1/Step 2. Why are there two phases identified as Cpx?

> Answer: Because a single solution model (Cpx) predicts the stability of two compositionally distinct phases of matter, i.e., a solvus. In this case, the phases are known petrographically as ompacite and augite.

2/Step 3

a) CO2: 0.00014, CH4: 0.91730, H2: 0.03916, CO: 0.00000, H2O: 0.04340 (molar)

b) ferrous_M1_aug := (0.0554 + 0.1604)/2
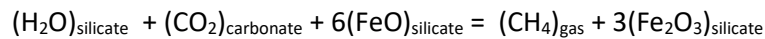ferric_M1_aug := (0.0155 + 0.0158)/2
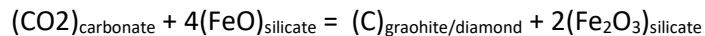ferric_ferrous_M1_aug := 0.145
ferrous_M1_omph := (0.0013 + 0.1423)/2
ferric_M1_omph := (0.0474 + 0.0054)/2
ferric_ferrous_M1_omph := 0.368

c) The overall process can be attributed to a reaction of the form
$$(H_2O)_{silicate} + (CO_2)_{carbonate} + 6(FeO)_{silicate} = (CH_4)_{gas} + 3(Fe_2O_3)_{silicate}$$
This reaction follows from the consideration that the initial bulk composition can be defined entirely of reduced oxide components, LHS). Despite the consequent absence of any excess oxygen, ferric iron and methane form by reduction of H2O and CO2. I often think of this process as being driven by the stability of ferric iron. The reality is there is no single driving factor, one might as well say the process is driven by the instability of H2O. In the present case the reaction is not representative of a natural process because we configured the problem incorrectly so as to preclude the stability of graphite. When the problem is properly configured, as done later in the tutorial, ferric iron forms by reducing CO2, as occurs in natural settings, a process that can be schematized by the reaction
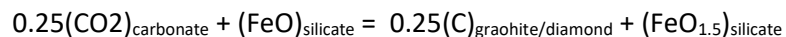$$(CO2)_{carbonate} + 4(FeO)_{silicate} = (C)_{graohite/diamond} + 2(Fe_2O_3)_{silicate}$$
Again, my wording suggests iron is the agent, but one could say with equal validity that CO2 oxidizes the iron. There are no true agents in thermodynamics other than the 2nd law.

3/Step 5

a) 0.06 wt%

b) The tutorial script suggests a different, equally valid, route to solving this problem than I outline here. As carbon is the only redox variable species besides iron in the system, ferric iron must form by the reaction
$$0.25(CO2)_{carbonate} + (FeO)_{silicate} = 0.25(C)_{graohite/diamond} + (FeO_{1.5})_{silicate}$$
Thus, n_ferric = 0.25 n_diamond = 0.0118 mol, n_ferrous = n_FeO – n_ferric = 1.3582, and n_ferric/n_ferrous = 0.00869.

4/Step 6

mu_O2$_{component}$ = -386421. J/mol, G0_O2$_{species}$ = -82162. J/mol, log10(f_O2) = -23.61

5/Step 7

a) solute molality = 16.92

b) Delta_pH = 1.827, the fluid is basic.

    c) The mass fraction of silica in the fluid is 3.926%

6/Step 8.

    a) solute molality = 14.48
    b) Delta_pH = 1.927
    c) The mass fraction of silica in the fluid is 4.326% (or something like this)

The differences are of marginal significance, an important consideration besides mass-balance is that simple back-calculation will output results even if they are implausible, whereas lagged speciation will not output implausible speciation (i.e., the algorithm reports lagged speciation has failed when such results are obtained).

7/Step 10. Trivial

8/Step 12. Trivial, ca 4.25+/-0.75 kbar, 850+/-150 K

9/Step 13. Trivial. Speciation plot +1.

10/Step 14. Trivial (at least in Matlab).