

Calculation of Solidification of Steels Under Back-diffusion Conditions Using ChemSheet

R. Pajarre

VTT - Technical Research Centre of Finland

Abstract

Behaviour of a solidifying metal alloy depends both on the system thermodynamics and diffusion and convection. Assuming diffusion is fast enough to maintain a uniform composition both in liquid and solid states, the system reaches chemical equilibrium in all temperatures, while fast diffusion/convection in a liquid state and negligible diffusion in solid state leads to the Scheil cooling behaviour. Both of these cases are easily calculated using FactSage or ChemSheet. Applying additional constraints, similar to those used for reaction kinetic calculations, an intermediate case where some of the constituents in the solid state mixtures are allowed to equilibrate with the liquid, while others are considered inert can also be solved using ChemSheet. This paraequilibrium pathway is known to be often a reasonable approximation for the solidifying steels, where the actual metallic constituents in solid solutions diffuse with much slower rate than the interstitial solutes like C and N.