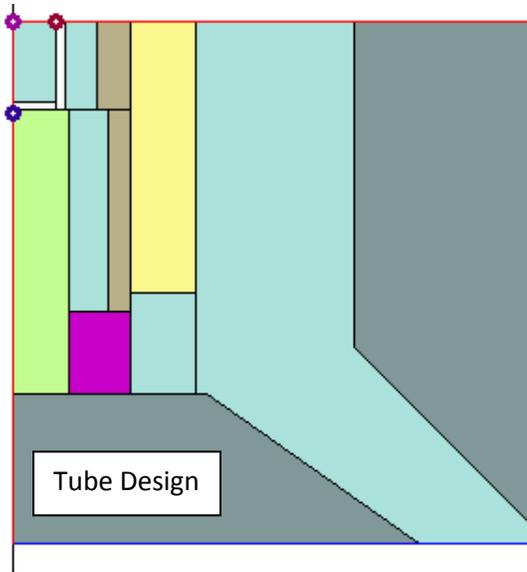
- a. Select the "model" drop down menu, then "Modify Assembly". Select "inner cap" as the name of the part and "zirconia" as the material.



- b. Select “reset the temperature and initialize”. Then converge to 1200°C again.
 - c. Copy and paste a print screen of the model with thermal gradients into a file you can print out and turn in.
 - d. How are these temperature gradients different from the first model?
14. How do you think the thermal gradient will be affected if we use a more thermally conductive material in the insulating sleeve?
15. Re-run the experiment replacing the zirconia insulating sleeve with magnesia. Print-screen this new image to turn in with this assignment.
- a. Was the outcome as you expected?
 - b. Why do you think this new configuration might be detrimental to the anvils?

There are two major types of cell designs; the one we have been working with is a *box* design. In tube designs the furnace extends all the way through the assembly. Let’s examine one of these assemblies. . .

16. Click on “File” then “open a cell assembly (CAS) file”. Open the Bayreuth file you downloaded.
17. What major differences do you see between this new tube assembly and the box design we looked at earlier?



18. What is the furnace sleeve and cap of the tube design made of?
19. How do you think the shape of these components will change the thermal gradient?
20. Converge to 1200°C on this new assembly. Are there more or less isotherms than the box design? Why do you think this is?
21. Noting the difference in sample size between the two assemblies, is the sample in this assembly more evenly heated than the box design? Explain your answer.