

Thermo-Calc Software

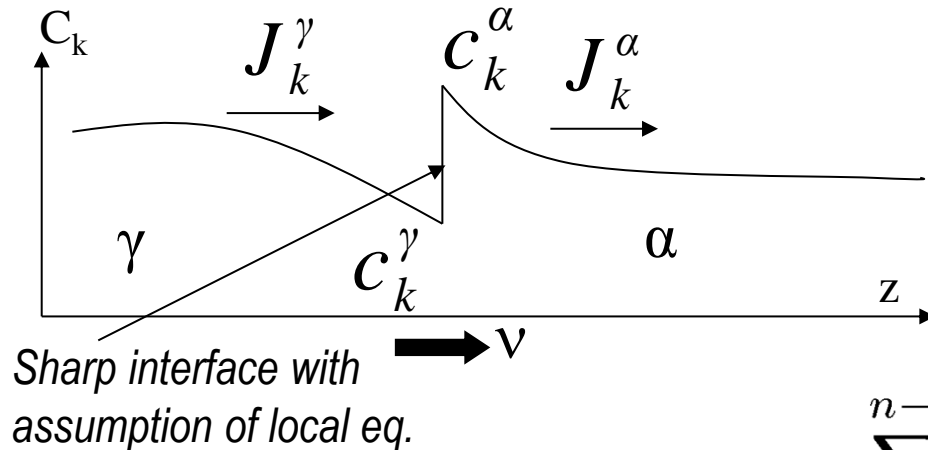
A new general model for diffusion controlled growth in DICTRA

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



n-1 Flux Balance Equations:

$$v (c_k^\alpha - c_k^\gamma) = J_k^\alpha - J_k^\gamma$$

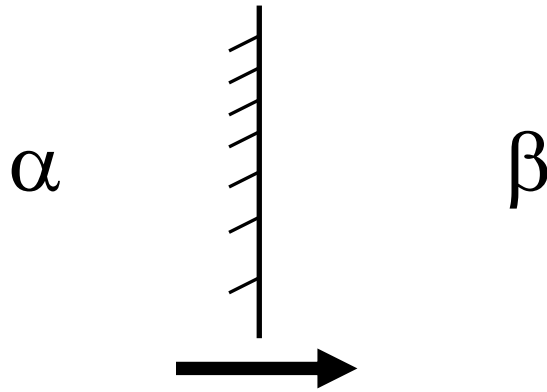
F-B Equations solved as:

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

- ❑ 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.

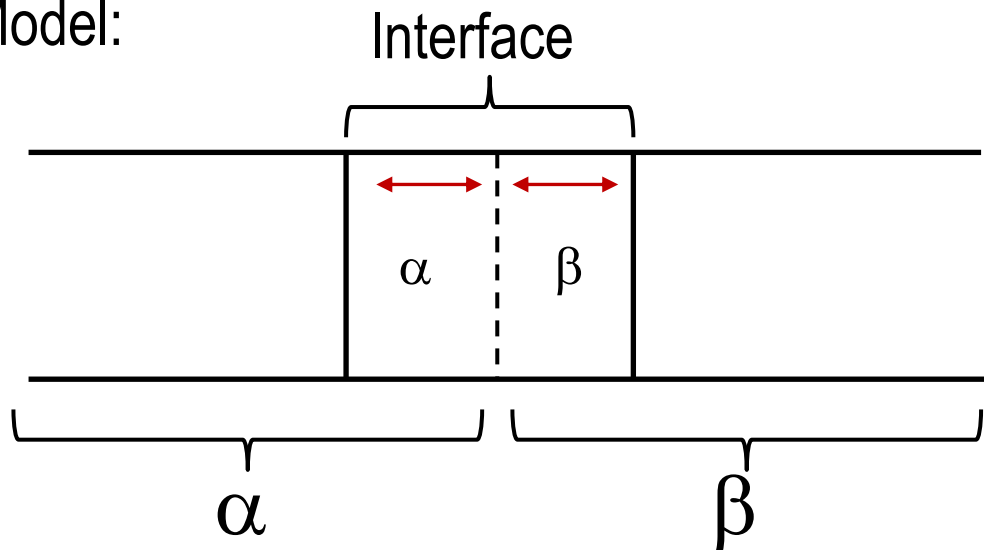
New moving phase boundary model



Model assumptions:

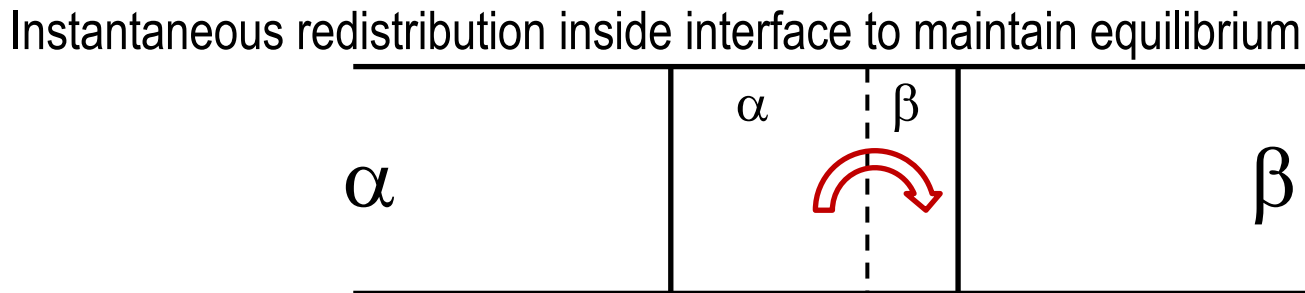
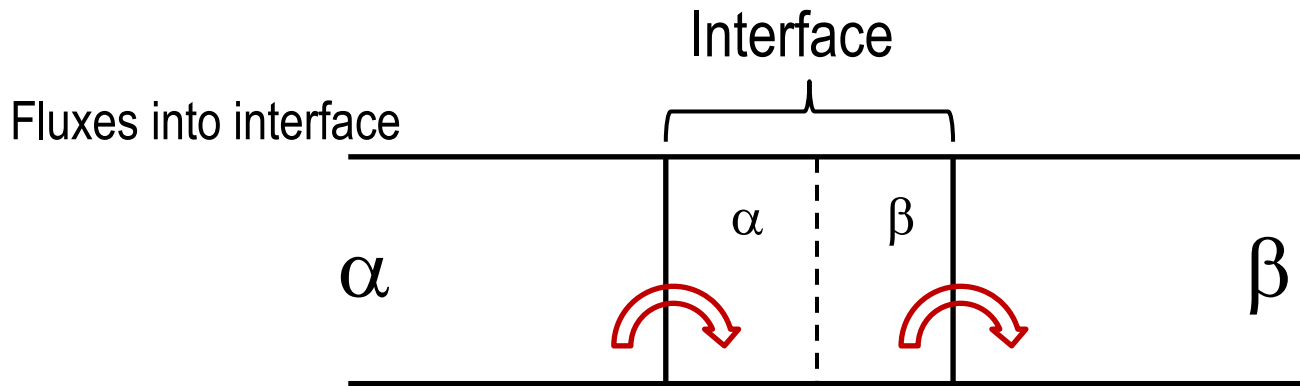
- Interfaces have a constant, finite width
- Local equilibrium holds at / in interfaces
- Infinitely fast kinetics in interfacial finite volume

Model:

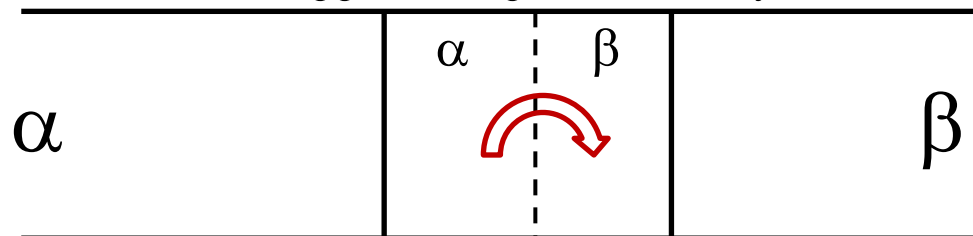


The interfacial finite volume extends the same distance into both phases; it contains 50% α and 50% β

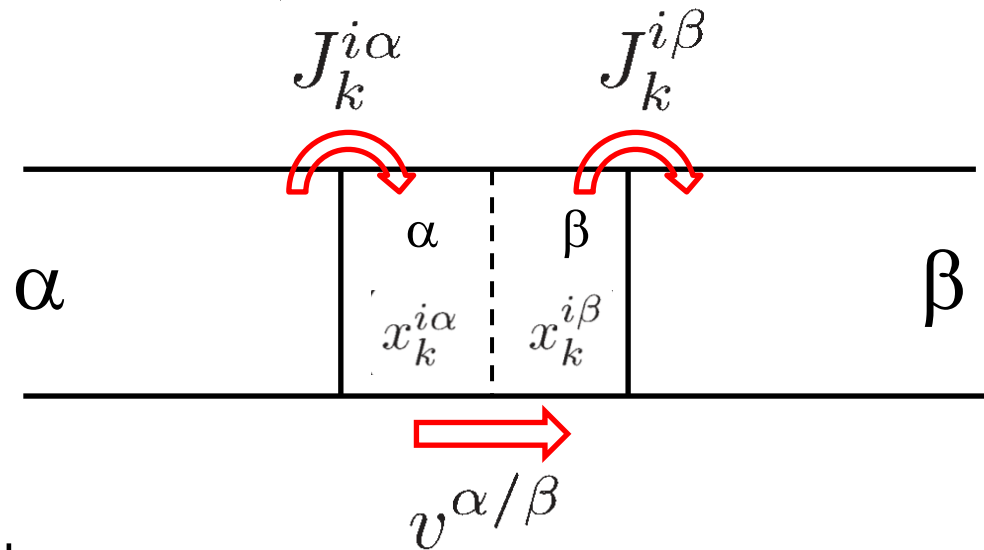
Conceived sequence of events leading to interface migration



The interface finite volume is dragged along convectively



Volume-fixed fluxes:



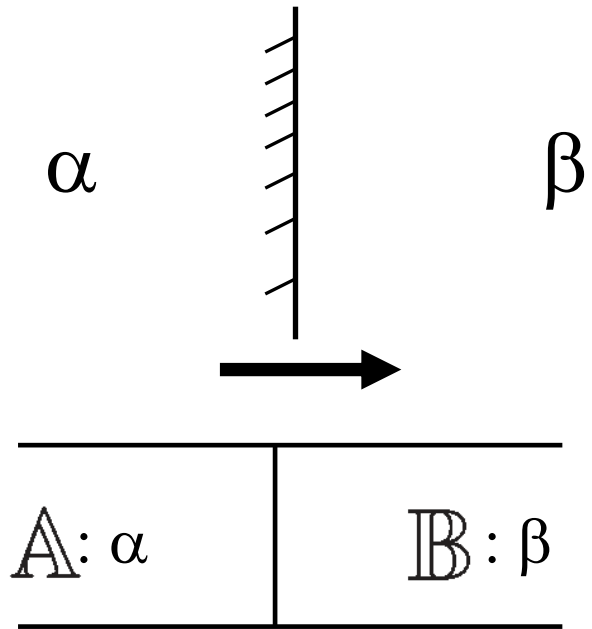
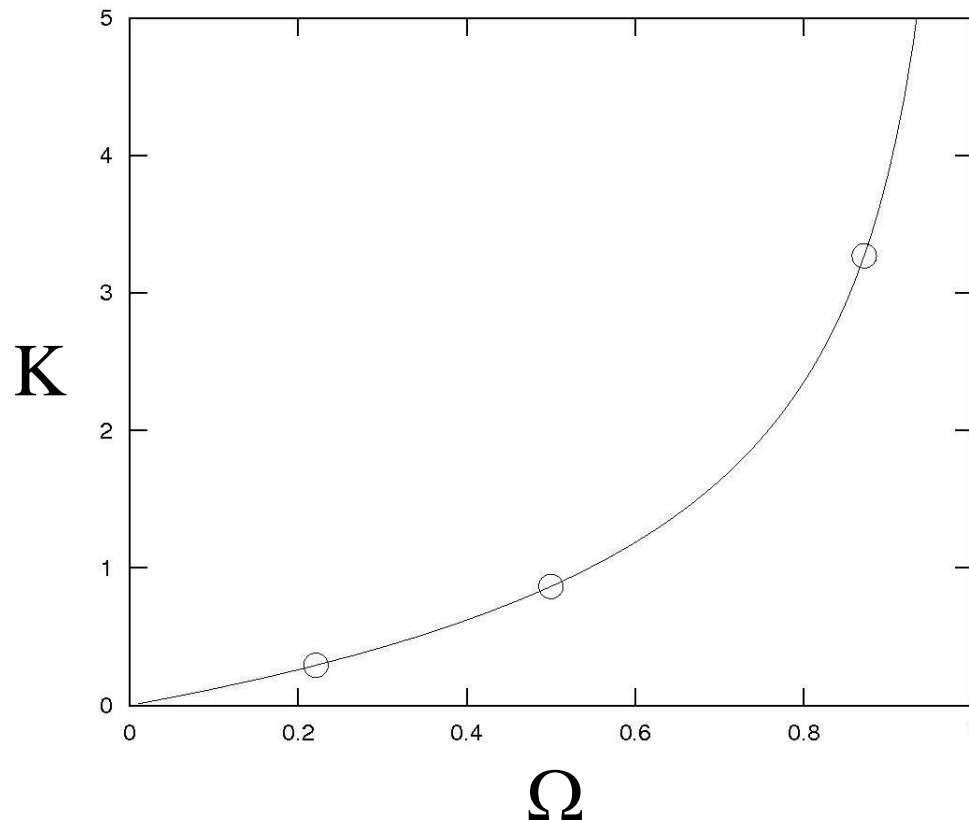
Interface velocity given by:

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

Validation – analytical case

Binary system, ideal solutions
Growth of α from supersaturated β

Circles: simulation
Line: analytical solution



α thickness S

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

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

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

”Classic” DICTRA moving phase boundary model

Sharp (zero width) interface

Find state at interface by solving set of flux balance equations

$$v (c_k^\alpha - c_k^\gamma) = J_k^\alpha - J_k^\gamma$$
$$k = 1, \dots, n - 1$$

Finite element method (FEM)

Fast and efficient

New model

Finite width interface

Explicit expression for interface velocity

Finite volume method (FVM)

Robust

Automatic switching between the models implemented

New moving phase boundary model

Generalize

Three sets of phases:

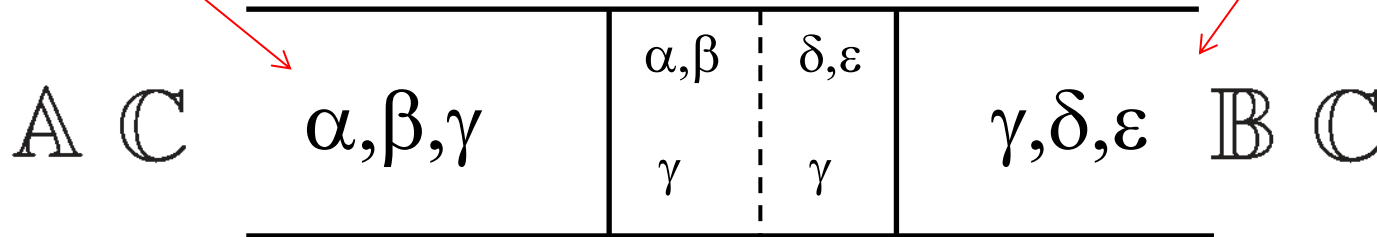
\mathbb{A} : α, β Allowed only on the left side of the interface

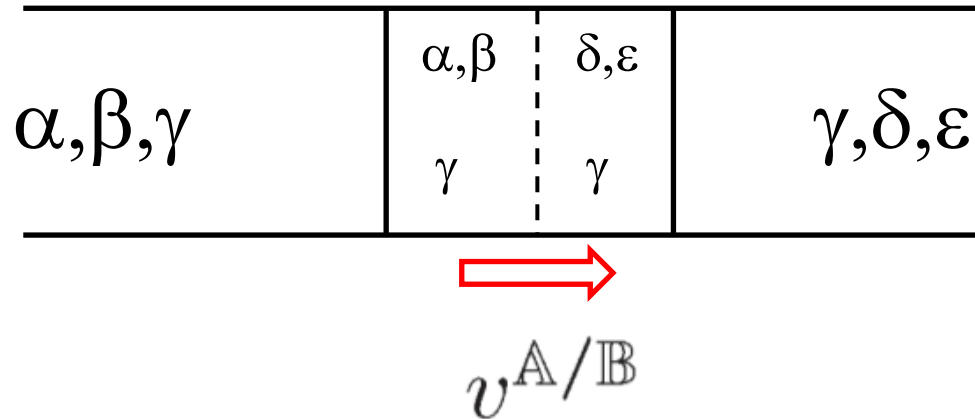
\mathbb{B} : δ, ε Allowed only on the right side of the interface

\mathbb{C} : γ Allowed on both sides of the interface

Multiphase mixture
 α, β, γ allowed

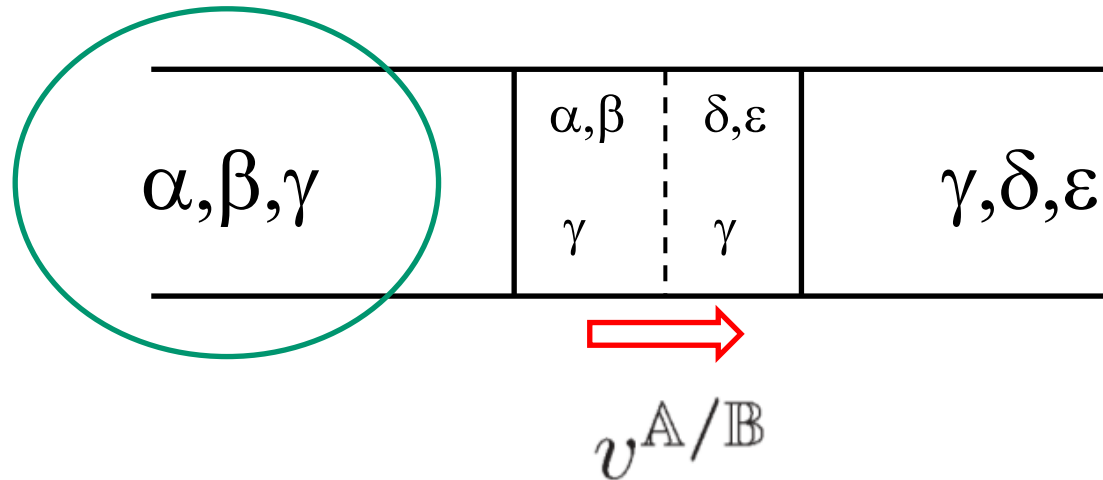
Multiphase mixture
 $\gamma, \delta, \varepsilon$ allowed





Interface velocity given by:

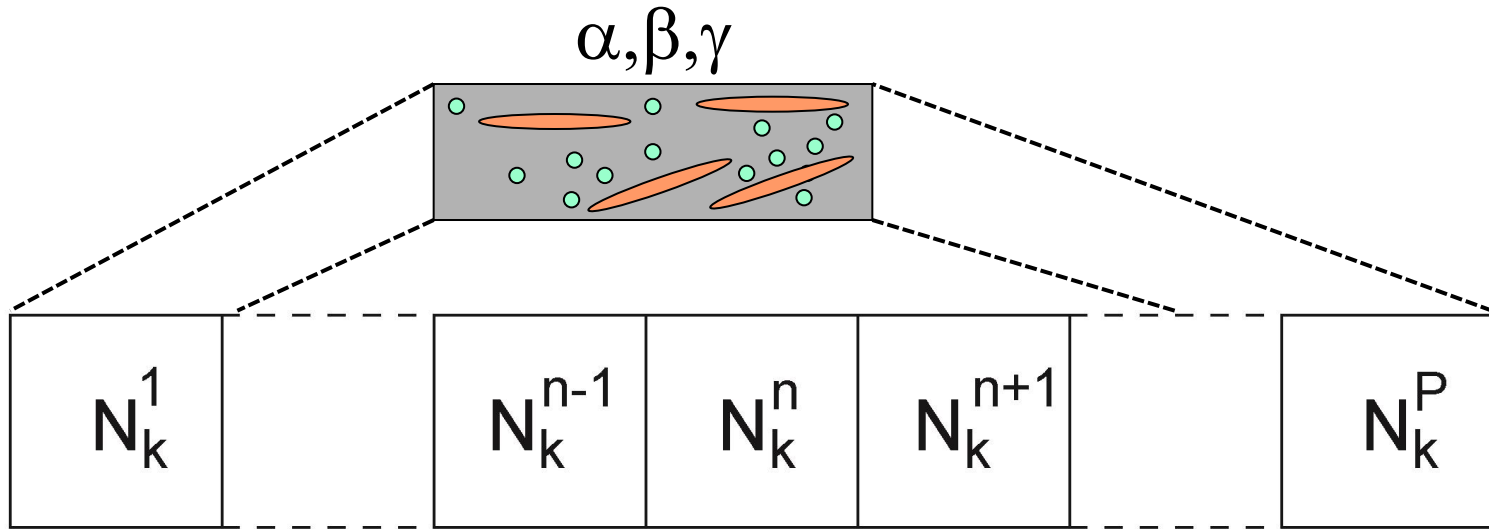
$$\frac{v^{A/B}}{V_S} = \frac{\sum_{\alpha \in A} \sum_k \frac{\partial f^\alpha}{\partial N_k} [J_k^{iA} A(z^{iA}) - J_k^{iB} A(z^{iB})] - \sum_{\delta \in B} \sum_k \frac{\partial f^\delta}{\partial N_k} [J_k^{iA} A(z^{iA}) - J_k^{iB} A(z^{iB})]}{\sum_{\alpha \in A} \sum_k \frac{\partial f^\alpha}{\partial N_k} [u_k^{iA} A(z^{iA}) - u_k^{iB} A(z^{iB})] - \sum_{\delta \in B} \sum_k \frac{\partial f^\delta}{\partial N_k} [u_k^{iA} A(z^{iA}) - u_k^{iB} A(z^{iB})]}$$



Interface velocity given by:

$$\frac{v^{A/B}}{V_S} = \frac{\sum_{\alpha \in A} \sum_k \frac{\partial f^\alpha}{\partial N_k} [J_k^{iA} A(z^{iA}) - J_k^{iB} A(z^{iB})] - \sum_{\delta \in B} \sum_k \frac{\partial f^\delta}{\partial N_k} [J_k^{iA} A(z^{iA}) - J_k^{iB} A(z^{iB})]}{\sum_{\alpha \in A} \sum_k \frac{\partial f^\alpha}{\partial N_k} [u_k^{iA} A(z^{iA}) - u_k^{iB} A(z^{iB})] - \sum_{\delta \in B} \sum_k \frac{\partial f^\delta}{\partial N_k} [u_k^{iA} A(z^{iA}) - u_k^{iB} A(z^{iB})]}$$

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



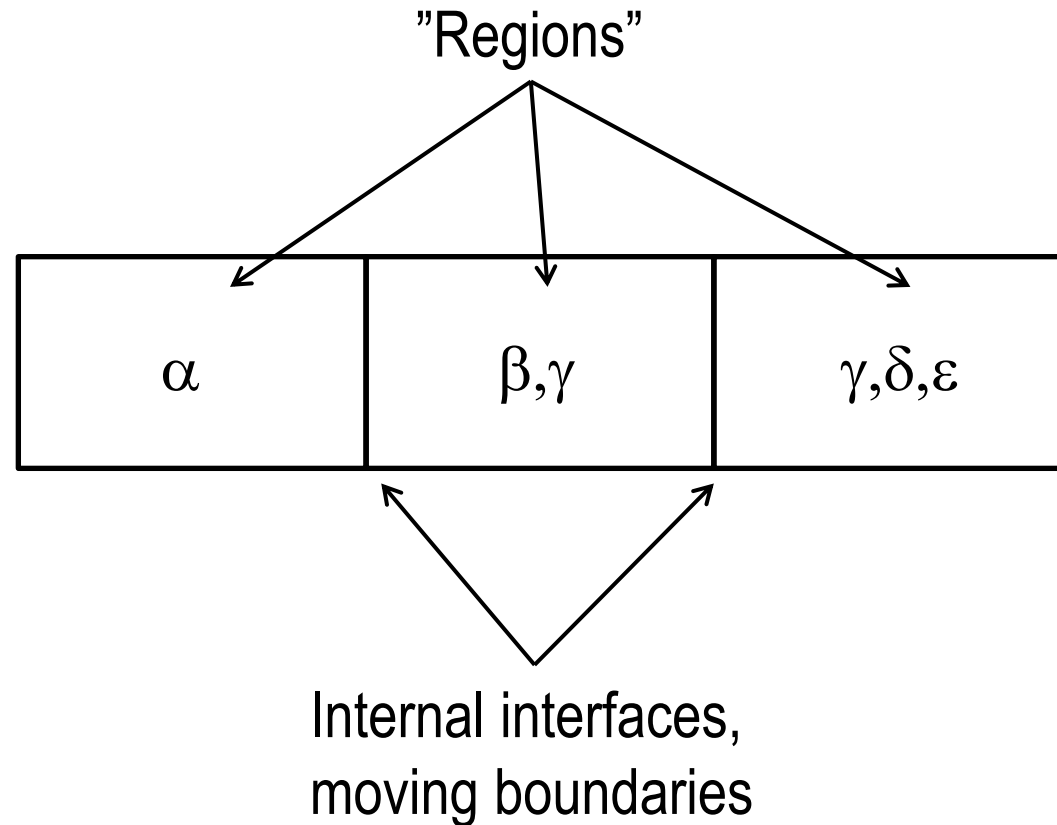
Equilibrium calculation
for each slice

Phase fractions
Phase compositions
Chemical potentials
Mobilities

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

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

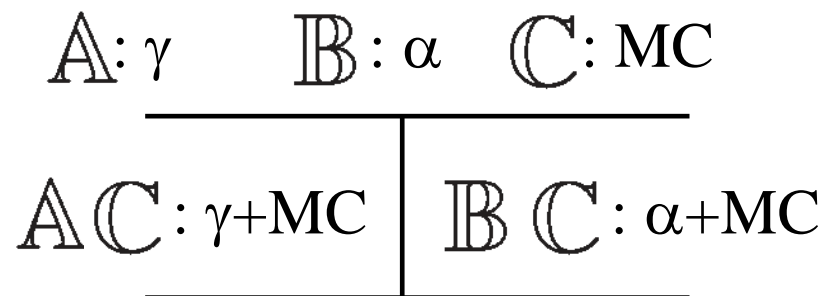
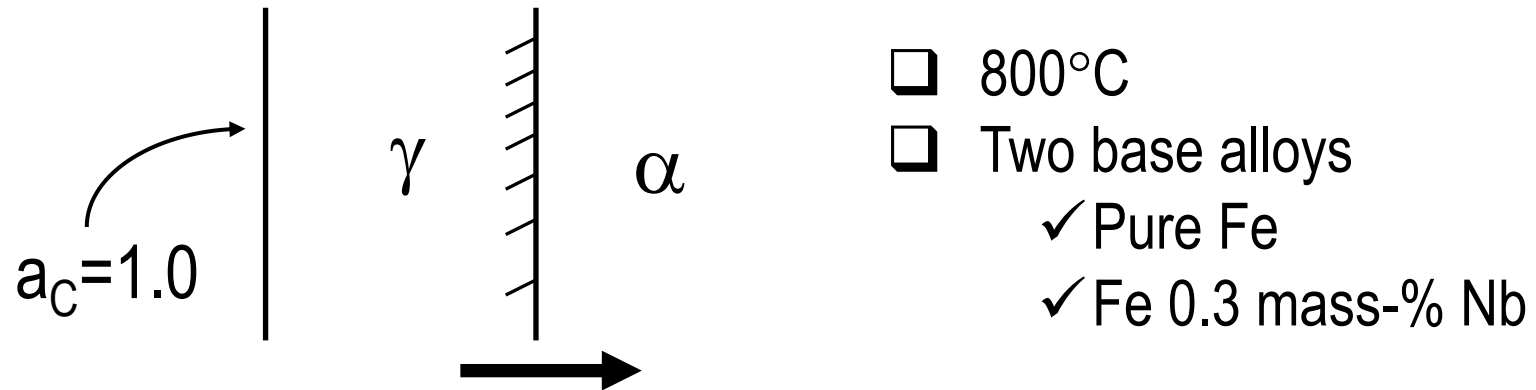
"Effective" $[M_k x_k]$ from combining rules



Arbitrary set of
phases in each region

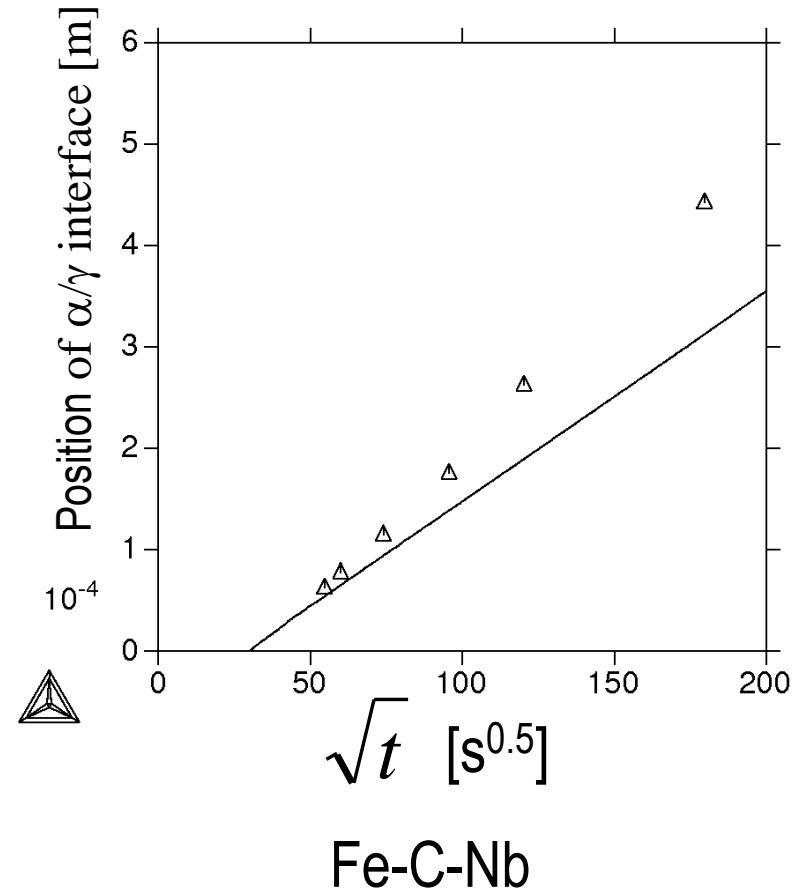
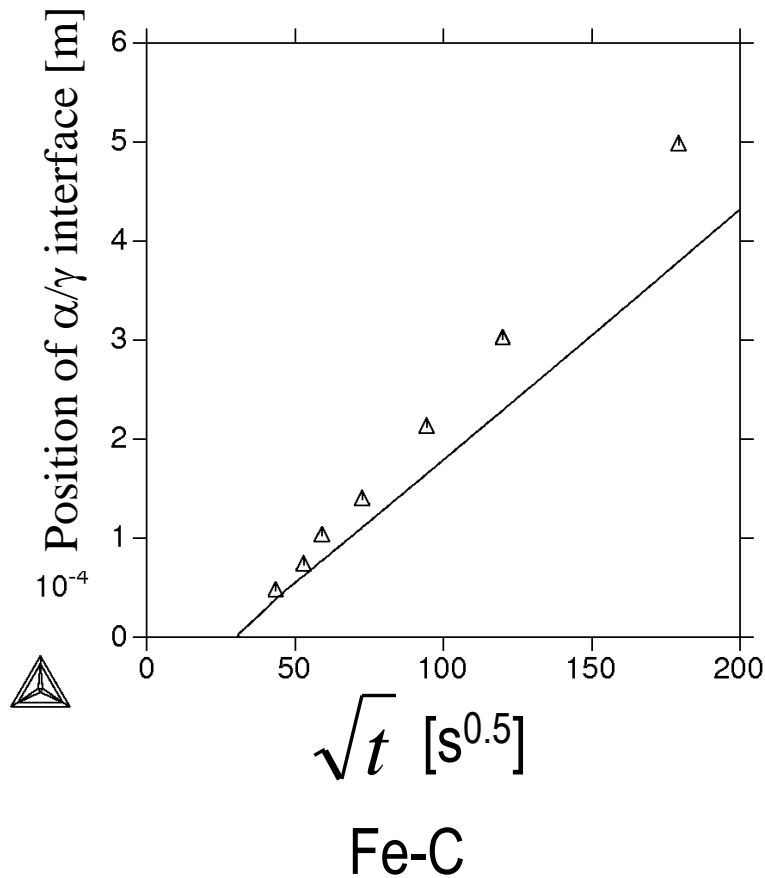
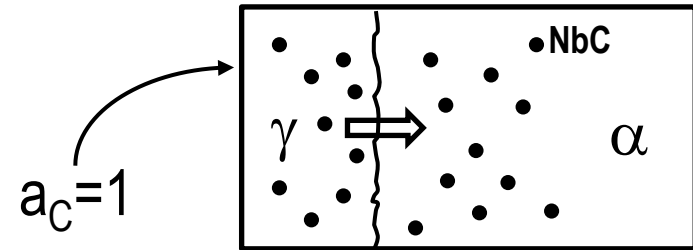
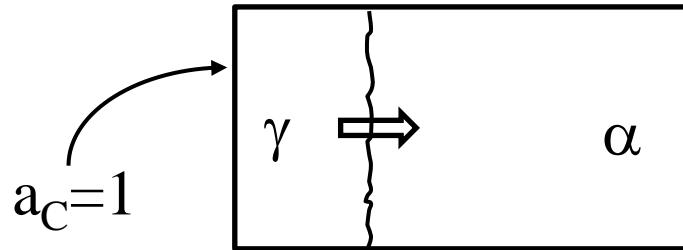
Remaining requirement: one unique phase in each region

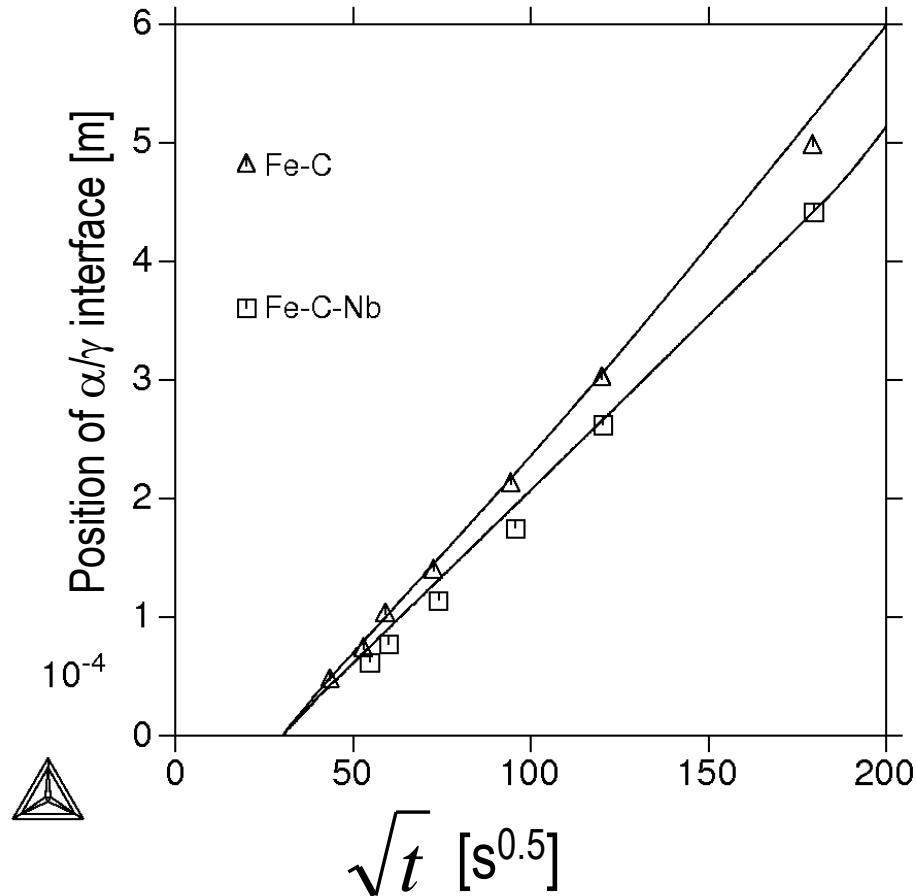
Carburization of steel accompanied by $\alpha \rightarrow \gamma$ transformation



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

Carburization of steel





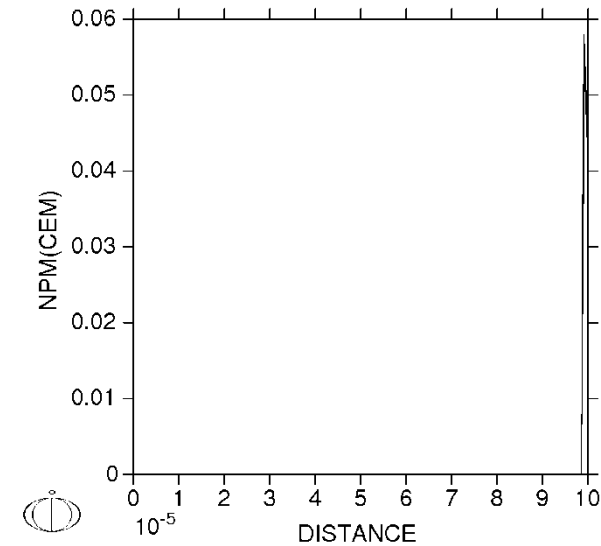
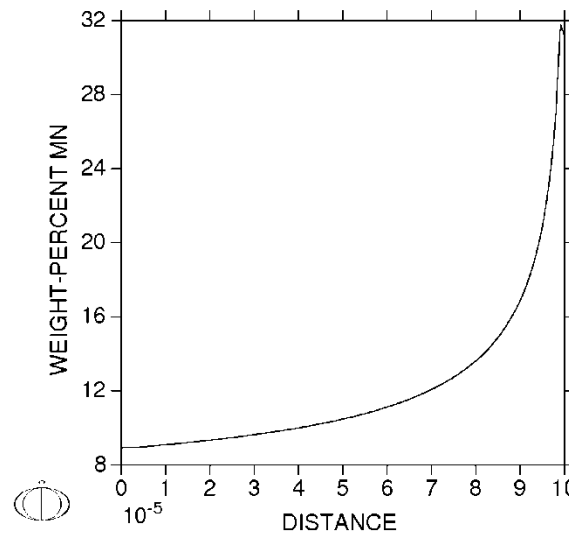
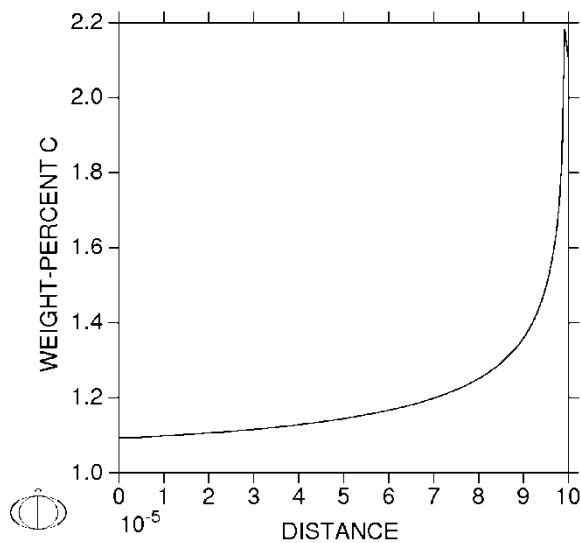
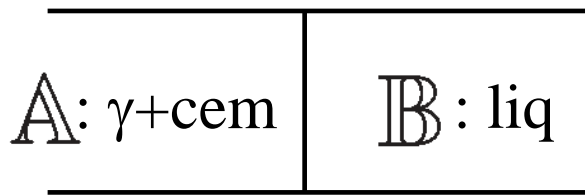
Increased mobility of carbon in austenite and ferrite by factor 2

Solidification and homogenizing

Hadfield steel Fe 1.2 C 12 Mn

100 μm domain

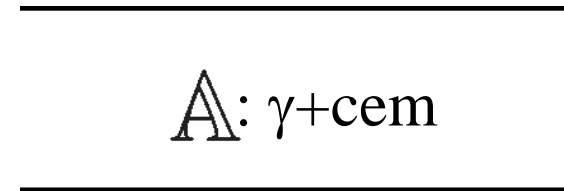
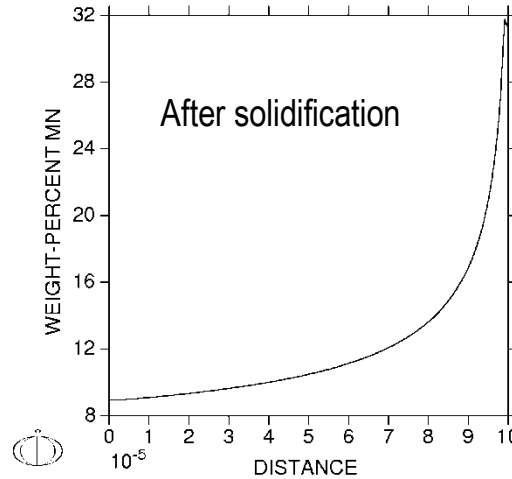
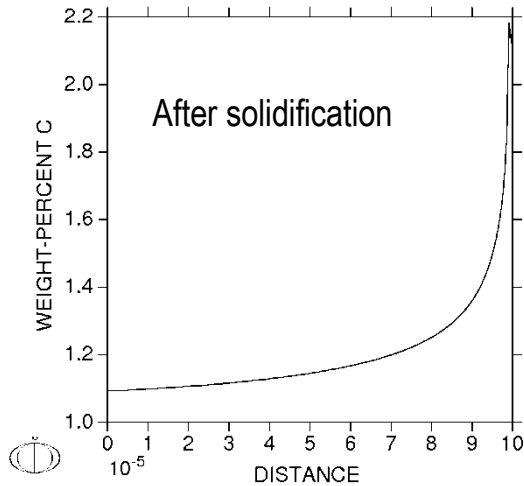
Cooling rate 1 K/s during solidification



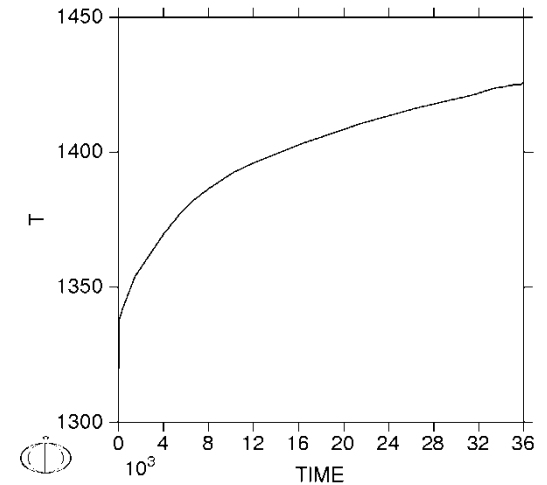
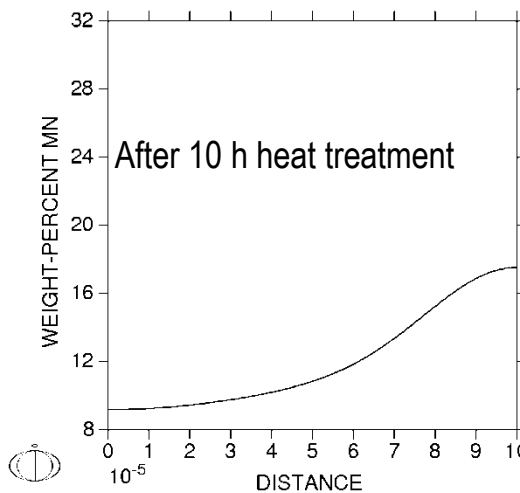
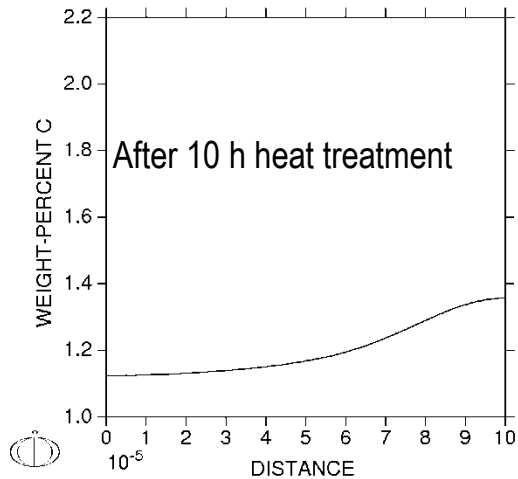
Profiles after solidification

Solidification and homogenizing

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

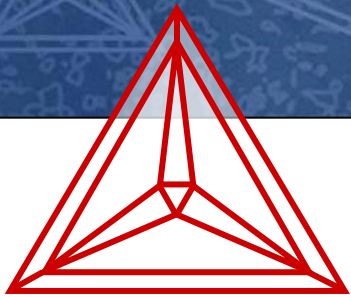


Target:
10 K below T_m



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

- ❑ 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



Thermo-Calc Software

Thank You!