Coupling Thermochemistry to Classical Solidification Modelling

Haritz Sarriegi[1], Konrad Weiß[2]

[1]Mondragon Technical University
[2]RWP, Roetgen

Abstract

Thermophysical and physical properties of liquid and solid phases during solidification are critical data in the modelling of casting simulations. These simulations require high quality information concerning these properties. This information encloses the fraction solid transformed, enthalpy release, thermal conductivity, volume and density, all as function of temperature. However, the number of alloys for which such information is available is limited, primarily due to the difficulty in experimentally determining these properties during the solidification process.

ChemApp subroutines have been programmed to achieve a coupling of calculated thermophysical properties with the WinCast (FEM) solidification simulation program. Two programs have been generated and one can easily apply their results in WinCast. These programes compute thermophysical properties for straightforward use as input variables when running a casting simulation. Calculation accuracy has been improved since four different latent heat releasing modes can be computed by the programs developed. Thus different casting technologies can be simulated with more precision.

The joint use of WinCast, a program for classical modelling of casting and solidification processes, and ChemApp, the programmer's library for thermochemical calculations, has been found to overcome several of the problems described above. The effect of changing the alloying elements or cooling rate on the thermophysical properties of six different steel grades has been computed and it has been shown that variation of C content may alter the latent heat of solidification for a micro alloyed steel within a given composition range by about 8%. According to the IDS software package cooling rate variations should not change the thermophysical properties at liquidus temperature, but joint calculations with

ChemApp and WinCast demonstrate that this is not true, the properties at liquidus temperature do vary.

Increase in solidification time has been reported when C, Cr and Ni contents as well thermophysical input properties for the casting simulation vary. The latent heat release is the thermophysical property with greatest influence on casting simulation results, achieving about 25% increment on solidification time when the latent heat released increases by 20%. Density and specific heat values do not increase solidification time as much as latent heat release except for stainless steels. On the other hand, thermal conductivity changes decrease solidification time a little for all cases. Solidification time increments or decrements are greater for slow cooling zones than for rapid cooling zones, when such simulation parameters change.