Segregation and Microstructure in Continuous Casting Shell

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Objectives

•Develop a fast, simple microsegregation model for the solidification of multicomponent steel alloys.

• Implement model into other macroscopic models such as heat flow and thermal-stress analysis (CON1D and CON2D) and apply models to continuous casting.

Simple Microsegregation Model

-based on the Clyne-Kurz model;
-extended to account for multiple components, columnar dendrite microstructure, coarsening and δ/γ transformation.

$$f_S = \frac{1}{1-\beta k}\left(1-\left[\frac{C_L}{C_o}\right]^{(1-\beta k)/(k-1)}\right)$$

where $$\beta = 2\alpha^+\left[1-\exp\left(-\frac{1}{\alpha^+}\right)\right]-\exp\left(-\frac{1}{2\alpha^+}\right),$$

$$\alpha^+ = 2(\alpha+\alpha^C) \text{ and } \alpha^C = 0.1$$

$$\alpha = \frac{D_S t_f}{X^2} \qquad t_f = \frac{T_{liq}-T_{sol}}{C_R}$$

Assumption for Simple Model

1. Complete diffusion in the liquid phase.

2. Local equilibrium at the solid-liquid interface.

3. The equilibrium partition coefficient of solute elements applies at the solid-liquid interface and is constant throughout solidification.

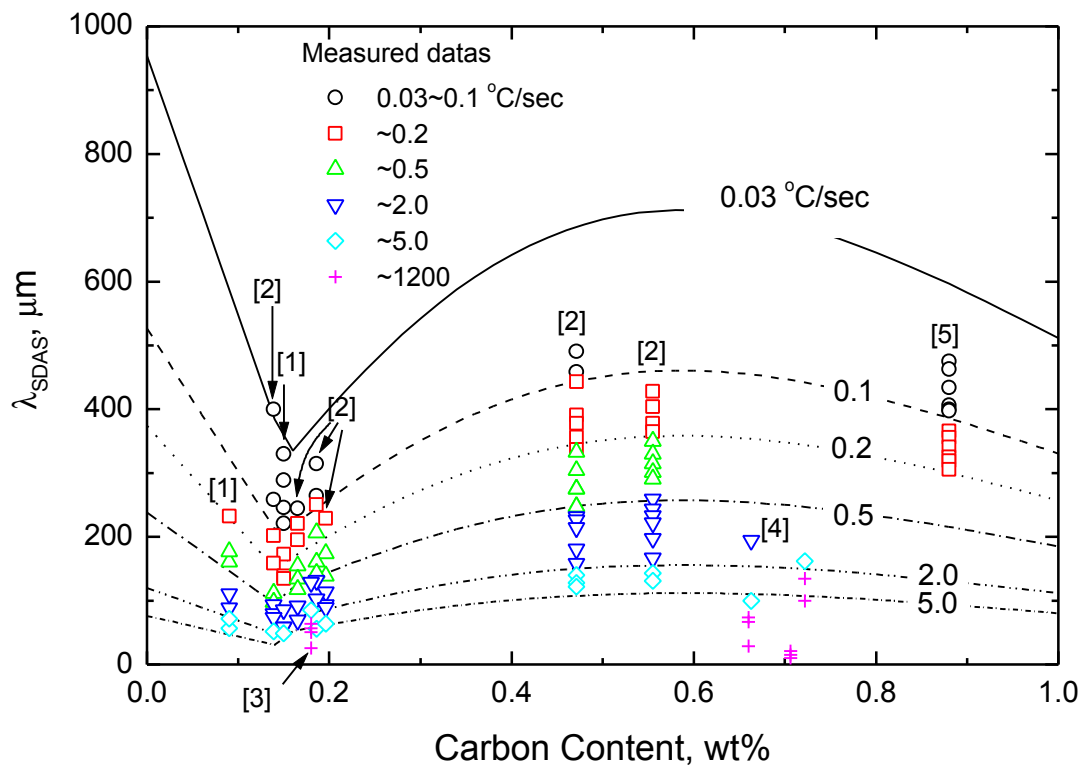
4. Nucleation undercooling effects are negligible.

5. Fluid flow effects are negligible.

Secondary Dendrite Arm Spacing Model

$$\lambda_{SDAS}\,(\mu m) = (169.1 - 720.9\,C_C)\,C_R^{-0.4835} \qquad \text{for } C_C \le 0.15$$

$$= 143.9\,C_R^{-0.3616}\,C_C^{\,(0.5501-1.996C)} \qquad \text{for } C_C > 0.15$$



C_R = cooling rate (°C/sec)
C_C = carbon content (wt%)

References

1. H. Jacobi et al. : Steel Res., 1999, v70, p. 357.
2. B. Weisgerber et al. : Steel Res., 1999, v70, p. 362.
3. M. Imagumbai et al. : ISIJ Int., 1994, v34, p.574.
4. D. Senk et al. : Steel Res., 1999, v70, p. 368.
5. A. Suzuki et al.: Nippon Kinzoku Gakkaishi, 1968, v32, p.1301.

Multicomponent Alloy Effect

**** Liquid temperature for a given liquid composition at the solid-liquid interface***

$$T(^{o}C) = 1536 - 78 \cdot \%C - 7.6 \cdot \%Si - 4.9 \cdot \%Mn - 34.4 \cdot \%P - 38 \cdot \%S$$

where %X (X = C, Si, Mn, P, S) is the liquid concentration at the solid-liquid interface.

**** Initial guess (equilibrium solidus temperature)***

=> Solidus temperature, T_{sol}, is given when $f_S = 1.0$

Peritectic Phase Transformation Effect

*** *Starting temperature of d/g transformation***

$$T_{start}^{\delta/\gamma}(^{o}C) = T_{Ar4} = 1392 + 1122 \cdot \%C - 60 \cdot \%Si + 12 \cdot \%Mn - 140 \cdot \%P - 160 \cdot \%S$$

where $\%X\ (X = C, Si, Mn, P, S) = k_X^{\delta/L} \cdot C_{L,X}^{\delta}$

*** *Ending temperature of d/g transformation***

$$C_{L,C} \geq 0.53 wt\%C$$

*** *Solid fraction of d- and g-phase in the solid***

$$^{\delta}f_S = \left(\frac{f_{end}^{\delta/\gamma} - f_S}{f_{end}^{\delta/\gamma} - f_{start}^{\delta/\gamma}} \right)^2 \cdot f_S \quad \text{and} \quad ^{\gamma}f_S = f_S - {}^{\delta}f_S$$

*** *Average liquid concentration during the d/g transformation***

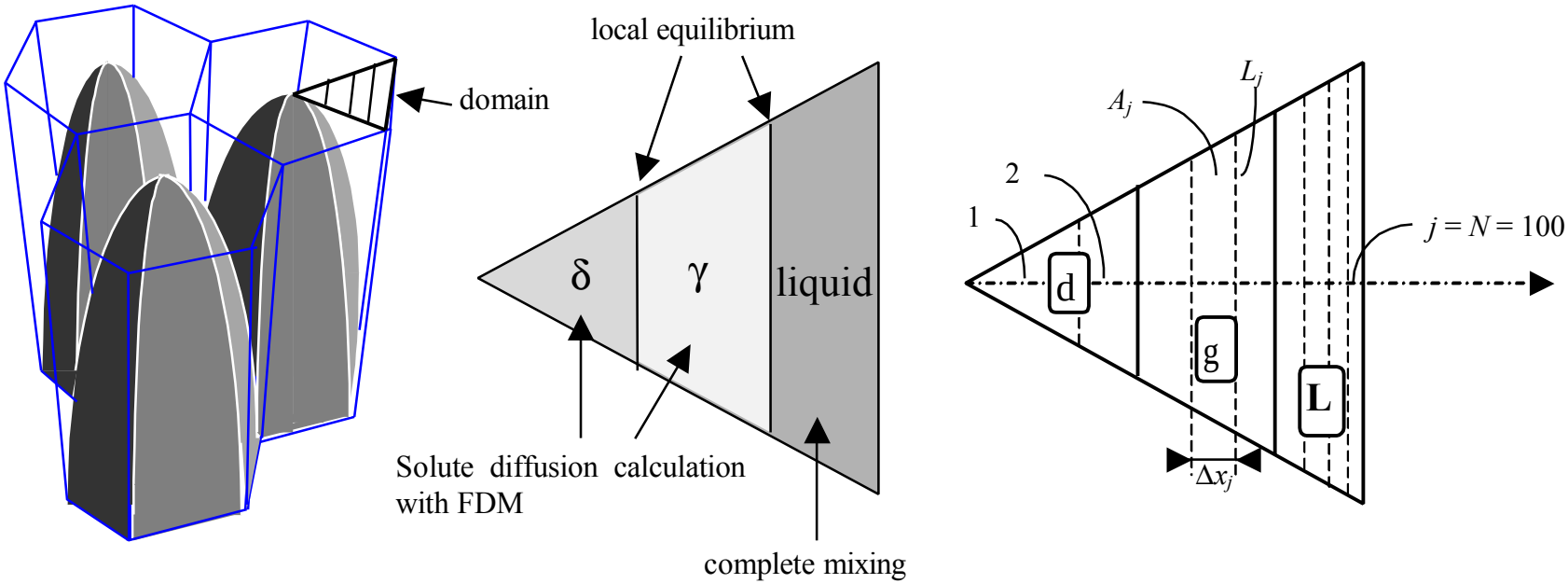
$$C_{L,i}^{ave} = \frac{^{\delta}f_S}{f_S} \cdot C_{L,i}^{\delta} + \frac{^{\gamma}f_S}{f_S} \cdot C_{L,i}^{\gamma}$$

Equilibrium Partition Coefficient and Diffusion Coefficient of Solute Elements

Element	$k^{d/L}$	$k^{g/L}$	D^{d} (cm^2/sec)	D^{g} (cm^2/sec)
C	0.19	0.34	0.0127exp(-19450/RT)	0.0761exp(-32160/RT)
Si	0.77	0.52	8.0exp(-59500/RT)	0.3exp(-60100/RT)
Mn	0.76	0.78	0.76exp(-53640/RT)	0.055exp(-59600/RT)
P	0.23	0.13	2.9exp(-55000/RT)	0.01exp(-43700/RT)
S	0.05	0.035	4.56exp(-51300/RT)	2.4exp(-53400/RT)

*** R is gas constant in cal/mol and T is temperature in K.**

1-D Finite-Difference Model for Microsegregation

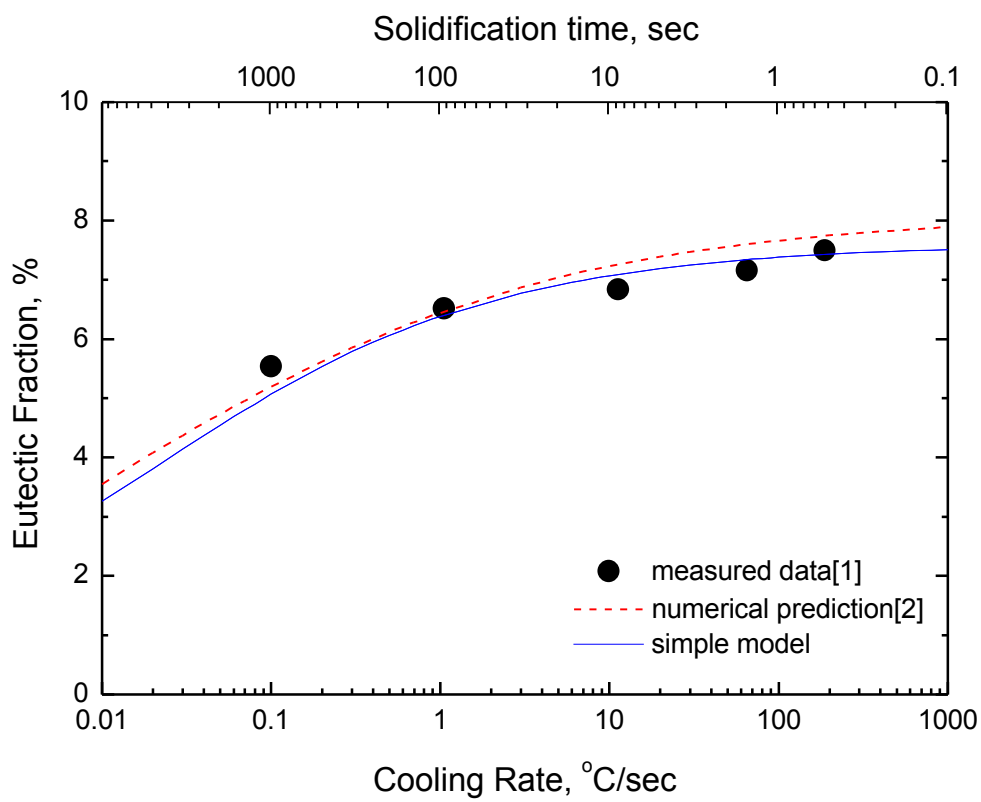


*** Diffusion equation and initial and boundary conditions for calculation.**

$$\frac{\partial C_{S,i}}{\partial t} = \frac{\partial}{\partial x}\left(D_{S,i}(T)\frac{\partial C_{S,i}}{\partial x} \right)$$

I. C. $C_{S,i} = k^{S/L} \cdot C_{o,i}$ at $t = 0$ B.C. $\frac{\partial C_{S,i}}{\partial x} = 0$ at $x = 0, \lambda_{SDAS}/2$

Validation (Case 1)



Al-4.9%Cu alloy system

$C_L = 33.2\%\text{Cu}$

$k = 0.145$

$D_S\ (\text{cm}^2/\text{sec}) = 5 \times 10^{-9}$

$\lambda_{\text{SDAS}}\ (\mu\text{m}) = 46.6 \cdot C_R^{-0.29}$

$T_{liq}\ (^{o}\text{C}) = 660 - 3.374 \cdot C_o$

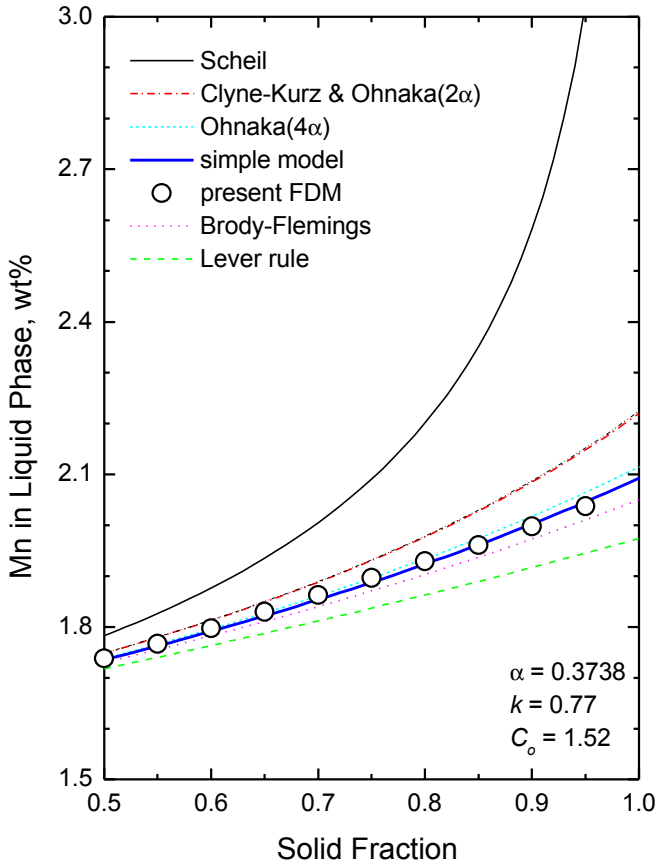
References

1. Sareal et al. : Metall. Trans. B, 1986, v17A, pp. 2063-73.
2. Voller et al. : Metall. Tarns. A, 1999, v30A, pp. 2183-89.

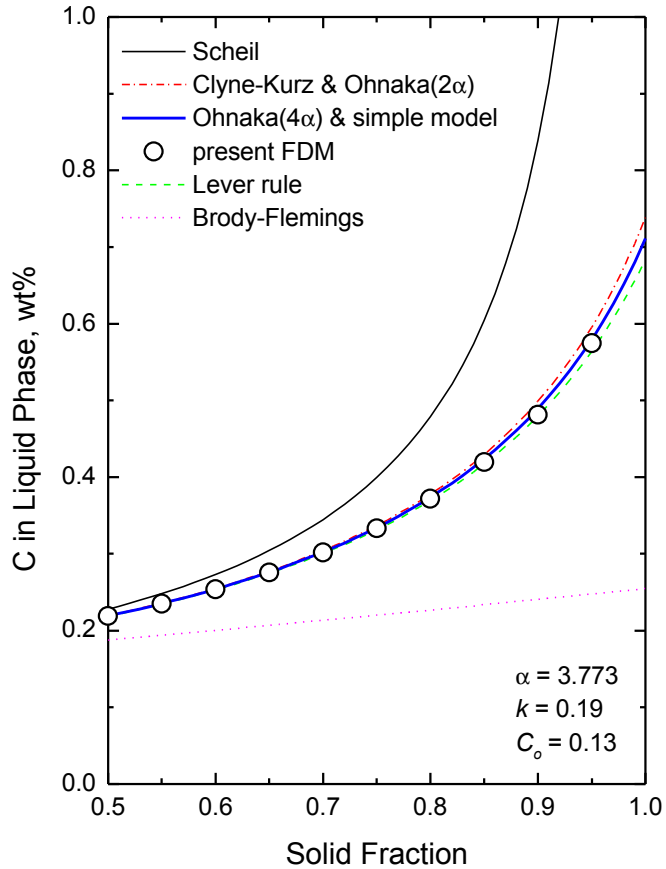
Validation (Case 2)

0.13%C-0.35%Si-1.52%Mn-0.016%P-0.002%S

$C_R = 0.045\ ^oC/sec$

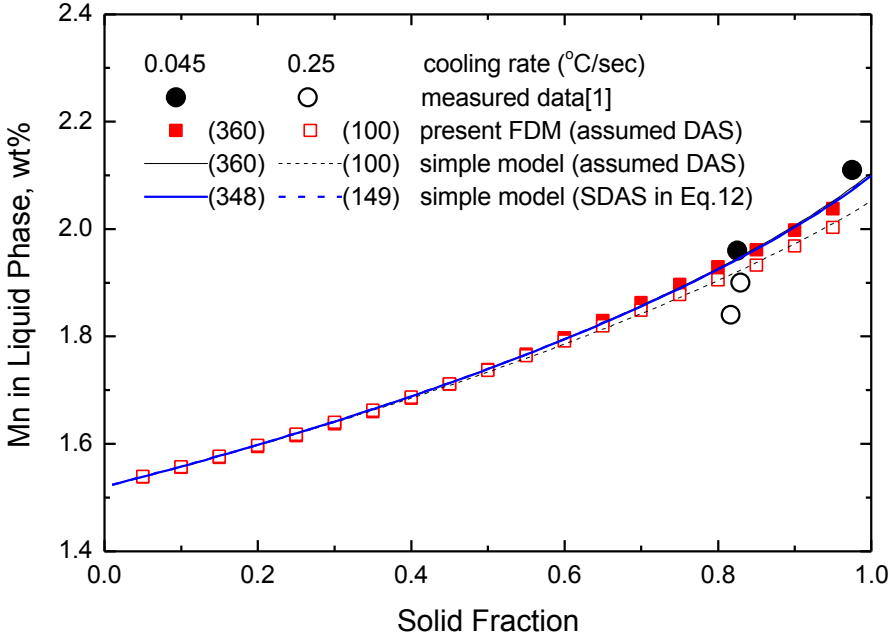


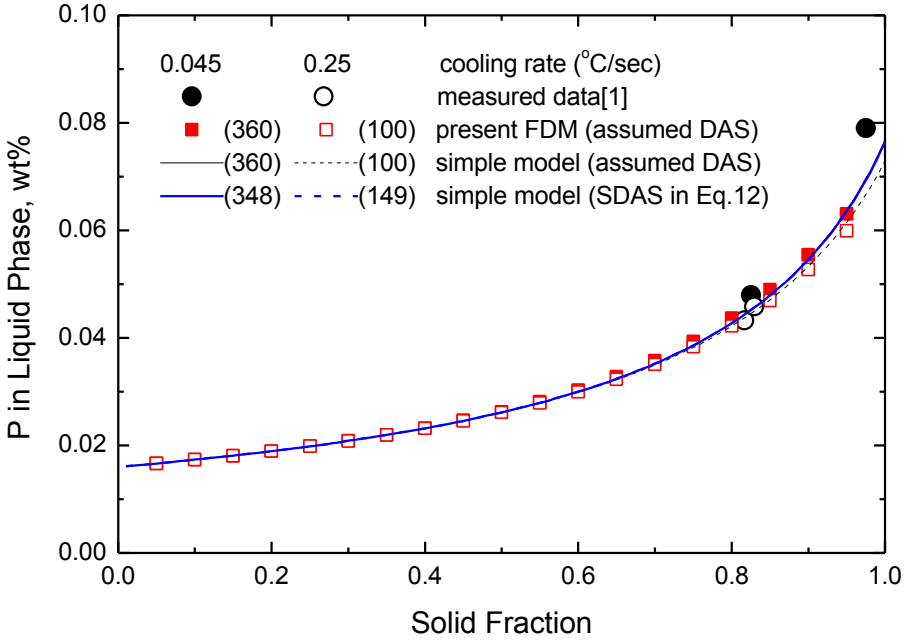
$C_R = 0.25\ ^oC/sec$



Validation (Case 3)

0.13%C-0.35%Si-1.52%Mn-0.016%P-0.002%S



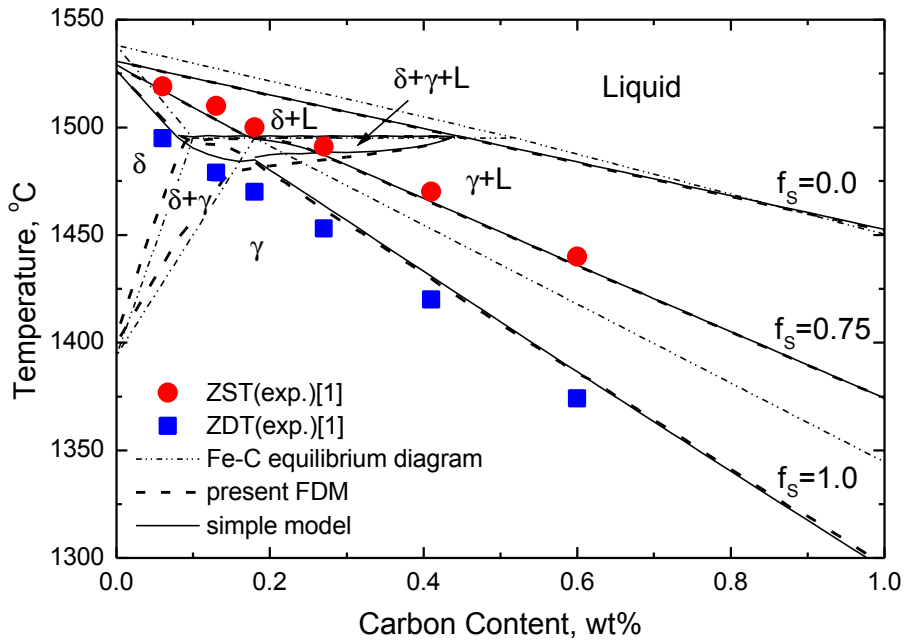


Reference

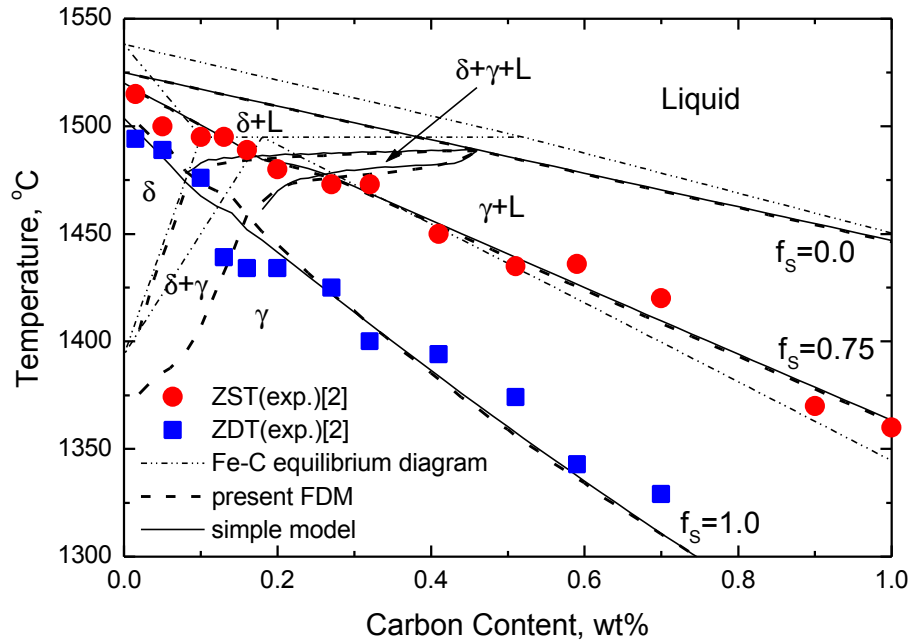
1. T. Matsumiya et al. : Trans. ISIJ, 1984, v24, pp. 873-82.

Validation (Case 4)

0.015%Si-1.05%Mn-0.0009%P-0.0008%S
C_R = 0.17 °C/sec



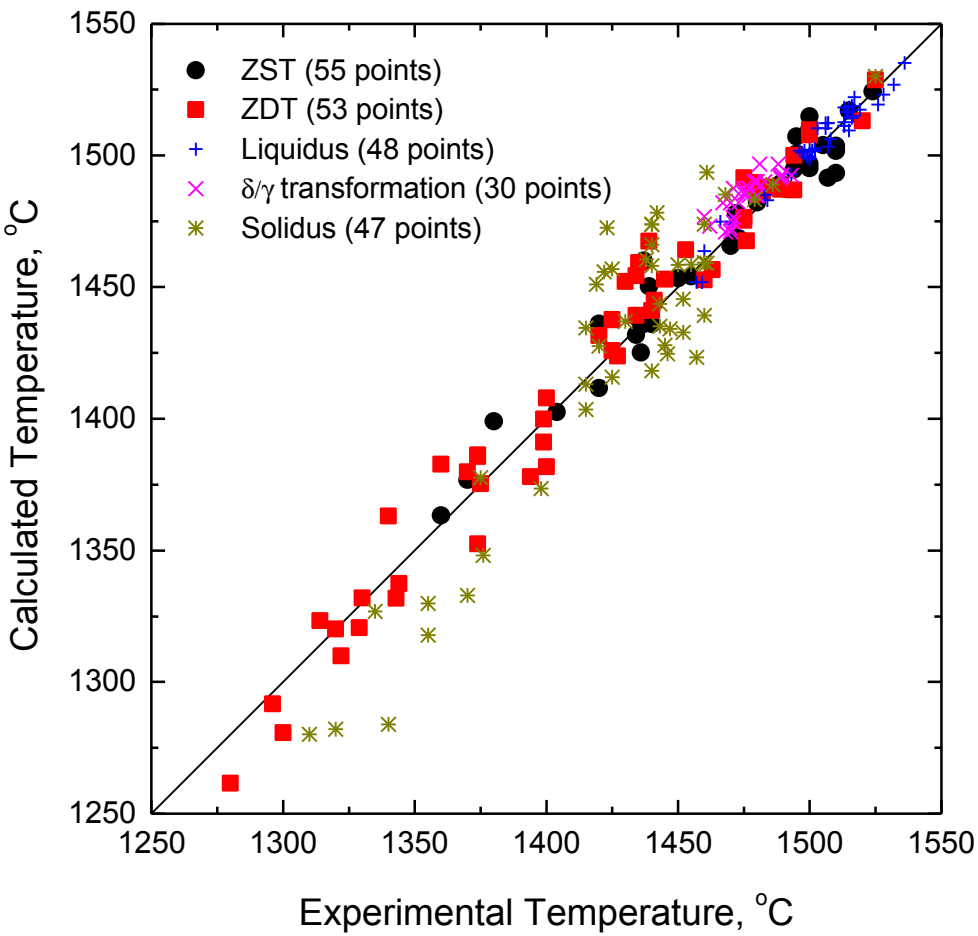
0.34%Si-1.52%Mn-0.012%P-0.015%S
C_R = 10.0 °C/sec



Reference

1. G. Shin et al. : Tetsu-to-Hagane, 1992, v78, pp. 587-93.
2. E. Schmidtmann et al. : Arch. Eisenhuttenwes., 1983, v54, pp. 357-62

Validation (Case 5)



1. Hot Tensile Tests

- Zero Strength Temp.[1-4]
- Zero Ductility Temp.[1-5]

2. Differential Thermal Analysis

- Liquidus Temp.[6-9]
- Solidus Temp.[6-9]
- peritectic Temp. [6-8]

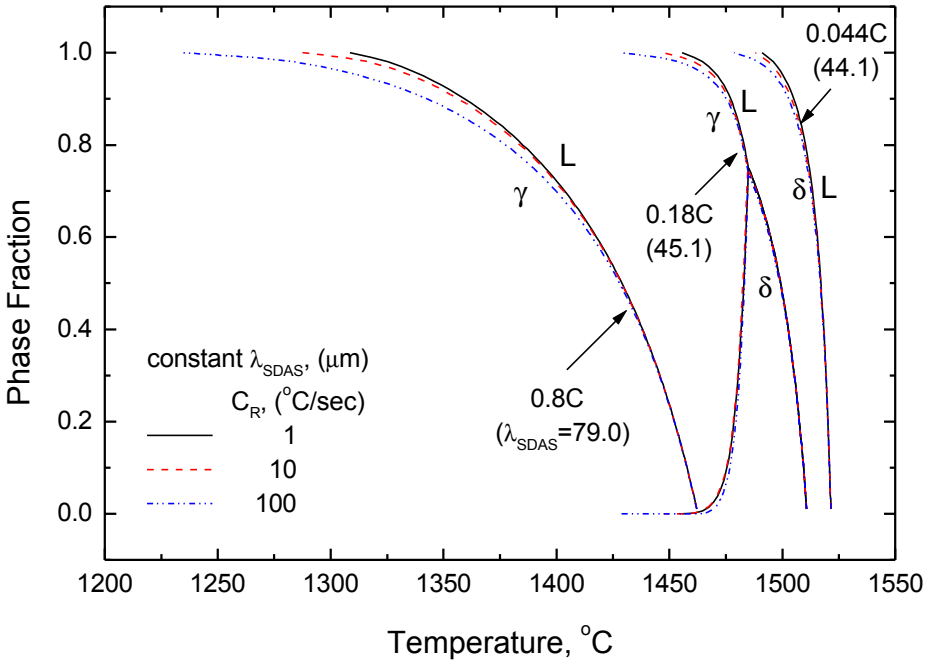
References

1. G. Shin et al. : Tetsu-to-Hagane, 1992, v78, p. 587..
2. D. J. Seol et al : ISIJ Int., 2000, v40, p.356.
3. E. Schmidtmann et al : Acrh. Eisenhuttenwe., 1983, v54, p. 357.
4. T. Nakagawa et al. : ISIJ Int., v35, p. 723.
5. H. G. Suzuki et al. : Trans. ISIJ, 1984, v24, p. 54.
6. A Guide to the Solidification of Steels, 1977.
7. L. Ericson : Scand. J. Metall., 1977, v6, p. 116.
8. S. Kobayashi : Trans. ISIJ, 1988, v28, p. 535.
9. POSCO data.

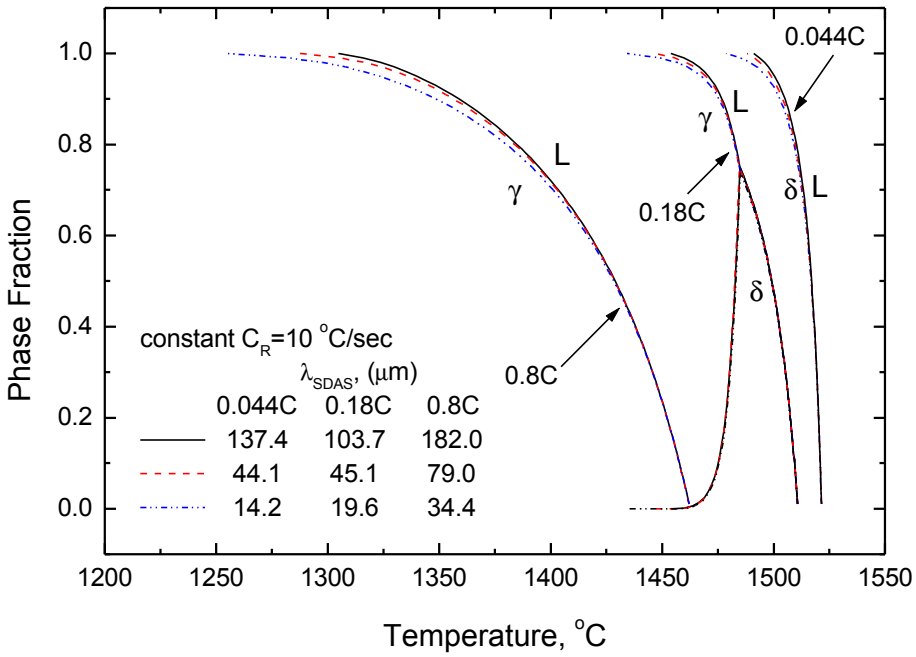
Effects of C_R and l_{SDAS} on Segregation

(by Simple Model)

Effect of C_R (l_{SDAS} = const.)



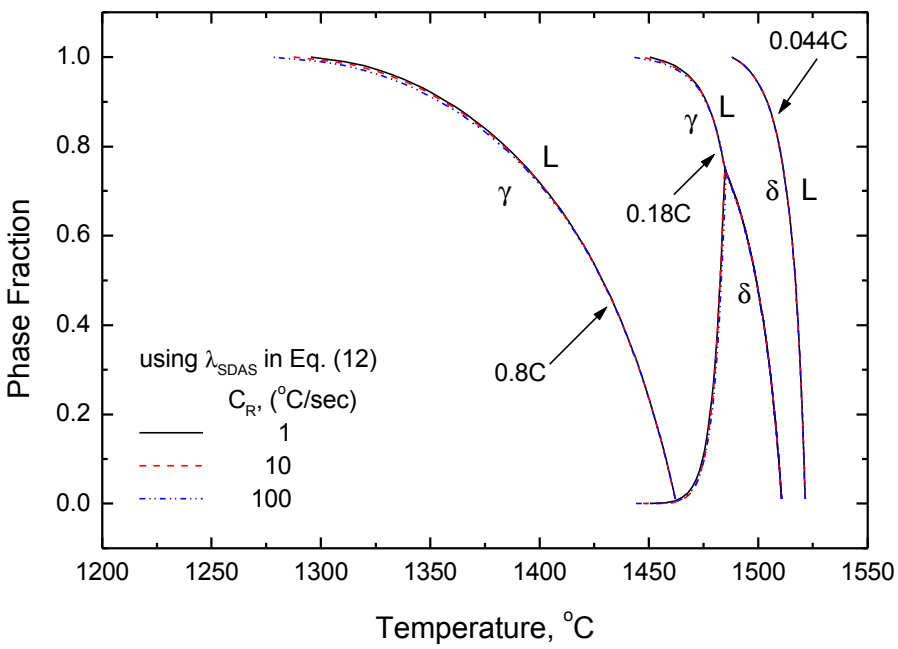
Effect of l_{SDAS} (C_R = const.)



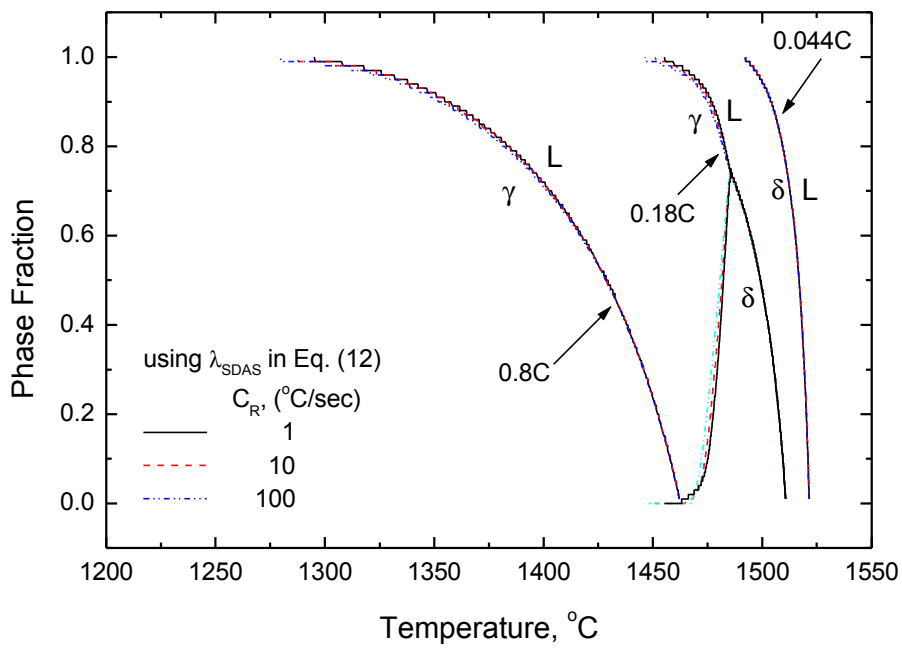
* Composition :0.044%C, 0.18%C, 0.8%C (-0.34%Si-1.52%Mn-0.012%P-0.015%S)

Combined Effects of C_R and l_{SDAS} on Segregation

By Simple Model



By Finite Difference Model



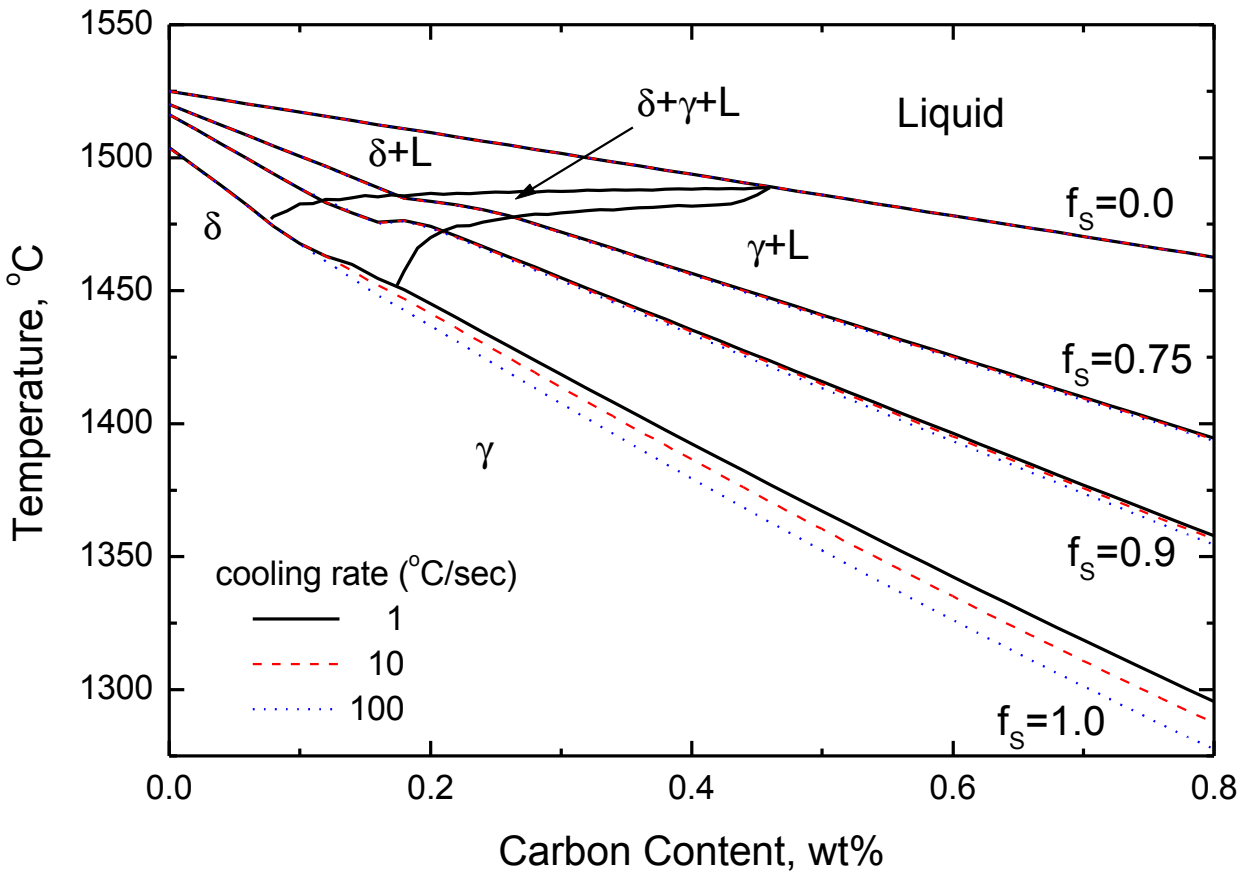
* Composition :0.044%C, 0.18%C, 0.8%C (-0.34%Si-1.52%Mn-0.012%P-0.015%S)

Calculated Solidus Temperatures using Simple Model for Plain Carbon Steels

	0.044wt%C		0.18wt%C		0.8wt%C	
C_R	λ_{SDAS}	T_{sol}	λ_{SDAS}	T_{sol}	λ_{SDAS}	T_{sol}
1. Constant secondary dendrite arm spacing						
1	44.1	1491.00	45.1	1455.64	79.0	1308.44
10	44.1	1487.86	45.1	1447.13	79.0	1287.40
100	44.1	1478.39	45.1	1428.13	79.0	1234.14
2. Constant cooling rate						
10	137.4	1478.55	130.7	1434.06	182.0	1254.72
10	44.1	1487.86	45.1	1447.13	79.0	1287.40
10	14.2	1490.99	19.6	1454.00	34.4	1304.75
3. Combined effects of cooling rate and secondary dendrite arm spacing						
1	137.4	1487.93	130.7	1450.38	182.0	1295.43
10	44.1	1487.86	45.1	1447.13	79.0	1287.40
100	14.2	1487.78	19.6	1442.83	34.4	1277.52

Non-equilibrium Phase Diagram Calculated with Simple Model

0.34%Si-1.52%Mn-0.012%P-0.015%S



Conclusions

1. A simple microsegregation model based on the Clyne-Kurz model developed.

2. A new equation for l_{SDAS} proposed.

$$l_{SDAS}\,(\mu m) = (169.1 - 720.9\,C_C)\,C_R^{-0.4835} \qquad \text{for } C_C \leq 0.15$$
$$= 143.9\,C_R^{-0.3616}\,C_C^{\,(0.5501-1.996C)} \qquad \text{for } C_C > 0.15$$

3. T_{sol} is lowered significantly with independent increases in either C_R or l_{SDAS}.

4. The effect of C_R less than 100 ^{o}C/sec on phase fraction evolution is insignificant in low alloy steels with less than 0.1wt%C, or for phase fractions below 0.9 in other steels

5. Phosphorus and sulfur have a significant effect on solidus temperature due to their enhanced segregation near the final stage of solidification.

6. The simple analytical model presented easily and efficiently incorporate micro-segregation phenomena into solidification calculations for use in advanced macroscopic models.

Applications with CON1D

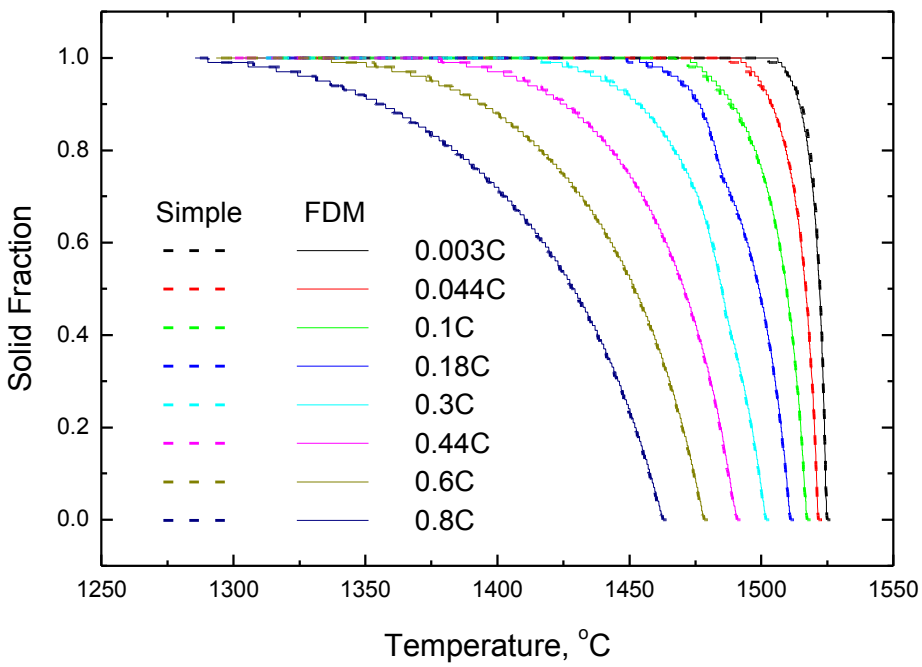
*** Conditions for Calculation**

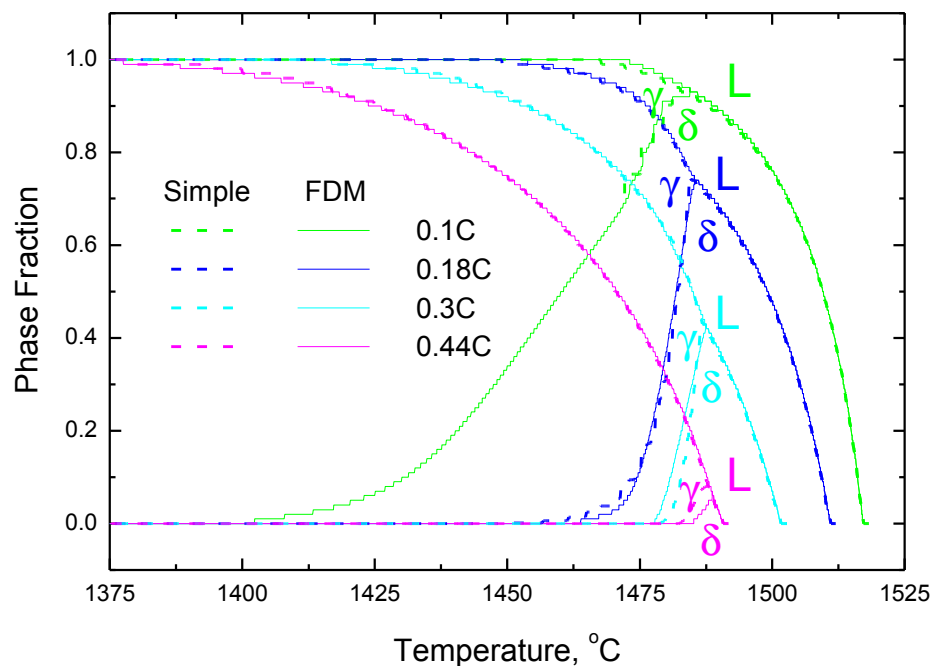
- **Steel compositions : %C-0.34%Si-1.52%Mn-0.012%P-0.015%S**
- **Casting speed : 1.524 m/min**
- **Slab dimension : 960 mm * 132.1 mm**
- **Working mold length : 1096 mm**
- **Superheat : 1 ^{o}C**

*** Predicted T_{liq} and T_{sol} at strand surface using simple model (after iteration)**

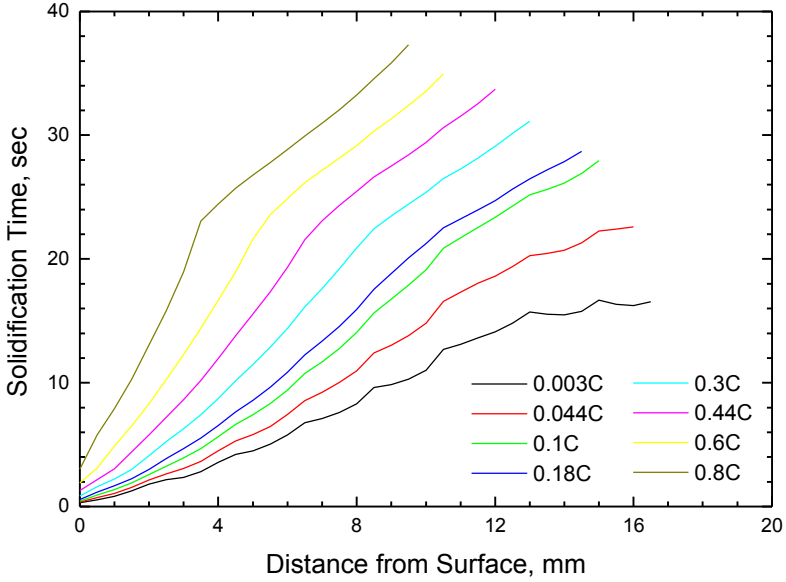
C (wt%)	0.003	0.044	0.1	0.18	0.3	0.44	0.6	0.8
t_f (sec)	0.303	0.350	0.437	0.575	0.846	1.268	1.862	2.862
C_R (^{o}C/sec)	73.5	96.6	114.1	120.5	113.0	97.8	82.5	65.1
l_{SDAS} (mm)	20.0	14.4	9.36	18.3	27.6	35.9	40.6	40.2
T_{liq} (^{o}C)	1524.8	1521.6	1517.2	1511.0	1501.6	1490.7	1478.2	1462.6
T_{sol} (^{o}C)	1502.5	1487.7	1467.3	1441.7	1406.0	1366.7	1324.5	1276.4

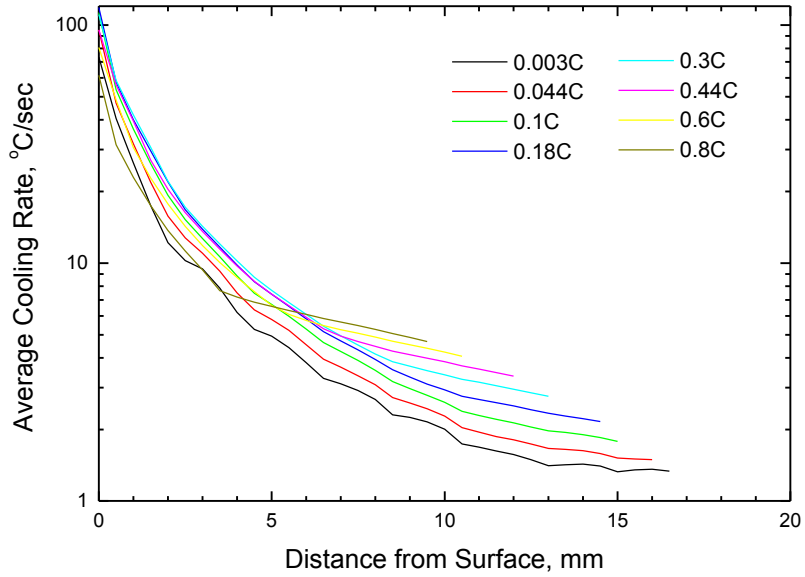
Prediction of Phase Fraction
(at 10 mm from surface)

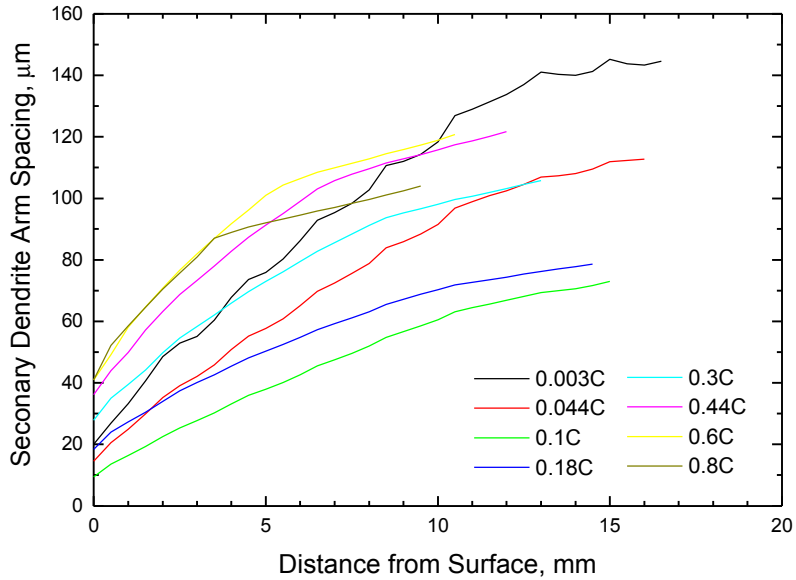




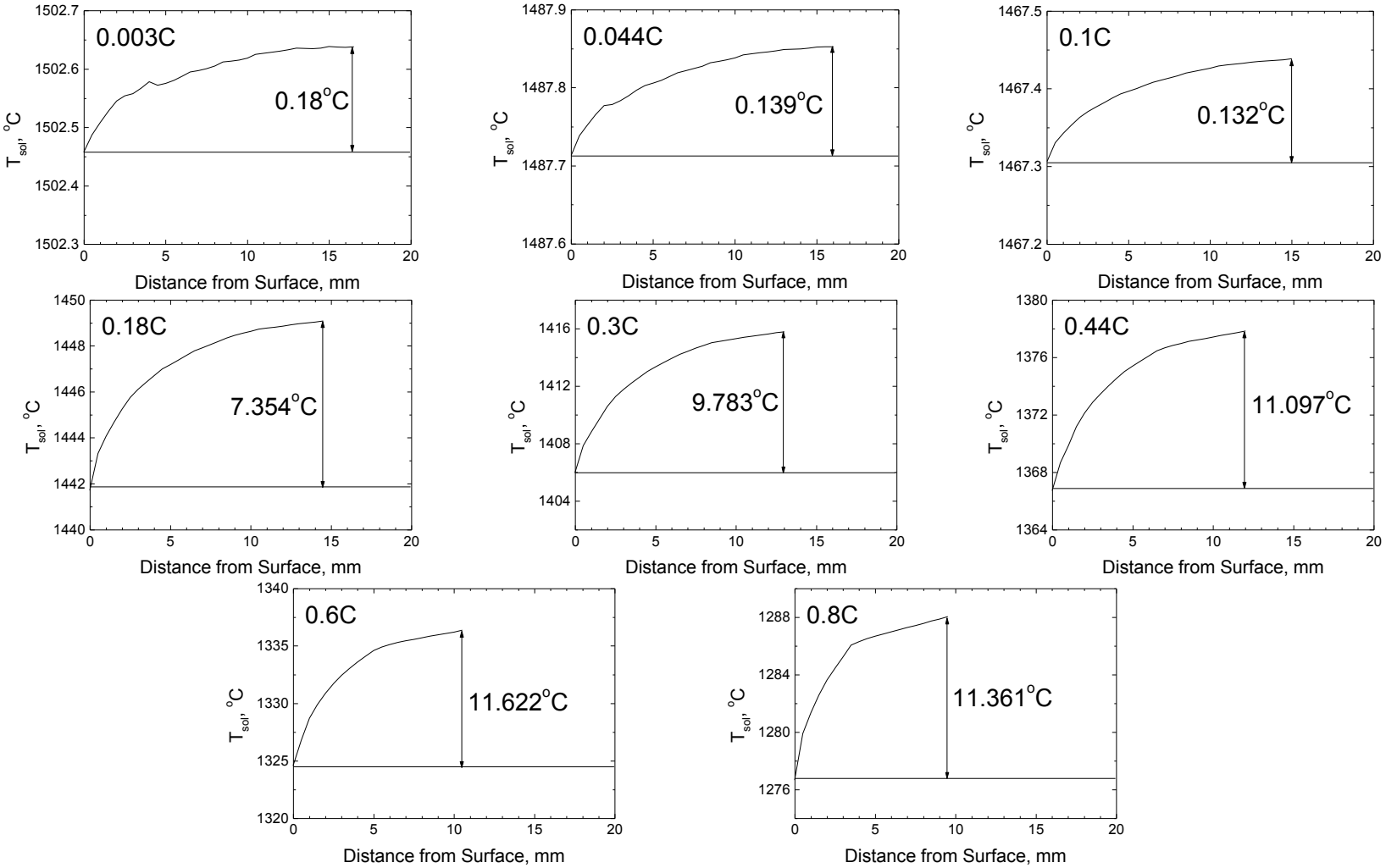
Prediction of t_f, C_R and l_{SDAS} Profiles







Predicted Effect of Carbon Content on T_{sol} Variation through Shell Thickness at Mold Exit



Microsegregation Model Implemented into CON1D

new outputs: t_f, C_R, l_{SDAS} and T_{sol} profiles

Future Work

(1) Maximum $C_{L,i}$ (composition between dendrites) and minimum $C_{S,i}$ (composition at dendrite trunks)

(2) Non-equilibrium phase diagrams

(3) Stainless steel

(4) Macrosegregation