Geometrical Acceleration of Complex Equilibrium Calculations for Integration in High-Temperature Models

Willem Roos*, Alfred Bogaers, Johan Zietsman
University of Pretoria
Ex-Mente (South Africa)

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The inclusion of high-temperature multiphase, multicomponent equilibrium calculations into multiphysics and process models can provide significant insight into a system. Direct integration of equilibrium calculations is in many cases, however, infeasible due to extreme computational expense. The computation time of a single equilibrium calculation increases non-linearly as the number of system components increases. In a simulation where thousands or even millions of equilibrium calculations are required it becomes infeasible to include thermochemical properties. Acceleration methods have been developed by others such as ten Cate et al [1], and Voskov [2], to address this problem.

Our acceleration method takes advantage of the fact that a phase diagram is a geometrical representation of a thermochemical system and builds on the work initiated by Zietsman [3] where phase region boundaries are discretised and the calculated thermochemical properties are stored thereon for later recall. The extractive metallurgy systems that we work with involve 10 to 16 system components, which presents us with a 10- to 16-dimensional phase diagram. The problem is that for complex systems the phase diagram is composed of hyper-volume phase regions and hyper-surface phase region boundaries. In this work, we discuss our generic accelerator and its performance of recalling thermochemical properties of the Ilmenite system (C-Fe-O-Ti) and a simplified steelmaking system (C-Ca-Fe-O-Si) for the integration into models.

[1] ten Cate, A., Geurts, B.J., Muskulus, M., Köster, D., Muntean, A., van Opheusden, J., Köster, N., Muntean, A., Peschansky, A., Vreman B. and Zegeling, P. (2008) 'Modeling and Simulation of Phase-transitions in Multicomponent Aluminum Alloy Casting', Proceedings of the sixty-third European Study Group Mathematics with Industry, pp.117-139.

[2] Voskov, D.V. and Tchelepi, H.A. (2009) 'Tie-simplex Based Mathematical Framework for Thermodynamical Equilibrium Computation of Mixtures With an Arbitrary Number of Phases', Fluid Phase Equilibria, 283 (1), pp.1-11.

[3] Zietsman, J.H. (2016) 'Efficient Storage and Recall of Slag Thermochemical Properties for Use in Multiphysics Models', Advances in Molten Slags, Fluxes, and Salts: Proceedings of the 10th International Conference on Molten Slags, Fluxes and Salts 2016, pp.635-644.