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## CALPHAD-based Thermodynamic and Kinetic Simulation of Secondary Steelmaking with Focus on Inclusion Formation and Modification

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The evolution of steel and slag chemistry in function of secondary metallurgy process parameters can be simulated with good accuracy using Thermo-Calc's TCOX CALPHAD database and the effective equilibrium reaction zone (EERZ) model that accounts for reaction kinetics.

An interesting aspect of such simulations is tracking the formation and modification of endogenous nonmetallic inclusions throughout the process. The TCOX database contains thermodynamic descriptions of all important non-inclusions allowing their amount and composition to be calculated in function of evolving steel chemistry.

Most inclusions form during deoxidation of the steel. But slag entrainment during tapping is also an important source of inclusions. During secondary metallurgy these inclusions will be gradually removed from the steel by flotation, but their minerology will also change over time in function of the changing steel chemistry. Inclusions can be modified intentionally: solid Al2O3 (Corundum) inclusions can be transformed into liquid Ca-Al-Oxides by calcium treatment. But they can also change without making any additions: Al2O3 might transform into MgAl2O4 Spinel due to MgO pickup from the ladle lining. Oxygen activity in the steel is an important driver for the type of inclusions that are formed. A high oxygen partial pressure will directly result in the formation of oxide inclusions. A very low oxygen activities will drive S out of the steel into the slag, leading to the dissolution of sulfide inclusions. At the same time most other elements, notably Si, will be reversed out of the slag back into the steel with potentially unwanted effects.

It will be shown how Thermo-Calc and the TCOX database can be used to calculate the thermodynamic stability of inclusion in function of steel chemistry, temperature and oxygen activity and how kinetic simulations can shed light on the evolution of inclusions in function of time during secondary steel making.

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