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A new general model for diffusion controlled growth in DICTRA

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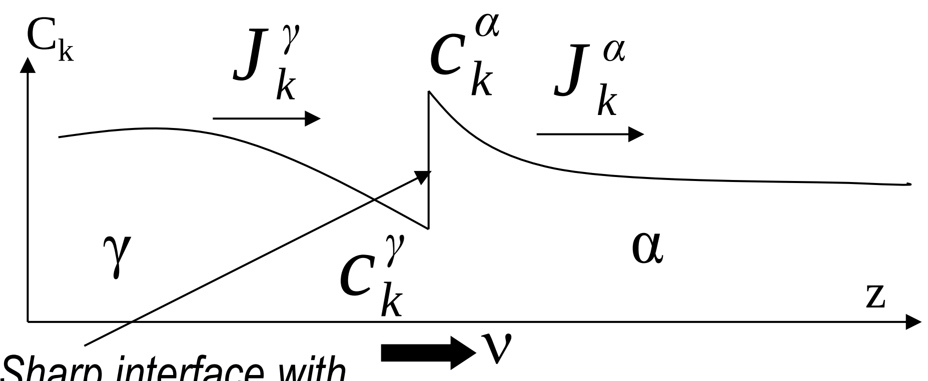
EUROMAT2013, September 8-13, 2013 · Sevilla, Spain

Background and motivation

DICTRA – a software package for simulating diffusion controlled transformations in 1D



Sharp interface with assumption of local eq.

n-1 Flux Balance Equations:

$$v\left(c_k^{\alpha} - c_k^{\gamma}\right) = J_k^{\alpha} - J_k^{\gamma}$$

F-B Equations solved as:

$$\sum_{k=1}^{n-1}\left[v\left(c_k^{\alpha} - c_k^{\gamma}\right) - \left(J_k^{\alpha} - J_k^{\gamma}\right)\right]^2 < \varepsilon$$

- ❑ Multiple phases was not allowed on either side of an interface
- ❑ Moving phase boundary problems are sometimes sensitive to starting values

The purpose of the new model is to generalize the software and increase the numerical robustness.

New moving phase boundary model

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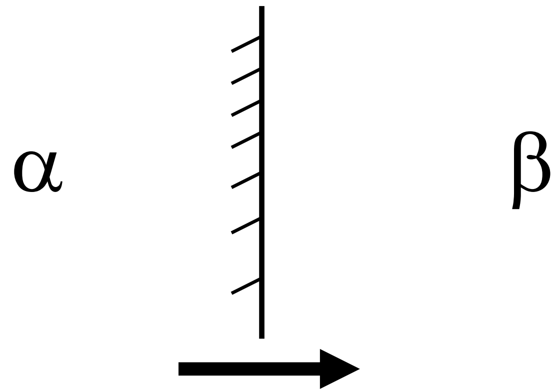
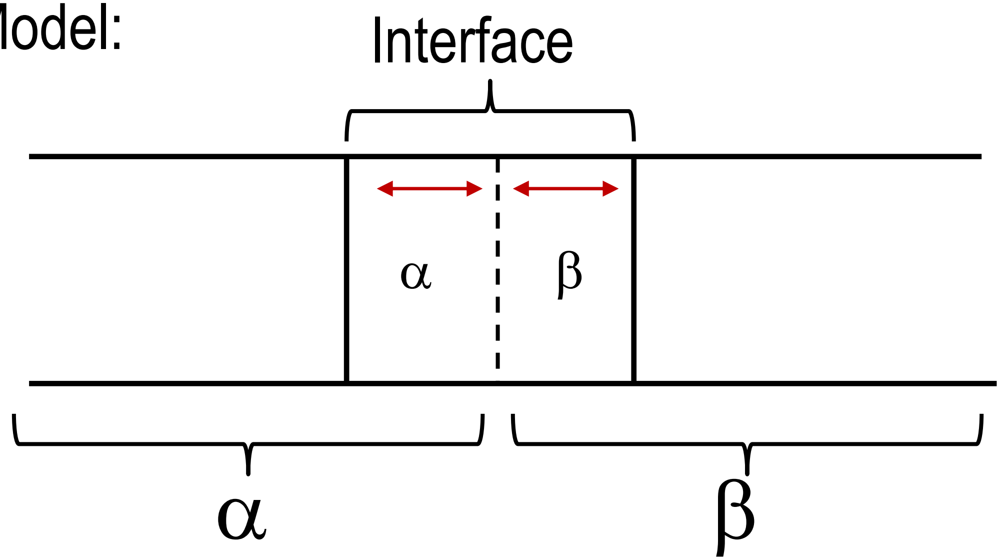


Model assumptions:

- Interfaces have a constant, finite width
- Local equilibrium holds at / in interfaces
- Infinitely fast kinetics in interfacial finite volume

Model:



The interfacial finite volume extends the same distance into both phases; it contains 50% α and 50 % β

New moving phase boundary model

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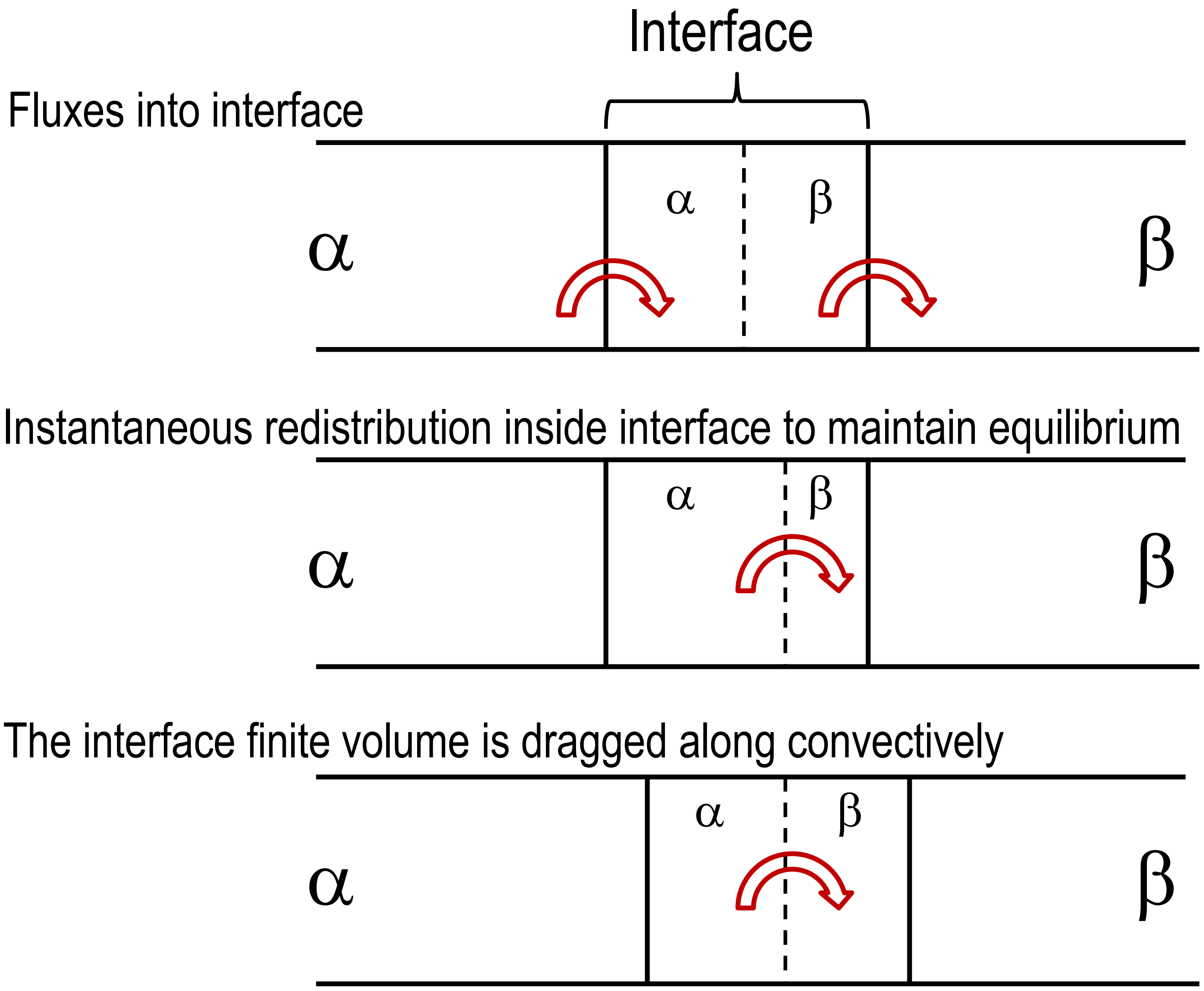
Conceived sequence of events leading to interface migration



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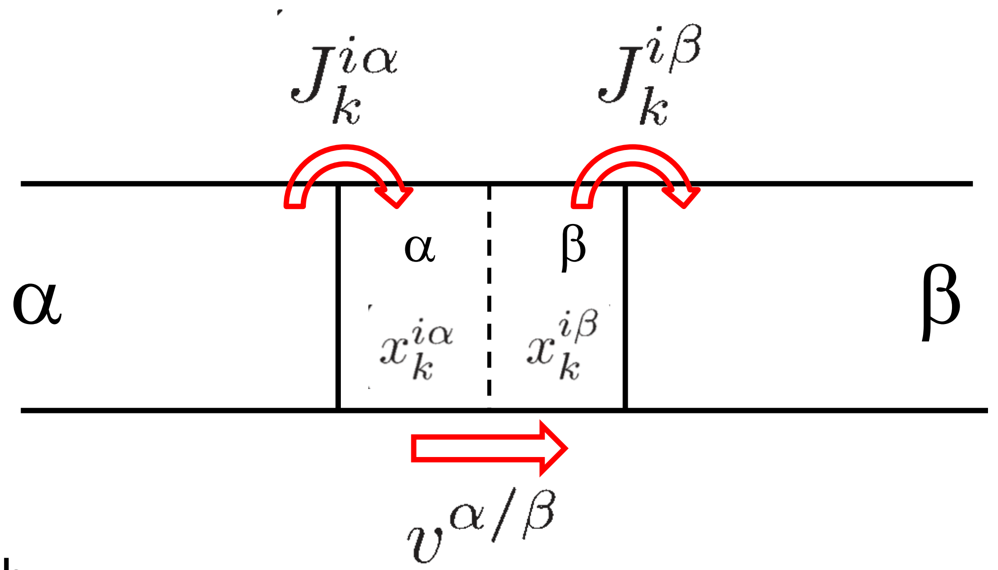
Volume-fixed fluxes:



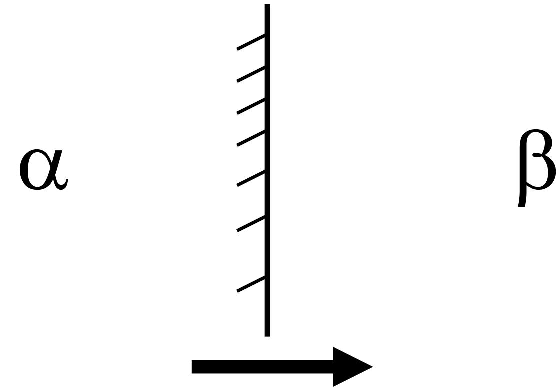
Interface velocity given by:

$$v^{\alpha/\beta} = V_m \frac{\sum \frac{\partial f^{\alpha}}{\partial N_k}\left(J_k^{i\alpha} - J_k^{i\beta}\right)}{\sum \frac{\partial f^{\alpha}}{\partial N_k}\left(x_k^{i\alpha} - x_k^{i\beta}\right)}$$

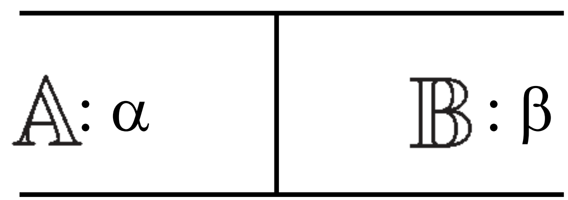
Larsson, Reed, Acta Mater 56(2008)3754

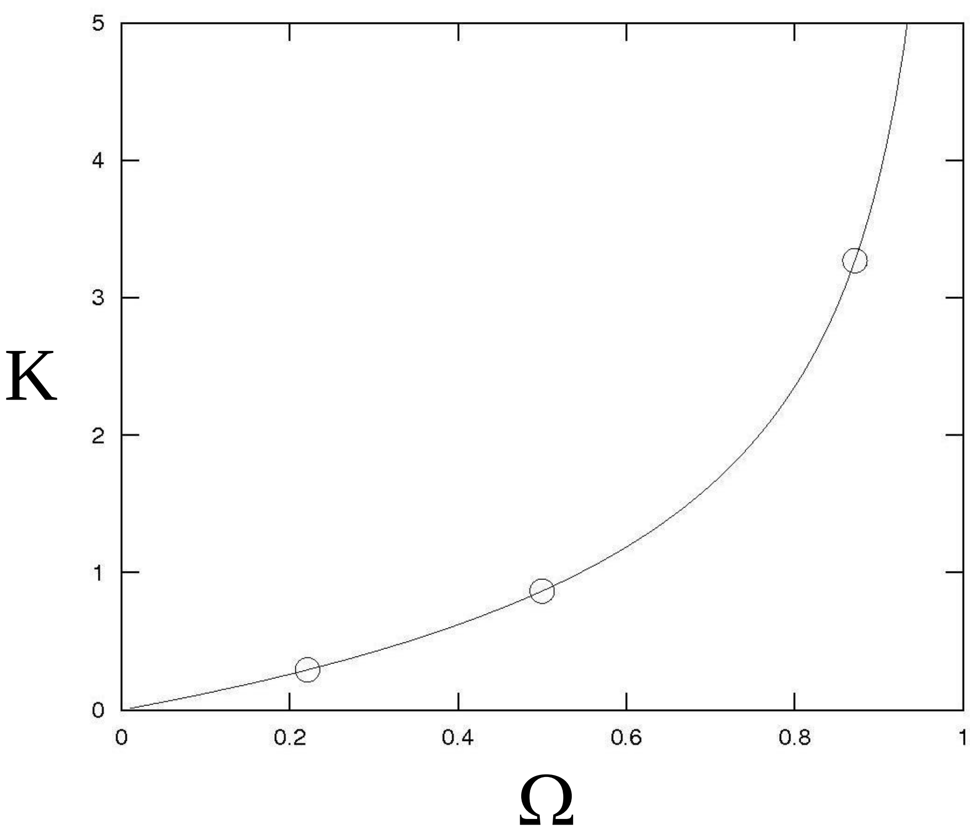
Validation – analytical case

Binary system, ideal solutions
Growth of α from supersaturated β



Circles: simulation
Line: analytical solution





α thickness *S*

$$S = K\sqrt{Dt}$$

$$K = \frac{2}{\sqrt{\pi}}\Omega\frac{\exp\left(-K^2/4\right)}{\left(1 - \operatorname{erf} K/2\right)}$$

$$\Omega = \frac{c^\beta - c^\infty}{c^\beta - c^\alpha}$$

Comparison of models

”Classic” DICTRA moving phase boundary model	New model
Sharp (zero width) interface	Finite width interface
Find state at interface by solving set of flux balance equations	Explicit expression for interface velocity
Finite element method (FEM)	Finite volume method (FVM)
Fast and efficient	Robust

$$v\left(c_k^{\alpha}-c_k^{\gamma}\right)=J_k^{\alpha}-J_k^{\gamma}$$

$$k=1,\ldots,n-1$$

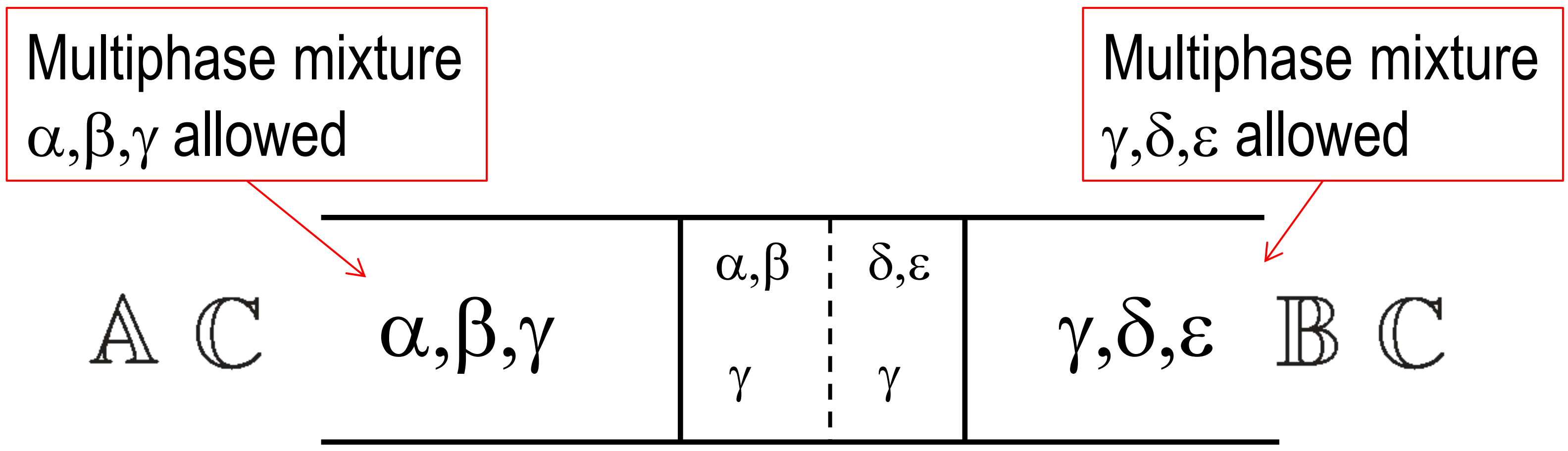
Automatic switching between the models implemented

New moving phase boundary model

Generalize

Three sets of phases:

$\mathbb{A}$: α,β	Allowed only on the left side of the interface
$\mathbb{B}$: δ,ε	Allowed only on the right side of the interface
$\mathbb{C}$: γ	Allowed on both sides of the interface



New moving phase boundary model

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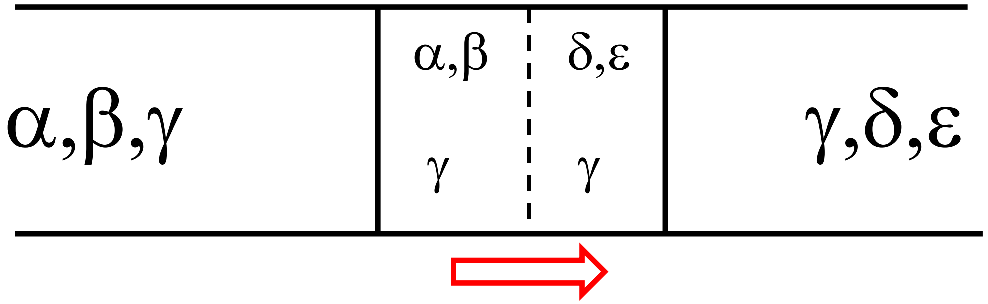

$$v^{\mathbb{A}/\mathbb{B}}$$

Interface velocity given by:

$$\frac{v^{\mathbb{A}/\mathbb{B}}}{V_S} = \frac{\sum_{\alpha\in\mathbb{A}}\sum_{k}\frac{\partial f^{\alpha}}{\partial N_k}\left[J_k^{i\mathbb{A}}A\left(z^{i\mathbb{A}}\right) - J_k^{i\mathbb{B}}A\left(z^{i\mathbb{B}}\right)\right] - \sum_{\delta\in\mathbb{B}}\sum_{k}\frac{\partial f^{\delta}}{\partial N_k}\left[J_k^{i\mathbb{A}}A\left(z^{i\mathbb{A}}\right) - J_k^{i\mathbb{B}}A\left(z^{i\mathbb{B}}\right)\right]}{\sum_{\alpha\in\mathbb{A}}\sum_{k}\frac{\partial f^{\alpha}}{\partial N_k}\left[u_k^{i\mathbb{A}}A\left(z^{i\mathbb{A}}\right) - u_k^{i\mathbb{B}}A\left(z^{i\mathbb{B}}\right)\right] - \sum_{\delta\in\mathbb{B}}\sum_{k}\frac{\partial f^{\delta}}{\partial N_k}\left[u_k^{i\mathbb{A}}A\left(z^{i\mathbb{A}}\right) - u_k^{i\mathbb{B}}A\left(z^{i\mathbb{B}}\right)\right]}$$

New moving phase boundary model

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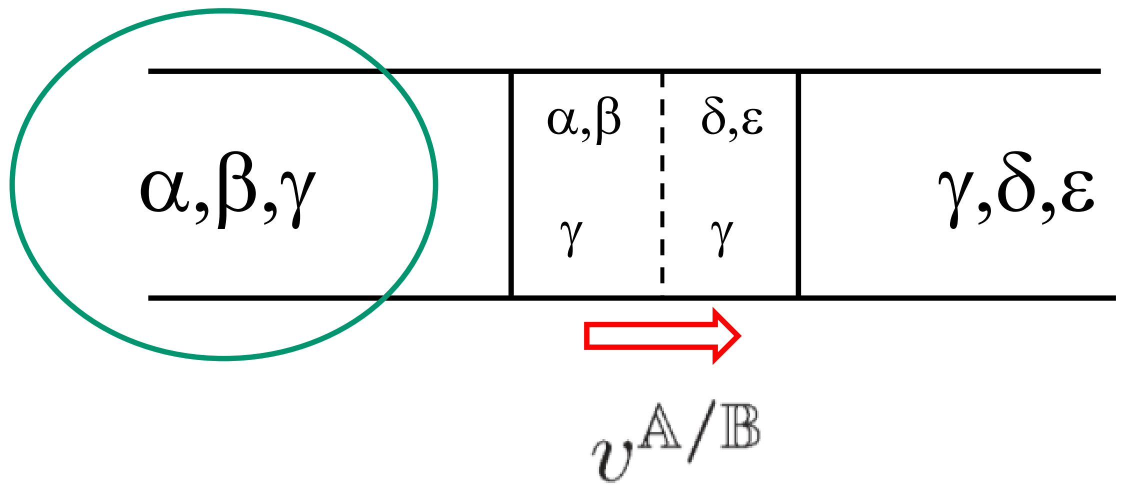
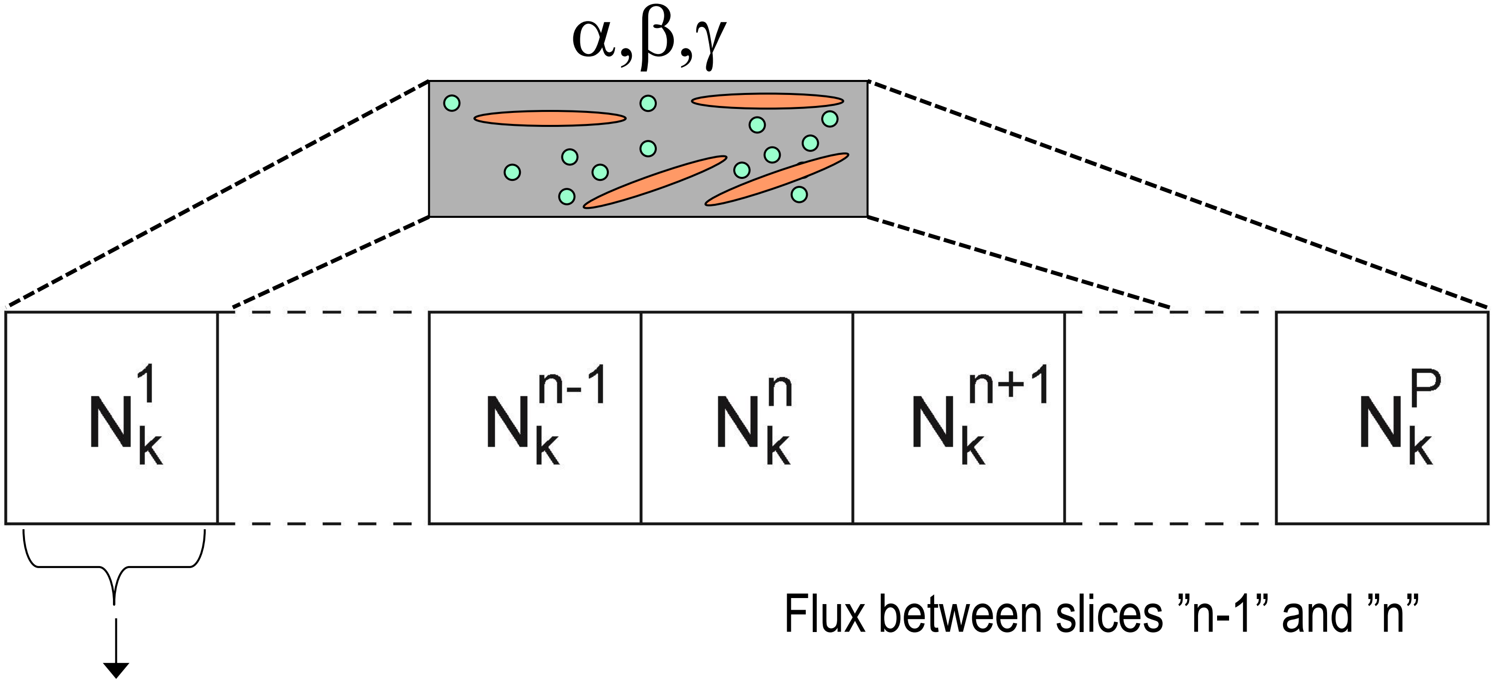


Interface velocity given by:

$$\frac{v^{\mathbb{A}/\mathbb{B}}}{V_S} = \frac{\sum_{\alpha\in\mathbb{A}}\sum_{k}\frac{\partial f^{\alpha}}{\partial N_k}\left[J_k^{i\mathbb{A}}A\left(z^{i\mathbb{A}}\right) - J_k^{i\mathbb{B}}A\left(z^{i\mathbb{B}}\right)\right] - \sum_{\delta\in\mathbb{B}}\sum_{k}\frac{\partial f^{\delta}}{\partial N_k}\left[J_k^{i\mathbb{A}}A\left(z^{i\mathbb{A}}\right) - J_k^{i\mathbb{B}}A\left(z^{i\mathbb{B}}\right)\right]}{\sum_{\alpha\in\mathbb{A}}\sum_{k}\frac{\partial f^{\alpha}}{\partial N_k}\left[u_k^{i\mathbb{A}}A\left(z^{i\mathbb{A}}\right) - u_k^{i\mathbb{B}}A\left(z^{i\mathbb{B}}\right)\right] - \sum_{\delta\in\mathbb{B}}\sum_{k}\frac{\partial f^{\delta}}{\partial N_k}\left[u_k^{i\mathbb{A}}A\left(z^{i\mathbb{A}}\right) - u_k^{i\mathbb{B}}A\left(z^{i\mathbb{B}}\right)\right]}$$

Diffusion in multiphase mixtures

Homogenization approach allow us to account for diffusion in more than one phase



Equilibrium calculation for each slice

↓

Phase fractions
Phase compositions
Chemical potentials
Mobilities

Flux between slices "n-1" and "n"

$$J_k = \frac{-1}{V_m}\sqrt{[M_k x_k]^{eff}_{n-1}\,[M_k x_k]^{eff}_{n}}\,\frac{\Delta\mu_k}{\Delta z}$$

"Effective" $[M_k x_k]$ from combining rules

Larsson, Engström, Acta Mat 54(2006)2431
Larsson, Höglund, Calphad 33(2009)495

DICTRA setup using new model

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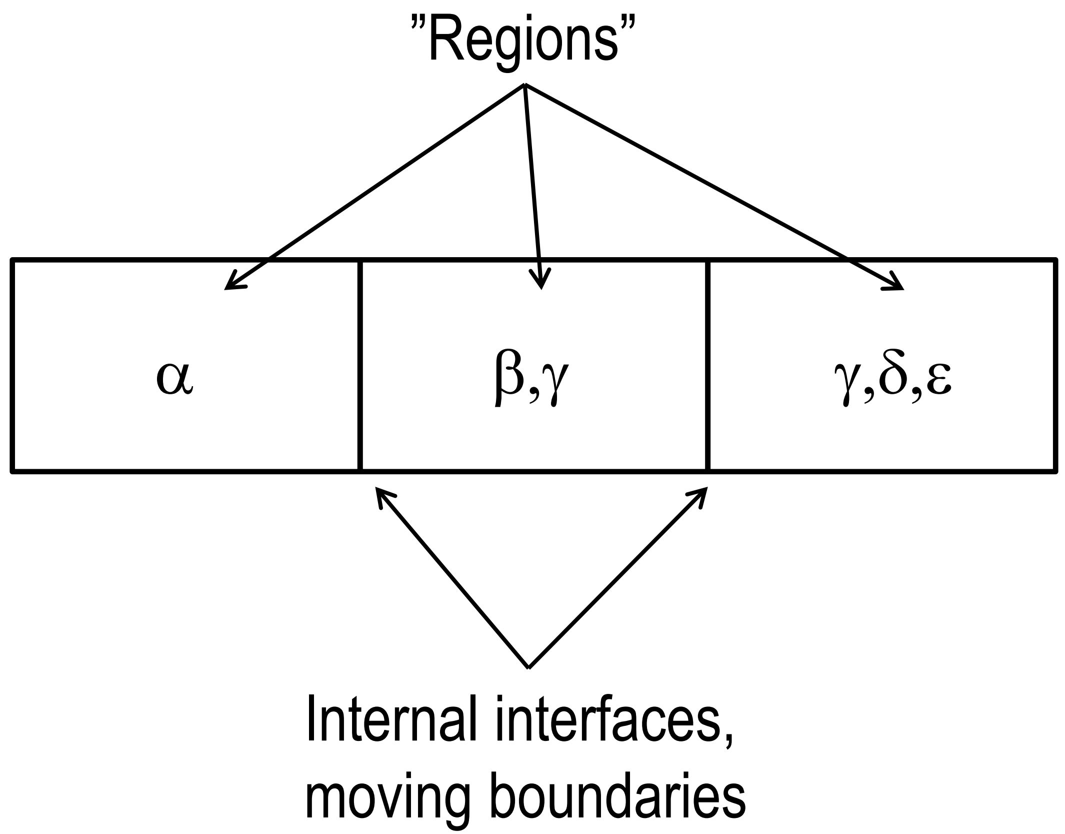
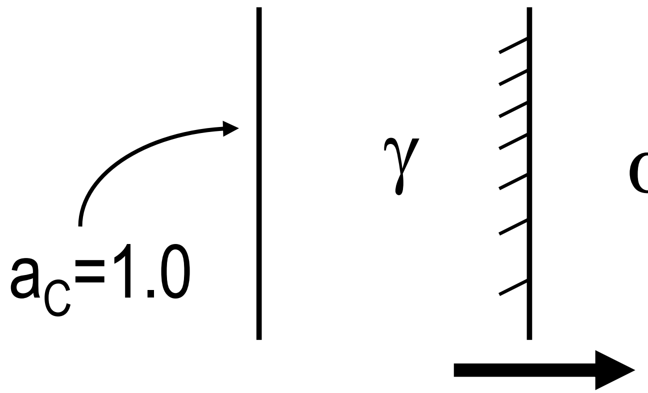


Arbitrary set of phases in each region

Remaining requirement: one unique phase in each region

Carburization of steel accompanied by α→γ transformation



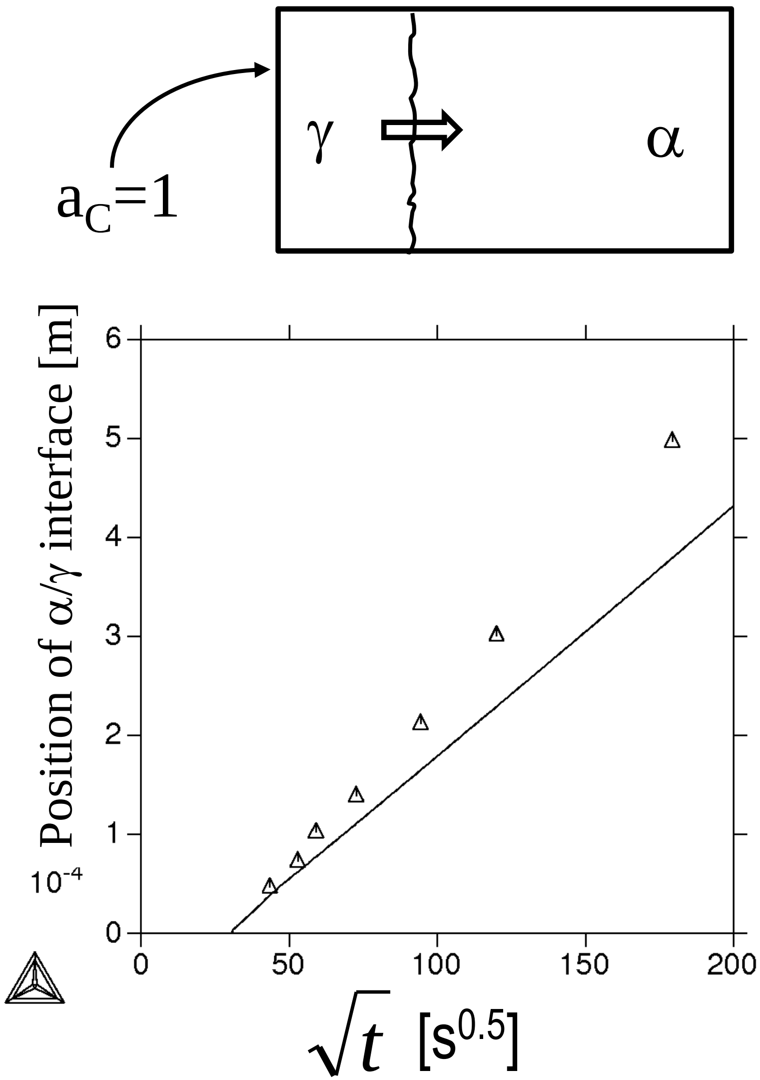
- 800°C
- Two base alloys
  - ✓ Pure Fe
  - ✓ Fe 0.3 mass-% Nb

𝔸: γ 𝔹: α ℂ: MC

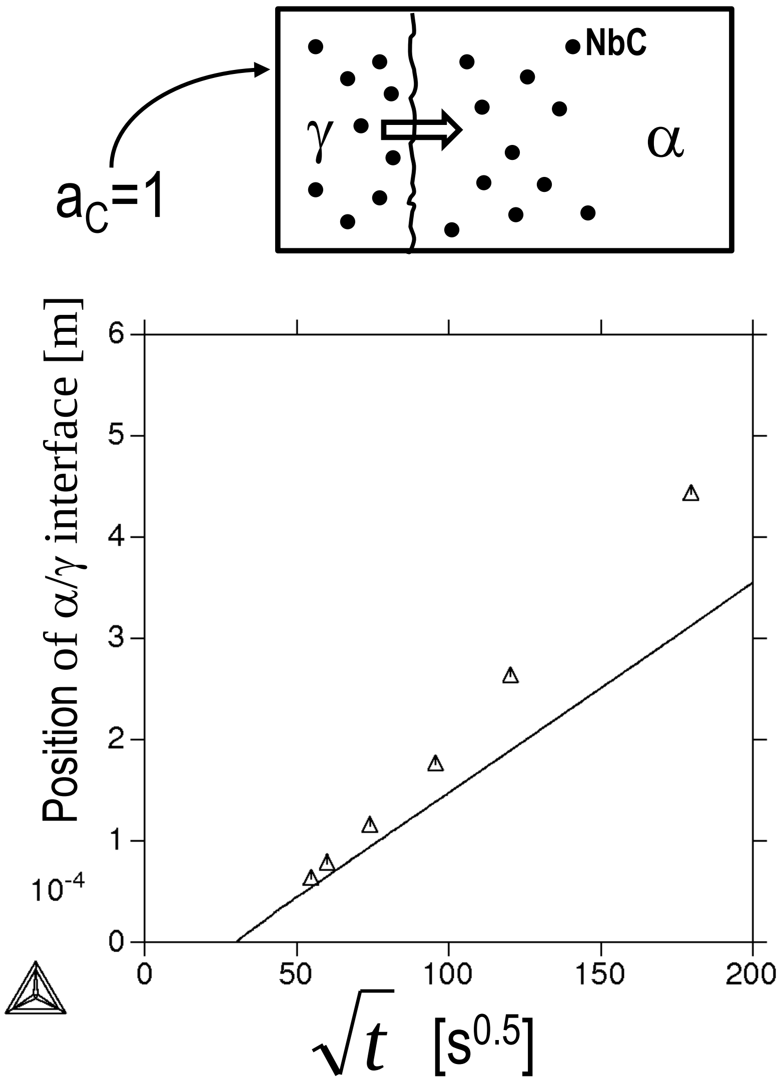
𝔸ℂ: γ+MC	𝔹ℂ: α+MC

Experiments by Togashi and Nishizawa, J Japan Inst Met 40(1976)12

Carburization of steel



Fe-C



Fe-C-Nb

Carburization of steel

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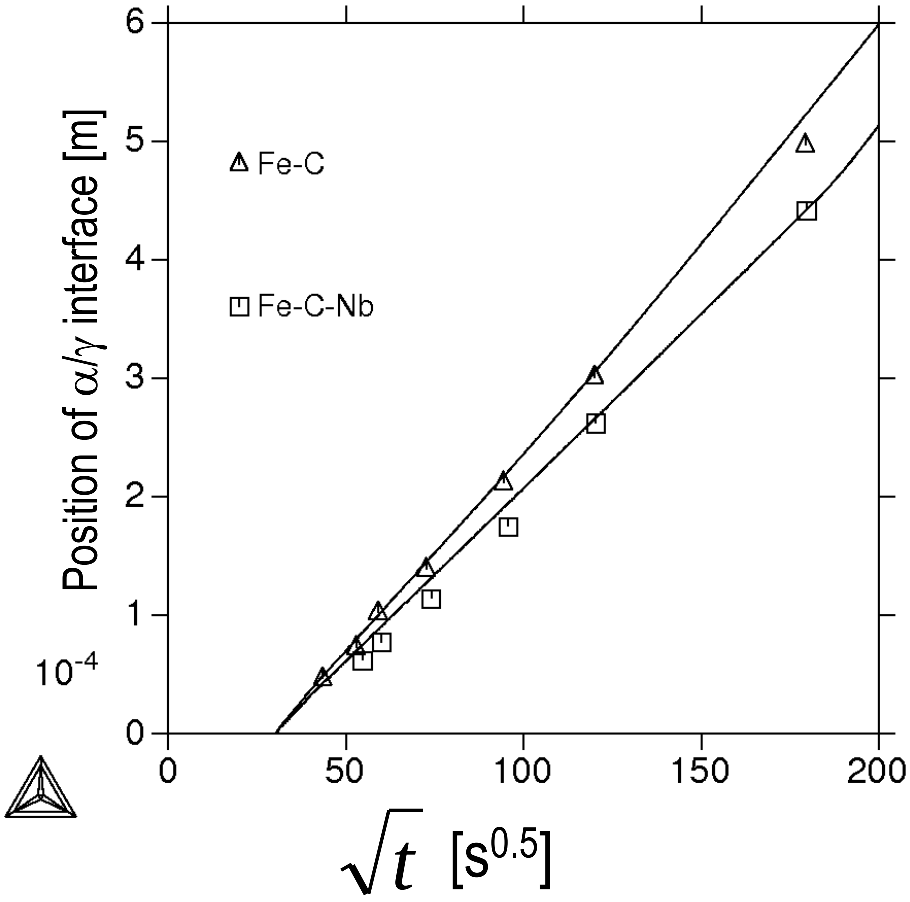


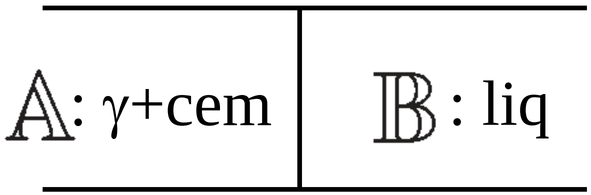
Increased mobility of carbon in austenite and ferrite by factor 2

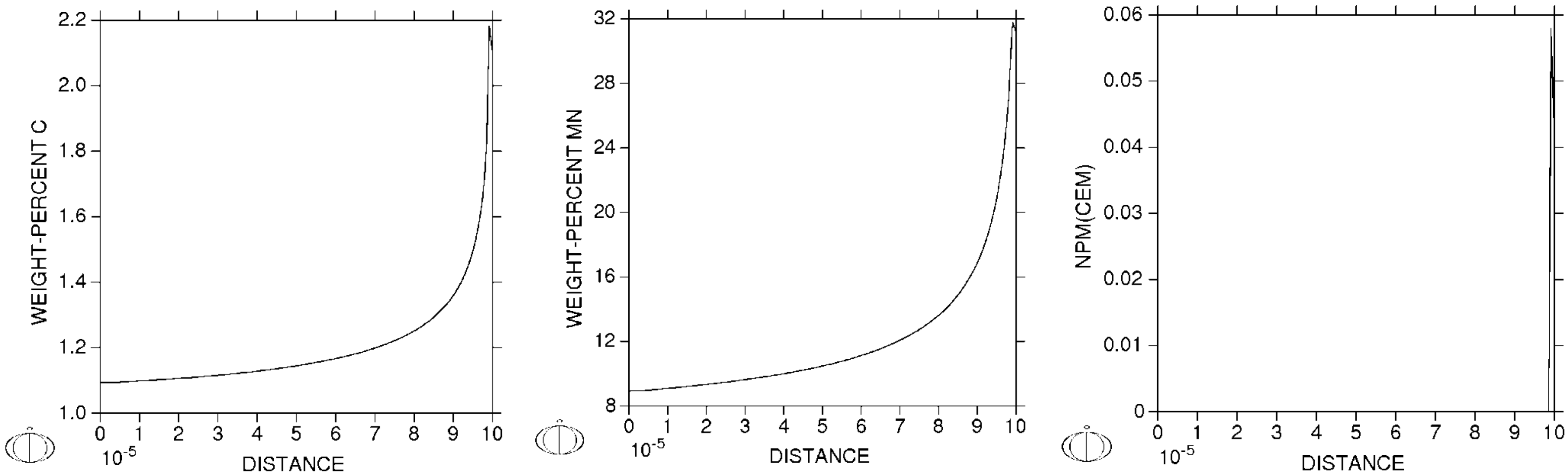
Solidification and homogenizing

Hadfield steel   Fe 1.2 C 12 Mn

100 μm domain

Cooling rate 1 K/s during solidification





Profiles after solidification

Solidification and homogenizing

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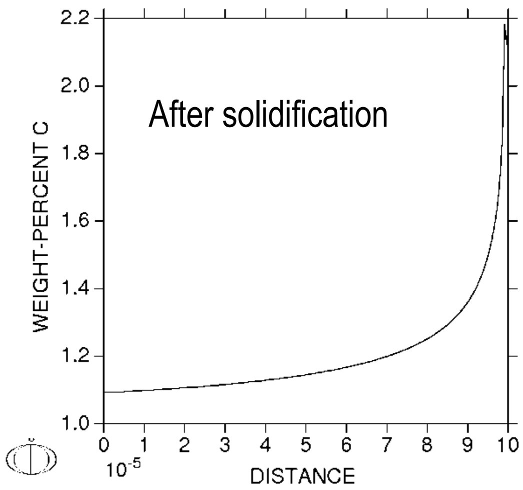
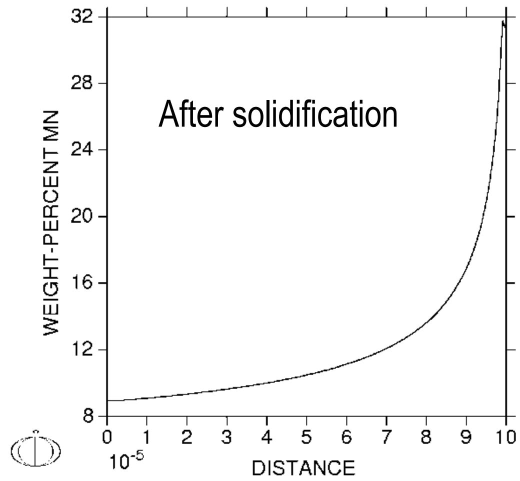
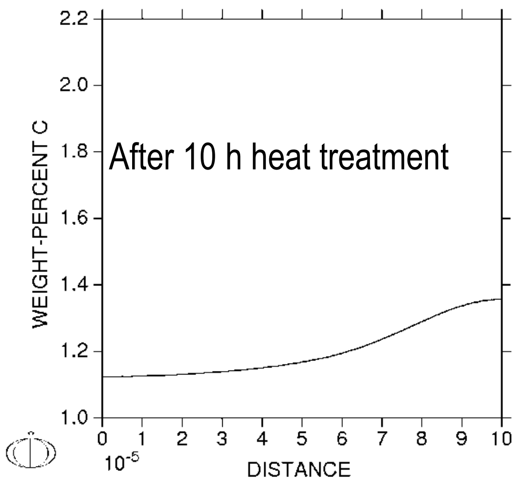
Utility: Set a target temperature as function of incipient melting temperature

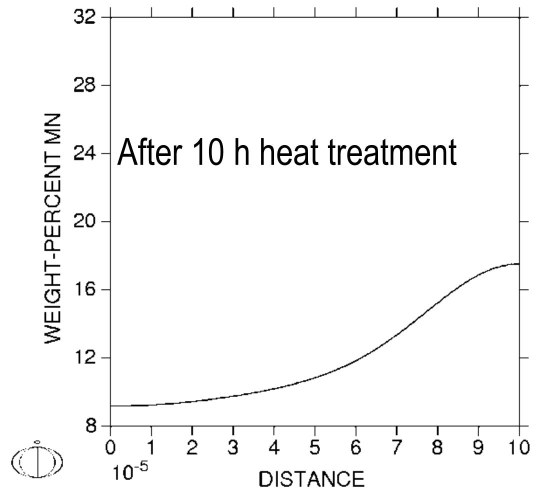


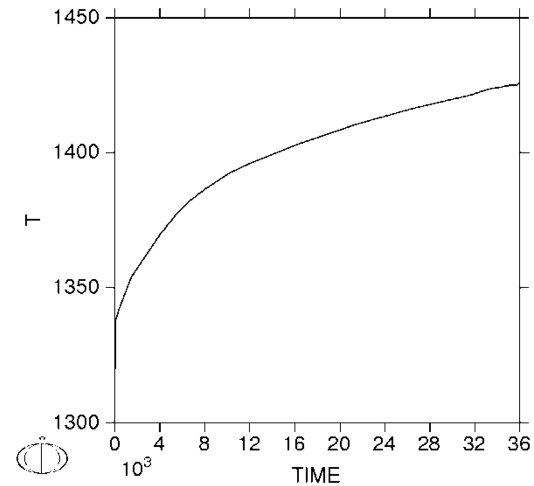


A: γ+cem

Target:
10 K below T_m







See also: Warnken, Larsson, Reed, Mat Sci Tech 25(2009)179

Summary

- ❑ New moving phase boundary model implemented in Dictra
  - ✓ More robust, but also much slower, than classic model
  - ✓ Simulations can be set up in a very general way

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Thank You!