
# Introduction of Dictra

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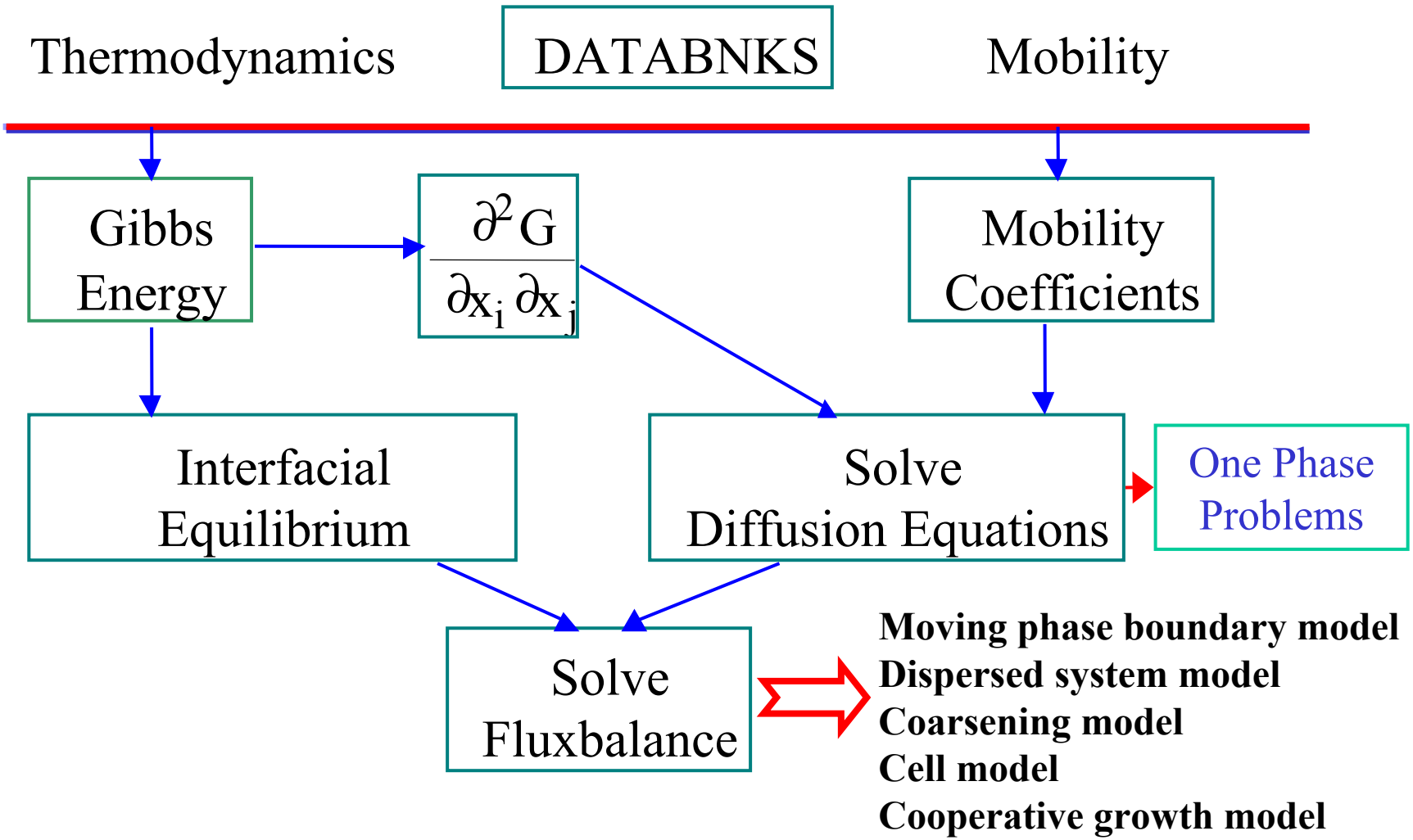
With help from Thermo-Calc Software, Stockholm, Sweden

# What is DICTRA?

- Software package for simulation of diffusional reactions in multicomponent alloys.

- The result of more than 20 years and 60 man-years R&D at KTH in Stockholm, Sweden, in cooperation with the Max-Planck Institute für Eisenforchung in Düsseldorf, Germany.

# Numerical Procedure of Dictra



# Features

- Linked to Thermo-Calc for thermodynamics
  - Has all modules in Thermo-Calc plus a Dictra module.
- Based on thermodynamics and mobility databases.
  - Quantitative description of multicomponent diffusion
  - Mobility for simple phases and *ordered B2 phase*
  - Diffusion through stoichiometric phases (*new in Version 22*)
- Written in FORTRAN, using finite difference method, runs on most plattforms.
- Geometry: One dimensional
- Three types of phase interface
  - Local equilibrium
  - Finite interface mobility
  - Interfacial energy

# Atomistic Treatment of Diffusion

- For crystalline phases it's usually believed that diffusion occurs through a vacancy exchange mechanism.
- Assuming that there is a random distribution of vacant sites and that the number of vacancies is everywhere adjusted to equilibrium, it's possible to derive the following expression for the flux of k in a lattice-fixed frame of reference:

$$J_k^L = -c_k y_{va} M_{kva} \nabla \mu_k$$

  - where $M_{kva}$ is some kinetic factor which gives the rate of exchange if there is a vacancy adjacent to a k atom.

# Phenomenological equations

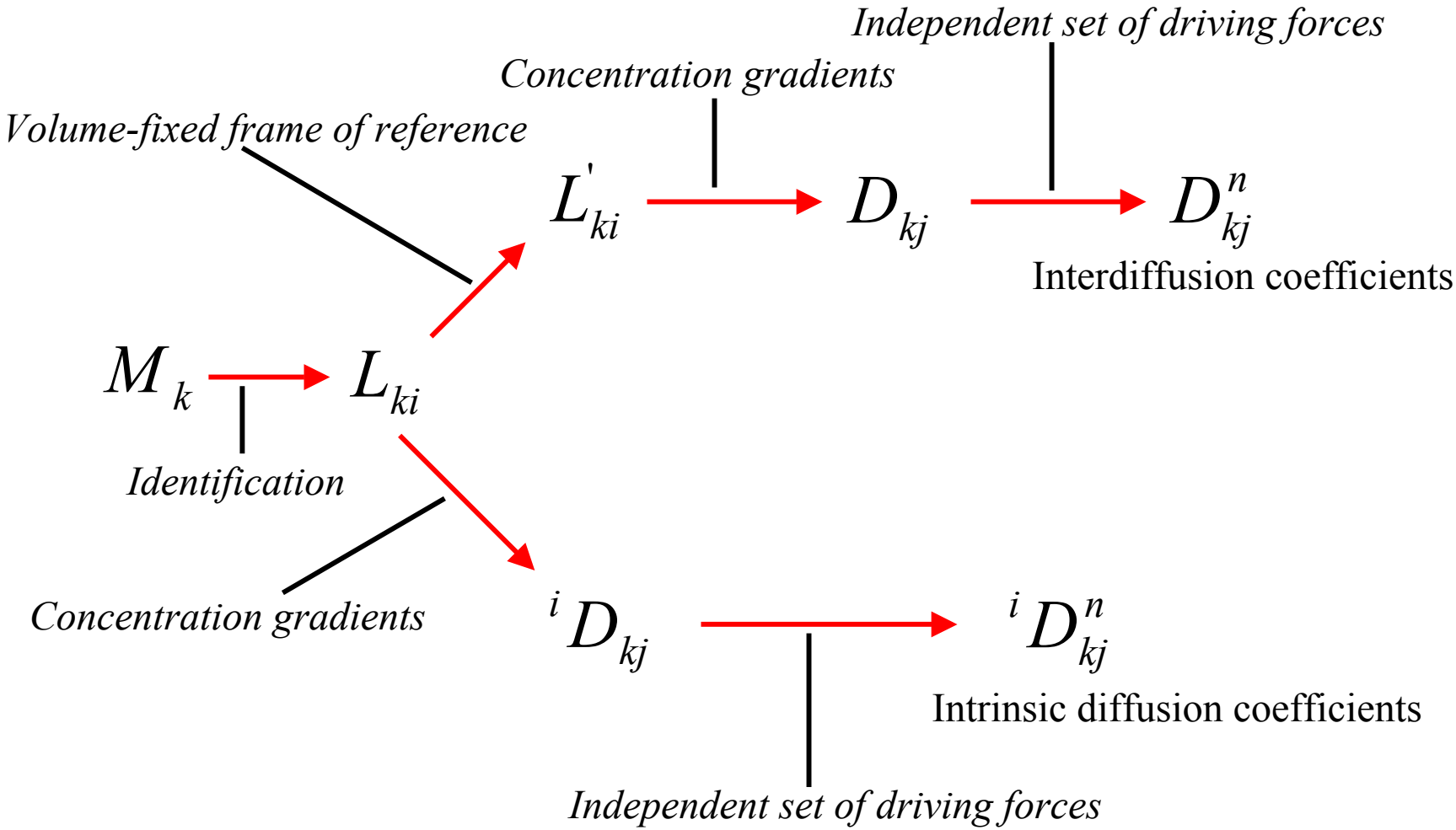
$$J_k^L = -\sum_{i=1}^{n} L_{ki} \frac{\partial \mu_i}{\partial z} - L_{1T} \frac{\partial T}{\partial z} - L_{1P} \frac{\partial P}{\partial z} - L_{1\phi} \frac{\partial \phi}{\partial z}$$

They are called phenomenological since they steam from no model, but from the observed conditions of equilibrium.

If we choose to consider an isothermal, isobaric and isopotential system we have:

$$J_k^L = -\sum_{i=1}^{n} L_{ki} \frac{\partial \mu_i}{\partial z} \qquad \left( J_k^L = -L_{kk} \frac{\partial \mu_k}{\partial z} \right)$$

# From Mobility to Diffusibity



# Kinetic databases

**Possible experimental information**

$^{i}D_{kj}^{n}$ **Intrinsic diffusion coefficient**

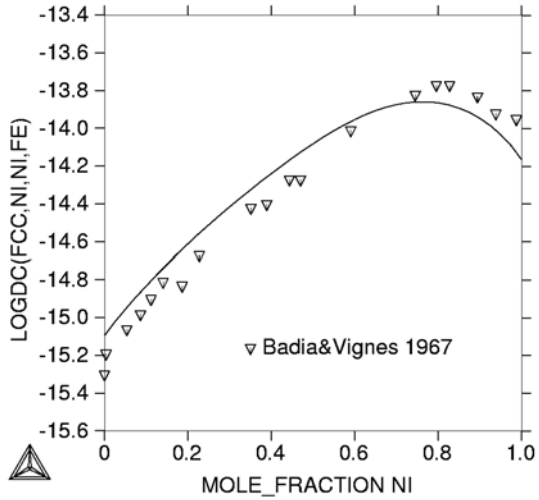
DI(phase,k,j,n)
LOGDI(phase,k,j,n)

$D_{A}^{*}$ **Tracer diffusion coefficient**

DT(phase,A)
LOGDT(phase,A)

$\tilde{D}_{kj}^{n}$ **Interdiffusion coefficient**

DC(phase,k,j,n)
LOGDC(phase,k,j,n)



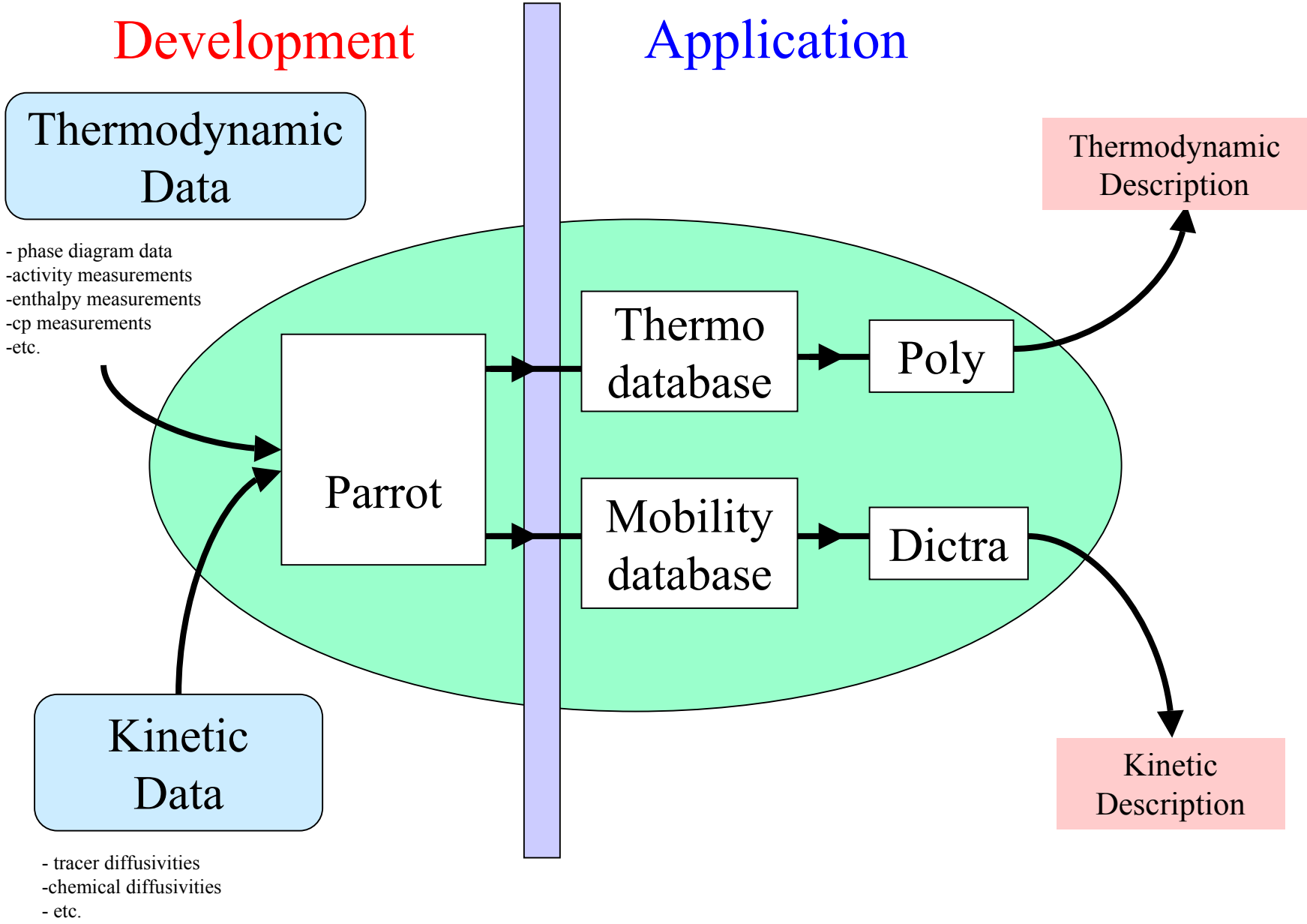

**Kinetic database**

$$RT\ln(RTM_i)$$

# Modeling

$$M_i = \frac{1}{RT}\exp\left(\frac{\Delta G_i}{RT}\right) \qquad \Delta G_i = -Q_i + RT\ln(M_i^0)$$

$$\Delta G_i = \sum_j \sum_m y_j^I y_m^{II} \Delta G_i^{j:m} + \sum_j \sum_{k>j} \sum_m y_j^I y_k^I y_m^{II} \Delta G_i^{j,k:m}$$
$$+ \sum_j \sum_n \sum_{m>n} y_j^I y_n^{II} y_m^{II} \Delta G_i^{j:n,m}$$


Development
Application
Thermodynamic Data
- phase diagram data
-activity measurements
-enthalpy measurements
-cp measurements
-etc.
Parrot
Thermo database
Mobility database
Poly
Dictra
Thermodynamic Description
Kinetic Data
- tracer diffusivities
-chemical diffusivities
- etc.
Kinetic Description

# Modeling Steps

- Understand the system and select experimental data
  - Search and read all references
- Create a setup file for the system
  - Define parameters
- Create an experimental data file
  - Make a pop file (or called dop file)
- Evaluate mobility model parameters
  - Use Parrot
- Compare experimental and calculated results
  - Use Dictra module
- Make a mobility database
  - add to an existing database

# Mobility Databases

## MOB2

The most general diffusion database

Could be used for Steels/Fe_alloys, Ni-alloys,Al-based alloys, and more.

75 Elements: Ag, Al, Am, As, Au, B, Ba, Be, Bi, C, Ca, Cd, Co, Cr, Cs, Cu, Dy, Er, Fe, Ga, Gd, Ge, Hf, Hg, Ho, In, Ir, K, La, Li, Lu, Mg, Mn, Mo, N, Na, Nb, Nd, Ni, Np, Os, P, Pa, Pb, Pd, Pr, Pt, Pu, Rb, Re, Rh, Ru, S, Sb, Sc, Se, Si, Sm, Sn, Sr, Ta, Tb, Tc, Te, Th, Ti, Tl, Tm, U, V, W, Y, Yb, Zn and Zr

Phases with diffusion data: **BCC_A2, CEMENTITE, FCC_A1, FE4N, HCP_A3, LIQUID**

*Assessed data for the following binary systems*

**BCC_A2: C-Fe, C-Cr, Cr-Fe, Cr-N, Cr-Ni, Fe-N, Fe-Ni**
**FCC_A1: Al-Cr, Al-Ni, C-Fe, C-Ni, Cr-Fe, Cr-Ni, Fe-N, Fe-Ni, Fe-Si**
**HCP_A3: C-Fe, Fe-N**
**FE4N: C-Fe, Fe-N**

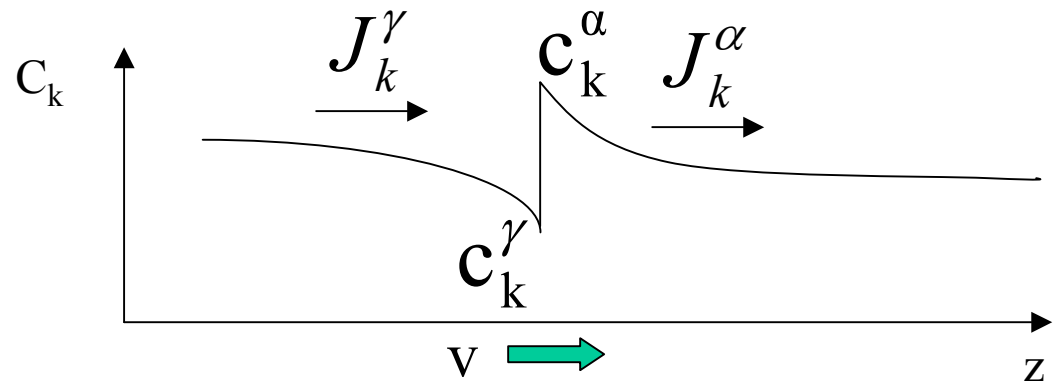
*Assessed data for the following ternary systems*

**BCC_A2: C-Cr-Fe**
**FCC_A1: Al-Cr-Ni, C-Cr-Fe, C-Fe-Ni**

*Assessed data for the following higher order systems*

**BCC_A2: C-Cr-Fe-N-Ni**
**FCC_A1: C-Cr-Fe-Ni**

# Sharp Interface

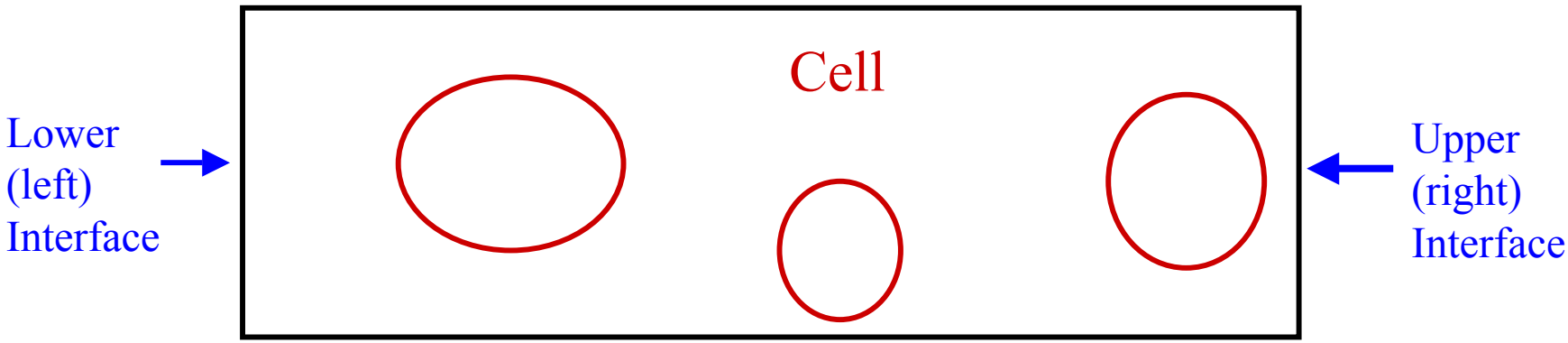



Unknowns: Tie-line, specified by n-2 $a_i$ or $\mu_i$
Velocity of phase boundary, v

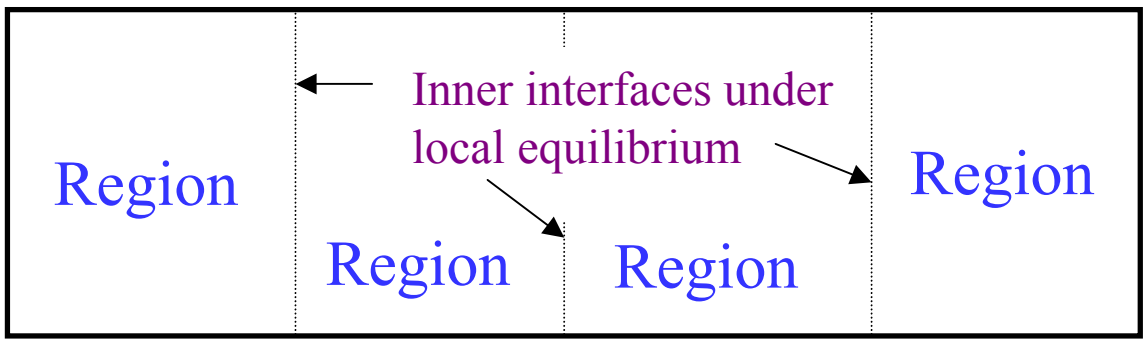
Equations: n-1 flux-balance equations, $v(c_k^\alpha - c_k^\gamma) = J_k^\alpha - J_k^\gamma$

Software: Dictra

# System


Cell
Lower
(left)
Interface
Upper
(right)
Interface

# Cell


Inner interfaces under
local equilibrium
Region
Region
Region
Region

# Boundary conditions in DICTRA

- **Boundary Conditions can be specified as functions of time, temperature and pressure.**
- **Different functions may be used in different time intervals.**

**Example of conditions are:**

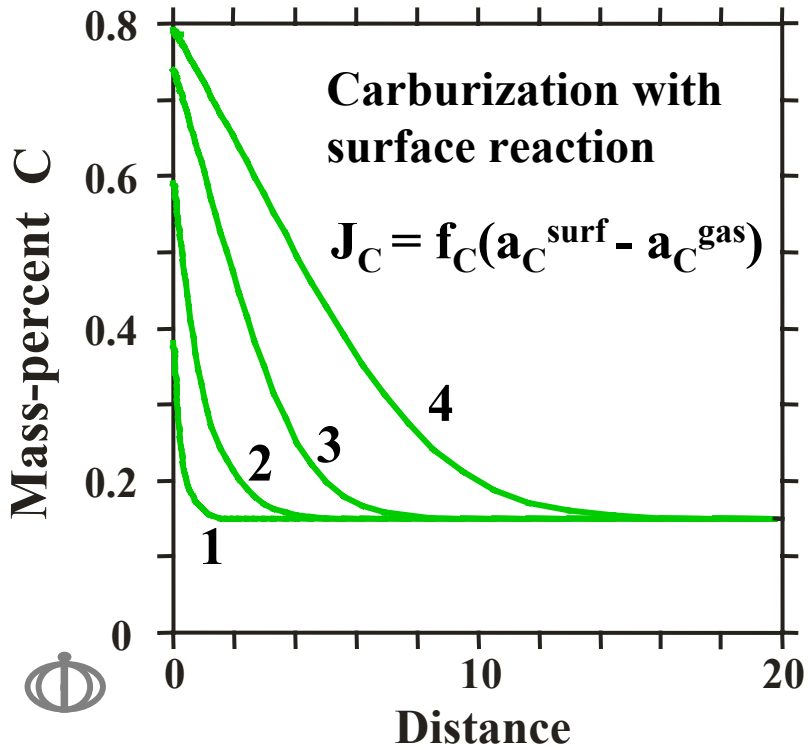
– Closed system (default)

– Sate variable expressions

– Flux conditions

– Mixed conditions

**Application example:**

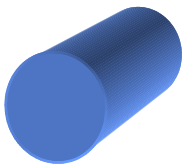


# ENTER_GEOMETRICAL_EXPONENT

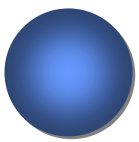
Command that determines the geometry of the system. The program handles problems that can be reduced to 1-dimensional geometries. Default value is zero, i.e. planar geometry.

Exponent Geometry

**0** **Planar geometry.**
This corresponds to an infinitely wide plate of a certain thickness.



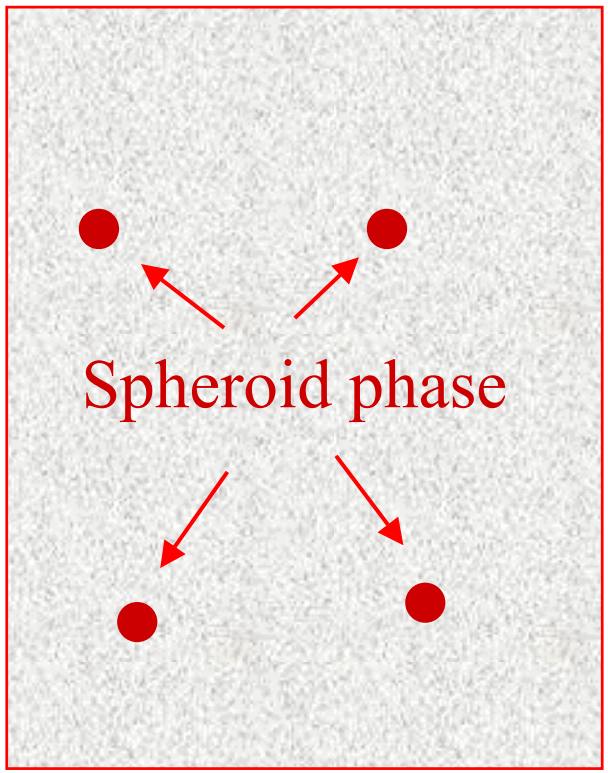
**1** **Cylindrical geometry.**
This corresponds to an infinitely long cylinder of a certain radius.



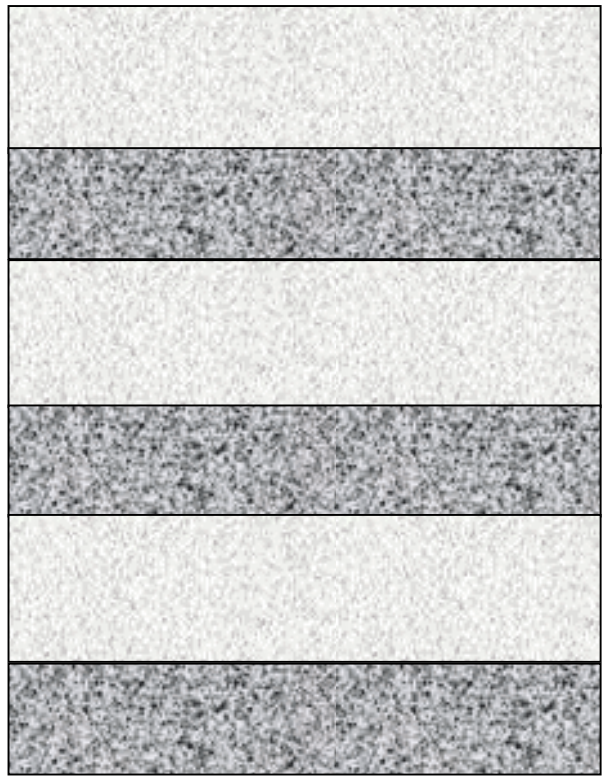
**2** **Spherical geometry.**
A sphere with a certain radius.

# Region

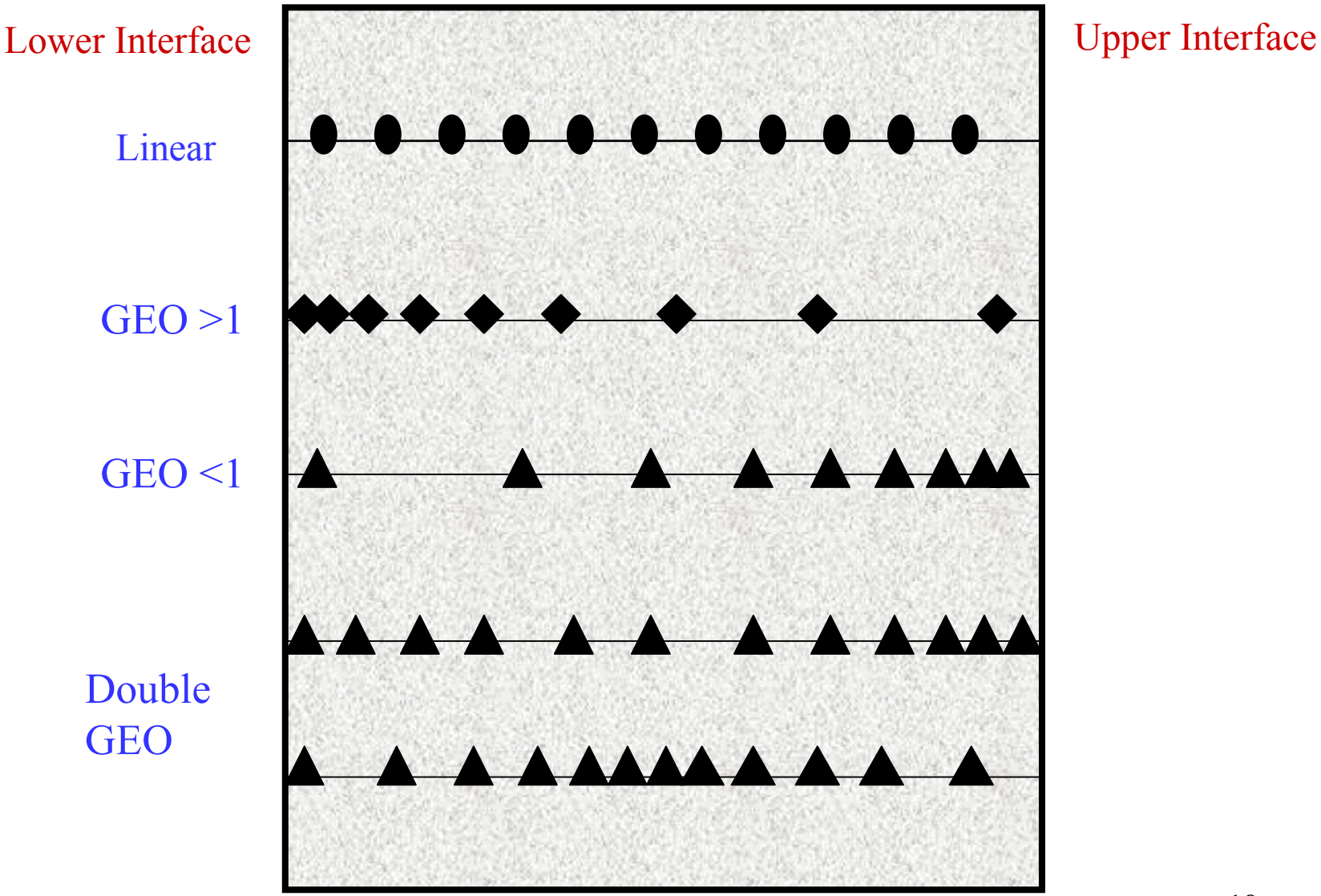
Matrix phase




Lamella phase



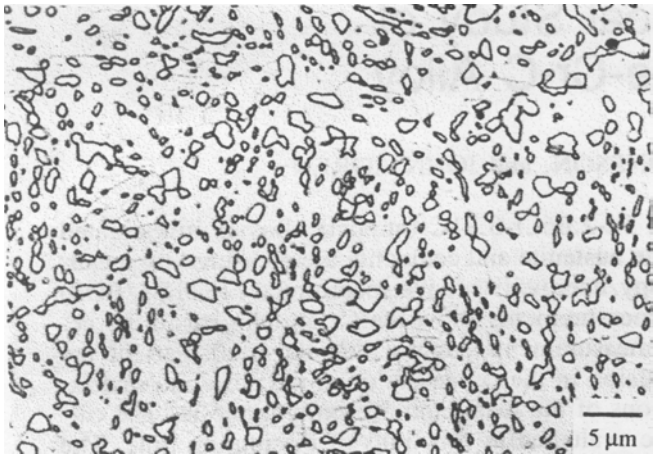
# Grid points

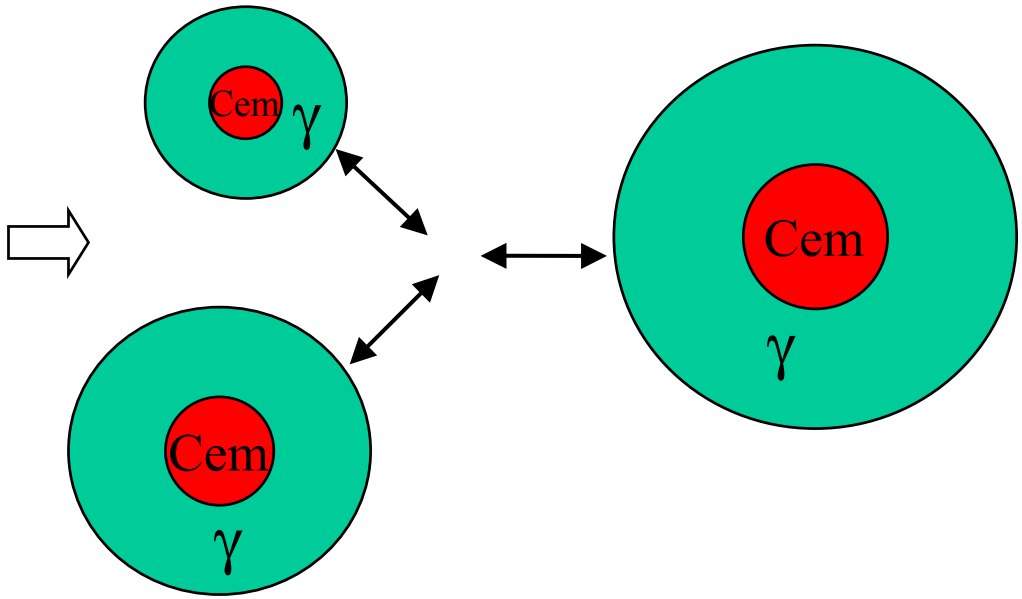

Lower Interface
Upper Interface
Linear
GEO >1
GEO <1
Double GEO

# Cementite dissolution in a Fe–Cr-C alloy

## Cell calculation with size-distribution

Dissolution of cementite at 910C (or 1183K):

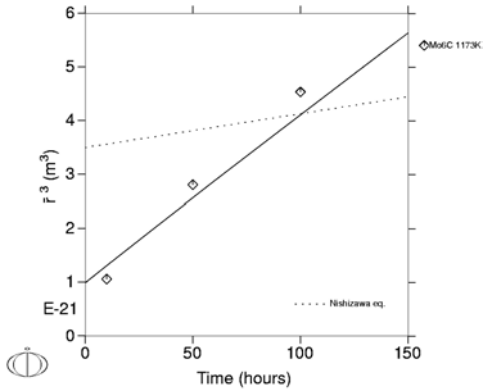


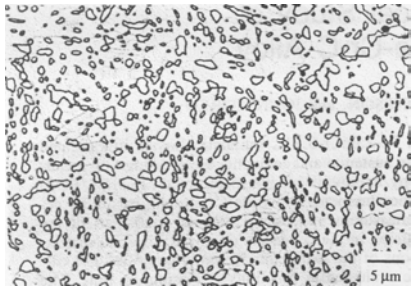

Instead of assuming an average particles size as in previous example, we will perform the simulation for a particle distribution using three cells of different sizes.

# Some DICTRA applications

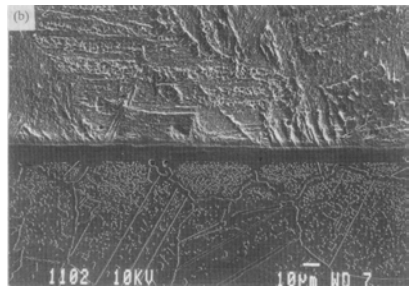
## Coarsening



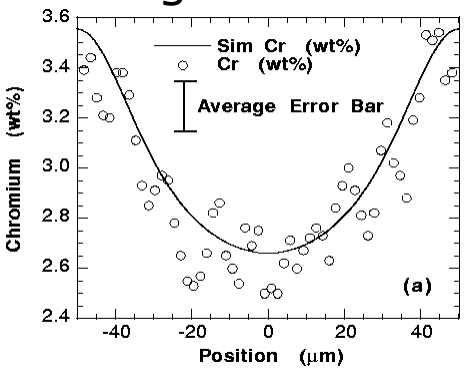

## Carbide dissolution




## Carbon diffusion in a weld between two steels

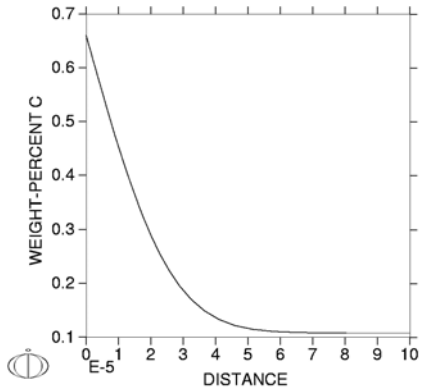



## Microsegregation during solidification




Lippard et al. *Metall. Mater. Trans. B* 1998

## Carburizing



# More DICTRA applications

- Homogenisation of alloys
- Carburization and decarburization
- Carburization of alloys
- Nitriding of steels
- Diffusion during sintering of cemented carbides
- Nitrocarburizing of steels
- Austenite/ferrite diffusional transformations in steels
- Growth or dissolution of individual particles
- Transient liquid phase bonding of alloys
- Calculation of TTT-diagrams
- Interdiffusion between coating/substrate
- Coarsening of a particle distribution
- Gradient sintering of cemented carbides
- Growth of pearlite in alloyed steels
- Sigma phase precipitation in stainless steel
- Post weld heat treatment of welds between dissimilar materials

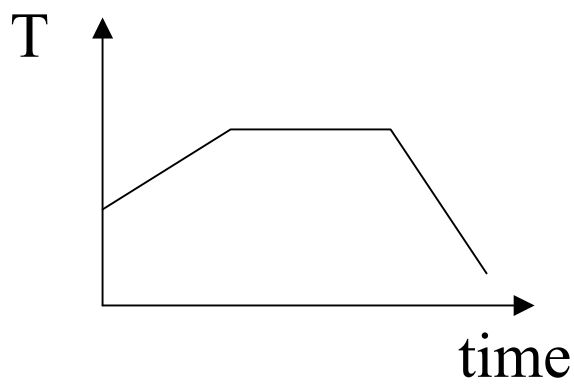
# Input of T and c

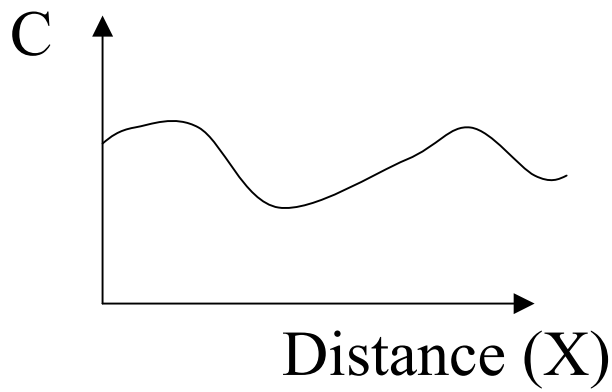
- Temperature (T) can be entered as a function of time

- Many different functions can be used (+, -, *, **, SQRT(X), EXP(X),LOG(X),SIN(X))

- Concentration can be entered as a function of distance or read from a file

- Many functions e.g. error-functions (erf(x)) and heavy-side step functions (hs(x))



# Summary

- DICTRA integrates the thermodynamic database and atomic mobility databases and solves one-dimensional diffusion equations in multicomponent systems.
- DICTRA can be used to develop atomic mobility databases using various experimental diffusion data.
- DICTRA can treat interface migrations with finite interfacial mobility and diffusion through stoichiometric phases.
- Any comments/questions, contact liu@matse.psu.edu.