- MTDATA Miscalculation – by Jee Hyun Kang

MTDATA is useful for simulating equilibrium state for any system. However, it is only useful when you use it properly. When MTDATA has completed the calculation, the calculation results should be carefully examined. This text is to inform you about the one case which results in inappropriate calculation.

Sometimes, MTDATA gives you 2 different results for the similar temperature range. You can easily realize this by Figure 1. Upper and lower graphs were obtained by calculation for the exactly same composition of steel and similar range of temperature (upper: 490~750℃, lower: 500~750℃). However, you can see that 2 graphs are completely different for the lower range of the temperature. The upper one is the wrong calculation and the lower graph is the one that is based on the correct calculation. Moreover, cases like this come up frequently. The warning sign of the case is discontinuous data points (upper). You must reconsider when you do NOT get smooth curve.

This problem is likely to occur in the lower temperature range. This is because the equilibrium thermodynamic data accessed by programs such as MTDATA and Thermocalc are usually measured at high temperatures and have to be extrapolated to low temperatures. It is not therefore wise to start a calculation from a low temperaturere and proceed to one that is high. The reverse is likely to give a better result. Hence, it cannot be overemphasized that you had better make your calculation from higher temperature to lower temperature. For instance, not from 500℃ to 700℃, but from 700℃ to 500℃. It is recommended to calculate from one phase region or liquid region even though a huge amount of calculation is needed.



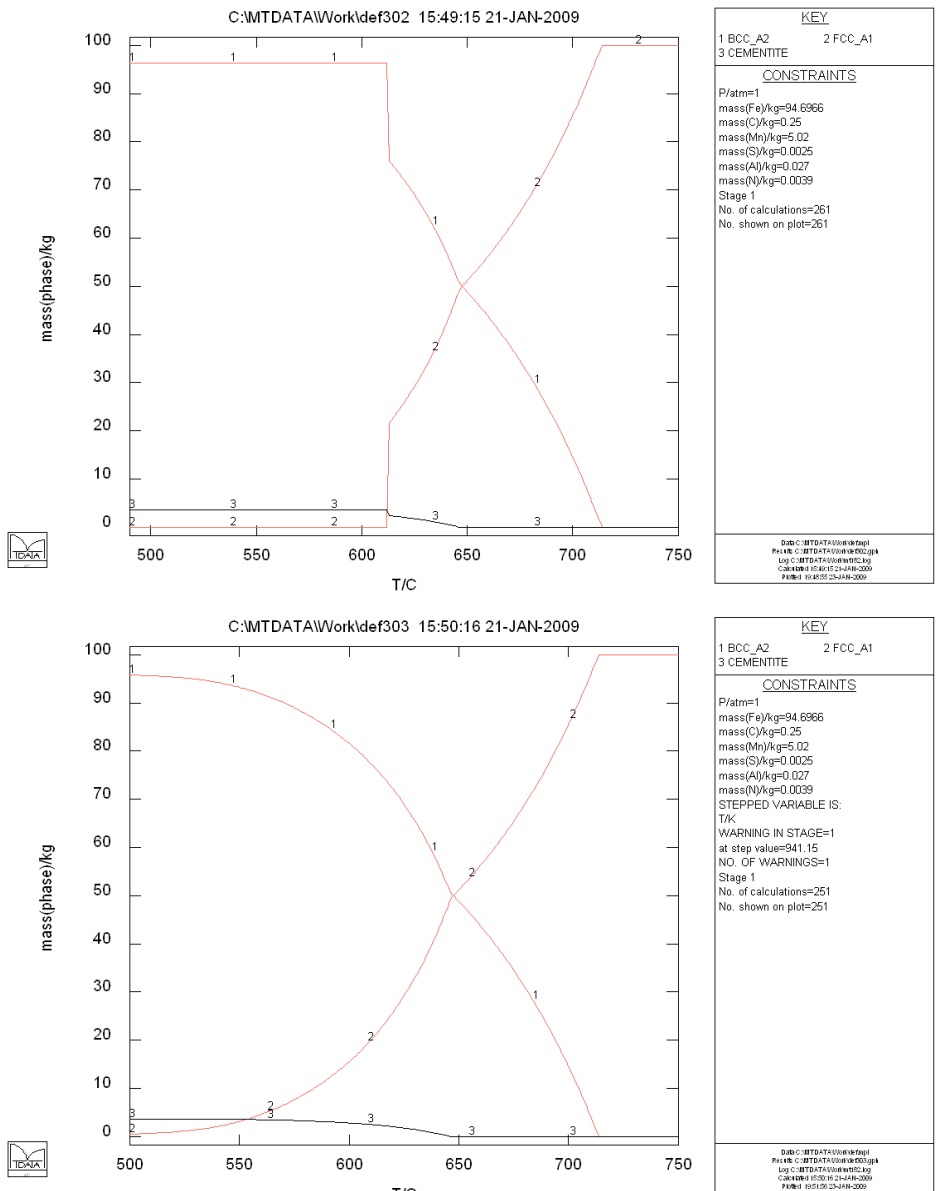**Figure. 1**

In conclusion, <span style="color:red">when giving temperature range, it is recommended to start from high temperature to low one</span> and <span style="color:red">WATCH OUT for the weird graph W/O SMOOTHNESS.</span>