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Advances in Modeling of Steel Solidification with IDS

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Abstract. IDS (Inter-Dendritic Solidification) is a thermodynamic-kinetic software package that simulates phase changes, compound formation/dissolution, and solute distribution during solidification of steels as well as during their cooling/heating process after solidification. The software package also simulates solid-state phase transformations related to the austenite decomposition process at temperatures below 900/600 °C, and calculates thermophysical material properties from the liquid state down to room temperature. These data are needed in other models, such as heat transfer and thermal stress models, whose reliability heavily depends on the input data. The software package also features a database for thermodynamic, kinetic and microstructure data, as well as for several material properties. Owing to the short calculation times, the IDS tool is suitable for online applications. This paper presents IDS and its modules with the latest developments and validations, along with examples of modeling results.

1. Introduction

IDS is a thermodynamic-kinetic solidification package for steels [1] developed since 1984. It has been validated with extensive data from solidification experiments, with good results [2]. The calculations of the IDS package are made in one volume element set on the side of a dendrite arm [1] based on two assumptions: (1) The dendritic structure formed throughout the strand is regular. (2) There are no strong liquid flows causing macrosegregation. Due to the simple-format thermodynamic sub-models of the IDS package and the simultaneous solution of thermodynamic, kinetic and material balance equations during the simulation, the calculation times of IDS are relatively short.

2. Description of the IDS model

The present IDS package includes six calculation modules: (1) SOL (solidification), (2) ADC (austenite decomposition), (3) MAT (material properties), (4) GAS (hydrogen and nitrogen behavior), (5) PRF (precipitate formation at the ferrite/austenite phase interface), and (6) SCA (oxide scale formation). It also includes an extensive database containing the thermodynamic, kinetic, microstructure and material data needed in calculations. In addition, an additional module for QIS (steel quality indices) is under development to provide information about the sensitivity for various casting problems, such as cracking. Figure 1 shows the main input and output data of the offline version of IDS, as well as its modular structure. Also included is the coupling of IDS with some other model packages, discussed later in the text.



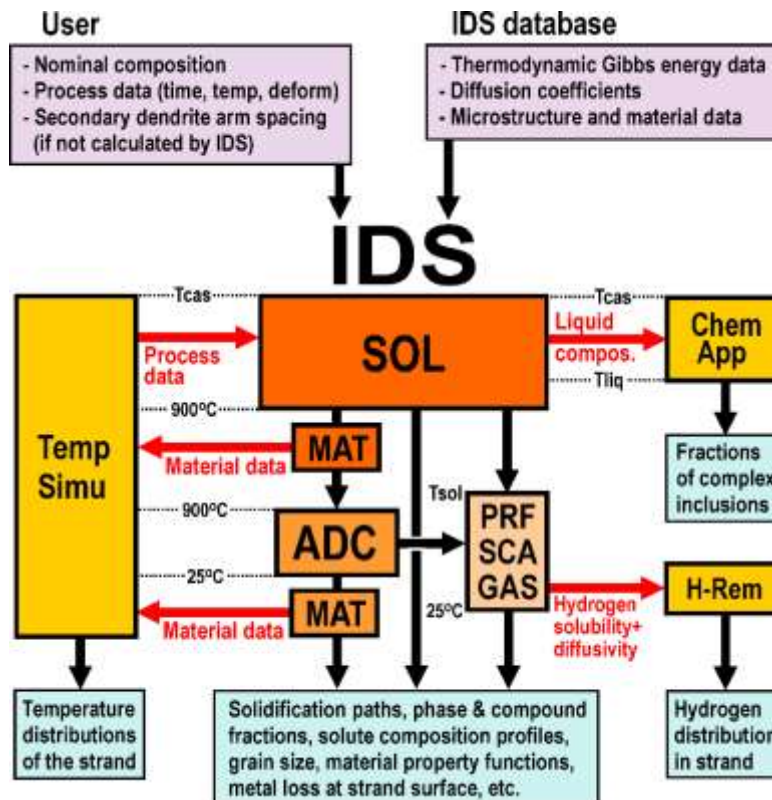


Figure 1. Main input and output data of the offline IDS model package and its modules and their coupling to other model packages.

2.1. SOL module

The SOL module is the main module of the IDS package. It is applied in the temperature range 1,600–900 °C for low-alloy steels and 1,600–600 °C for high-alloy steels. The steel is regarded as high-alloy steel whenever at least one of the following conditions for the nominal composition is true: wt%Cr \geq 5, wt%Ni \geq 5, wt%Mn \geq 5, wt%Mo \geq 3 or wt%Si \geq 3. The module applies thermodynamic chemical potential equality equations (all components), interfacial material balance equations including Fick's first law of diffusion (solutes), and a finite difference application of Fick's second law of diffusion (solutes). The computational routine has been described in [1].

Using the IDS input data (see Figure 1), the SOL module simulates or calculates the following phenomena: (1) solidification of steel (ferritic, austenitic, and peritectic solidification); (2) enrichment or impoverishment of solutes in liquid; (3) formation of various compounds (inclusions) from liquid; (4) homogenization of solute microsegregation below the solidus; (5) ferrite-austenite transformation below the solidus; (6) formation and dissolution of eutectic ferrite (in high-alloy steels only); (7) formation and dissolution of various compounds (precipitates) below the solidus; and (8) growth of austenite grains.

The possible solute or impurity components and their recommended maximum compositions (wt%) are given for low-alloyed (L) and high-alloyed (H) steels as: C = 3.5(L), 1.5(H); Mn = 5(L), 25(H); Cr = 5(L), 30(H); Mo = 3(L), 6(H); Ni = 5(L), 25(H); Al, Cu, Si = 3; Nb, Ti, V, N = 0.5; P, S = 0.05; Ca, Ce, Mg = 0.02, and B, O, H = 0.005. For the present, the possible compounds (precipitates) of the simulation are: AlN, BN, CrN, Cr₂N, Si₃N₄, TiB₂, CaS, MgS, H₂(g), N₂(g), FeMo₂B₂, Fe₃Mo₃C, FeNbB, Ti₂CS, (Mn,Fe)S, (C,N)Nb, (C,N)Ti, (C,N)V, (Cr,Fe)₂B, (Fe,X)₂B (X=Cr,Mn, Ni, V), (Cr,Fe)₂₃C₆, (Cr,Fe)₇C₃, (BC)₆Fe₂₃, (Fe,X)₃C (X=Cr,Mn,Mo), (Cr,Ni)₈Fe₉ (~sigma), together with several simple oxides.

2.2. ADC module

The ADC module is used for low-alloy steels in the temperature range 900–25 °C to simulate the decomposition of austenite to proeutectoid ferrite or cementite, pearlite, bainite and BCT martensite. Also simulated is the formation or dissolution of different precipitates (see the compounds of the SOL module). The ADC module applies thermodynamic chemical potential equality equations of paraequilibrium condition, material balance equations of carbon, boron, and nitrogen for the ferrite/austenite interface advancing in a spherical austenite grain, and regression formulas optimized from the German and British CCT measurements and some additional measurements on boron steels. In these formulas, the influencing solutes are C, Si, Mn, Cr, Mo, Ni, and B. Using the IDS input data (see Figure 1), the ADC module simulates or calculates the following phenomena: (1) fractions of austenite and its decomposition phases, (2) formation and dissolution of various precipitates, (3) A_{e3} and A_{eC} temperatures, and (4) austenite grain growth.

Due to the limited solute contents in the original CCT data, the recommend composition ranges for the ADC calculations are relatively low. A tentative suggestion is to apply compositions of $0.001 < \text{wt\%C} < 3.5$, $\text{wt\%Si} < 1$, $\text{wt\%Mn} < 2$, $\text{wt\%Cr} < 3$, $\text{wt\%Mo} < 1$, and $\text{wt\%Ni} < 3$, while the compositions of the other solutes (taking no action in the CCT formulas) should be as low as possible. In further work, the present CCT formulas will be re-optimized to include a much larger set of CCT measurements for alloys with higher solute contents, and also including two new solutes: Al and Cu.

For high-alloy steels, the ADC module is used in the temperature range 600–25 °C, and the only decomposition phases are BCT and HCP martensites. In this case, the recommended composition ranges are the same as those of the SOL module, and no simulation is made for the compound formation.

2.3. MAT module

The MAT module calculates temperature and time functions for important material properties using the material data of the IDS database and the phase fractions and compositions calculated by the SOL and ADC modules. Here, the most important material properties are enthalpy, thermal conductivity, and density, which are needed as input data in other model packages in order to simulate the macroscopic heat transfer in a strand. In the case of enthalpy, the thermodynamic Gibbs energy data of the IDS database is used directly, and in the case of other material properties, the regression parameters optimized for the database are used. The advantage of the method is that discontinuities caused by different phase changes are automatically included in the material property functions. The present IDS package calculates material data for the Tempsimu package [3], but the data can be “tailored” to other packages, as well. The new MAT module also calculates the strain rates at different stress values (0.1–400 MPa) and the elastic modulus for the considered steel, as a function of temperature. Calculations are made also to give the surface tension and the stacking fault energy (in high-alloyed steels).

2.4. PRF module

The PRF module is applied to simulate the precipitate formation at the ferrite/austenite phase interface, if present in the steel. Only the final amounts of the precipitates are reported (at 25 °C) together with the temperature and time intervals of their appearance and disappearance. This output data gives an opportunity to study the tendency of Cr (enriching strongly on the ferrite side of the boundary in stainless steels) to form Cr carbides or even Cr nitrides, and their possible effect on cracking.

2.5. GAS module

The GAS module is applied to simulate the behavior of gaseous elements (H and N) in solid steels below the solidus. Temperature (and time) functions are calculated for (1) solubility of H and N in solid (ferrite and austenite), (2) excess (insoluble) composition of H and N in solid, and (3) diffusion coefficients of H and N in solid. Above the solidus, part of H and N may take a gaseous form, leading to porosity formation in the mushy zone. This is handled by the SOL module, allowing gaseous $\text{H}_2(\text{g})$ and $\text{N}_2(\text{g})$ “compounds” to form from the liquid phase. The gas formation depends on the ferrostatic pressure in

the liquid phase and its decrease from the mushy zone shrinking. The resulting H and N contents (their solubility at the solidus) thus represent the start composition of the GAS simulation.

2.6. SCA module

The SCA module is applied to simulate oxide scale formation on the surface of the continuous casting strand, depending on the oxygen pressure. This module is a typical furnace treatment application of continuous casting. Temperature and time functions are calculated for (1) metal loss, (2) oxide phase weight gain, and (3) approximate fractions of different oxide types. In addition, the oxide type, whether it is detrimental or not, is tentatively characterized.

2.7. Database

During this decade, a great amount of new thermodynamic, kinetic and microstructure data has been stored in the IDS database to make IDS simulations for different steel grades. Also included are new material data parameters permitting the calculation of thermal conductivity, density, viscosity, surface tension, strain rate, and elastic modulus for these steels as a function of temperature. All these data have been verified with experimental measurements. Most of the data is the Gibbs energy data of solution phases and compounds taken from thermodynamic assessments of iron-based alloys.

2.8. Coupling of IDS to other model packages

The IDS package can be coupled with some other model packages: ChemApp, H-Rem and Tempsimu, as illustrated in Figure 1. ChemApp [4] is a thermodynamic programming library that can be used to simulate the formation of multiphase inclusions in the liquid steel. H-Rem is a package for calculating the hydrogen distribution in continuous casting slabs. The model is used to find optimal holding temperatures and times for different strand geometries, which can decrease the hydrogen content of the strand to an acceptable level. Tempsimu [3] is a package that simulates the heat transfer in continuous casting strands. In this case, IDS calculates the temperature functions of the material property data (including liquidus and solidus temperatures) for Tempsimu, while Tempsimu calculates the nodal process data (time, temperature, deformation) of the strand for IDS. The deformation effect comes from the bending and unbending processes. In online processes of continuous casting, the output of IDS can be used in casting and strand simulators visualizing the state of the strand for the user. So far, IDS and online version of Tempsimu, called CastManager, have been installed in four slab casters for online use.

2.9. Latest developments of IDS.

During the two last years, several steps have been made to improve the IDS package. Some essential improvements are summarized below.

2.9.1. Database. The thermodynamic and material property data of the IDS database has been extended considerably in comparison to earlier work [1]. The focus in the thermodynamic data has been on systems containing nitrogen, and high-alloyed systems. In the material properties, the focus has been on the calculation of new properties (such as strain rates (as a function of stress), elastic modulus and stacking fault energy), and on new optimizations for thermal conductivity, density, surface tension and secondary dendrite arm spacing (SDAS).

2.9.2. Extension of IDS to cast irons. The recommended maximum carbon composition of low-alloyed steels has been increased from 1.5 to 3.5 wt% C, to extend the applicability of IDS simulations to cast irons. Also, the material property algorithms have been updated in this respect. The calculations have been validated with numerous temperature measurements on cast irons [2]. Note that IDS cannot simulate the morphology of cast iron, but only the formation of graphite and cementite phases from liquid and austenite. The effect of nodularity on thermal conductivity, however, can be taken into account.

2.9.3. Cooling/heating processes and precipitation. The IDS procedure linking a complex cooling/heating curve to the simulation of precipitation, phase transformation, and scale formation in steels has been improved. Particularly, the problems related to the sensitivity of the precipitation calculations to diverge (as a result of sudden changes from cooling to heating and vice versa) have been solved. Also, the treatment of precipitate formation itself has been improved, to get a clear “nose” for their formation. This makes it possible to seek a critical cooling rate above which we get no formation for a precipitate. The results have been validated with experimental measurements.

2.9.4. Solidus of high-alloyed steels. In heavily alloyed steels beyond the recommended composition ranges of the SOL module, the solidus may sometimes get far too low and even crash the simulation. That trend has now been reduced by specific thermodynamic modifications made close to the solidus temperature, when its value gets exceptionally low.

2.9.5. Eutectic ferrite. The treatment of the eutectic formation has been simplified and allowed for any high-alloyed steels, including their equilibrium solidification. In the latter case, the extension concerns only the purely austenitic solidification, since there is no entrance from the austenitic solidification back to the ferritic solidification in IDS. In other words, the simulation of eutectic ferrite formation is then the only way to get ferrite back in the structure.

3. Validation and results

The calculations of the IDS model have been validated with numerous experimental measurements of solidification [2]. Table 2 summarizes the average deviation between calculated and measured temperatures of liquidus (T_{LIQ}), austenite formation (T_{AUS}), zero-strength (T_{ZST}), and solidus (T_{SOL}) of low-alloyed and stainless steels, and for the residual ferrite contents of stainless steels (ferrite content). The agreement is reasonably good, and much better than can be obtained with analytic literature equations, e.g. for the liquidus and solidus temperatures.

Table 1. Average deviation between IDS calculations and measurements for steels [2].

Alloy type	Number of measurements	Average deviation				
		T_{LIQ}	T_{AUS}	T_{ZST}	T_{SOL}	Ferrite content
Ternary Fe–X–C alloys	283	5.6 °C	7.4 °C	5.6 °C	10.5 °C	1.11%
Ternary Fe–Cr/Ni–X alloys	274	3.9 °C				
Steels	387	3.2 °C				
Steels	47					
Low-alloyed steels	25					
Steels	170					
Stainless steels	93					

Figure 2 shows examples of calculations mimicking phenomena in continuous casting and reheating furnace. The figure shows how (a) some precipitates form in an AISI 410-type stainless steel (containing exceptionally 0.1%C and 0.1%Nb), and how (b) the metal loss proceeds in the slab surface of the 0.15% C, AISI 410 and AISI 316 steels, as the applied cooling/heating histories are those shown in the upper figures. Figure 2a reveals the importance of fixing the cooling/heating history and the straightening (or bending) position so that fewer precipitates would form in the latter region. Otherwise, the probability for cracks may clearly increase. Figure 2b shows that in the case of low-alloyed carbon steels, a high holding temperature in combination with a high oxygen pressure leads to higher metal loss. In ferritic stainless steel (AISI 410), the metal loss is much smaller, and it is smaller still in AISI 316 austenitic stainless steel. The weaker oxidation in the latter steels is due to the formation of protective layers of Cr_2O_3 and MoO_2 oxides. The cases are illustrative and not from any real industrial process.

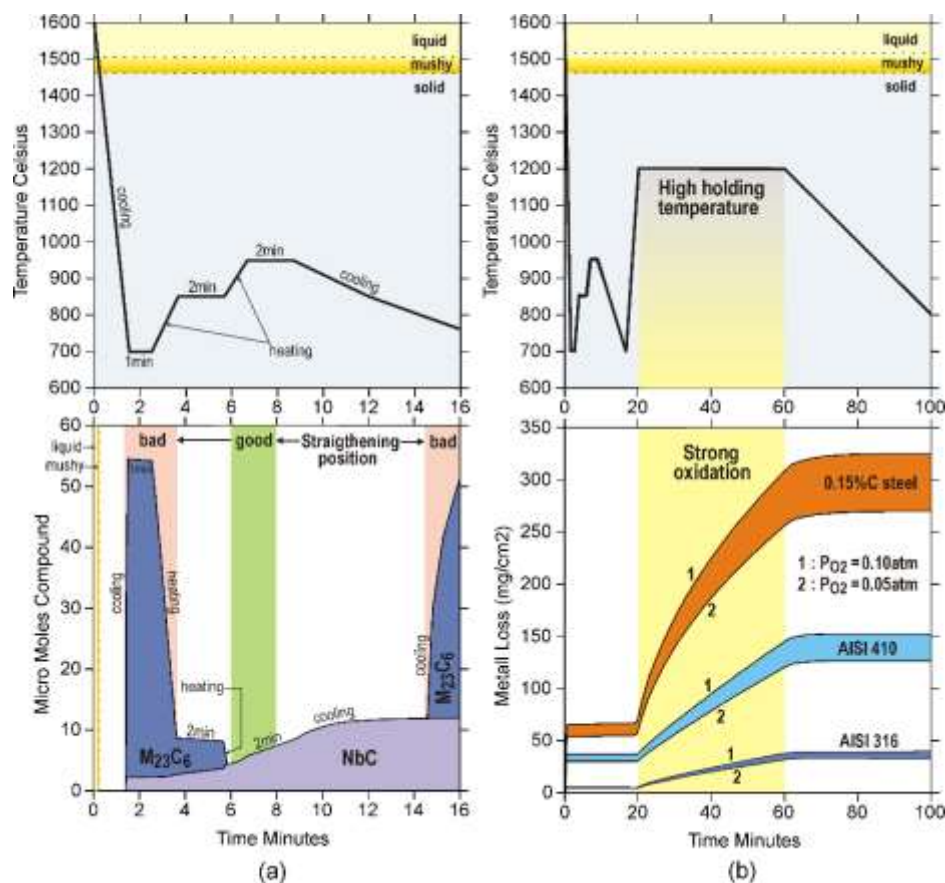


Figure 2. Effect of temperature histories (upper figures) on the formation of precipitates in (a) AISI 410-type stainless steel containing 0.1%C and 0.1%Nb, and (b) on the metal loss in a plain carbon steel (0.15%C) and in AISI 410- and 316-type stainless steels.

4. Conclusions

The aim of this paper was to present IDS and its modules with the latest developments. Validation of the model suggests a good match with experimental data for different steel grades. The latest developments have been directed at extending the thermodynamic and material property database as well as improving the descriptions for cooling/heating processes and precipitation, solidus of high-alloyed steels and eutectic ferrite formation. Owing to its short calculation times, IDS is suitable for online applications of continuous casting.

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