COMSOL CONFERENCE 2016 BOSTON

Modeling Scheil Cooling – Thermodynamic and Multiphysics Simulation

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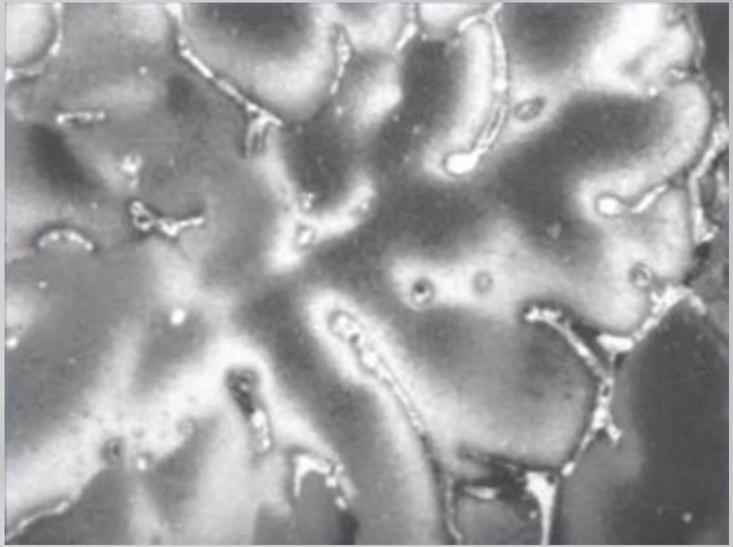
M4dynamics

Multicomponent Solidification

<u>The Problem</u>:

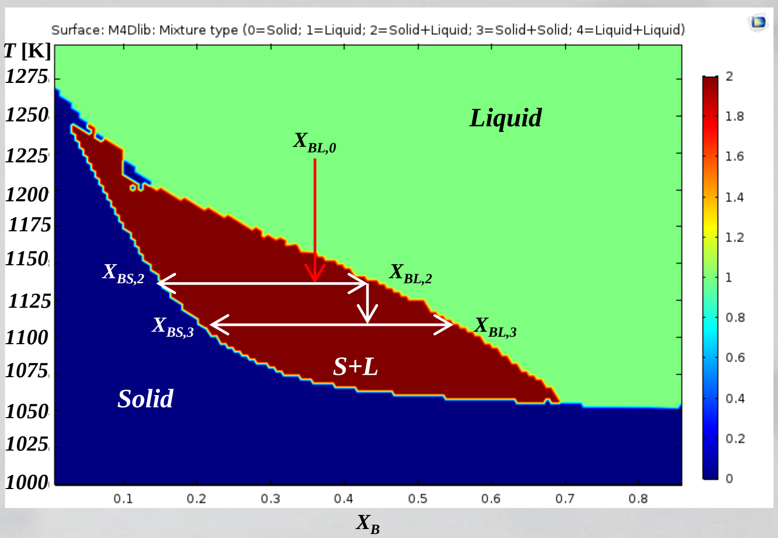
- Process depends on both Temperature and composition
- Most system are highly non-ideal (metal alloys, mattes, slags)
- During real solidification, solid doesn't equilibrate with residual liquid → non uniform solid concentration



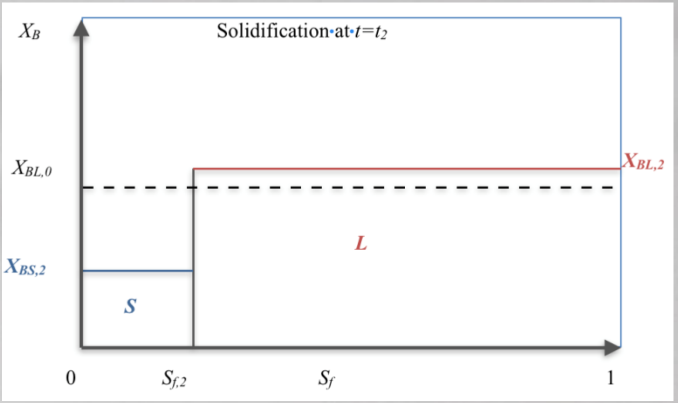
Coring in Al cast. Picture from Prof. David Dye, Imperial College, MSE104 course notes, 2012.

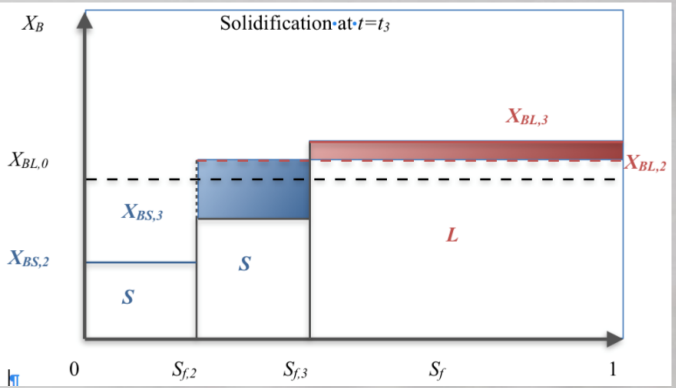
Multicomponent Solidification

- Rapid cooling Concept



Phase diagram for binary alloy, calculated in COMSOL using M4Dlib





Implementation in COMSOL

- The real solidification model was implemented using 0D ODE module → the same concept can later be applied to 1,2,3D
- Three variables were defined:
- T : Temperature $\frac{\partial T}{\partial t} = R$
- S : Solid fraction $S = S_f(T, X)$ ← from M4Dlib
- XB : Composition of component B $\frac{\partial X_{B,L}}{\partial t} = R_{B,L}$

Source Term: “enrichment”

- Balance from solidification from t_2 to t_3:

$$\left(S_{f,3} - S_{f,2}\right)\left(X_{BL,2} - X_{BS,3}\right) = \left(X_{BL,3} - X_{BL,2}\right)\left(1 - S_{f,3}\right)$$

↓

$$\frac{\partial X_{BL}}{\partial t} = \frac{(X_{BL} - X_{BS})}{L_f}\frac{\partial S_f}{\partial t}$$

Scheil Equations:

- Balance from solidification from t_2 to t_3:

$$(S_{f,3} - S_{f,2})(X_{BL,2} - X_{BS,3}) = (X_{BL,3} - X_{BL,2})(1 - S_{f,3})$$

$$K_{B_{S,L}} = \frac{X_{BS}}{X_{BL}}$$

$$(1 - K_{B_{S,L}}) \int_0^{S_f} \frac{dS_f}{(1 - S_f)} = \int_{X_{B0}}^{X_{BL}} \frac{dX_{BL}}{X_{BL}}$$

$$X_{BL} = X_{B0}(1 - S_f)^{(K_{B_{S,L}} - 1)}$$

$$X_{BS} = K_{B_{S,L}} \cdot X_{B0}\,(1 - S_f)^{(K_{B_{S,L}} - 1)}$$

Results – Scheil Cooling

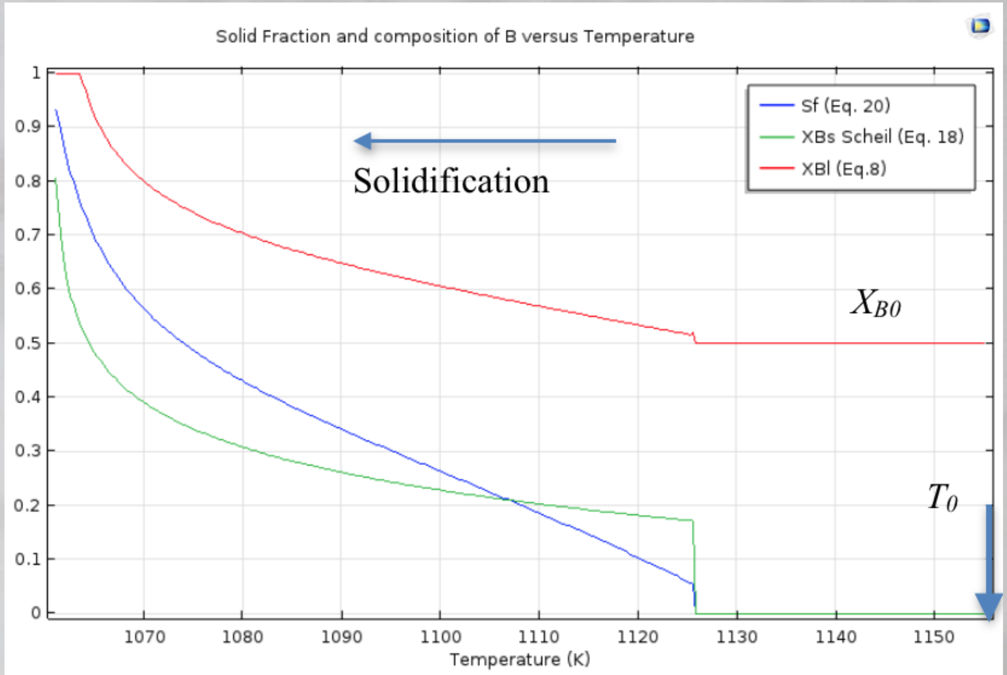
- Initial conditions:

  T_0=1155K

  X_{B0}=0.5

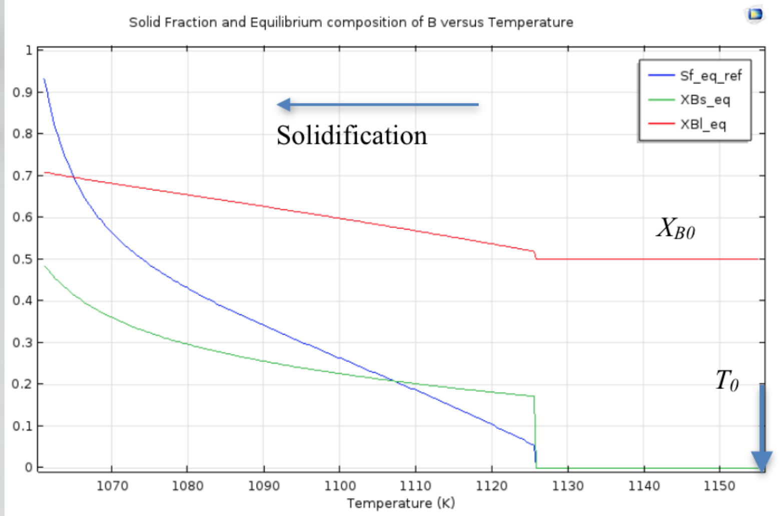
- $T_{liquidus}$ = 1127K
- Final solid comp.:

  X_{BS} = 0.8 (> 0.5)



Scheil vs Equilibrium Solidification

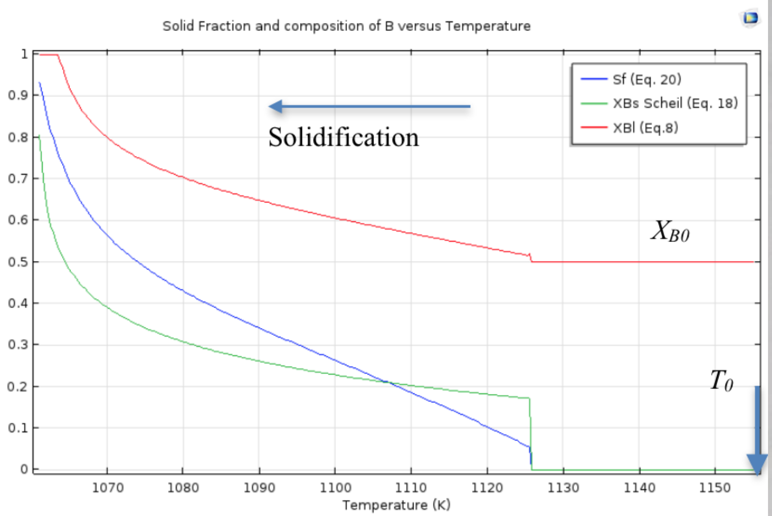
Equilibrium



- $T_{solidus}$ = 1061K
- Final solid comp.:

  X_{BS} = 0.5

Scheil



- $T_{solidus}$ = 1061K
- Final solid comp.:

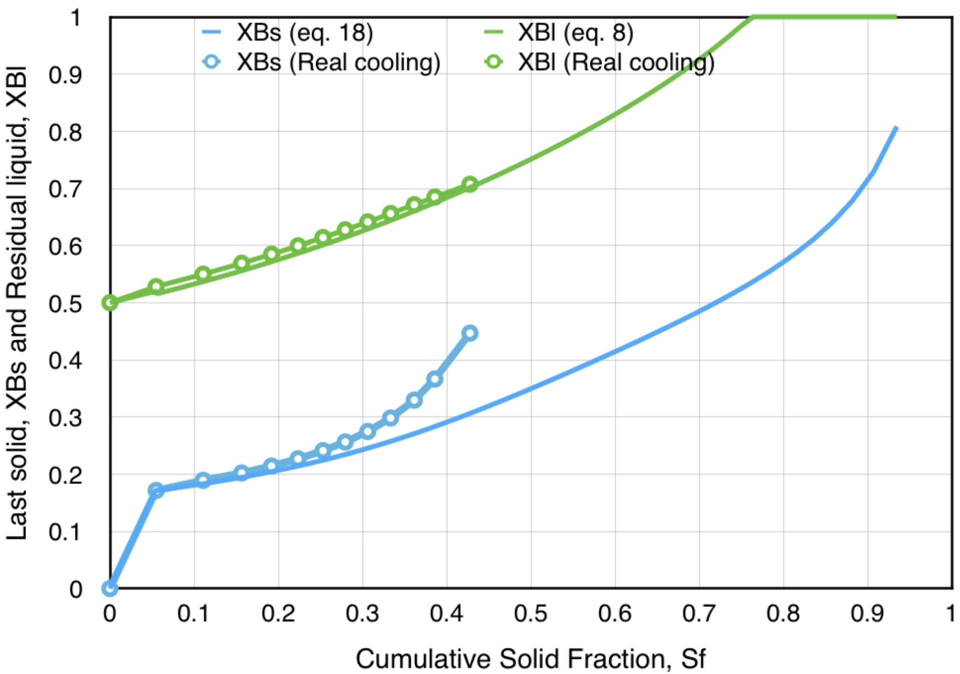
  X_{BS} = 0.8 (> 0.5)

Scheil vs Real Solidification

Scheil approx. assumes constant partition: $K_{BS,L}$.
Instead:

$$-ln(1-S_f) = \int_{X_{B0}}^{X_{BL}} \frac{dX_{BL}}{X_{BL}(1-K_{B_{S,L}})}$$

- Real solidification:
  - $T_{solidus}$ = 1055K



Conclusions

- Scheil Cooling has been implemented using COMSOL Multiphysics and M4Dlib
- The model has been solved using a 0D ODE model for three variables: T, S_f and X_B.
- A source term describing the “enrichment” of liquid was derived to calculate XB based on thermodynamic functions.
- There are still some limitations to this model that has been solved in M4Dlib but yet to be implemented in external library for COMSOL:
  - Lf → 0
  - Constant partition K