

Balancing Reactions Using CSpace

CSpace does a number of things, including plotting and projecting phases in composition space, but right now we want to use it's matrix capabilities to balance reactions. As an example we shall attempt to balance the reaction:



Because both hydrous and carbonate minerals are involved, we know that H₂O and CO₂ are involved in the reaction as well, but let's suppose that we don't know whether they are released or consumed by the reaction.

| | Var_1# | Var_2# | Var_3# | Var_4# | Var_5# | Var_6# | Var_7# |
|----|--------|--------|--------|--------|--------|--------|--------|
| 1 | | | | | | | |
| 2 | | | | | | | |
| 3 | | | | | | | |
| 4 | | | | | | | |
| 5 | | | | | | | |
| 6 | | | | | | | |
| 7 | | | | | | | |
| 8 | | | | | | | |
| 9 | | | | | | | |
| 10 | | | | | | | |
| 11 | | | | | | | |

CSpace uses a spreadsheet-like interface in which we generate a matrix of phases vs. components. When we open CSpace the spreadsheet looks like this:

First we must enter our data. We make the components as columns and phases as rows. To be orderly, and to be able to check for mistakes, we carefully label the columns and rows at the onset. Column labels (Var_1#, Var_2#, ...) can be changed by double-clicking the label cell. An input window then asks you to "Edit Variable Name", and we can overtype the default with labels of our choice. Because the first column will contain the names of the phases in our reaction, we may enter the label: Phase#. The # sign indicates that the data in the column are labels, and not numeric variables to be used in calculations. The phases in our reaction all belong to the system: CaO-MgO-SiO₂-H₂O-CO₂ ("CMS-HC"), and we can proceed to re-label the columns to conform to this system (in any order):

| | Phase# | SiO2 | MgO | CaO | CO2 | H2O | Var_7# |
|----|--------|------|-----|-----|-----|-----|--------|
| 1 | | | | | | | |
| 2 | | | | | | | |
| 3 | | | | | | | |
| 4 | | | | | | | |
| 5 | | | | | | | |
| 6 | | | | | | | |
| 7 | | | | | | | |
| 8 | | | | | | | |
| 9 | | | | | | | |
| 10 | | | | | | | |
| 11 | | | | | | | |

We next label our rows with phase names. To change the data in a cell, move the cursor to the cell and hit the enter key, then type the data for that cell and hit enter again. You can correct mistakes by re-entering the data. We can determine the number of moles/molecules of each component in a phase from the mineral formula. For example, tremolite has 2 molecules of CaO, 5 molecules of MgO, 8 or SiO₂, and 1 of H₂O. The completed data input looks like this:

| Phase# | SiO2 | MgO | CaO | CO2 | H2O | Var_7# |
|--------|------|-----|-----|-----|-----|--------|
| 1 Tr | 8 | 5 | 2 | 0 | 1 | |
| 2 Dol | 0 | 1 | 1 | 2 | 0 | |
| 3 Di | 2 | 1 | 1 | 0 | 0 | |
| 4 Mgs | 0 | 1 | 0 | 1 | 0 | |
| 5 H2O | 0 | 0 | 0 | 0 | 1 | |
| 6 CO2 | 0 | 0 | 0 | 1 | 0 | |
| 7 | | | | | | |
| 8 | | | | | | |
| 9 | | | | | | |
| 10 | | | | | | |
| 11 | | | | | | |

Now it's time to perform the matrix analysis. Select the Matrix Analysis Wizard (MAW) from either the icon or the toolbar (under Matrix). In the input box, select Phase# for the Case (object) labels and leave (None) for comments. Then click on Next. We then select the rows that we want to include in the matrix. Click on the gray cell "1" at the left end to highlight the first row, and then click on the icon with the blue arrow at the bottom of the MAW window to include it in the matrix. You should see 00001 as the Case and Tr as the Phase# in the MAW window. Continue to add all six rows to our matrix. Then click on Next in the MAW window. You can now open the Text Pad window by clicking on the icon in the main CSpace window. The matrix should be displayed in the Text Pad. We are not doing any fancy weighting, so click Next again in the MAW window. We are also not doing any modeling, so click Next again. At the bottom of the present MAW window there should be a button labeled "Univariants". Click on this button to get the reaction stoichiometry. At the bottom of the Text Pad window you should see:

Rank of Working Set is: 5
 Working Set contains 1 rank+1 column selections ("univariants")
 "Univariant" relation(s): (unfiltered)

| Tr | Dol | Di | Mgs | H2O | CO2 | |
|--------|--------|---------|---------|---------|---------|---|
| 1.0000 | 2.0000 | -4.0000 | -3.0000 | -1.0000 | -1.0000 | 1.0000 Tr + 2.0000 Dol = 4.0000 Di + 3.0000 Mgs + 1.0000 H2O + 1.0000 CO ₂ |

indicating that the reaction is balanced as:

