DISCUSSION

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Keith Reynard: The calculations you describe appear to involve complex optimization algorithms and extensive data. Can you cite examples where predictions you have made have been subsequently confirmed by laboratory experiment or industrial data.

Tom Barry (author's response): The accuracy of predictions made using MTDATA has been confirmed on numerous occasions. Nevertheless, verification by experiment is always useful as I will illustrate. Reference 1 of the paper contains a diagram of the calculated liquidus surface for the $KCl-CaCl_2-ZnCl_2$ system, predicted on the basis of critically assessed data for the binary systems. The superimposed experimental data were not available at the time of the calculations but clearly confirm them and enable the diagram and other associated calculations to be used with confidence. Sometimes there are discrepancies. In a collaborative project with British Steel, undertaken in connection with the modelling of continuous casting, predictions were within a few degrees for Fe-Cr-Ni-Mn-Si-C steels but not where Cr and Si were both present in significant amounts. The discrepancies were traced to data for the Cr-Si system for which the data had been estimated because few reliable experimental data were available. It was possible to improve the data for Cr-Si using the results from the multicomponent system but more direct experiments have been put in hand.

Some years ago we undertook a series of calculations for an industrial company in connection with pilot plant testing of corrosion rates in gas atmospheres containing C, H, O, N, S and Cl. The agreement between the chemical analyses and calculated amounts of CO, CO_2, H_2, H_2O, CH_4, H_2S, HCl, etc was always very good, so that on one occasion when the temperature sensor in the experiment failed we were able to provide an estimate of the operating temperature, probably to better than 5°C and hence save the results of a costly retrial. A characteristic of this system is that, even when the gas phase reaches internal equilibrium, it may become supersaturated with respect to precipitation of carbon, which requires a catalyst. Either the metastable or the stable equilibrium may be calculated by omitting or including the condensed phases of carbon.