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Thermodynamic study of non-metallic inclusion formation in SAE 1141 steel

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ABSTRACT

The main purpose of this paper is the thermodynamic study of non-metallic inclusion formation in the CC tundish for SAE 1141 steel. The specific purposes are: 1) obtaining inclusions as function of steel composition and casting temperature. 2) establishing steel chemical composition to form less harmful inclusions to the SAE 1141 steel castability. Simulations using the commercial software FactSage and databases were carried out. Results showed both different solid oxides and liquid phase formation in inclusions by varying calcium content in the steel. Thus, it was possible: 1) to determine both the inclusion composition as a function of aluminum and calcium content of SAE 1141 steel. 2) to establish a range of calcium content in which inclusions are formed predominantly by liquid phase. 3) to calculate percentage of liquid and solid phases in inclusions, and oxides composition as well.

Keywords: SAE 1141 steel, inclusions, calcium treatment, FactSage.

1 INTRODUCTION

Additions of calcium-based alloys are largely employed to control composition, distribution and morphology of remaining non-metallic inclusions in the steel. The greatest benefit of that practice is to minimize clogging occurrence during the continuous casting (CC), that is, to increase heats castability in the steel mill.

Another advantage of inclusions treatment with calcium is to have influence on the control of sulfides morphology. Sims' classification provides three specific types of sulfides which can be found in steels. Among them, type II MnS inclusions are found in steels with both low oxygen and Al content. Such type of inclusion precipitates along primary grain-boundaries during steel solidification. Thus, the primary goal of controlling the morphology of sulfides is to eliminate type II sulfide inclusions by forming (Ca, Mn)S, according to Kiessling [1].

Firstly, addition of Ca modifies oxide inclusions and later, it either forms CaS or converts MnS to (Ca, Mn)S. Inclusions of (Ca, Mn)S precipitate at higher temperatures than those of type II MnS (elongated MnS sulfides), according to Faulring [2].

Inclusions of high melting point, such as Al_2O_3 and CaS, can work as nucleation sites for MnS making sulfides thinly dispersed in the steel matrix. Yaguchi [3] describes a study performed with a base steel (SAE 1030 - 0.06%S) with large sulfides inclusions concentrated on the as cast product. Formation of sulfide lines in the matrix can be observed in the forged product. In the steel with addition of Ca and Mg, sulfide inclusions became both thin and globular, and thinly dispersed in the forged product, as well.

For the production of special steels (as those intended for automotive industry) quality requirements are above average, whether compared to the most part of commercial steels. According to Kirsch-Racine *et al.* [4], the present tendency is the production of both aluminum killed and resulfurized steels. The former, to answer clients demand, regarding both grain size and fatigue resistance, and the latter to improve machinability for the production of mechanical components. In this way, such steels are considered critical in relation to their production in steel mill, since contents of some of their elements (Al, S, O, Ca) must be controlled.

Thus, the general purpose of this work is the thermodynamic study of non-metallic inclusions formation in the CC tundish for SAE 1141 steel. Specific purposes are: 1) obtaining phases and compounds formed in inclusions due to chemical composition and CC temperature employed for SAE 1141 steel. 2)

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establishing conditions of steel chemical composition for producing less harmful inclusions to the SAE 1141 steel castability.

2 MATERIALS AND METHODOLOGY

2.1 Materials

SAE 1141 quality combines both good conformability and machinability in the same steel grade. It is widely employed in forging segments to produce components with both relative complexity and mechanical demand, such as forks and shaft ends for automotive industry, according to Capellari [5] SAE 1141 steel is classified by SAE-AISI as resulfurized carbon steel. The chemical composition used was obtained from a series of industrial heats, as it is showed in Table 1.

Table 1: Chemical composition of SAE 1141 steel in mass percentage (wt %).

C	Si	Mn	S	Al*	Ca*	Cr	Ni	P	O_{total}*
0.40	0.16	1.52	0.101	21.23	5.57	0.17	0.08	0.019	24.5

*Al, Ca and O total (total oxygen) in ppm.

2.2 Methodology

Based on previous studies by Bielefeldt *et al.* [6], thermodynamic simulations were performed with the commercial software FactSage and databases. Simulations were carried out by using both global chemical composition and average temperature of SAE 1141 steel in the CC tundish. The result obtained is the steel composition and non-metallic inclusions (oxides and sulfides) at the temperature of 1,520 ^{o}C, during CC.

Thermodynamic study was performed with the commercial software FactSage 5.5. A general description of the software and databases was carried out by Bale et al [7, 8], as well as current modifications.

The following databases were used, described according to FactSage Database Documentation [9]:

- Ftoxid – FS50 database was extended and optimized from 2000 to 2003 and divided into FToxid, FTsalt, FThall, FTmisc and Fthelg. Ftoxid database contains data for both stoichiometric solids and liquids, and oxide solutions of 20 elements (as well as for diluted solutions of S, SO_4, PO_4, H_2O/OH, CO_3, F, Cl, I, in melting slag phase). Among several sub-systems of solutions in Ftoxid, FToxid-SLAGA was used. It contains oxides of Al, As, B, Ca, Co, Cr(II), Cr(III), Cu(I), Fe(II), Fe(III), Ge, K, Mg, Mn, Na, Ni, Pb, Si, Sn, Ti(III), Ti(IV), Zn, Zr + F, Cl, S in diluted solution (<10%). For calculations, the following compounds were taken into consideration: FeO, MnO, SiO_2, CaO, Al_2O_3, NiO, CaS, FeS, MnS, Fe_2O_3, CrO, Cr_2O_3, NiS.
- FSStel – Database primarily directed for iron-rich compounds. Among several sub-systems in FSStel, FSstel-FE-L was used. Liquid-iron phase which includes the elements: Al, B, Bi, C, Ca, Ce, Co, Cr, Fe, Mg, Mn, Mo, N, Nb, Ni, O, P, Pb, S, Sb, Si, Te, Ti, V, W, Zn, Zr. For calculations, the following compounds were taken into consideration: Fe, C, Cr, Al, Mn, Ni, P, S, Si, O, AlO, Al2O, CrO, Cr2O, MnO, SiO, FeS, MnS, Ca, CaO, CrS, NiS, CaS.

For calculating liquid windows, both FToxid-SLAGA (for oxides and CaS) and FSstel-FE-L (for steel) solution databases were employed in the FactSage Equilib module.

Before calculating, liquid window boundaries (or area) were determined as follows:

1) By calculating calcium-aluminates saturation line ($CaOAl_2O_3$, $CaO_2Al_2O_3$), considering a minimum of 30 and 35% of CaO in inclusions.

2) By calculating CaS saturation lines: maximum of 5 and 10% of CaS.

Furthermore, a more detailed analysis of liquid window was carried out, taking into account the following reasons:

1) There are few studies on oxide inclusions in resulfurized steels treated with calcium;

2) It could be interesting to establish percentages of both inclusions liquid and solid phases in liquid windows, what could increase knowledge not only on casting, but also on a wider control of phase formation in inclusions;

3) A major fraction of solids in oxide inclusions can help controlling the morphology of manganese sulfides (MnS), mainly to avoid forming elongated sulfides (type II), according to Wakoh [10];

4) As stated by Fuhr *et al.* [11], according to industrial results, castability problems more evidently occur when solid inclusions proportion is higher than 60-70%.

Considering reasons presented above, a different approach was adopted in order to make possible calculating either the formation or not of solid phases. In this case, besides employing solutions databases, stoichiometric pure solids (FactSage FS50 databases) were used as well, what was not possible with only solutions databases.

3 RESULTS AND DISCUSSION

Figure 1 shows the junction of two approaches described on the methodology:

1) Liquid window calculated for SAE 1141 steel;

2) Curve points from the beginning of liquid phase formation, 40% of liquid phase and 100% of liquid phase.

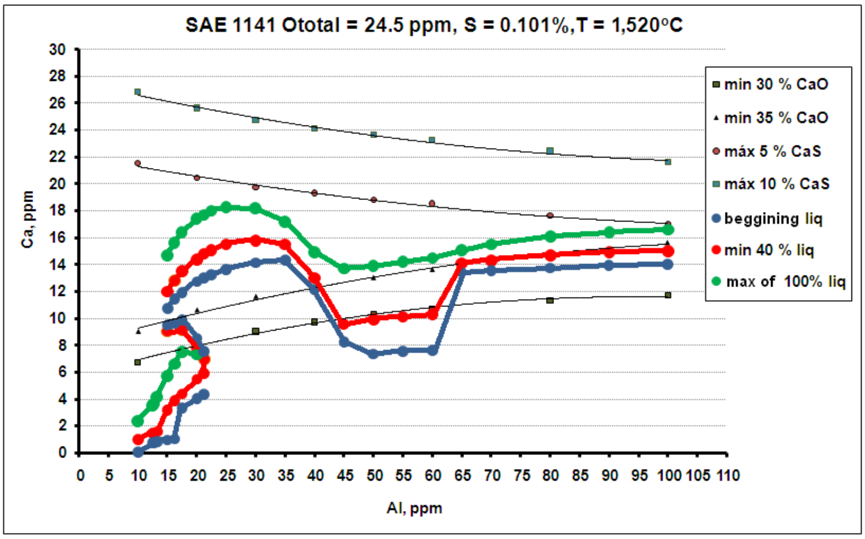


Figure 1: Liquid window for SAE 1141 steel and liquid phase formation. O_{total} = 24.5 ppm and T = 1,520 ºC.

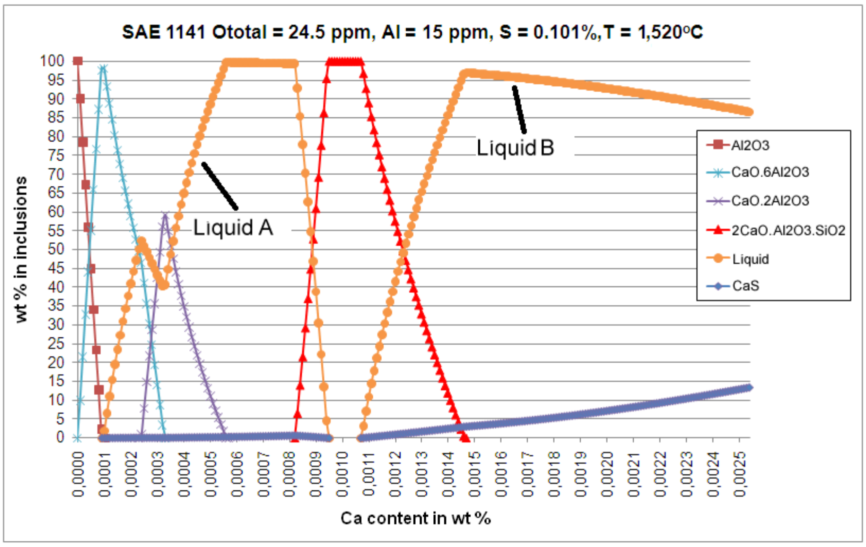


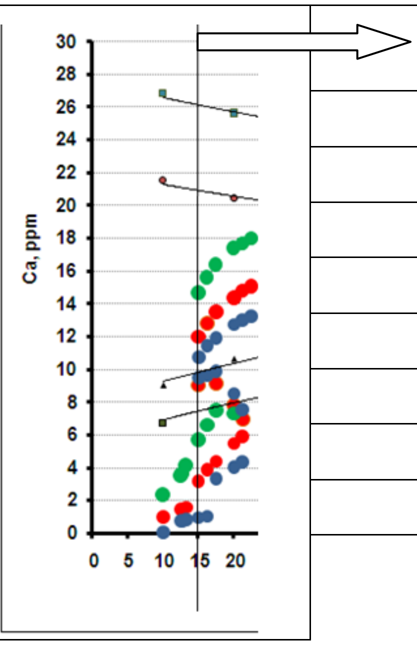
Figure 2: Mass percentage (wt %) of oxides and CaS in inclusions x SAE 1141 steel calcium content for Al = 15 ppm and O_{total} 24.5 ppm.

One can observe in Figure 1 that, from 10 ppm to around 45 ppm of Al, there is a great difference between both formation curves of 35% of CaO and liquid fraction points. From 45 ppm of Al, formation curves of 35 % of CaO and liquid fraction points coincide. Determination of liquid fraction points was obtained from graphics of oxides mass fractions in inclusions x steel Ca content. See Figures 2, 3 and 7 to 9.

Figures 2, 3 and 7 to 9 show the mass percentage of varied oxides and CaS in inclusions, depending on total calcium content. Each figure takes into consideration a fixed Al content. It is possible to analyze curves of both solid oxides and liquid phase - for selected points - as showed in Figure 1.

In order to understand better how points from Figure 1 were obtained, Table 2 shows a cut from Figure 1, highlighting curve points in 15 ppm of Al, as an example. Values of each selected point were obtained from Figure 2.

Table 2: Points of liquid fraction for SAE 1141 steel with 15 ppm Al.

	Points in line of 15 ppm Al	Ca content in ppm
	Beginning of liquid A	0.9
	First minimum 40 %of liquid phase A	3.2
	Beginning 100% of liquid phase A	5.7
	Second minimum 40 %of liquid phase A	9.0
	End of liquid phase A	9.5
	Liquid beginning B	10.7
	Minimum 40 % of liquid phase B	12.0
	Beginning 100% of liquid phase B	14.7

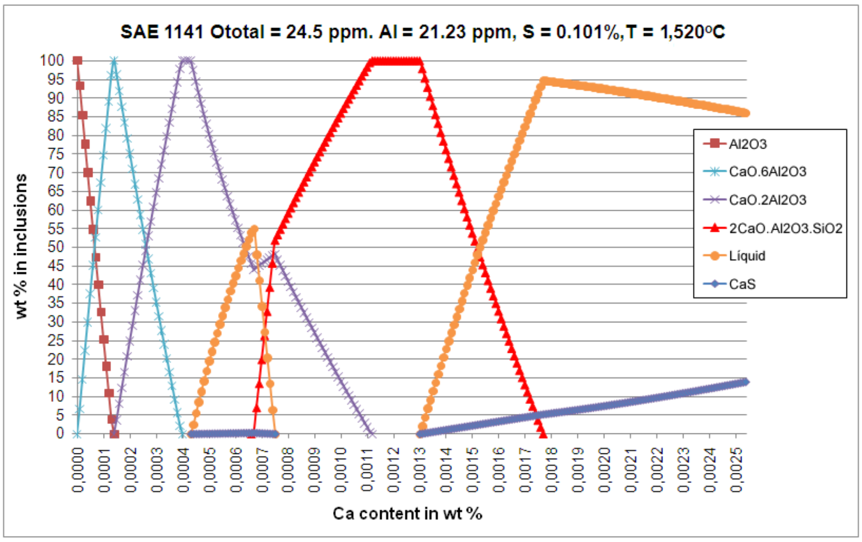


Figure 3: Mass percentage (wt %) of oxides and CaS in inclusions x SAE 1141 steel calcium content for Al = 21.23 ppm and O_{total} 24.5 ppm.

Among 10 ppm and little above 20 ppm Al, there are two peaks forming 100% of liquid phase, according to Figures 2 and 3.

Figure 3 regards Al = 21.23 ppm, which is heats average collected in the plant. There are two zones of liquid phase, however, the first one (between 4 and 8 ppm of calcium) is smaller than the second one (initiating in 13 ppm of calcium). In the first zone, heats sampled in the plant are located, and the liquid phase coexists with inclusions of $CaO._2Al_2O_3$.

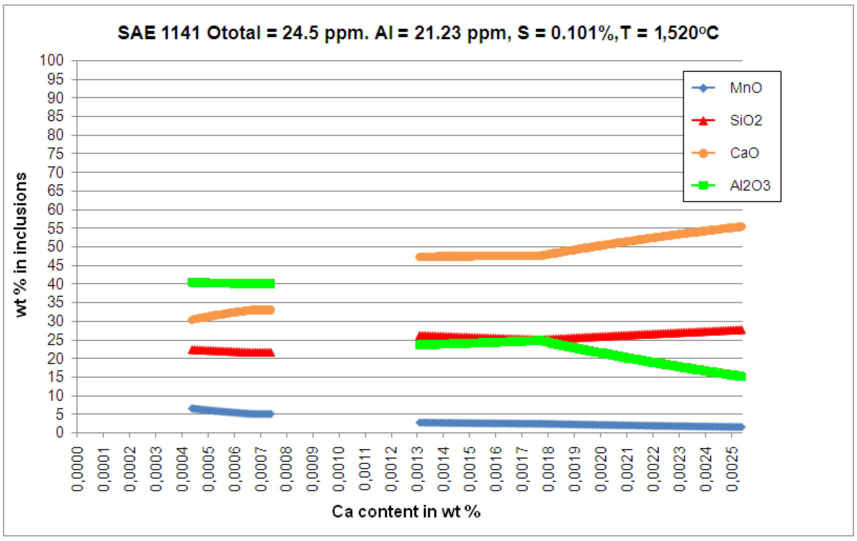


Figure 4: Composition of liquid phase for SAE 1141, Al = 21.23 ppm and O_{total} = 24.5 ppm.

Figure 4 shows a liquid phase composition in mass percentage %. Considering both content of Al = 21.23 ppm and O_{total} = 24.5 ppm, and other conditions for SAE 1141 steel. If the first zone is compared to the second one, both an increase of CaO content and a decrease of Al_2O_3 occur, with increasing of calcium content (from 17.7 ppm of Ca). SiO_2 content remains practically constant.

Figure 5 shows both Ca and O contents dissolved in steel as function of total calcium content. Moreover, dissolved Ca contents are multiplied by 100, while oxygen ones, by 10. Figure 6 shows dissolved Al in steel as function of total calcium content. In figures 5 and 6 both Al = 21.23 ppm and O_{total} = 24.5 ppm contents and other conditions for SAE 1141 steel were taken into consideration. In these figures - for average total calcium content of 5.7 ppm - values obtained were: O = 11.5 ppm, $\underline{Ca}$ = 0.085 ppm and $\underline{Al}$ = 10.6 ppm.

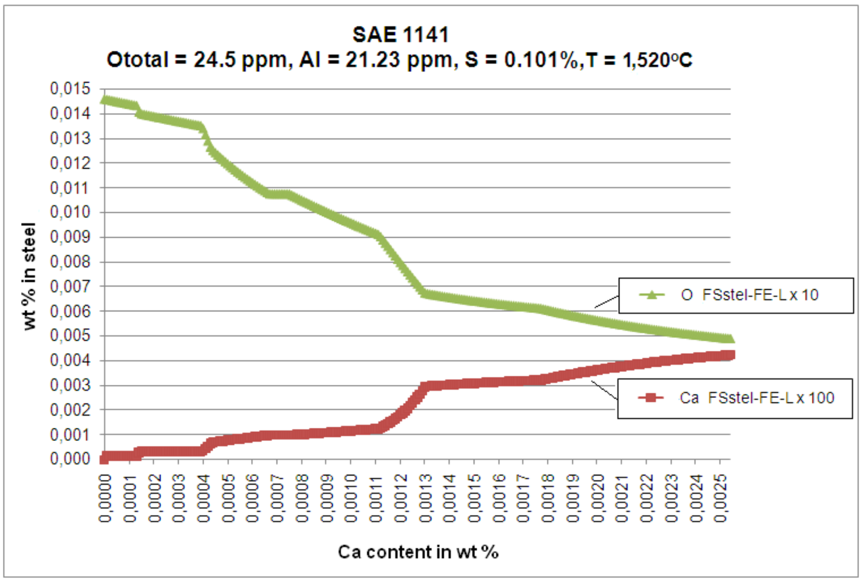


Figure 5: Dissolved Ca and O content depending on Ca content for SAE 1141 steel**,** Al = 21.23 ppm and O_{total} = 24.5 ppm.

Figure 7 (Al = 30 ppm) shows the only formation of a liquid phase zone (from 14.1 ppm of Ca), coexisting with calcium-silicate inclusions $2CaOAl_2O_3SiO_2$ (Gehlenite).

In Figure 8, there is not Gehlenite formation. Liquid phase starts with lower calcium contents. In Figure 9, for Al = 80 ppm, $CaOAl_2O_3$ formation occurs; with a new increase of calcium content necessary to form liquid phase.

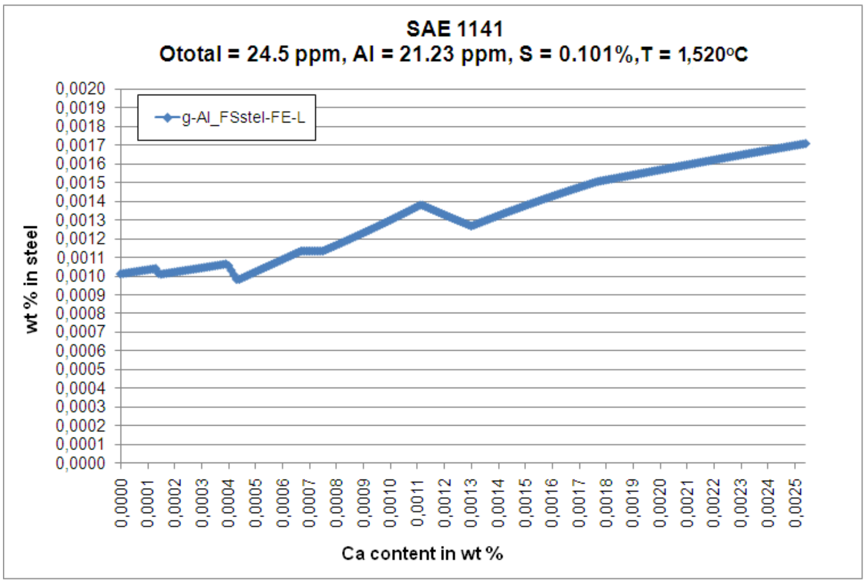


Figure 6: Dissolved Al content depending on Ca content for SAE 1141 steel Al = 21.23 ppm and O_{total} = 24.5 ppm.

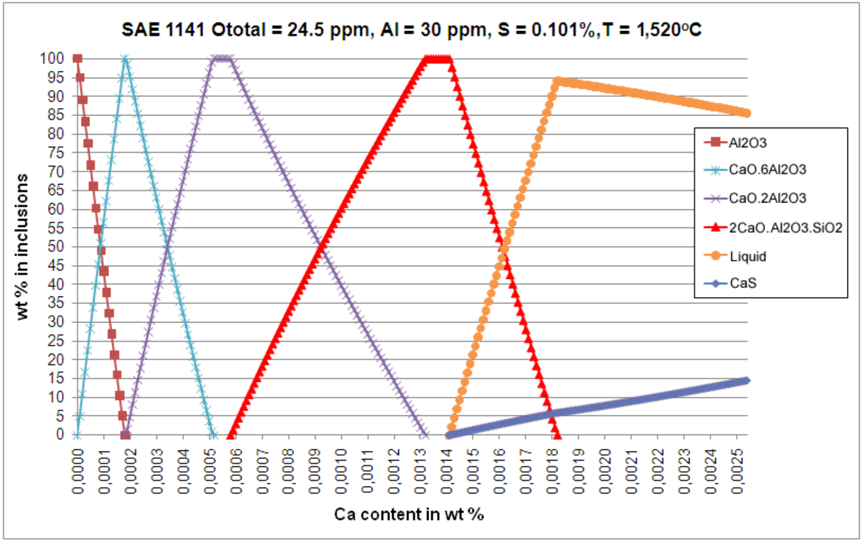


Figure 7: Mass percentage (wt %) of oxides and CaS in inclusions x calcium content in SAE 1141 steel for Al = 30 ppm and O_{total} = 24.5 ppm.

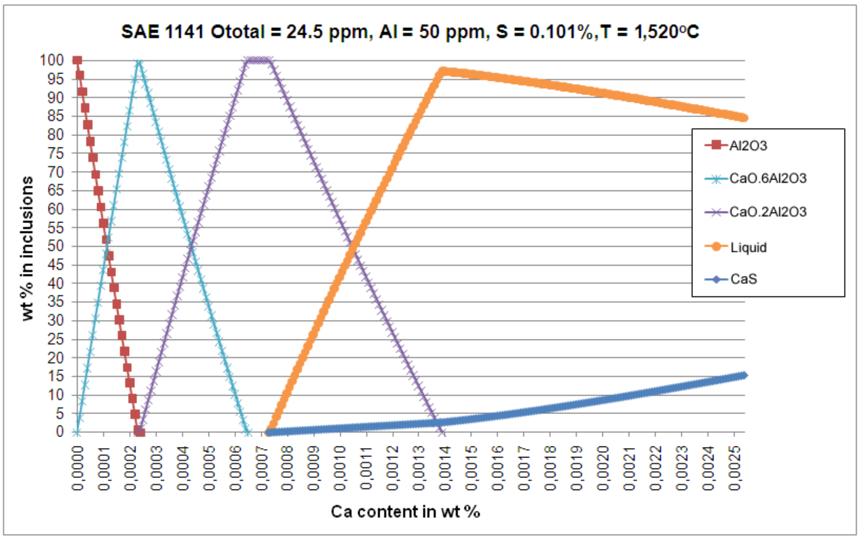


Figure 8: Mass percentage (wt %) of oxides and CaS in inclusions x calcium content in SAE 1141 steel for Al = 50 ppm and O_{total} = 24.5 ppm.

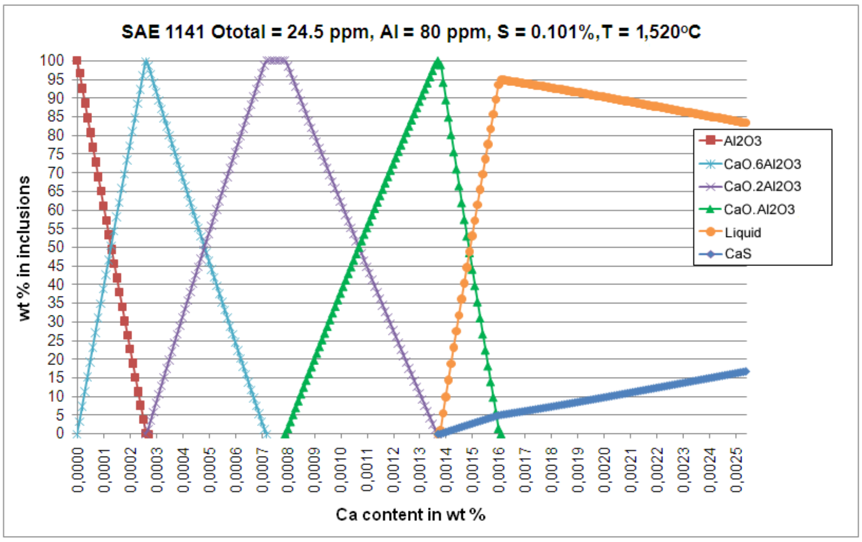


Figure 9: Mass percentage (wt %) of oxides and CaS in inclusions x calcium content in SAE 1141 steel for Al = 80 ppm and O_{total} = 24.5 ppm.

4 CONCLUSIONS

For SAE 1141 steel conditions, ranging from 10 ppm to around 45 ppm of Al, there is a great difference between formation curves of 35% of CaO, and the points of liquid fraction. However, from 45 ppm of Al, they coincide.

There are two peaks of 100% liquid phase formation, from 10 ppm and little above 20 ppm of Al.

Considering Al = 21.23 ppm, O_{total} = 24.5 ppm and average total calcium content of 5.7 ppm, the following values obtained from dissolved elements in steels were: $\underline{O}$ = 11.5 ppm, $\underline{Ca}$ = 0.085 ppm and $\underline{Al}$ = 10.6 ppm.

For Al = 50 ppm, there is not Gehlenite formation, and the liquid phase starts with lower calcium content.

However, for Al = 80 ppm, formation of $CaO.Al_2O_3$ occurs, backing to increase the calcium content necessary to form the liquid phase.

Both conditions of chemical composition for obtaining window of liquid inclusions and the influence of aluminum content on forming inclusions for SAE 1141 steel were satisfactorily evaluated.

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