Accelerating Thermochemical Equilibrium Calculations for Multiphysics Modelling Applications

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High temperature thermochemical equilibrium calculations are computationally expensive, taking up to several seconds to complete on currently available hardware. Integrating such calculations into a multiphysics model to describe thermochemical behaviour in combination with fluid flow and heat transfer, will in most cases result in a model that cannot be solved with the available computating resources.

This problem can be alleviated by pre-calculating, storing, recalling and interpolating the required data. If recall and interpolation can be done rapidly, the time required to obtain the results can be reduced by several orders of magnitude. Some researchers have implemented this approach on systems with a small number of components. Pyrometallurgical processes, however, involve many system components, including Al-C-Ca-Cr-Fe-Mg-Mn-N-O-Si-Ti in significant amounts.

An acceleration approach is demonstrated for binary and ternary slag systems. Options for integrating the algorithm into multiphysics framework are also evaluated.