## Influence of Chemical Composition on Macro-Segregation in AISI 4340 Forging Products

O.Bogdan<sup>1</sup>, *Industrial Soft Montreal, Canada* bogdan@castingsnet.com

## Abstract

The analysis goal was to check if the chemical composition of AISI 4340 steel grade offers conditions of avoiding A-segregation and material heterogeneity in forging products made using 50 tons ingots. To this purpose the computer program SimCADE v.2.0 is employed to simulate the solidification process. In these numerical experiments, cooling and solidification rate have been correlated with the criterion value calculated by A-segregation prediction module of the solidification software. The mathematical model is based on the chemical composition of the steel and the A-segregation mechanism proposed by Suzuki and Miyamoto. Numerical analysis shows that if the chemical composition of steel poured into 50 tons ingot with the given geometry is in the limits of AISI 4340 steel grade specification, the steel will develop macro-segregation. Also, the results show that the carbon and silicon content increase the macro-segregation area. Instead, a higher molybdenum content decrease the A-segregation area size. The results are useful for both, steel and forgings manufacturers and semimanufactured or forging products buyers as well. Using the manufacturing records as input data for the simulation software, the buyer may choose a forging product with higher homogeneity of mechanical properties.

## **1** Introduction

It is known that one of the most important factors that affect the final quality of forging products is the solidification process. Macro-segregation commonly known as A-segregation, often found in large steel ingots, present channels enriched by sulfur, carbon, phosphorus and is one of the reasons why the mechanical properties of the product are anisotropic. A-segregation form in the zone of columnar grains at the regions with structure characterized by the transition from the columnar grains to large equiaxed grains.

Manufacturing a forging product with a high homogeneity of mechanical properties is impossible without a strict control of A-segregation and solidification process variables. In order to better understand how these

<sup>&</sup>lt;sup>1</sup> O.Bogdan has been for ten years with the Research & Design Department, IMGB (Doosan IMGB SA)

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parameters are influenced by chemical composition variation, we realized a series of numerical simulations, applied the Suzuki and Miyamoto criterion and measured the A-segregation area size. From all parameters that have influence on the segregation process, in this paper, we are focused on the effect of C, Si, Mn, P, S, Ni, Cr and Mo on A-segregation.

# 2 The mathematical model used to simulate the solidification process

The equation used to describe the heat flow during the solidification process in two coordinates for the transient regime is the following:

$$\frac{\partial}{\partial x} \left[ \lambda(T) \frac{\partial T}{\partial x} + \lambda(T) \frac{\partial T}{\partial y} \right] = \rho C_p \frac{\partial T}{\partial t}$$
(1)

where T represents temperature,  $\lambda$  - conductivity, C - specific heat, t - time and  $\rho$  - density. The initial condition (2) and boundary condition (3) attached to Equation (1) to get a complete model are:

$$T = T_0, t = 0$$
 (2)

$$\lambda(\frac{\partial T}{\partial x}n_{x} + \frac{\partial T}{\partial y}n_{y}) + \alpha(T - T_{0}) = 0, \quad \forall P(x, y) \in S_{\alpha}$$
(3)

where  $T_o$  represent temperature at initial moment and  $\alpha$  is the heat transfer coefficient on the surface  $S_{\alpha}$ .

During the solidification process a significant factor is the latent heat which works like an external source of heat. To get a valuable model it is necessary to include this factor in our mathematical model. There is a lot of methods to include this external source in the heat transfer model. We use the following relation:

$$C_1' = C_1 + \frac{L}{\delta T}$$
(4)

where C'<sub>1</sub> represents the specific heat which include the latent heat, C<sub>1</sub> - specific heat without latent heat, L - latent heat and  $\delta T$  - the differences between liquidus and solidus temperatures.

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Because the analytical equations cannot be used to realize the computer program it is necessary to transform it into an integral model. Knowing the differential equation (1), initial (2) and boundary condition (3) the integral equation for mathematical model is:

$$\pi = \int_{V} \frac{1}{2} \left[ \lambda_{\tau} \left( \frac{\partial T}{\partial x} \right)^{2} + \lambda_{\tau} \left( \frac{\partial T}{\partial y} \right)^{2} \right] dV + \int_{V} \rho C_{p} \frac{\partial T}{\partial x} dV + \int_{S_{\alpha}} \frac{\partial T}{\partial x} dV + \int_{S_{\alpha}} \frac{\partial T}{\partial x} dS$$
(5)

Having in view that the analyzed domain V can be broken into finite elements with quadrilateral shape, using the linear functions we can describe the temperature with the following equation:

$$\hat{T}(x, y, t) = N_1(x, y)T_1(t) + N_2(x, y)T_2(t) + N_3(x, y)T_3(t) + N_4(x, y)T_4(t)$$
(6)

where  $N_1(x,y)$ ,  $N_2(x,y)$ ,  $N_3(x,y)$  and  $N_4(x,y)$  represents shape functions and  $T_1(t)$ ,  $T_2(t)$ ,  $T_3(t)$  and  $T_4(t)$  the temperatures in finite element nodes. With this last relation and imposing the stationary conditions for Equation (5), we have the following equation:

$$\sum_{1}^{n} \left( \int_{V^{e}} \mathbf{B}^{\mathrm{T}} \mathbf{D} \mathbf{B} \mathbf{T}^{e} d\mathbf{V} + \int_{V^{e}} \rho C_{p} \frac{\partial}{\partial t} \mathbf{N} d\mathbf{V} + \int_{S_{\alpha}^{e}} \mathbf{N}_{N^{\mathrm{T}}} \mathbf{T}^{e} d\mathbf{S} + \int_{S_{\alpha}^{e}} \alpha T_{\alpha} \mathbf{N}^{\mathrm{T}} d\mathbf{S} = 0$$
(7)

This equation can now be written as follows:

$$K_1^{e} \dot{T}^{e} + (K_2^{e} + K_3^{e}) \cdot T = K_4^{e}$$
(8)

After assembling all elements of analyzed domain we get the equations:

$$K_{1}\dot{T} + (K_{2} + K_{3}) \cdot T = K_{4}$$
(9)

To obtain the temperatures in transient regime we use finite differences method. The equation which gives the initial temperatures for a new cycle of computing is:

$$\left(\frac{2}{\Delta t}K_{1}+K_{2}+K_{3}\right)\cdot T_{n+1}=\left(\frac{2}{\Delta t}K_{1}-K_{2}-K_{3}\right)\cdot T_{n}+\left(K_{4,n+1}+K_{4,n}\right)$$
(10)

Using the last equation we can compute all temperatures at time t+dt if we know the temperature at time t.

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## 3 The computer program

Using the mathematical model described, we have developed a computer program to simulate the heat transfer during the solidification process. The software simulates cooling and solidification of metal in the mold so that the effects of various manufacturing parameters and environmental conditions upon the solidification process can be examined.

The computer program, shown in Picture 1, written in C++ language, take in account the internal sources and variation of material properties with temperature. The software uses over 450.000 finite elements to get an accurate geometrical description of the domain. The necessary time to compose the problem and solve the equation system is about 60 seconds for a PC computer system.

The successive approximation method with a variable suprarelaxation factor is used to solve the equation system. The software has routines for automeshing the analyzed geometry and displays results in the graphical mode.





The main simulation system of the software consists of three processors: - the pre-processor module for reading the 3D CAD drawing of the analysis model and automatic generation of the finite element mesh,

- a simulator for the solidification process and,

- the post-processor module to display the results.

The software has been tested for industrial conditions in slab reheating and casting solidification applications.

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## **4 A-segregation Prediction Module**

The segregation in the columnar zone is much influenced by the cooling and solidification rate. To define the A-segregates occurring conditions K.Suzuki and T.Miyamoto proposed the following Equation (11), based on solidification rate V (mm/mm) and cooling rate R ( $^{\circ}C/min$ ):

$$\mathsf{R} \cdot \mathsf{V}^{1.1} \le \alpha \tag{11}$$

K.Suzuki and T.Miyamoto have investigated at Muroran Research Center, The Japan Steel Works Ltd. (JSW) a 0.7 % carbon steel and obtained  $\alpha$  = 8.75; however, the value  $\alpha$  is depending upon chemical composition. Using the Equation (11), the chemical composition of the analyzed steel, liquid diffusion and solid diffusion equation applied for carbon and Scheil's equation applied for all elements except carbon, we have developed the prediction module attached to the simulation software SimCADE. For AISI 4340 steel with the following chemical composition:

Γ	%C	%Si	%Mn	%P	%S	%Cr	%Mo	%Ni
	0.40	0.35	0.60	0.01	0.002	1.20	0.25	1.50

the calculated value  $\alpha$  is 0.63 and is shown in Picture 2. Because the R•V<sup>1.1</sup> values (red curve) does intersect critical value  $\alpha$  (blue line), the



A-segregates <u>will occur</u> in the steel with the given chemical composition and poured into a 1700mm medium diameter ingot.

To quantitatively appreciate influence of the chemical composition on Asegregation, we have defined the value Rs, the ratio between area affected by segregation and the longitudinal section area of the ingot.

The following numerical experiments will calculate the area affected by segregation, Rs for AISI 4340 steel ingot.

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## **5** Numerical experiments

## 5.1 Initial conditions, boundary conditions, material properties and simulation results

The limits of the chemical composition of AISI 4340 steel grade are shown in Table 1. Liquidus and solidus temperature taken in simulation have been 1490°C and 1430°C, respectively.

%C	%Si	%Mn	%Cr	%Mo	%Ni
0.36~	0.10~	0.45~	1.00~	0.20~	1.30~
0.44	0.35	0.70	1.40	0.35	1.70

The emissivity values on the outside surface of the mold has been assumed to be function by temperature and estimated at 0.75 - 0.95. The value of the heat transfer convection coefficient on the outside surface of the mold has been 15 kcal/m<sup>2</sup>h°C. The upper surface of the ingot has been considered as insulated. The material data of the mold and AISI 4340 steel used in these numerical experiments are given in Table 2. The geometry data of the ingot used in these simulations is shown in Table 3.

Table 2.Materials and thermal properties used in simulation

	Conductivity	Specific heat	Latent heat	Density
	W/m°K	J/kg°K	kJ/kg	kg/m³
35NCD16	33.0	480	267.0	7800
Mold (Grey Iron)	59.0	460	-	7000

Table 3.	Geometry	<sup>,</sup> data	of the	ingot
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Medium diameter	Body Height	H/D ratio	Taper Ratio
[mm]	[mm]		[%]
1700	2250	1.5	9.0

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Pouring and mold temperature taken into account has been 1600°C and 20°C, respectively. The transitory regime have been used to calculate solidification and cooling rate The iso-solidus curves are shown in Figure 1.



Figure.1 Iso-solidus curves for 1700mm medium diameter ingot

#### 5.2 Influence of C content on A-segregation

To check if the carbon content offers conditions for A-segregation appearance in the 1700mm medium diameter ingot, the segregation module of the software has been employed to calculate the critical value  $\alpha$  for carbon content between 0.36C and 0.44C. The other elements taken in consideration have been:

%Si	%Mn	%P	%S	%Cr	%Mo	%Ni
0.35	0.60	0.01	0.002	1.20	0.25	1.50

The results of the simulations are shown in Figure 2 a, b, c. As seen in this figure, there is a strong A-segregation in AISI 4340 steel poured into 1700mm medium diameter ingot. A-segregation zone ratio Rs is 46%, 55%, 60% for the carbon content of 0.36C, 0.40C and 0.44C, respectively. Because the values of the solidification and cooling rate calculated for analyzed ingot size are lower than the critical value  $\alpha$ , the A-segregation will occur.

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a) Simulation result for 0.36C b) Simulation result for 0.40C c) Simulation result for 0.44C Figure 2. A-Segregation for carbon content between 0.36C and 0.44C

A high carbon content, through the solidification range, is one of the factors that increase the critical value  $\alpha$  and the A-segregation area size. The segregation zone strongly increase with the increase of carbon content.

#### 5.3 Influence of Si content on A-segregation

To check if into 1700mm diameter ingot the A-segregation will occur for silicon in the limits of the steel specifications, three simulations with Si between 0.10Si and 0.35Si have been made. The other elements taken into consideration have been:

%C	%Mn	%P	%S	%Cr	%Mo	%Ni
0.40	0.60	0.01	0.002	1.20	0.25	1.50

The results of simulation are shown in figure 3 a, b, c. As seen, A-segregation will occur in the 1700mm medium diameter ingot. Because the solidification and cooling rate calculated for 1700mm medium diameter



a) Simulation result for 0.10Si b) Simulation result for 0.23Si c) Simulation result for 0.35Si Figure 3. Simulation results for Si content between 0.10Si and 0.35Si

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ingot is lower than the critical value  $\alpha$  calculated with the silicon content in the limits of the steel specification, the A-segregation will occur.

The Rs values are 45%, 60% and 70% for 0.10Si, 0.23Si and 0.35Si, respectively. The segregation zone strongly increase with the increase of silicon content.

#### 5.4 Influence of Mn content on A-segregation

To analyze the influence of manganese content on A-segregation, three simulations with 0.45Mn, 0.58Mn and 0.70Mn have been made. The other elements taken into account are in the following table:

%C	%Si	%P	%S	%Cr	%Mo	%Ni
0.40	0.35	0.01	0.002	1.20	0.25	1.50

In all three simulations made with the Mn content in the limits of the AISI 4340 steel specification, the 1700mm diameter ingot does have A-segregation area size unmodified. The Mn content has a low influence on A-segregation.

#### 5.4 Influence of P content on A-segregation

The phosphorous content used to calculate the critical value  $\alpha$  and make the simulations has been 0.01P, 0.02P and 0.03P. The other elements have been:

%C	%Si	%Mn	%S	%Mo	%Cr	%Ni
0.40	0.35	0.60	0.002	0.25	1.20	1.50



The results of simulation are shown in figure 4 a, b, c. As seen, A-segregation will occur in the 1700mm medium diameter ingot. Because

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the solidification and cooling rate calculated for 1700mm medium diameter ingot is lower than the critical value  $\alpha$  calculated with the steel composition and P content given before, the A-segregation will occur. The Rs values, the ratio between segregation area size and longitudinal section of the ingot, are 40%, 42% and 44% for 0.01P, 0.02P and 0.03P, respectively.

#### 5.5 Influence of S content on A-segregation

The numerical experiments concerning the analysis of sulfur content influence on A-segregation have been made with the following values: 0.002S, 0.01S, and 0.02S. In this case, the other elements have been:

%C	%Si	%Mn	%P	%Mo	%Cr	%Ni
0.40	0.35	0.60	0.01	0.25	1.20	1.50

The results of simulation are shown in figure 5 a, b, c.



Figure 5. A-segregation function by sulfur content

Because the solidification and cooling rate calculated for 1700mm medium diameter ingot is lower than the critical value  $\alpha$  calculated with the steel composition and S content values given before, the A-segregation will occur in this ingot.

The Rs values, the ratio between the area affected by segregation and the longitudinal section of the ingot are 34%, 42% and 44% for 0.002S, 0.01S and 0.02S, respectively. Because the sulfur content directly influences the A-segregation zone size, a lower content is recommended.

#### 5.6 Influence of Mo content on A-segregation

In the following numerical experiments, the molybdenum content was between 0.20Mo and 0.35Mo. The other elements taken in consideration have been:

%C	%Si	%Mn	%P	%S	%Cr	%Ni
0.40	0.10	0.60	0.01	0.002	1.20	1.50

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The Figure 6 a, b, c shows the results of simulations.



Figure 6. A-segregation area function by molybdenum content

It is known that an increased Mo content has a strong influence on inhibition of the segregation process. As seen in Figure 6, even at the upper limit allowed by the specification, the A-segregation will occur. Because a high molybdenum content reduces the A-segregation zone size, a Mo content at the upper limit it is recommended.

#### 5.7 Influence of Ni and Cr content on A-segregation

The nickel content used to calculate the critical value  $\alpha$  has been 1.30Ni, 1.50Ni and 1.70Ni. The other elements are in the following table:

%C	%Si	%Mn	%P	%S	%Mo	%Cr
0.40	0.35	0.60	0.01	0.002	0.25	1.20

In the chrome experiments, the simulation has been made using the following values: 1.00Cr, 1.20Cr and 1.40Cr. The other elements taken into account are in the following table:

%C	%Si	%Mn	%P	%S	%Mo	%Ni
1.20	0.35	0.60	0.01	0.002	0.25	1.50

Because, in all these experiments, the critical value  $\alpha$  has higher values than the solidification and cooling rate for 1700mm diameter ingot, the A-segregation will occur.

The Ni and Cr content does have low influence on the A-segregation process in the AISI 4340 steel ingot. If there is not another reason to keep

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their content values high, to cut the ferro-alloys consumption, a lower value for Ni and Cr content for steel making may be used.

## 6 Conclusions

Influence of C, Si, Mn, P, S, Ni, Cr and Mo have been analyzed to check if there are conditions for A-segregation appearance and material heterogeneity in AISI 4340 forging products made from 50 tons, 1700mm medium diameter ingot. The following results were obtained:

- (1) Because the solidification and cooling rate for the analyzed ingot size and geometry are lower than the critical value  $\alpha$  calculated using the steel elements in the specification limits, the A-segregation will occur and the material of the forging product is not homogenous;
- (2) A high carbon content increases the critical value  $\alpha$  and the A-segregation area size. The segregation area size strongly increases with the increase of carbon content;
- (3) The A-segregation zone strongly increase with the increase of the silicon content as well. To reduce the segregation zone a lower silicon content is recommended;
- (4) The manganese content has a low influence on A-segregation zone and can be established having in view the technological reasons;.
- (5) Because the phosphorous and sulfur content directly influence the segregation area size a lower value is recommended;
- (6) Molybdenum reduces the A-segregation area size. For the analyzed ingot, even at the maximum value of the molybdenum content allowed by specification, the A-segregation will occur. To reduce the A-segregation zone and increase the homogeneity of the forging product, a molybdenum content at the upper limit is recommended;
- (7) Nickel and chrome content has a low influence on the segregation process. If there is not another reason to keep their values high, to minimize the ferro-alloys consumption, for AISI 4340 steel grade poured in 1700mm medium diameter ingot, a lower content of these elements may be taken in consideration for steel making;
- (8) Using the proposed ingot shape and size, it is not possible to have AISI 4340 steel ingot free of macro-segregation and homogeneous forging product only by changing the chemical composition of the steel;

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(9) To obtain AISI 4340 forging products free of segregation and homogenous material, the manufacturer has to find out other ways to increase the solidification rate. For example, changing the ingot shape and size may be a solution that can fix the problem;

Using the simulation software to check the quality of the forging products or to optimize the chemical composition of the steel according to the ingot size, the manufacturer can control the intensity of segregation process in order to lower the ferroalloy consumption and minimize the A-segregation area size and increase the homogeneity of forging products.

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