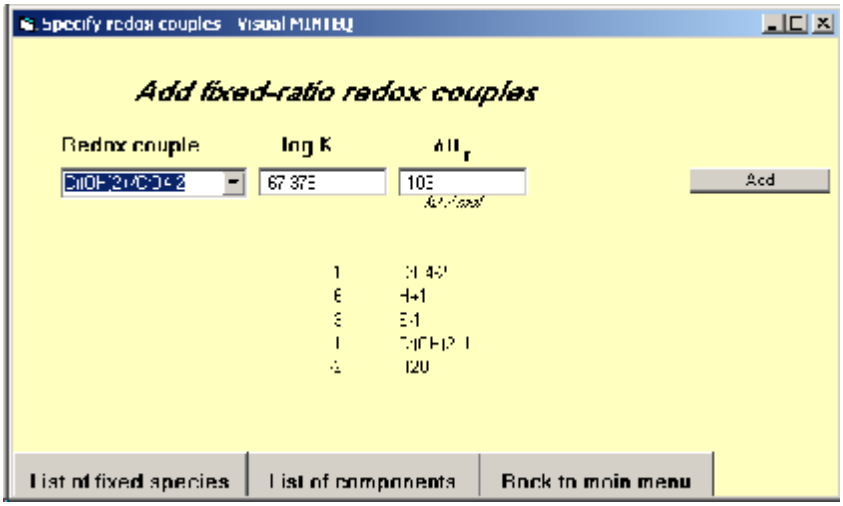
ENTERING REDOX PROBLEMS IN VMINTEQ:

Add the basic "recipe" ingredients as usual (for example, Cr042-, K+, H+, etc. You can ignore CO2 at low pH.

To "switch on" redox reactions, you need to go to the Redox tab on the main menu, and get "sellect from list window and find the Cr(iii)/Cr(VI) couple, which is in the form of the main species near neutral pH:



Note that Vminteq will then set a FIXED pe of 8.0. This is NOT what you want, since you want a computed pe. But Vminteq needs a COMPLETE reaction in order to calculate pe. In a soultion of pure H2O and chromate, what is the reduced component that can get oxidized by Cr(VI)?

In aqueous acid-base chemistry there is always at least one component that can take up or give up protons and that is H2O. The same is true of aqueous redox chemistry with respect to the electron: Your chromate wants to oxidize something, so it always can, in principle, oxidize what? When you oxidize this component, what common gas do you get? Now, you won't find this redox couple in the redox part, but you will find the gas you need among the choices of gases at fixed partial pressure, and I bet you can figure out the appropriate partial pressure needed. Once you do that, you'll have a complete (full cell) redox reaction and your pE will be definable by VMINTEQ.

Now, you must tell Vminteq NOT to fix the pe, but instead compute it. Go to the Parameters menu, (See next page). Switch from Fixed pe to pe/Eh computed. Since this is very oxic, choose a pe guess of at least 14, and since its somewaht acidic, try something like 16 or so, as shown. Then save.

By the way, once you add the Fe(II), you'll need to assume (realistically) that Fe(II) is the reductant of choice for chromate, so you need to completely delete that other (gaseous) species from the system. Otherwise you'll get unrealistic results. I.e., put in Fe2+ as a reductant (and specify the Fe2/Fe3 couple) and get rid of the gas that is produced in the earlier parts of the project.