SOLIDIFICATION IN SQUARE SECTION

SOLIDIFICACION EN SECCIÓN CUADRADA

CARLOS HERNÁN SALINAS LIRA¹

ABSTRACT

The objective of the present work is to develop a numerical model to analyze melting solidification process considering the natural convection phenomena to an alloy metal in a square section. Physical medium is taken as incompressible Newtonian fluid with isotropy thermal properties where the heat is transferred by conduction and convection, including de thermal phase change phenomenon. The last one is modeled by the improvement procedure, called Enthalpy Model, based on the fraction solid function which liberates the latent heat according to fraction of solid particles generated using as parameter the temperature level. The mathematical model is based on a non-linear second order differential partial equation system: Momentum, continuity, heat transfer equations and a set of auxiliary expressions with the purpose of equation system closure or applied the boundary and interface condition. The numerical model is based on Volume Finite Method in body fitted coordinates with a SIMPLER scheme to join pressure and velocities. The strategy study allows the two-dimensional solidification of alloy aluminum (Non-Isothermal Solidification) in square section. Unsteady state results are shown in the way: Streamlines and isotherms compared with available data after performing a consistency analysis.

KEYWORDS: Phase Change, Natural Convection, Alloy Aluminum, Enthalpy Model, Finite Volume Method.

1. INTRODUCTION

This paper presents a study about solidification of alloy aluminum that is known in the literature as solid-liquid phase-change problem. Considerable researches have been focused in this problem because of their scientific and practical significance in material processing: Purification of metal, continuum casting, high temperature super conducting crystals, etc. (See Rohatgi, 1988 and Murphy *et al.*, 1988). The physical aspects of solidification process are reviewed by Beckerman and Viskanta (1993) with a discussion of the principal topic in numerical simulation at macroscopic scale. Explicit modeled by average volume method are given.

The classical analytical analysis for the solidification problem is so called Stephan Problem, which accept solution for few limited cases that are reviewed by Alexiades and Solomon (1993). The simplest problem is to study heat transfer by conduction without convection effects (Lazaridis, 1970;

¹Departamento de Ingeniería Mecánica, Facultad de Ingeniería, Universidad del Bío-Bío, Av. Collao 1202, Concepción, Chile. E-mail: casali@ubiobio.cl

Hsiao, 1985). Today with the improvement of computational fluid dynamics it has been possible to analyze the convection effects through direct numerical simulation using several finite methods (Kurz and Fisher, 1998). One of the first investigations in this line was presented by Sparrow *et al.* (1977).

The historical of finite methods has two basic direction: The fixed grid methods are easier which are used mainly by researchers who work with Finite Difference and Finite Volume (Wolff and Viskanta, 1988) techniques. The second direction is the multi domain method naturally preferred by researchers who use Finite Elements Analysis (McDaniel and Zabaras, 1994). Adaptive grid techniques and explicitly determination of interface are required in the last case. Furthermore, the most recent research using mixed numerical model like Average Volume Method (Bekerman and Viskanta, 1993) or by explicit determination of interface using a fixed grid as presented by Chun and Park (2000). Relative merit of fixed grid and multi domain methods has been discussed in literature (Salcudean and Aduallah, 1988; Lacroix and Voller, 1990).

Of course, the simple domain solution in a fixed grid for any kind of numerical method is easier to work and it saves computer time. The problem with explicit determination of front tracking are convection effects of grid moving and high curvature of interface position which can produced instability in the numerical solution and introduced unnecessary errors. However, the problem is not how to discrete the mathematical model, but how to simulate the latent heat liberation, that happens at micro scales, to produce desirable macroscopic physical effects. This is specially important in mushy zone for non-isothermal solidification and capturing front tracking for isothermal solidification. For instance, the Enthalpy Method like presented by Swaminathan and Voller (1993) gives the same

tools to work in a simple and consistent way for macroscopic formulation.

In this work the improvement enthalpy method is used for modeling the interchange of latent heat where the sensible heat is increased by latent heat liberated according to a liquid-solid phase-change fraction as function of temperature. The domain is discrete in a fixed grid without explicit formulation for interface. The mushy zone is modeled by partial latent heat liberation and modification the viscosity according to an inverse relation of solid-fraction in the solid-liquid temperature range. Solid boundaries are fixed to finite volumes, which has temperature under solid temperature.

Two dimension non-linear heat transfer, momentum and continuity equations form a second order non-linear partial differential system equation which is solved by numerical procedure using finite volume method with algorithms developed by authors in Salinas (1996) and Moraga and Salinas (1999). For instance, results of Non-isothermal solidification of alloy aluminum in a square section problem are shown by unsteady isothermal and streamline curves, previous to a grid size consistency analysis.

2. THE PHYSICAL PROBLEMS

The physical liquid-solid phase-change problem for alloy aluminum in square section studied is showed in the Fig. 1 with properties summarized in table I. The Fig. 1 shows a schematic view of alloy aluminum solidification in square section considering as boundary condition three adiabatic wall and imposed cold temperature at fourth left vertical wall. The initial condition for this non-isothermal phase-change problem are the rest flow and temperature equal to 700 [°C] considering at left vertical wall an imposed cold temperature equal to 500°C.



Figure 1. Scheme of liquid-solid phase-change problems in square section.

3. THE MATHEMATICAL MODEL

The mathematical model for two dimension liquid-solid phase-change problem, included the natural convection, in a simple domain solution considering alloys aluminum material is based on the Continuity, Linear Momentum and energy equations is presented by Eqs.(1-4). It is supposed incomTable 1. Physical properties of alloy aluminum.

Properties	Alloy Aluminum
Density	2500 [kg/m ³]
Conductivity	100 [W/m ºC]
Specific heat	1000 [W/Kg °C]
Phase-change enthalpy	4.0*10 ⁵ [J/kg °C]
Solid temperature	550 [ºC]
Liquid Temperature	650 [ºC]
Dynamic viscosity	2.5*10 ⁻³ [kg/m s]
Thermal expansion coefficients	4.0*10 ⁻⁵ [1/°C]

pressible Newtonian fluid with properties constants (See table I) except the density evaluated as linear function of temperature by Boussinesq approximation. The enthalpy method (Swaminathan and Voller, 1993) is used to model the phase-change latent heat liberation by using a liquid-solid fraction function (Raw and Lee, 1991).

$$\frac{\mathbf{u}}{\mathbf{x}} + \frac{\mathbf{v}}{\mathbf{y}} = \mathbf{0} \tag{1}$$

$$\left[-\frac{u}{t} + u - \frac{u}{x} + v - \frac{u}{y}\right] = -\frac{1}{x} + \frac{\mu}{x} \left[-\frac{2}{x}u + -\frac{2}{y}u\right]$$
(2)

$$\left[\frac{v}{t} + u - \frac{v}{x} + v - \frac{v}{y}\right] = -\frac{1}{y} + \frac{\mu}{z} \left[\frac{2}{x} + \frac{2}{y}\right] + g \quad (T - T_{ref})$$
(3)

$$\left(c_{p}+L\frac{-f_{pc}}{T}\right)\left[-\frac{T}{t}+u\frac{-x}{x}+v-\frac{T}{y}\right] = -\frac{-x}{x}\left(-\frac{(k_{p}T)}{x}\right) + -\frac{-y}{y}\left(-\frac{(k_{e}T)}{y}\right)$$
(4)

Where: u, v, p and T are the dependent variables for the velocity components, pressure and temperatures respectively, and μ , , _e, L, f_{pc} and c_p are the material properties

of dynamic viscosity, density, effective thermal conductivity, phase-change enthalpy, liquid-solid fraction function and specific heat, respectively.

3.1. Initial and Boundary Conditions

fication of alloy aluminum in square section problem.

The initial and boundary condition are given below according to of non-isothermal solidi-

Initial condition
$$\begin{cases} u = 0 \\ v = 0 \\ T = 700 \text{ °C} \end{cases}$$

Boundary condition
$$\begin{cases} u = 0 ; v = 0 \text{ to } | \begin{array}{c} x = 0.0 , x = 0.05 \text{ m} ; 0.0 \text{ y } 0.05 \text{ m} \\ y = 0.0 , y = 0.05 \text{ m} ; 0.0 \text{ x } 0.05 \text{ m} \end{cases}$$
$$-\frac{T}{y} = 0 \text{ to } 0.0 \text{ x } 0.05 \text{ m } \text{ at } \begin{cases} y = 0 \\ y = 0.05 \end{cases}$$
$$-\frac{T}{x} = 0 \text{ to } 0.0 \text{ y } 0.05 \text{ m } \text{ at } x = 0.05 \end{cases}$$
$$T = 500 \text{ °C } \text{ to } 0.0 \text{ y } 0.05 \text{ m } \text{ at } x = 0 \end{cases}$$

For this formulation a linear liquid-solid fraction function is used with increased of

viscosity in mushy zone according to inverse function of liquid-solid fraction value.

Viscosity
$$\begin{cases} \mu & \text{to } T > T_{L} \\ -\frac{\mu}{f_{pc}} & \text{to } T_{S} & T_{L} \\ & \text{to } T < T_{S} \end{cases}$$

Where the T_L and T_S are the temperature de liquid and solid of alloy respectively.

When the conductivity is space variable (mushy zone) then is necessary an improvement procedure to model correctly the heat transfer conduction which is performed by introduction next effective conductivity obtain of conductivity boundary condition in interfaces (See Moraga and Salinas, 1999). This way, the following expression for interface temperature T_w and effective conductivity k_e see Fig. 2, are obtained according to evaluated in a conservative form the heat flow in each face of the finite volume elements.

$$T_{W} = \frac{n_{p}k_{s}T_{s} + n_{s}k_{p}T_{p}}{n_{p}k_{s} + n_{s}k_{p}}$$
(5)

$$K_{e} = \frac{n k_{s} k_{p}}{n_{p} k_{s} + n_{s} k_{p}}$$
(6)

Solidification in Square Section / Carlos Hernán Salinas L.



Figure 2. Interface Scheme.

The Eqs. (1-4) form a system of four partial differential equations that model fluid mechanics and heat transfer of liquid-solid phase-change process under initial and boundary condition described above. This mathematical model is solved in a numerical form as explained in the next section.

4. NUMERICAL MODEL

The computational fluid dynamics algorithm was developed by the author in Salinas (1996) and modified to include the calculation of heat transfer in Moraga and Salinas (1999). In this section the main aspect of the algorithms, particular values of parameters are given.

The algorithm is developed in body fitted coordinates system generated by a Poisson equation with the stretching function described in Thompson *et al.* (1985) and implemented in Salinas (1996). After transforming the system of equations the Finite Volumes Method (FVM) is applied to obtain the discrete system of equations. To couple the continuity and Navier-Stokes equations the SIMPLER algorithm

(Patankar, 1980) is used. A staggered grid is used to represent the variables considering T, p and physical properties in the center of each control volume while the velocity components and heat fluxes are calculated in the faces of the finite volumes. The terms of diffusion (second order derivatives) and Laplacian operator are calculated through a central difference scheme, the convection terms (first order derivatives) are evaluated through the power law interpolation (Patankar, 1980), and the transient terms are calculated in an implicit way by using a backwards difference procedure. The non-linear system equation is linearized by using values of the properties obtained in the previous iteration and Crank-Nicolson procedure for the convection terms (Lapidus and Pinder, 1982). Afterwards the linear systems of equations are solved by the iterative Gauss-Seidel method with successive relaxation. Relaxation factors equals to 0.65, 0.55 and 0.55 for p, T, u and v, respectively are used. Generally not more that three SIMPLER cycles and around 10³ iterations for each linear system are adequate in order to obtain convergence with maximum local deviation for u, v, p and T equal to 7.0E-3%.

5. VALIDATIONS OF FLUID MECHANICS AND HEAT TRANSFER CALCULATIONS

The transient evolution of natural convection of air in a square cavity (Satya Sai and Seetharamu, 1994) was used to validate the fluid mechanics and heat transfer. The results for Rayleigh numbers equal to 10⁴, 10⁵ and 10⁶ are presented in Moraga and Salinas (2000).

A consistence analysis is performed to study convergence. For this instance non-

isothermal solidification problem is used showing results in the Figs. 3-5. In the Fig. 3 and Fig. 4 can see a good convergence in relation to grid size 40x40 in relation to coarse grid 20x20 and fine grid 60x60 when is analyzed local center vertical velocity and centerline temperature at indicated time. In transient temperature at center point, showed by Fig. 5 for several grid size, is observed a convergence to grid size 40x40 too which is very close to temperature curve obtained with grid size equal 60x60. This convergence study can been concluded that a grid size 60x60 is good grid to used.



Figure 3. Centerline temperature v/s grid size at t=50 s.

Solidification in Square Section / Carlos Hernán Salinas L.



Figure 4. Vertical centerline velocity v/s grid size at t=50 s.



Figure 5. Center time temperature v/s grid sizes.

6. RESULTS AND DISCUSSION

After the consistency analysis was performed the prediction for natural convection and heat transfer for three liquid-solid phasechange problems was accomplished. For all problem a uniform grid size 60x60 with constant time step are used

Unsteady results of Non-isothermal solidification in square section obtained by the present model are presented in Fig. 6. It shows streamlines and isotherms for Gr=1.0e7, Pr=0.025, St=0.5 at t=10, 40 and 80 s. Can be observed that fluid flow have a complex and strongly unsteady development with secondary vortex in upper region and right under corner for initial times (showing at=10 s). After that only one vortex is formed as showed in the figure at t=40 s and t=80 s. This results are very similar to the one presented by Cruchaga and Celentano (1997). Notice that, in this work is not predicted the secondary vortex.



Figure 6. Isotherms and streamline for alloy aluminum solidification. (Gr=1.0e7, t=10,40 y 80 s, Pr=0.025, St=0.5, Grid size 60x60, dt=0.01 s)

7. CONCLUSION

A numerical model has been developed to solve the liquid-solid phase change problem for non-isothermal solidification process.

Consistent numerical analysis for unsteady temperature curve is performed. This study, convergence results using grid size equal to 60x60 was obtained.

Numerical results of non-isothermal solidification process of alloy aluminum in a square section are similar to available numerical data.

Secondary vortex are predicted by the present method.

9. ACKNOWLEDGMENT

Financial support for this study provided by Universidad del Bío-Bío through grant FPI Nº 0152112 is greatly appreciated.

8. BIBLIOGRAPHY

- ALEXIADES, V. and SOLOMON, A.D., 1993. *Mathematical Modeling of Melting and Freezing Processes*, chap. 2, Hemisphere Publishing Corporation, Washington.
- BECKERMANN C. and VISKANTA R., 1993, "Mathematical Modeling of Transport Phenomena During Alloy Solidification", *Appl. Mech. Rev*, vol 46, N^o 1, pp 1-27.
- CHUN, C.K. and PARK, S.O., 1999. "A Fixed Grid Finite-Difference Method for Phase-Change Problems", *Numerical Heat Transfer*, Part B, 38:59-73,200.
- CRUCHAGA M. and CELENTANO D., 1997. "Thermally Coupled Incompressible Flow Formulation With Phase-Change Effects", Tenth Inter. Conference on Thermal Problem, U.K.
- HSIAO, J.S., 1985. "An Efficient Algorithm for Finite Difference Analyses of Heat Transfer with Melting and Solidification", *Numer. Heat Transfer*, 8: 653-666.
- KURZ, W. and FISHER, D., 1998. "Fundamentals of Solidification", Trans Tech Publications, Aedermannsdorf, Switzerland.
- LACROIX, M. and VOLLER, V.R., 1990. "Finite

Difference Solution of Solidification Phase Change Problems: Transformed versus Fixed Grids", *Num. Heat Transfer*, Part B, Vol. 17, pp. 25-41.

- LAPIDUS, L. and PINDER, G.F., 1982. Numerical Solution of Partial Differential Equations in Science and Engineering, John Wiley & Sons, Inc.
- LAZARIDIS, A., 1970. "Numerical Solution of the Multidimensional Solidification (or Melting) Problems", *Int. J. Heat Mass Transfer*, Vol. 13, pp 1.459-1.477.
- MCDANIEL, D.J. and ZABARAS, N., 1994. "A Least-squares Front-Tracking Finite Element Method Analysis of Phase Change with Natural Convection", *Int. J. For Num. Methods in Engineering*, Vol. 37, 2.755-2.777.
- MORAGĂ, N.O. and SALINAS, C. H., 1999. "A Numerical Model for Heat and Fluid Flow in Food Freezing", *Numerical Heat Transfer*, Part A, 35: 495-518.
- MORAGA, N.O. and SALINAS, C. H., 2000. "Numerical Study of Unsteady 2d Natural Convection and Solidification of a Food Inside a Freezing Chamber", *Num. Heat Transfer*, Part A, 37: 755-777.
- MURPHY, D.W., JOHNSON, D.W., JIN, S. and HOWARD R.E., 1988. "Processing Techniques for the 93K Superconductor Ba₂Ycu₃O₄", *Sci* 241, 922-930.
- PATANKAR, S.V., 1980. *Numerical Heat Transfer* and Fluid Flow, Hemisphere Publishing Corporation, Washington, DC.
- RAW, W.Y. and LEE, S.L., 1991. "Application of Weighting Function Scheme on Convection-Conduction Phase Change Problems", *Int. J. Heat Mass Transfer*, Vol. 34, N^o 6, pp. 1.503-1.513.
- ROHATGI, P., 1988. Foundry Processing of Metal Matrix Composites, Modern Casting, April, pp 47-50.
- SALCUDEAN, M. and ADUALLAH Z, 1988. "On the Numerical Modeling of Heat Transfer During Solidification Processes", *Int. J. Numer. Meth*ods Engineering, Vol. 25, pp. 445-473.
- SALINAS, C.H., 1996. "Modelação de Escoamentos Tridimensionais em Geometrias Complexas", D. Sc. Thesis, COPPE/PENO, UFRJ, RJ-Brazil,.
- SATYA SAI, B.V.K. and SEETHARAMU, K.N., 1994. "Solution of Transient Laminar Natural Convection in a Square Cavity by an Explicit Finite Element Scheme", *Numerical Heat Transfer.* Part A, 25, 593-609.
- SPARROW, M., PATANKAR, S.V. and RAMADHYANI, S., 1977. "Analysis of Melting in Presence of Natural Convection in the Melt Region", *ASMEJ. Heat Transfer,* Vol. 99, pp. 520-526.

- SWAMINATHAN, C.R. and VOLLER, V.R., 1993. "On the Enthalpy Method", *Int. J. of Num. Heat Fluid Flow.* 3: 233-244.
- THOMPSON, J.F., WARSI, A. and MASTIN, C.W., 1985. "Numerical Grid Generation", *Elsevier Science.* Publishing.
- WOLFF, F. and VISKANTA, R., 1988. "Solidification of a Pure Metal at a Vertical Wall in the Presence of Liquid Superheat", *Int. J. Heat Mass Transfer*, Vol. 31, N^o 8, pp. 1.735-1.744.