NUMERICAL MACRO-MODELING OF SOLIDIFICATION

From the analysis of solidification based on the energy transport equation presented in the previous section, it was seen that analytical solutions of this equation are not always available. Significant simplifying assumptions must be used, assumptions that are many times debilitating to the point that the solution is of little engineering interest. Fortunately, with the development of numerical methods and their application to the solution of partial differential equations, the most complicated equations can be solved numerically. Numerical solutions rely on replacing the continuous information contained in the exact solution of the differential equation with discrete values. Discretization equations are derived from the governing differential equation.

Process modeling has become possible in a much larger extent than allowed by the use of analytical solutions. Process modeling has emerged as a practical industrial tool for the design of manufacturing processes, troubleshooting, and identifying the dependent and independent variables of the process.

Computer simulation of solidification is based on numerical solutions of energy, mass and momentum transport. Its main computational purpose is calculation of the evolution of the thermal and compositional field throughout the casting. To produce a solidification model the following steps are necessary:

- problem formulation
- discretization of governing equations
- solving of the system of algebraic equations

6.1 Problem formulation

Heat transfer (HT) modeling for a given casting - mold combination requires solving of the energy conservation equation for heat conduction with heat generation. Ignoring for the time being the convective term of the energy transport equation, the governing equation is:
\[
\frac{\partial T}{\partial t} = \alpha \nabla^2 T + \frac{\dot{Q}_{\text{gen}}}{\rho c}
\]  
(6.1)

The source term associated with the phase change, which describes the rate of latent heat evolution during the liquid-solid transformation given by Eq. 5.4 is:

\[
\dot{Q}_{\text{gen}} = \rho \Delta H_f \frac{\partial f_S(x,t)}{\partial \rho}.
\]  
(6.2)

To solve Eq. (6.1) an appropriate expression for \(f_S(x,t)\) must be found.

In one approach, the solution of the discretized energy transport equation at all the nodes or elements of the computational domain, is found by prescribing a solidification path, \textit{i.e.}, by assuming a relationship between \(f_S\) and \(T\). The fraction of solid is rewritten as \(\frac{\partial f_S}{\partial t} = \left(\frac{\partial f_S}{\partial T}\right) \left(\frac{\partial T}{\partial t}\right)\). Then, some functional dependency of the fraction of solid on temperature is assumed. Such typical assumptions include linear dependency for eutectics, and equilibrium or Scheil equation for dendritic alloys. For example, assuming that the composition field is governed by Scheil-type diffusion an equation for the fraction solid evolution can be derived as follows. The interface temperature depends on composition according to the relationships \(T_f - T_L = -mC_o\) or \(T_f - T_L = -mC^*_L\). The liquid composition is given by Scheil equation, \(C^*_L = C_o\left(1 - f_S\right)^{1-k}\). Then, \(f_S = 1 - \left(C^*_L/C_o\right)^{1/(1-k)}\) and finally:

\[
f_S = 1 - \left(\frac{T_f - T^*}{T_f - T_L}\right)^{1/(k-1)}
\]  
(6.3)

With these assumptions, Eq. (6.1) can be rewritten in several ways and solved by numerical techniques.

6.1.1 The Enthalpy Method

In the enthalpy method (Pham, 1986) for 1-D Eq. (6.1) is rewritten as:

\[
k \frac{\partial^2 T}{\partial x^2} = \left(\rho c - \rho \Delta H_f \frac{\partial f_S}{\partial T}\right) \frac{\partial T}{\partial t}
\]  
(6.4)

Defining the enthalpy as:

\[
H(T) = \int_0^T \rho c dT + \rho \Delta H_f \left[1 - f_S(T)\right]
\]

and substituting in the previous equation, we obtain: