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DENDRITIC SEGREGATION OF STEEL ALLOYS IN CONTINUOUS CASTING PROCESSES

Mario A. Storti, Norberto M. Nigro, and Sergio R. Idelsohn
Grupo de Tecnología Mecánica del INTEC
CONICET - Universidad Nacional del Litoral
Güemes 3450, 3000 Santa Fe, Argentina

RESUMEN

El problema de solidificacion de aleaciones en trenes de colada continua esta gobernado macroscopicamente por fenomenos asociados a: mecanica de fluidos, transferencia de masa y de energia y difusion doble. Los problemas de interes desde el punto de vista metalurgico son la macro y microsegregacion, contraccion volumetrica, formacion de poros, entre otros. Para poder abordar la resolucion de las ecuaciones de conservacion que plantea la mecanica del continuo, tanto para la transferencia de masa, momento y energia es necesario plantear un modelo para el flujo a dos fases que aparece dentro de la zona pastosa. En este trabajo nos hemos basado en un modelo continuo de flujo a dos fases presentado por Choudhary y Mazumdar resolviendo las ecuaciones de momento, continuidad y transporte de soluto, con un modelo de turbulencia algebraico para el liquido. Se presentan casos test y un analisis de sensibilidad a diferentes parametros de operacion.

ABSTRACT

Continuous casting alloys solidification is macroscopically governed by fluid flow, heat transfer, mass transfer and double diffusion phenomena. From a metallurgical point of view some of the main problems are the prediction of micro and macrosegregation, volumetric shrinkage and porosity formation. In order to solve the set of conservation equations corresponding to flow, heat and mass balances it is neccesary to model the two phase flow appearing at the mushy region. In this work we have adopted a continuum model presented by Choudhary and Mazumdar adding an algebraic turbulence model for liquid phase. We present several test problems and a sensitivity analysis for different operation parameters.

INTRODUCTION

Fluid flow coupled with heat and mass transfer principles are increasingly gaining acceptance as a means of improving the quality and yield of castings. The benefits to be derived from adopting such an approach range from slag- and dross-free gating system design to a desired microstructure of the finished product. In general the transport of heat, mass and momentum during solidification processing controls such varied phenomena as solute macrosegregation, distribution of voids and porosity, shrinkage effects and overall solidification time. These parameters, in turn, result in a variation of the mechanical, thermophysical and electrical properties of the solidified product. The complex nature of the coupling between heat and mass transport with fluid flow during solidification necessitates a fundamental understanding of the processes and the mechanisms of interaction in relation to empirical formulas and charts. Heat transfer by forced convection predominates during the filling stages. Once the mold cavity is filled, buoyancy-generated natural convective heat and mass transfer occur before the phase change. [1]

The principles of heat transfer by forced convection in continuous casting processes are caused by the molten steel alloy superheated charge that enters through a pouring nozzle. This mass flow generates a strong turbulent mixing at the upper part of the mold region and decays rapidly in the axial direction with almost negligible influence at the secondary part of the billet. Subsequent stages during the solidification of a binary alloy involve both phase change heat and mass transfer as well as buoyant thermosolutal convection [2].

With this approach it is possible to gain some macroscopic insight of solidification process. Following in complexity it is possible to introduce the modeling of microstructure or micromodeling. Analytical studies carried out by Fredriksson and Svensson [3] for eutectic gray, ductile and white iron were extended to hypoeutectic irons and to eutectoid transformation by Stefanescu and Kanetkar [4]. Su *et.al* [5] used a finite difference scheme combined with a model assuming growth of graphite spheroids controlled by diffusion of carbon through the austenite shell. More recently, similar development have been made for the dendrite growth of equiaxed grains [6][7][8] and the question about columnar to equiaxed transition has been addressed by Hunt [9].

This work deals with macrosegregation of solute elements during solidification of metal alloys in continuous casting processes. The importance of this research is associated with the great influence of macrosegregation phenomenon on the quality of the casting products. It is well known that both micro and macrosegregation produce compositional heterogeinity that is responsible for the nonuniformity of mechanical properties of products decreasing the metal quality. Although the general level of segregation in continuously casting processes is less than in conventional cast metal, significant axial macrosegregation is often observed in continuously cast billets. Even though micro and macrosegregation can occur in continuously cast steel, macrosegregation of C,P and S causes more serious quality problems compared with microsegregation because the annealing process can eliminate most of the microstructures but it is not possible to produce a redistribution of solutes in order to eliminate the compositional heterogeinity [10]. In this paper the molten steel is modelled by incompressible Navier-Stokes equations coupled with an energy balance with mushy phase change including the concentration balance for only one solute (carbon). The momentum equations contain two bouyancy terms (double diffusion) that represent the effects of temperature and concentration gradients on the local density and produce natural convection. Both terms are introduced with a Bousinesq model [10]. The equations were closed with constitutive laws for newtonian fluids, an algebraic turbulence model for viscosity and conductivity corrections [11][12] and a thermodynamic phase diagram for Fe-C alloys. It uses a viscosity augmented model for mushy region treatment [13].

MATHEMATICAL MODELLING OF MACROSEGREGATION

The mathematical modelling of solidification processes of steel alloys with macrosegregation is established from the conservation laws applied to the whole domain considering that the two phases are represented by a one phase fluid model. The basic principle of the two-fluid approach is the development of separate governing equations for each phase (solid and liquid) which are then coupled through interface transfer terms [13].
A schematic plot of the geometric details is shown in figure 1. We have considered both square and round billet casting systems without submerged entry nozzle. The molten metal is poured continuously into the mold through a nozzle and the strand is drawn away at a constant casting speed. The liquid velocity at the inlet nozzle was assumed constant and in balance with that corresponding to the outlet section.
The development of the mathematical model was based on the following assumptions [10]:

_The problem was assumed to be at steady state with respect to a fixed coordinate system.
_For the sake of computational cost we have restricted to plane and axisymmetric 2D geometries.
_Only the vertical part of the caster section was considered and the strand curvature due to bending was ignored.
_(C_p, ρ) in liquid and solid phases were assumed to be equal
_The carbon steel considered in this simulation was assumed to be a binary Fe-C alloy.
_Local thermodynamic equilibrium during solidification was assumed to prevail in this study
_An incompressible newtonian fluid was assumed and turbulence effects were approximated using an algebraic model.[11][12]
_The latent heat of $\delta - \gamma$ transformation compared to the latent heat of fusion was considered to be negligible.
_The effect of strand deformation (bulging) on solute distribution was neglected.
_Effect of mould oscillation was ignored
_The free surface at the top of the caster was assumed to be plane. This is a reasonable assumption because the meniscus is covered with a protective slag layer through which negligible heat was assumed to be lost.

The main numerical ingredients of the algorithm are:
_Petrov-Galerkin finite element formulation
_SUPG-PSPG for incompressible Navier-Stokes equations
_stabilized SUPG for advection dominated flows in energy and solute balances
_phase change term computed through nodal entalpies, auxiliary variables in the scheme.
_underrelaxed Newton-Raphson with direct solver at each iteration step.

NUMERICAL EXAMPLES

Continuous casting solidification of Fe-C alloy.: Figure 1 and 2 show the geometrical description of the process and the boundary conditions applied to the numerical problem. We follow the numerical examples of Aboutalebi et.al [10] to validate our development and to compare the two models. As it was mentioned above our model differs from the Aboutalebi's one in the mushy region

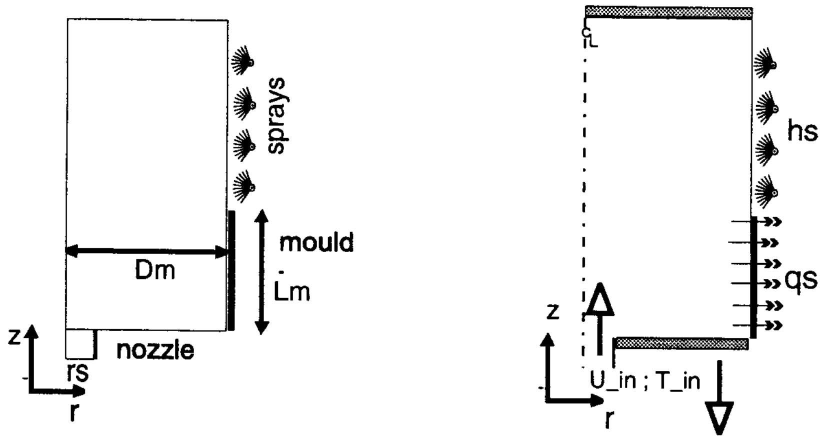

Figure 1: Continuous casting process
1.a) (left) Geometric description
1.b) (right) Boundary conditions

treatment and in the turbulence model. We have used augmented viscosity and an algebraic turbulence model [11,12] while Aboutalebi et.al [10] have used a porous media and a $k-\epsilon$ turbulence model. We have simulated only the round billet case and the geometrical data are similar to those included in Table I. Table II summarizes the boundary conditions and Table III presents physical properties.

Table I: Geometrical data

	geometrical parameter	round	square
D_m	Mould diameter - width (m)	0.11	0.133
L_m	Mould length (m)	0.5	0.5
$2r_s$	Nozzle diameter (m)	0.03	0.03
U_0	Casting speed (m/s)	0.0317	0.0254
	Simulated length (m)	6	6

Table II: Boundary conditions

Boundary	U_1	U_2	Temperature
Nozzle	0	U_{in}	T_{in}
Meniscus	$\frac{\partial U_1}{\partial n}=0$	0	$\frac{\partial T}{\partial n}=0$
Mould	0	U_0	$q_s=[2.67-0.33\sqrt{z/U_0}]\,10^6$
Spray	0	U_0	$q_s=h_s(T-Ts)$
Centerline	0	$\frac{\partial U_2}{\partial n}=0$	$\frac{\partial T}{\partial n}=0$
Outlet	$\frac{\partial U_1}{\partial n}=0$	$\frac{\partial U_2}{\partial n}=0$	$\frac{\partial T}{\partial n}=0$

Table III: Physical data

	Physical data	
ρ	Density $[Kg/m^3]$	7020
μ_l	Molecular viscosity $[Kg/ms]$	$6.2\,10^{-3}$
ΔH_f	Latente heat content $[J/Kg]$	$0.270\,10^{6}$
C_p	Specific heat $[J/Kg^\circ C]$	680
κ	Thermal conductivity $[W/m^\circ C]$	34
$\Delta\beta_T$	Thermal volumetric expansion coefficient $[\frac{1}{^\circ C}]$	10^{-4}
$\Delta\beta_C$	Solutal volumetric expansion coefficient $[\frac{1}{^\circ C}]$	$4\,10^{-2}$
D_{liq}	Liquid mass diffusivity $[m^2/s]$	10^{-8}
D_{sol}	Solid mass diffusivity $[m^2/s]$	$1.6\,10^{-11}$
h_m	Mould convective heat transfer $[W/m^2/^\circ C]$	1270
h_s	Sprays convective heat transfer $[W/m^2/^\circ C]$	1080
T_s	Spray water temperature $[^\circ C]$	40
	Steel carbon content	0.8%
T_m	Melting point	$1567.3^\circ C$
T_0	Casting temperature	$1500^\circ C$
m_l	Liquidus line slope	$-115.4^\circ C$
k_p	Equilibrium partition ratio	0.48

We have simulated the above set for two different casting speeds, $U_0 = 0.03\,m/s$ and $U_0 = 0.01\,m/s$ with pouring velocities at nozzle of $U_{\text{in}} = 0.4898\,m/s$ and $U_{\text{in}} = 0.1632\,m/s$ respectively.
After doing some numerical experiments to test the convergence of the results for different meshes and for different locations of the outlet boundary we conclude that there is no great influence of the results with the coarseness of the mesh restricted to a minimim number of elements capable to represent the mushy region. On the other hand it is advisable to place the outlet boundary in regions where the metal had solidified completely. In the following examples we have used a mesh with about 2400 elements with refinement close to the meniscus and to the mould wall.
In all the experiments we have followed the suggestion of Choudhary et.al [11,12] to take half the turbulent viscosity correction at the submould part or sprays zone. This modification is due to the reduction of turbulence patterns at this region.

Example 1 - $C = 0.8\%$ and $U_0 = 0.03m/s$: Figure 2.a plots the solidified shell thickness and the mushy region width and figure 2.b shows the segregation ratio versus radial coordinate for three axial stations at $z = 0.5\,,\,1\,,\,2$ meters.
We may note that in the mould region ($z \leq 0.5$), there is a liquid pool with a high carbon mass diffusivity relative to the solid phase, enhanced by turbulent corrections, that produce an almost constant concentration within the pool with a smooth variation inside the mushy region to the solid part where the solute concentration presents some profile according to the low solid mass diffusivity.
We may also appreciate a very large mushy region for this operation condition

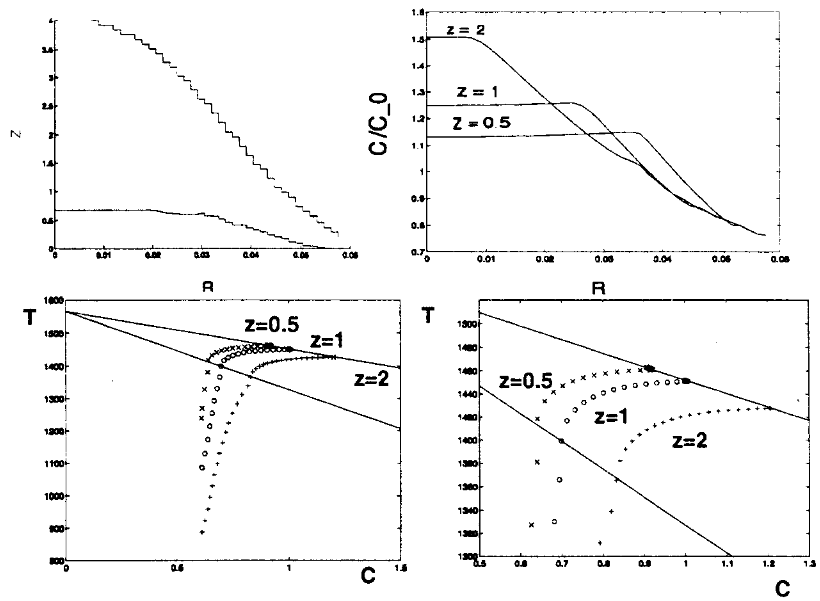

Figure 2: Example 1.
a) (upper-left) Solid shell thickness.
b) (upper-right) Macrosegregation $f_{mushy} = 100$.
c) (lower) Equilibrium diagram.

and the macrosegregation at $z = 2$mts reaches an increment of 50% over the nominal carbon concentration for this steel.
Figure 2.c shows the corresponding phase transformation for the three axial stations $z = 0.5$, $z = 1$, $z = 2$. They present a thermal gradient that deviate the isothermic transformation to another with a lower partition ratio than the nominal for each liquid temperature.

Example 2 - $C = 0.8\%$ *and* $U_0 = 0.01 m/s$: This example corresponds to take the same steel alloy but decreasing the casting speed to 0.01 m/s. This variation produces a longer period of time where heat flux is removed from the molten metal causing a faster solidification.
A numerical drawback of this example is related with the high Grashoff and Rayleigh numbers produced by this slower flow. They produce some difficulties associated with physical or numerical instabilities and we have decresead both the thermal and solutal volumetric expansion coefficient one order of magnitude to have similarities with the above example. After having the first solution with this data we did a kind of sensitivity analysis with double diffusion parameters trying to reach the original values for volumetric expansion coefficients. However we can not reach this limit and some future research should be done to have a better explanation of this phenomenon.
Figure 3.a shows the phases distribution with a thinner mushy region than in the above example and the whole section solidification is obtained at $z = 1.5$ meters. Figure 3.b plots the segregation ratio for this case. The mushy region is a little thinner and the macrosegregation is slightly bigger than the case with

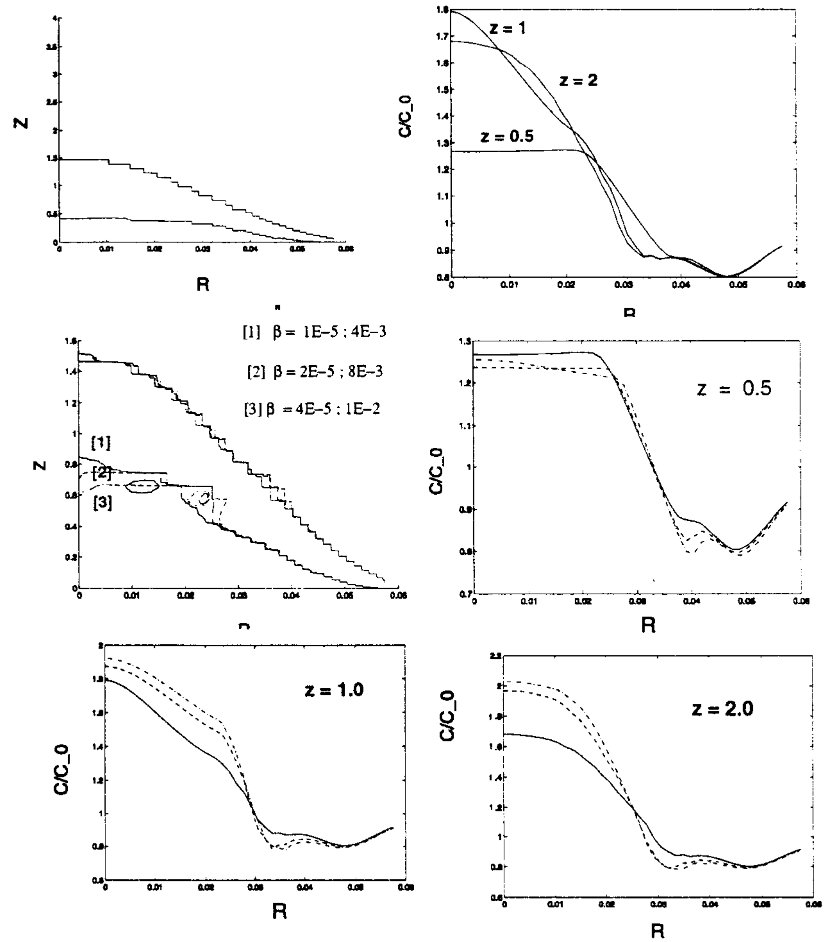

Figure 3: Example 2.
a) (upper-left) Solid shell thickness.
b) (upper-right) Macrosegregation.
c) (middle-left) Solid shell thickness.
d) (middle-right and lower) Macrosegregation.

$U_0 = 0.03$ m/s.
Figure 3.c shows the sensitivity analysis with double diffusion coefficients. It was found not a significant difference among the solutions get with three different volumetric expansion coefficients,

$$\text{case } \#1 : \beta_T = 10^{-5} \qquad \beta_T = 4 \times 10^{-3}$$
$$\text{case } \#2 : \beta_T = 2 \times 10^{-5} \qquad \beta_T = 8 \times 10^{-3}$$
$$\text{case } \#3 : \beta_T = 4 \times 10^{-5} \qquad \beta_T = 1 \times 10^{-2}$$

It is only remarkable that the larger the Grashoff number the bigger the secondary recirculation close to the mushy-liquid interface. This pattern suggests the presence of a physical or numerical instability that transform the original steady problem into another with unsteady behavior. The causes of this instability should be analyzed deeply but it is out of the scope of this paper.
Figure 3.d extends the above sensitivity analysis to the segregation ratio. For $z = 0.5$ there is no significant influence of these parameters but this conclusion changes with the axial coordinate. Specially at $z = 2$ meters we have more than 20% of difference between the case 1 and case 3.

CONCLUSIONS

This paper is part of a research project which goal is to predict by computational resources the coupled influence of fluid flow, heat and mass transfer on the macro and microsegregation in casting moulds. We have started with the development of a numerical method to solve the mathematical model associated with the peritectic and hypoeutectic Fe-C alloys macrosegregation yielded by continuously casting processes. Our conclusions are: a) results are acceptable qualitatively, b) global balances are satisfied, c) the segregation ratio agrees with the corresponding partition ratio coefficient for steel alloys, d) results are not to sensitive to the viscosity augmented factor, e) in contrast with a high sensitivity to the volumetric expansion coefficient. We have found that further improvements in the understanding of how the mushy region and turbulence model affect the results are needed in order to compare with other numerical results. Also it is neccesary to do some research about the physical or numerical instabilities arising from the Grashoff or Rayleigh number, here they are associated with double diffusion phenomena. Other future research topics of interest are multiple species, tridimensional simulation and microstructural evolution.

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