

# IDS

## Solidification Analysis Package for Steels

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# Content

- Aalto University and the Group of Metallurgy shortly
- IDS with case examples
- Future work

# Aalto University

With 20.000 students and 340 professors



Picture: Main building

## Fusion of 3 universities in 2010

- Helsinki University of Technology
- University of Art and Design Helsinki
- Helsinki School of Economics

# 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

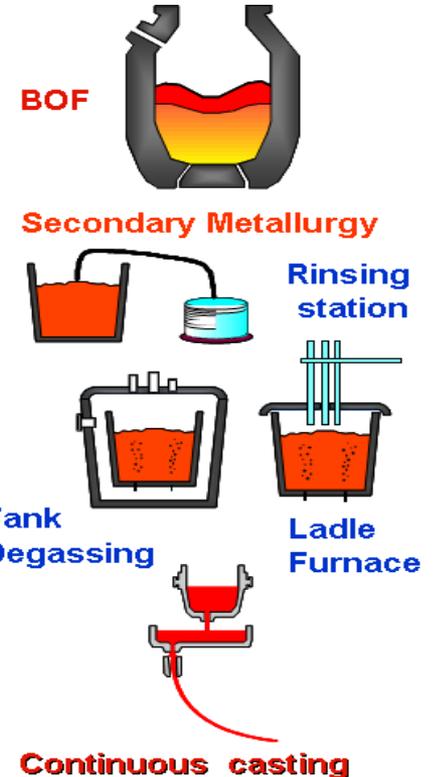
Copper industry: Mainly casting processes

Others: Many special projects (recycling,...)

## Special areas today:

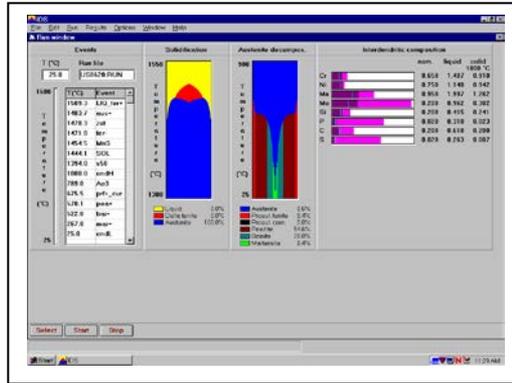
Mathematical modelling: in-house tools, commercial tools

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



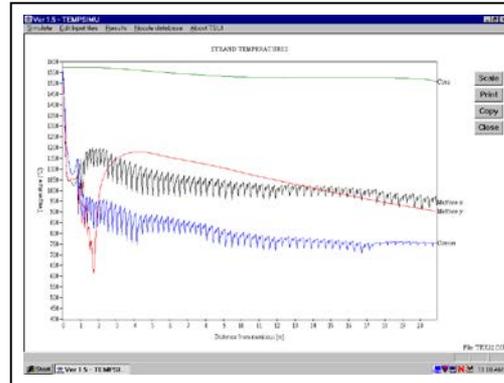
# Examples: Development of in-house software

IDS



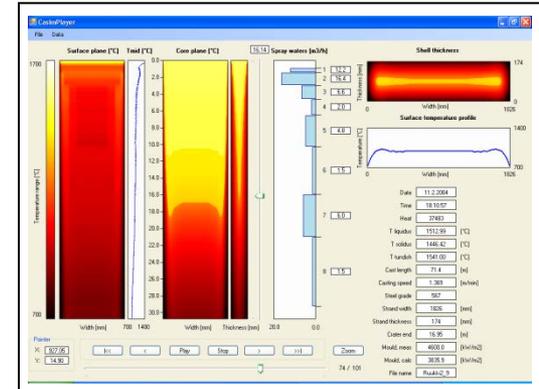
Solidification, phases, material properties and microsegregation from 1600 °C-25 °C

TEMPSIMU3D



Temperatures and solidification of strand in steady state casting conditions

CastManager (3D, on-line)



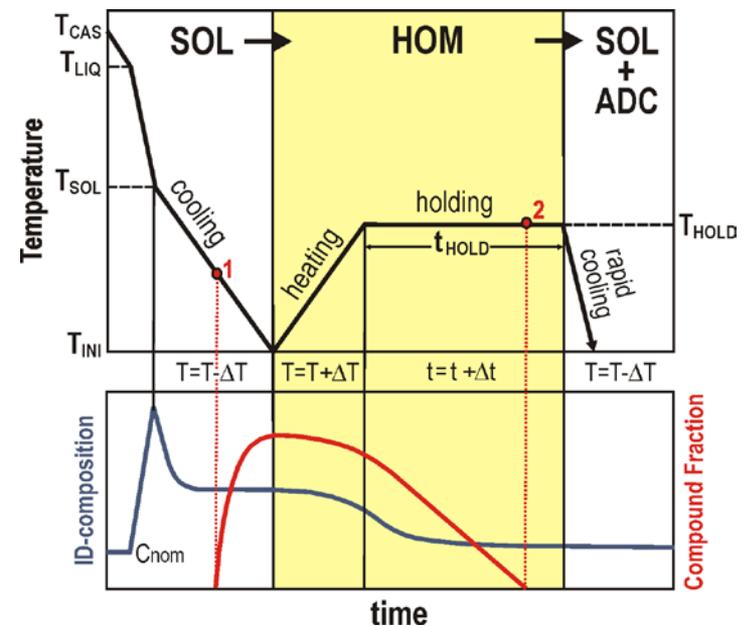
Temperatures and solidification of strand in dynamic casting conditions

# 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 led by Dr. Jyrki Miettinen

## INPUT

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

Element	Value	Element	Value	Element	Value
C	0.35	Cr	0.35	Nb	
Si	0.25	Ni	0.06	Ti	0.030
Mn	1.35	Mo	0.03	V	
P	0.01	Cu	0.10	Ca	
S	0.01	Al	0.03	B	0.003
		N	0.008	O	0.002
				H	0.0004

Run file: Example

Solidification     Austenite decomposition

Solidification:  Non-equilibrium,  Equilibrium

Cooling rate:  Constant,  Function

Composition file: Example

Cooling rate: 1.0

Dendrite arm diameter: SOL

ADC cooling rate: 0.1

ADC grain diameter: SOL

## 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

# IDS solidification physics

1) Diffusion in liquid is infinite, diffusion in solid follows Ficks II diffusion law

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

Experimental data bank

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

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

$$\longrightarrow J_i \approx M \frac{\partial \mu_i}{\partial x}$$

# IDS solidification physics

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.

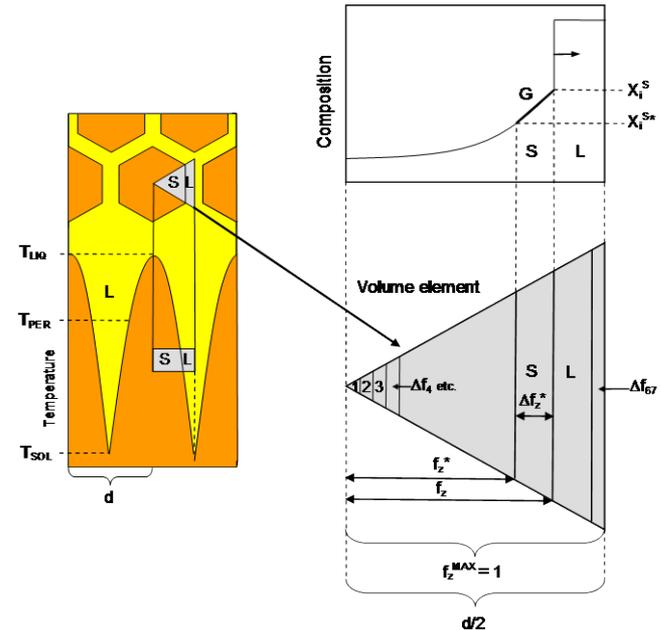
3) Phase stabilities are determined solving thermodynamic and mass transfer equations (ferrite, austenite, liquid, eutectic ferrite, compounds,...)

# IDS solidification physics

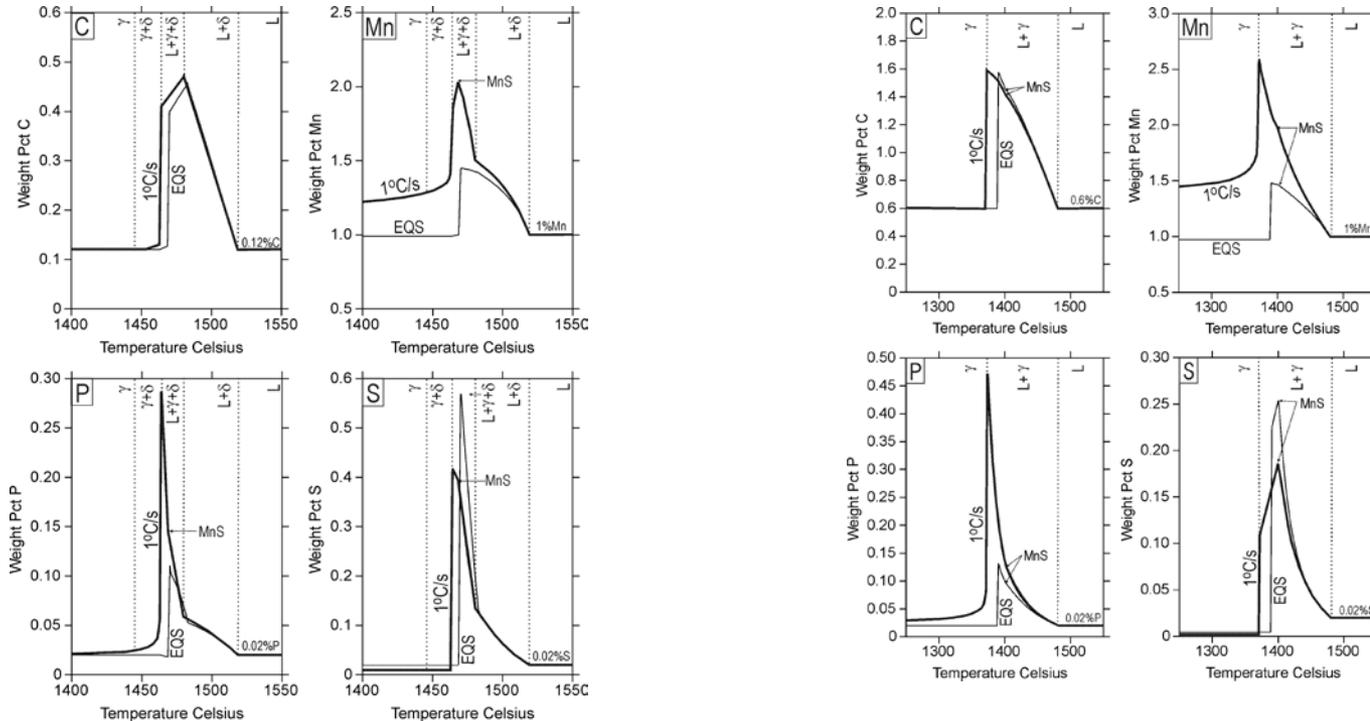
4) Volume-element (3D) has a **hexagonal form** in dendrite arm. Perpendicular to the growth direction, the volume element is described **with a triangle**. In the austenite region, the modeled element is a **3D sphere grain**.

5) During austenite to ferrite transformation, the **paraequilibrium condition** is assumed  $\rightarrow$  only interstitial elements (B, C,..) diffuse but larger substitutional not. Chemical potential equality equations 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 vs equilibrium model



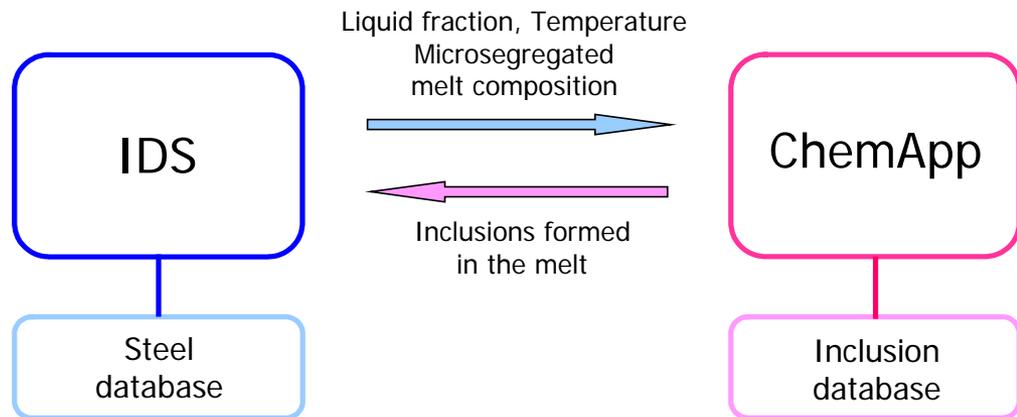
IDS results of microsegregation of the elements C, Mn, P and S in low carbon, C=0.12%, (left) and high carbon, C=0.6%, steel alloy (right). Other elements are 0.3%Si+1%Mn+0.02%P+0.02%S. The cooling rate in IDS was 1°C/s. Clear difference can be seen compared the IDS results with equilibrium calculations, EQS.

# Inclusions and precipitations in IDS

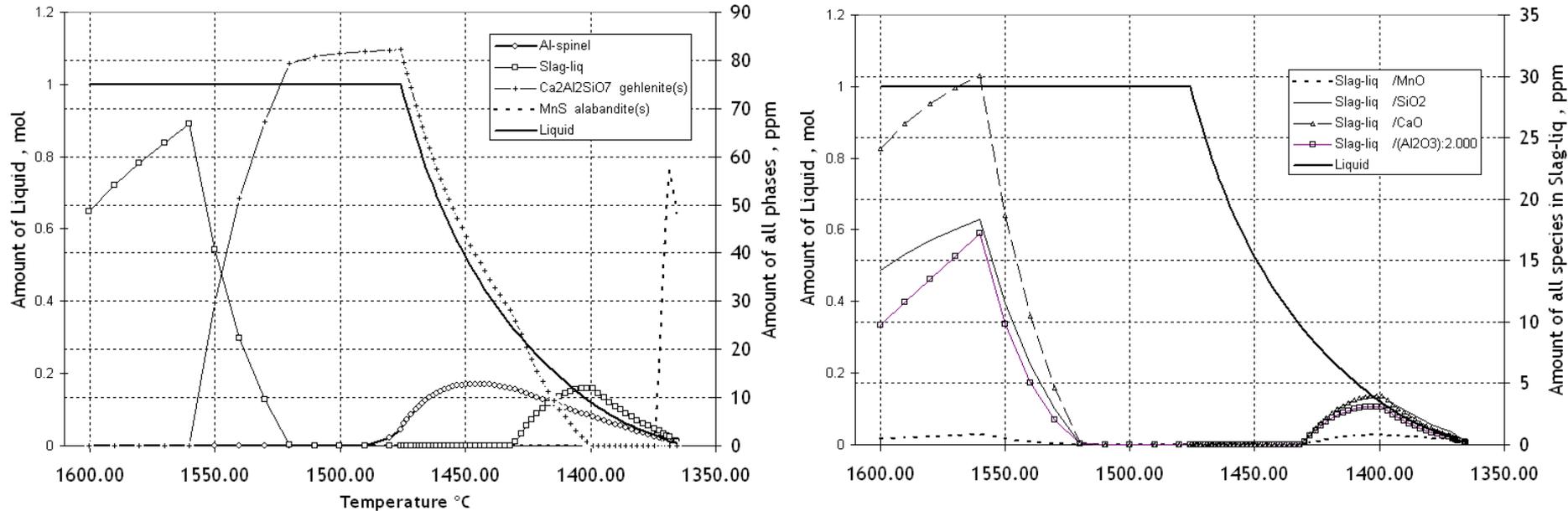
The formation of the following compounds can be simulated:

- **Stoichiometric binaries:** AlN, BN, B<sub>2</sub>O<sub>3</sub>(l), CaO, CaS, CO(g), H<sub>2</sub>(g), MgO, N<sub>2</sub>(g), SiO<sub>2</sub>, TiB<sub>2</sub>, TiO<sub>2</sub>, Ti<sub>2</sub>O<sub>3</sub>, VO
- **Stoichiometric ternaries:** Fe<sub>26</sub>Al<sub>9</sub>C<sub>5</sub>, FeMo<sub>2</sub>B<sub>2</sub>, FeNbB, Fe<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub>, Fe<sub>4</sub>Nb<sub>2</sub>O<sub>9</sub>, Ti<sub>2</sub>CS
- **Semistoichiometric ternaries:** (Mn,Fe)S, (Mn,Cr)S, (C,N)Nb, (C,N)Ti, (C,N)V, (Cr,Fe)<sub>2</sub>B, (Ni,Fe)<sub>3</sub>B, (Nb,Fe)O<sub>2</sub>, (Fe,X)<sub>2</sub>B (X=Cr,Mn,Ni,V), (Fe,X)<sub>3</sub>O<sub>4</sub> (X=Al,Cr,Mo,V), (Fe,X)<sub>2</sub>O<sub>3</sub> (X=Al,Cr,V), (Fe,X)<sub>0.947</sub>O (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.



# Case example: IDS+ChemApp



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

# Precipitations in IDS: Also nucleation and misfit energies are needed

Modified Gibbs energy expression

$$\Delta G_I^P = \frac{C_{INC} \cdot 10^{-7}}{D_{Me}^\phi(T)} = \text{barrier energy of incubation}$$

$$\Delta G_{MeX}^* = \Delta G_{MeX} + \Delta G_I^P + \Delta G_S^P$$

Thermodynamic Gibbs energy expression

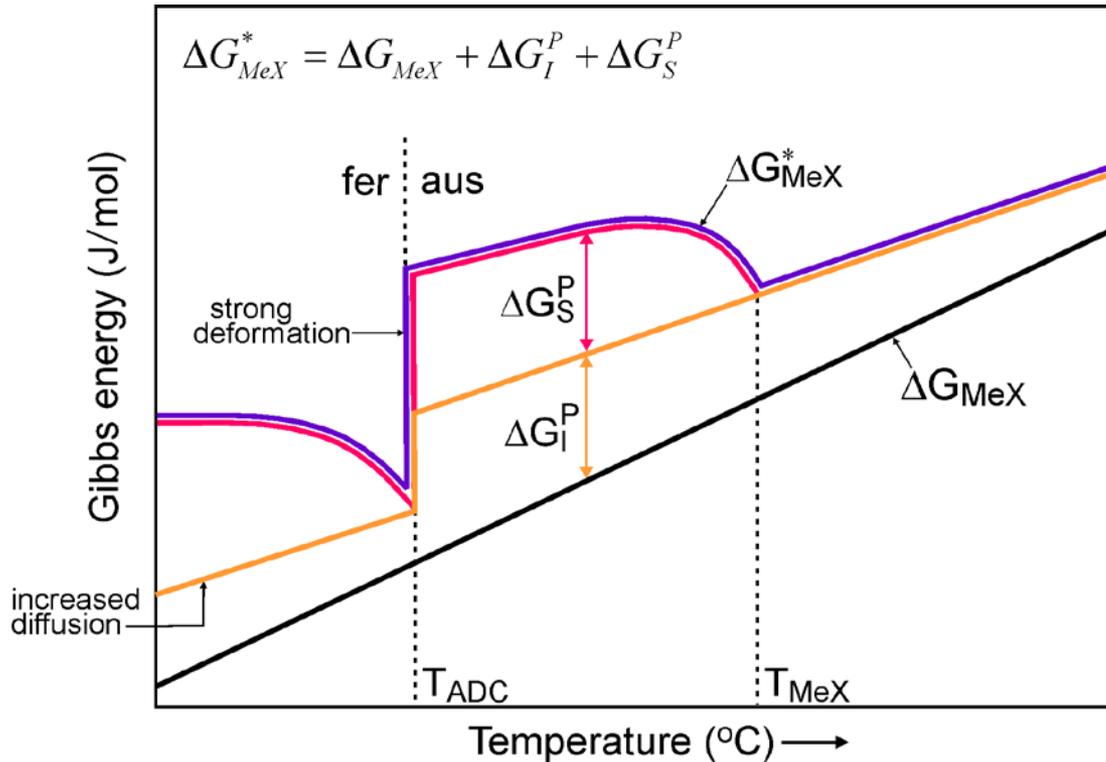
$$\Delta G_S^P = \frac{E}{1-\nu} \left( \frac{1}{3} \cdot \frac{V_{mol}^P - V_{mol}^M}{V_{mol}^M} \cdot C_{VMF} \cdot C_{ADC} \right)^2 \cdot V_{mol}^M \cdot (f^P)^{0.2} = \text{barrier energy of volume misfit}$$

Future: For more complex precipitations, we plan to apply ChemApp. Question: Can we add extra energies to ChemApp?

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

# Precipitation energies schematically

S=for misfit, I=for nucleation

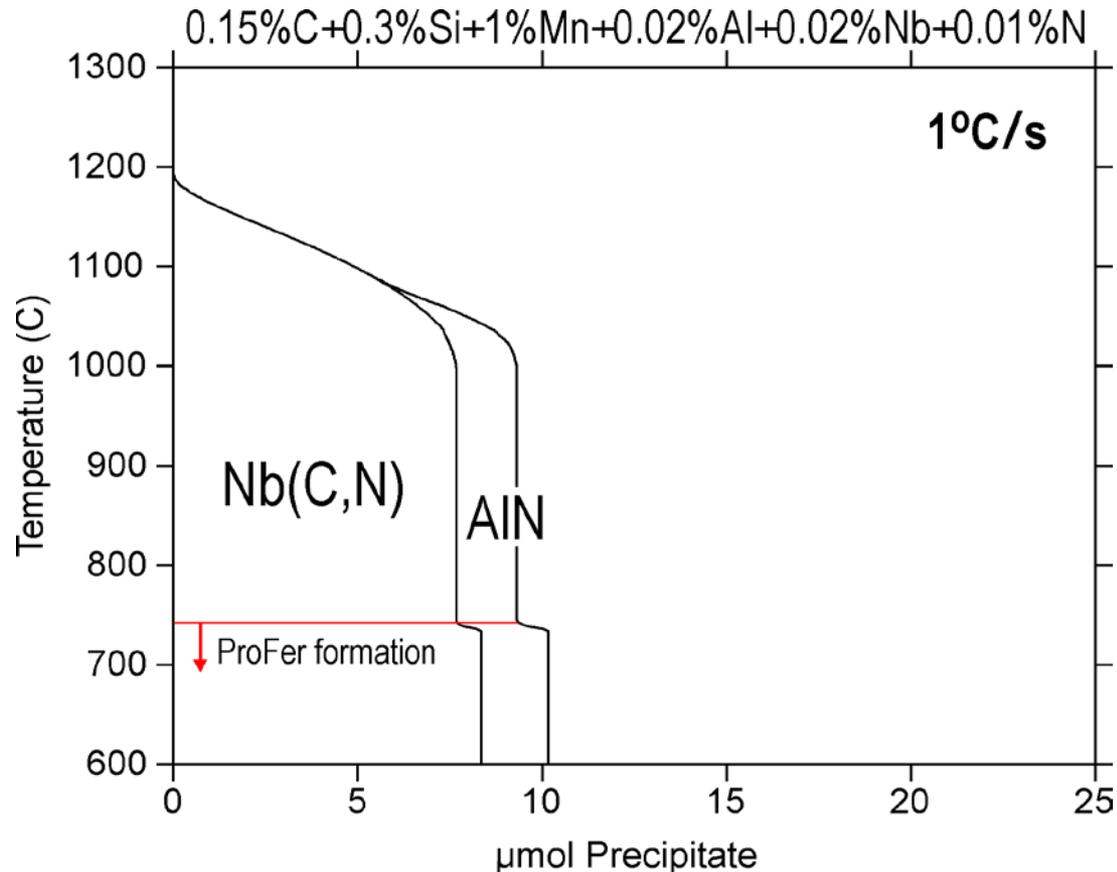


Nucleation energy increases with decreasing temperature, just due to the decreasing solute diffusion in austenite. In ferrite the diffusion increases → energy decreases.

Misfit energy increases after the start of the precipitate formation, at  $T_{MeX}$ .

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

# Case example: Precipitation



Note the suppressed growth at about 1000°C, which is due to the increasing values of barrier energies  $\Delta G_I^P$  and  $\Delta G_S^P$  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!!!!

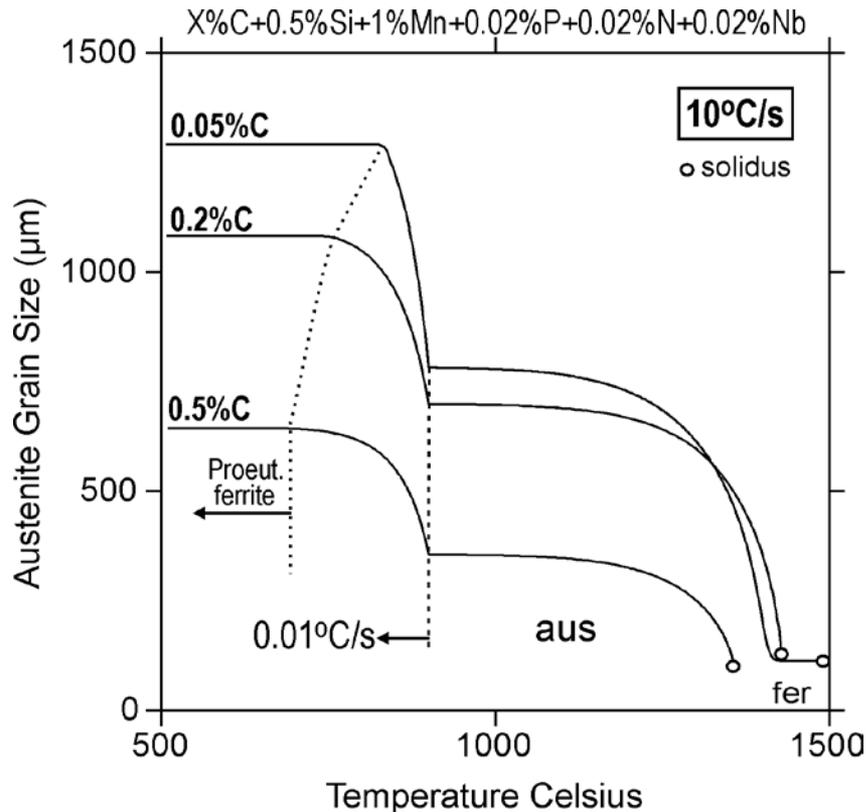
$$D(t + \Delta t) = D(t) + M_0^* \cdot \exp(-Q / R / T(t)) \cdot \left( \frac{1}{D(t)} - \frac{1}{D_{\max}} \right)^{\frac{1}{n_0} - 1} \cdot \Delta t$$

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

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 ( $\mu\text{m}$ ) at time  $t+\Delta t$  ( $\Delta t$ =time step in IDS simulation)
- $D(t)$  = grain size of the previous step, at time  $t$
- $D_{\max}$  = the maximal grain size (assumed as  $D_{\max}=8000\mu\text{m}$ )
- $M_0^*, n_0$  = grain boundary constants (assumed as  $n_0=0.5$  and  $M_0^*=4 \cdot 10^9 \mu\text{m/s}$ )
- $Q$  = activation energy (J/mol)
- $f^{fer}, f^{pre}$  = 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  $Q_0=165000 \text{ J/mol}$ )
- $C_{EQ}$  = carbon equivalent (estimated as  $C_{EQ}=\text{wt}\%C$ )
- $Q_{EQ}$  = increase of activation energy due to  $C_{EQ}$  (optimized as  $Q_{EQ}=25000 \text{ J/mol}$ )

# Case example: Grain size



As in all steels, the growth is quite effective at high temperatures and the growth is finally stopped by the formation of proeutectoid ferrite.

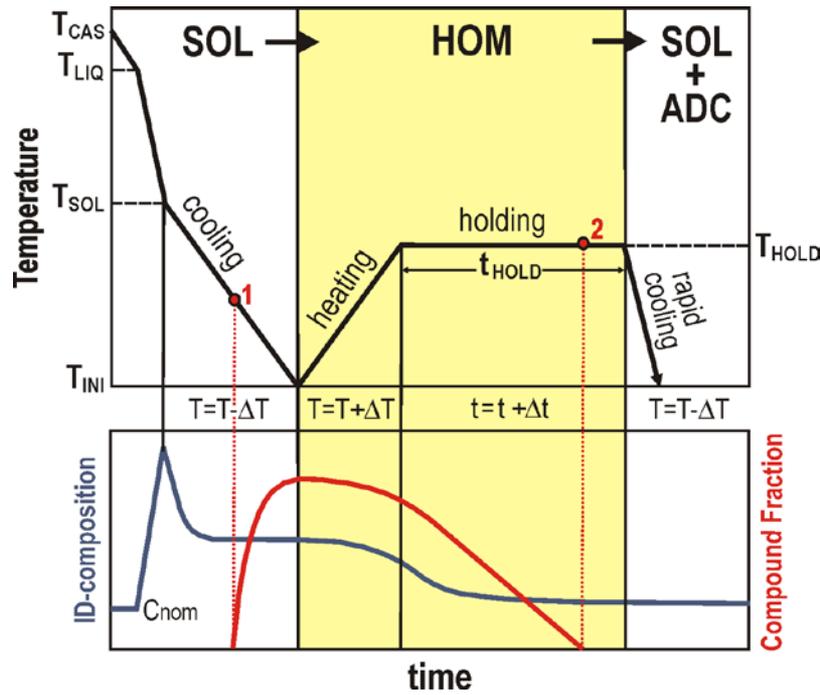
The effective growth is restrained by grain boundary ferrite and Nb(C,N) precipitations.

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

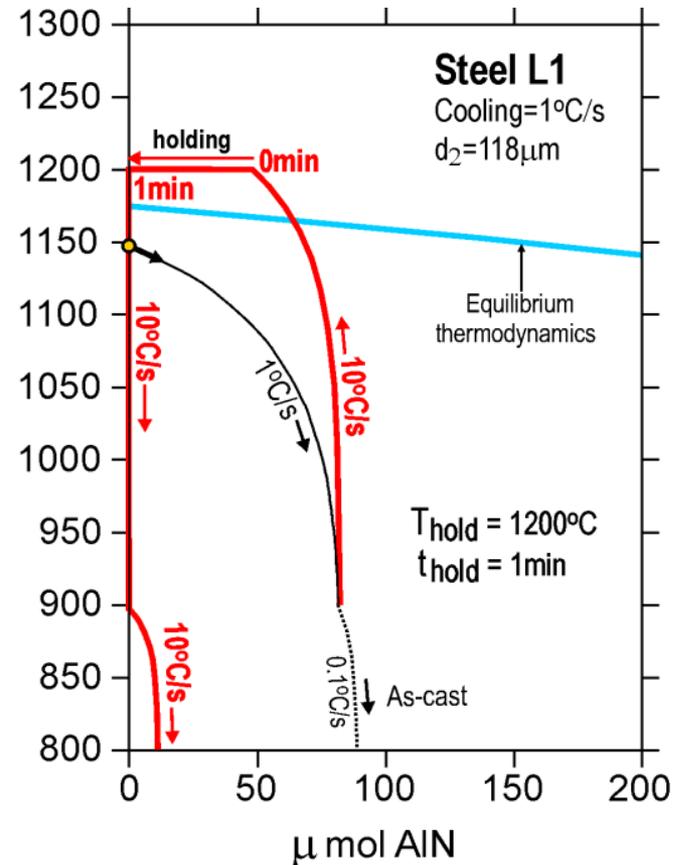
The final grain size in the 0.05wt%C alloy is highest because of the low amount of Nb(C,N), which restrains the grain growth.

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 10° C/s, reheating 10° C/s, holding 1 min 1200 °C, cooling 10° C/s

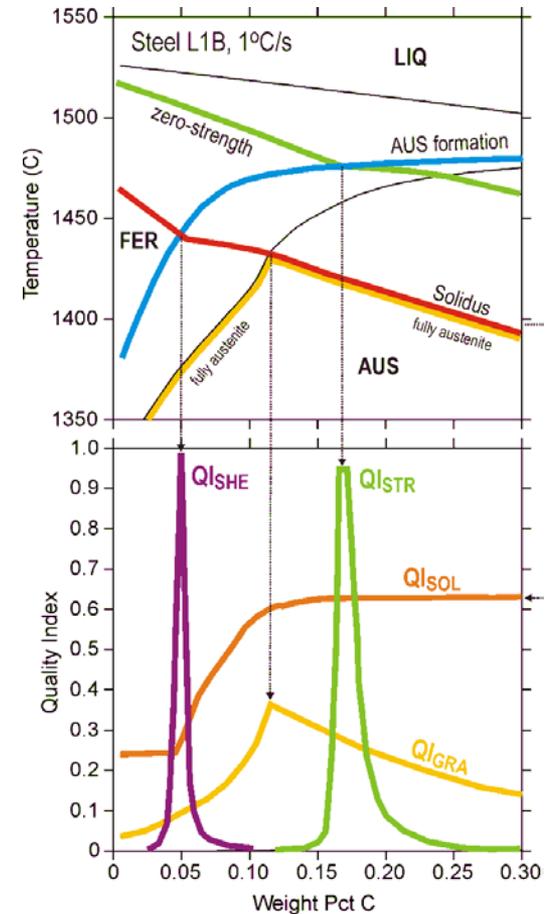
# IDS: Databanks

1. Thermodynamic Gibbs energy data. *Phases: liquid, ferrite, austenite, compounds and cementite. Components: Fe, C, Si, Mn, P, S, Cr, Mo, Ni, Cu, Al, N, Nb, Ti, V, Ca, B, O, H)*
2. Diffusion coefficients of solutes. *Phases: ferrite and austenite. Solutes: Si, Mn, P, Cr, Mo, Ni, Cu, Al, Nb, Ti, V, Ca (diffusion of B, C, H, N, O, S assumed extremely rapid)*
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*
5. CCT data. Parameters of CCT regression formulas. Components: C, Si, Mn, Cr, Mo, Ni. Applied in ADC simulations.

# 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

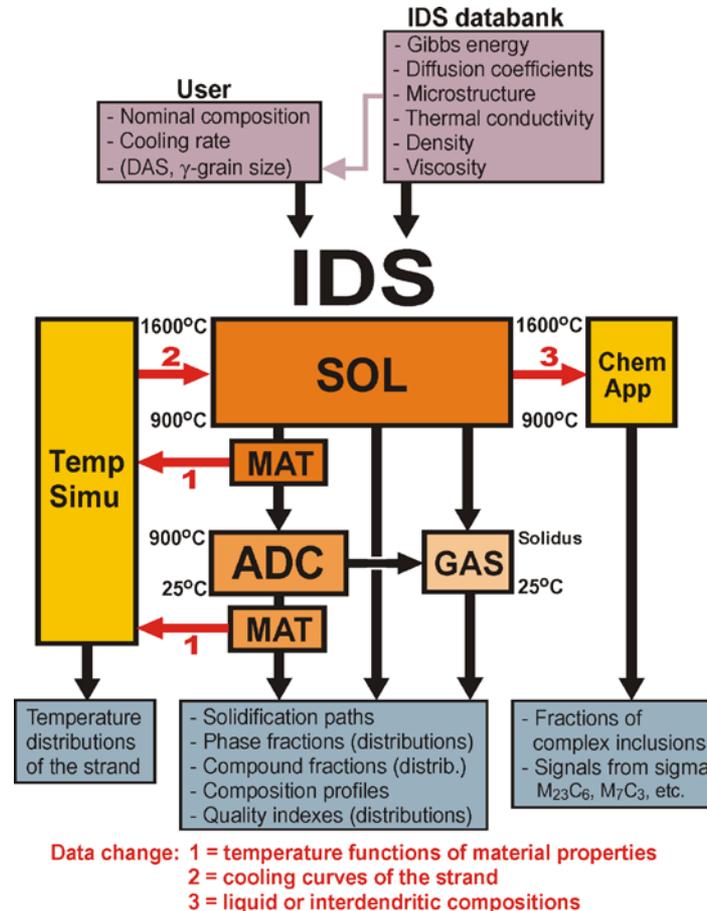
With **prediction of steel hot ductility** curve: Gleeble ductility curve.

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



# Future: Coupling with continuous casting process models - real-time software package

On-line: Process data, material ID

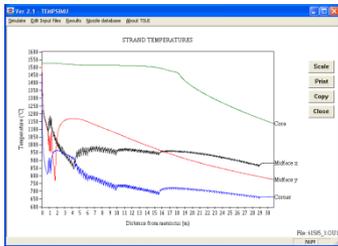
Continuous casting simulator

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

## On-line Continuous Casting Simulator



Tempsimu



Machine data

IDS – solidification and microstructure model

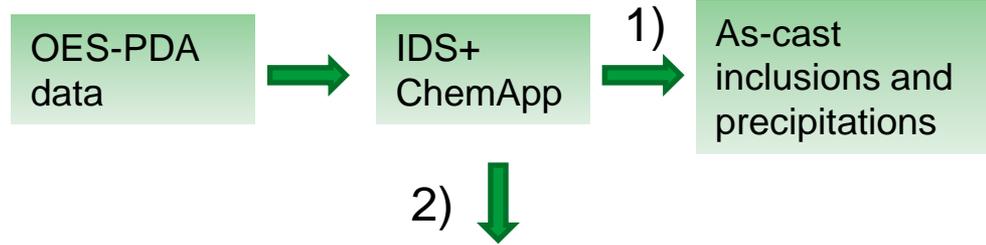


Material data

Output data

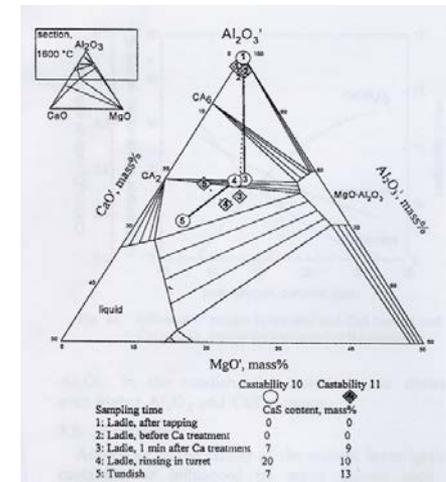
# More future plans

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