IDS

Solidification Analysis Package for Steels

Seppo Louhenkilpi, Prof.
Aalto University
School of Chemical Technology
Research Group Metallurgy

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Aalto University

With 20,000 students and 340 professors

Fusion of 3 universities in 2010
- Helsinki University of Technology
- University of Art and Design Helsinki
- Helsinki School of Economics

Picture: Main building
Research Group Metallurgy

Personnel:

Prof. Seppo Louhenkilpi
Two emeritus professors Lauri Holappa, Heikki Jalkanen
Now 15 other academic persons (4 post docs, 5 doctoral students, 6 M. Sc students)

Main research areas:

Steel industry: Processes from steelmaking to reheating, especially continuous casting and solidification
Copper industry: Mainly casting processes
Others: Many special projects (recycling, ...)

Special areas today:

Mathematical modelling: in-house tools, commercial tools
Why: the phenomena are so complex and new steel grades and metal alloys are produced all the time → advanced, special models and tools are strongly needed
Examples: Development of in-house software

IDS

Solidification, phases, material properties and microsegregation from 1600°C-25°C

TEMPSIMU3D

Temperatures and solidification of strand in steady state casting conditions

CastManager (3D, on-line)

Temperatures and solidification of strand in dynamic casting conditions
IDS tool

IDS (InterDendritic Solidification) is a thermodynamic-kinetic-empirical model package for the simulation of solidification and microstructure evolution (phase transformations, microsegregation, compound formation, etc) in steels from liquid to room temperature and during reheating.

IDS package includes the following modules:

- SOL: simulation of solidification
- ADC: simulation of austenite decomposition
- MAT: calculation of material properties
- GAS: calculation of hydrogen and nitrogen solubility, pressure and diffusivity
- HOM: simulation of homogenization
- Defect prediction module (for cracking,…)

IDS development work is leaded by Dr. Jyrki Miettinen.
IDS – Solidification and microstructure model

**INPUT**

Steel composition
Cooling rate
(Dendrite arm spacing and austenite grain size; default values available for these)

**OUTPUT**

Solidification phenomena
Microsegregations
Microstructure evolution
Inclusions
Precipitations
Pore formation

Thermophysical material properties
Thermal contraction
Liquid viscosity
Liquid/air surface tension
Solid/liquid interface energy
Hardness
Quality prediction

Chemical alloying elements included: C, Si, Mn, P, S, Cr, Mo, Ni, Nb, Ti, V, B, Al, Ca, Cu, N, O, H

Aalto University
School of Chemical Technology
1) Diffusion in liquid is infinite, diffusion in solid follows Ficks II diffusion law

\[ D \frac{\partial^2 C}{\partial x^2} = \frac{\partial C}{\partial t} \]

\[ D_i^\phi = D_i^{0\phi} \cdot \exp\left[-\frac{Q_i}{RT} + \sum_{j=2}^{n} b_{ij}^\phi x_j^\phi\right] \]

Experimental data bank

This is during solidification and also for homogenisation during cooling and reheating.

In the future: diffusion should be based on gradient of chemical potentials and mobilities, instead of concentration gradient and binary diffusion coefficients

\[ J_i \approx M \frac{\partial \mu_i}{\partial x} \]
2) At the solid/liquid interface, thermodynamic equilibrium is assumed and the distribution of the alloying elements is based on the chemical potentials. For each element, $i$:

$$\mu_i^S = \mu_i^L$$

For rapid solidification processes, more energies should be taken into account as the solid-liquid interfacial energy and the kinetics energies dealing with movement of the atoms at the interface.

3) Phase stabilities are determined solving thermodynamic and mass transfer equations (ferrite, austenite, liquid, eutectic ferrite, compounds,...)
IDS solidification physics

4) Volume-element (3D) has a hexagonal form in dendrite arm. Perpendicular to the growth direction, the volume element is described with a triangle. In the austenite region, the modeled element is a 3D sphere grain.

5) During austenite to ferrite transformation, the paraequilibrium condition is assumed → only interstitial elements (B, C,..) diffuse but larger substitutional not. Chemical potential equality equatations are used for interstitial element at the interface to calculate the distribution.

6) All the phase transformation temperatures for austenite decomposition is calculated with using statistical in-house expressions (=ADC module
IDS results of microsegregation of the elements C, Mn, P and S in low carbon, C=0.12%, (left) and high carbon, C=0.6%, steel alloy (right). Other elements are 0.3%Si+1%Mn+0.02%P+0.02%S. The cooling rate in IDS was 1°C/s. Clear difference can be seen compared the IDS results with equilibrium calculations, EQS.
Inclusions and precipitations in IDS

The formation of the following compounds can be simulated:

- **Stoichiometric binaries**: AlN, BN, B₂O₃(l), CaO, CaS, CO(g), H₂(g), MgO, N₂(g), SiO₂, TiB₂, TiO₂, Ti₂O₃, VO
- **Stoichiometric ternaries**: Fe₂₆Al₉C₅, FeMo₂B₂, FeNbB, Fe₂Mo₃O₈, Fe₄Nb₂O₉, Ti₂CS
- **Semistoichiometric ternaries**: (Mn,Fe)S, (Mn,Cr)S, (C,N)Nb, (C,N)Ti, (C,N)V, (Cr,Fe)₂B, (Ni,Fe)₃B, (Nb,Fe)O₂, (Fe,X)₂B (X=Cr,Mn,Ni,V), (Fe,X)₃O₄ (X=Al,Cr,Mo,V), (Fe,X)₂O₃ (X=Al,Cr,V), (Fe,X)_0.947O (X=Cr,Mn,V).

- Inclusions: calculation is based on the minimization of the Gibbs energies. For precipitations: see later.

IDS has not a ”slag model”, so liquid slags or more complex inclusions cannot be simulated. For that IDS has been coupled with ChemApp + databank, which is a thermodynamic library tool developed by GTT technologies, Germany.
Left: Formation of liquid and solid oxides and sulphides in liquid steel (above 1480°C) and in residual liquid steel during solidification (from 1480°C to 1370°C). High carbon (HC) steel. Right: Amount of components in liquid inclusions formed in HC steel in casting and solidification.

Case example: IDS+ChemApp
Precipitations in IDS: Also nucleation and misfit energies are needed

\[
\Delta G_{\text{MeX}} = \Delta G_{\text{MeX}_1} + \Delta G_{\text{I}}^P + \Delta G_{\text{S}}^P
\]

\[
\Delta G_{\text{I}}^P = \frac{C_{\text{INC}}}{D_{\text{Me}}(T)} \cdot 10^{-7} = \text{barrier energy of incubation}
\]

\[
\Delta G_{\text{S}}^P = \frac{E}{1-v} \left( \frac{1}{3} \frac{V_{\text{mol}}^P - V_{\text{mol}}^M}{V_{\text{mol}}^M} \cdot C_{\text{VMF}} \cdot C_{\text{ADC}} \right)^2 \cdot V_{\text{mol}}^M \cdot (f^P)^{0.2}
\]

= barrier energy of volume misfit

\[\text{C}_{\text{INC}} = \text{fitting coefficient of incubation (C}_{\text{INC}}=0.4)\]
\[D_{\text{Me}}(T) = \text{diffusion coefficient of metallic solute in phase } \phi \text{ at temperature } T \text{ (cm}^2/\text{s})\]
\[E = \text{Young modulus of the matrix (J/cm}^3\)]
\[v = \text{Poisson constant of the matrix (dimensionless, } =R/\text{Cp})\]
\[V_{\text{mol}}^M = \text{molar volume of the matrix (cm}^3/\text{mol})\]
\[V_{\text{mol}}^P = \text{molar volume of the precipitate (cm}^3/\text{mol})\]
\[C_{\text{VMF}} = \text{fitting coefficient of volume misfit (effect of dislocations, } C_{\text{VMF}}=0.6)\]
\[C_{\text{ADC}} = \text{coefficient describing the state of the austenite decomposition process}\]
\[\text{C}_{\text{ADC}}=1 \text{ before its start and } C_{\text{ADC}}=\text{fraction of decomposed austenite after its start}\]
\[f^P = \text{precipitate fraction “launching” the effect of volume misfit}\]
S = for misfit, I = for nucleation

Nucleation energy increases with decreasing temperature, just due to the decreasing solute diffusion in austenite. In ferrite the diffusion increases \( \rightarrow \) energy decreases.

Misfit energy increases after the start of the precipitate formation, at TMeX.

A sudden drop of volume misfit (down to the zero value) due to the strong deformation caused by the formation of proeutectoid ferrite in the austenite grain boundaries is caused by the high increase of dislocations. However, with the growing ferritic net, that deformation start to decrease and the volume misfit increases again.
Calculated fractions of Nb(C,N) and AlN in a low alloyed steel cooled with a constant rate of 1°C/s.

Note the suppressed growth at about 1000°C, which is due to the increasing values of barrier energies $\Delta G_{1P}$ and $\Delta G_{SP}$ at low temperatures.

Below the temperature of austenite decomposition (745°C), both energy values are dropped. This accelerates the growth again but not much, due to the limited time of diffusion.

Calculated fractions of Nb(C,N) and AlN in a low alloyed steel cooled with a constant rate of 1°C/s.
Austenite grain growth model in IDS

Pinning effect precipitations and ferrite must be included!!!!

\[ D(t + \Delta t) = D(t) + M_0^* \cdot \exp(-Q / R / T(t)) \cdot \left( \frac{1}{D(t)} - \frac{1}{D_{\text{max}}} \right)^{n_0 - 1} \cdot \Delta t \]

Where: \[ Q = (1 + (f_{\text{fer}})^{a_0} + (f_{\text{pre}})^{b_0}) \cdot Q_0 + C_{EQ} \cdot Q_{EQ} \]

The higher the ferrite and the precipitate fractions, the higher the activation energy \( Q \rightarrow \) the weaker the growth.

- \( D(t=0) = \lambda_1 \)
- \( D(t+\Delta t) = \) grain size (\( \mu m \)) at time \( t+\Delta t \) (\( \Delta t \)=time step in IDS simulation)
- \( D(t) = \) grain size of the previous step, at time \( t \)
- \( D_{\text{max}} = \) the maximal grain size (assumed as \( D_{\text{max}}=8000 \mu m \))
- \( M_0^*, n_0 = \) grain boundary constants (assumed as \( n_0=0.5 \) and \( M_0^*=4 \cdot 10^9 \mu m/s \))
- \( Q = \) activation energy (J/mol)
- \( f_{\text{fer}}, f_{\text{pre}} = \) fractions of ferrite and all precipitates (calculated by IDS)
- \( a_0, b_0 = \) fitting exponents (assumed as \( a_0=1 \) and \( b_0=0.35 \))
- \( Q_0 = \) fitting parameter of activation energy (optimized as \( Q_0=165000 \) J/mol)
- \( C_{EQ} = \) carbon equivalent (estimated as \( C_{EQ}=\text{wt}\%C \))
- \( Q_{EQ} = \) increase of activation energy due to \( C_{EQ} \) (optimized as \( Q_{EQ}=25000 \) J/mol)
As in all steels, the growth is quite effective at high temperatures and the growth is finally stopped by the formation of proeutectoid ferrite.

The effective growth is restrained by grain boundary ferrite and Nb(C,N) precipitations.

0.05wt%C grain growth starts later because to the high ferrite content of that alloy below the solidus.

The final grain size in the 0.05wt%C alloy is highest because of the low amount of Nb(C,N), which restrains the grain growth.

Calculated austenite grain growth in three low-alloyed steels containing 0.05%C, 0.2%C and 0.5%C and cooled with a rate 10°C/s above 900°C and with a rate 0.01°C/s below 900°C.
IDS: HOM-module

HOM module is applied to simulate the heating and holding periods: Compound (precipitate) growth or dissolution, Ferrite growth or dissolution, Growth of austenite grains.

Example for AlN: Cooling 1°C/s, reheating 10°C/s, holding 1 min at 1200°C, cooling 10°C/s.
IDS: Databanks


3. Microstructure data for DAS and grain

4. Thermophysical material data:
   - Enthalpy, specific heat and latent heat (derived from the Gibbs energy data)
   - Thermal conductivity. Phases: liquid and solid. Components: Fe, C, Si, Mn, Cr, Mo, Ni, Nb, Cu, V.
   - Density. Phases: liquid, ferrite, austenite and cementite. Components: Fe, C, Si, Mn, P, S, Cr, Mo, Ni, Cu, Al, Nb, Ti, V, B, O (liquid) and Fe, C, Si, Mn, Cr, Mo, Ni, Nb (solid phases).
   - Dynamic liquid viscosity. Components: Fe, C, Si, Mn, P, S, Cr, Mo, Ni, Cu, Al, Nb, Ti, V, B, O.
   - Surface tension (between liquid and air). Components: Fe, C, Si, Mn, P, S, Cr, Mo, Ni, Cu, Al, N, V, B, O.
   - Fusion entropy. Phases: ferrite and austenite. Components: Fe, C, Cr, Mo, Ni. For the calculation of solid/liquid interface energy

IDS – module: Defect prediction criteria

Nine (9) quality criteria developed: for cracks, hot spots, porosity, etc.

As a function of steel composition, cooling rate, temperature, taking into account the phase transformations, inclusions, etc.
IDS tool – future work

Now we are working with data bank extension to special new steel grades as high Mn, Si, Al steels. IDS has in-house Gibbs energy databank applying thermodynamic substitutional solution model

With grain growth model: validation and fine tuning of the model

With precipitation model: validation and fine tuning of the model

With prediction of steel hot ductility curve: Gleeble ductility curve.

With coupling IDS with process models

With quality criteria: algorithms and validation

Coupling IDS with ChemApp: for calculation of complex multiphase inclusions and precipitations, we are working with coupling IDS with ChemApp and corresponding databanks by GTT Technologies.
Future: Coupling with continuous casting process models - steady state software package

Data change:
1 = temperature functions of material properties
2 = cooling curves of the strand
3 = liquid or interdendritic compositions
Future: Coupling with continuous casting process models - real-time software package

On-line: Process data, material ID

Continuous casting simulator
3D transient heat transfer model for calculating temperature distribution during continuous casting

On-line Continuous Casting Simulator

IDS – solidification and microstructure model

Tempsimu

Machine data

Material data

Output data
More future plans

1) On-line inclusion model for ladle treatments before CC: coupling of ChemApp, IDS, flow model, etc

2) Prediction of clogging index in continuous casting: coupling of IDS+ChemApp

3) On-line analysis of OES-PDA data to get information about inclusions in liquid before casting: coupling of IDS+ChemApp

2) Inclusions at the sample in the melt state presented in the “slag triangle” → solid or liquid inclusions?
Thank You