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 $\delta/\gamma$ transformation.

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

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

\( \alpha^+ = 2(\alpha + \alpha^C) \) and \( \alpha^C = 0.1 \)

\[
\alpha = \frac{D_S t_f}{X^2} \quad t_f = \frac{T_{liq} - T_{sol}}{C_R}
\]
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

\[ \lambda_{SDAS} (\mu m) = (169.1 - 720.9 \ C_C) \ C_R^{-0.4835} \]

\[ = 143.9 \ C_R^{-0.3616} \ C_C (0.5501 - 1.996 C) \]

for \( C_C \leq 0.15 \)

for \( C_C > 0.15 \)

\[ C_R = \text{cooling rate (}^{\circ}\text{C/sec)} \]

\[ C_C = \text{carbon content (wt\%)} \]

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

\[ T(\degree C) = 1536 - 78 \cdot \%C - 7.6 \cdot \%Si - 4.9 \cdot \%Mn - 34.4 \cdot \%P - 38 \cdot \%S \]

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

* Initial guess (equilibrium solidus temperature)

\[ \Rightarrow \text{Solidus temperature, } T_{sol}, \text{ is given when } f_S = 1.0 \]
**Peritectic Phase Transformation Effect**

* **Starting temperature of \( \delta/\gamma \) transformation**

\[
T_{\text{start}}(^\circ \text{C}) = T_{\text{Ar}_4} = 1392 + 1122 \cdot \%C - 60 \cdot \%Si + 12 \cdot \%Mn - 140 \cdot \%P - 160 \cdot \%S
\]

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

* **Ending temperature of \( \delta/\gamma \) transformation**

\( C_{L,C} \geq 0.53 \text{wt}\%C \)

* **Solid fraction of \( \delta \)- and \( \gamma \)-phase in the solid**

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

* **Average liquid concentration during the \( \delta/\gamma \) transformation**

\[
C_{L,i}^{\text{ave}} = \frac{\delta f_s}{f_s} \cdot C_{L,i}^{\delta} + \frac{\gamma f_s}{f_s} \cdot C_{L,i}^{\gamma}
\]
# Equilibrium Partition Coefficient and Diffusion Coefficient of Solute Elements

<table>
<thead>
<tr>
<th>Element</th>
<th>$k^\delta/L$</th>
<th>$k^\gamma/L$</th>
<th>$D^\delta$ (cm$^2$/sec)</th>
<th>$D^\gamma$ (cm$^2$/sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.19</td>
<td>0.34</td>
<td>$0.0127\exp(-19450/RT)$</td>
<td>$0.0761\exp(-32160/RT)$</td>
</tr>
<tr>
<td>Si</td>
<td>0.77</td>
<td>0.52</td>
<td>$8.0\exp(-59500/RT)$</td>
<td>$0.3\exp(-60100/RT)$</td>
</tr>
<tr>
<td>Mn</td>
<td>0.76</td>
<td>0.78</td>
<td>$0.76\exp(-53640/RT)$</td>
<td>$0.055\exp(-59600/RT)$</td>
</tr>
<tr>
<td>P</td>
<td>0.23</td>
<td>0.13</td>
<td>$2.9\exp(-55000/RT)$</td>
<td>$0.01\exp(-43700/RT)$</td>
</tr>
<tr>
<td>S</td>
<td>0.05</td>
<td>0.035</td>
<td>$4.56\exp(-51300/RT)$</td>
<td>$2.4\exp(-53400/RT)$</td>
</tr>
</tbody>
</table>

* 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

\[ C_L = 33.2\% \text{Cu} \]
\[ k = 0.145 \]
\[ D_S (\text{cm}^2/\text{sec}) = 5 \times 10^{-9} \]
\[ \lambda_{\text{SDAS}} (\mu\text{m}) = 46.6 \cdot C_R^{-0.29} \]
\[ T_{\text{liq}} (^{\circ}\text{C}) = 660 - 3.374 \cdot C_o \]

References
Validation (Case 2)

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

\[ C_R = 0.045 \, ^{\circ}\text{C/sec} \]

\[ C_R = 0.25 \, ^{\circ}\text{C/sec} \]
**Validation (Case 3)**

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

![Graphs showing Mn and P in Liquid Phase vs. Solid Fraction](image)

**Reference**
Validation (Case 4)

0.015%Si-1.05%Mn-0.0009%P-0.0008%S  
$C_R = 0.17 \, ^\circ\text{C}/\text{sec}$

0.34%Si-1.52%Mn-0.012%P-0.015%S  
$C_R = 10.0 \, ^\circ\text{C}/\text{sec}$

Reference
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
9. POSCO data.
**Effects of $C_R$ and $\lambda_{SDAS}$ on Segregation**
(by Simple Model)

**Effect of $C_R$ ($\lambda_{SDAS} = \text{const.}$)**

- Constant $\lambda_{SDAS}$ (µm)
- $C_R$ (°C/sec)
  - 1
  - 10
  - 100

**Effect of $\lambda_{SDAS}$ ($C_R = \text{const.}$)**

- Constant $C_R$ = 10 °C/sec
- $\lambda_{SDAS}$ (µm)
  - 0.044C
  - 0.18C
  - 0.8C

*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 $\lambda_{SDAS}$ 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

<table>
<thead>
<tr>
<th>$C_R$</th>
<th>$\lambda_{SDAS}$</th>
<th>$T_{sol}$</th>
<th>$\lambda_{SDAS}$</th>
<th>$T_{sol}$</th>
<th>$\lambda_{SDAS}$</th>
<th>$T_{sol}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.044wt%C</td>
<td>0.18wt%C</td>
<td>0.8wt%C</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>44.1</td>
<td>1491.00</td>
<td>45.1</td>
<td>1455.64</td>
<td>79.0</td>
<td>1308.44</td>
</tr>
<tr>
<td>10</td>
<td>44.1</td>
<td>1487.86</td>
<td>45.1</td>
<td>1447.13</td>
<td>79.0</td>
<td>1287.40</td>
</tr>
<tr>
<td>100</td>
<td>44.1</td>
<td>1478.39</td>
<td>45.1</td>
<td>1428.13</td>
<td>79.0</td>
<td>1234.14</td>
</tr>
<tr>
<td>1</td>
<td>137.4</td>
<td>1478.55</td>
<td>130.7</td>
<td>1434.06</td>
<td>182.0</td>
<td>1254.72</td>
</tr>
<tr>
<td>10</td>
<td>44.1</td>
<td>1487.86</td>
<td>45.1</td>
<td>1447.13</td>
<td>79.0</td>
<td>1287.40</td>
</tr>
<tr>
<td>10</td>
<td>14.2</td>
<td>1490.99</td>
<td>19.6</td>
<td>1454.00</td>
<td>34.4</td>
<td>1277.52</td>
</tr>
<tr>
<td>1</td>
<td>137.4</td>
<td>1487.93</td>
<td>130.7</td>
<td>1450.38</td>
<td>182.0</td>
<td>1295.43</td>
</tr>
<tr>
<td>10</td>
<td>44.1</td>
<td>1487.86</td>
<td>45.1</td>
<td>1447.13</td>
<td>79.0</td>
<td>1287.40</td>
</tr>
<tr>
<td>100</td>
<td>14.2</td>
<td>1487.78</td>
<td>19.6</td>
<td>1442.83</td>
<td>34.4</td>
<td>1277.52</td>
</tr>
</tbody>
</table>

1. Constant secondary dendrite arm spacing
2. Constant cooling rate
3. Combined effects of cooling rate and secondary dendrite arm spacing
Non-equilibrium Phase Diagram
Calculated with Simple Model

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

Temperature, °C

Carbon Content, wt%

δ+L
δ+γ+L
δ
γ+L
γ
Liquid

cooling rate (°C/sec)

1
10
100

f_s = 0.0
f_s = 0.75
f_s = 0.9
f_s = 1.0
Conclusions

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

2. A new equation for $\lambda_{SDAS}$ proposed.

   \[
   \lambda_{SDAS} (\mu m) = \begin{cases} 
   (169.1 - 720.9 \ C_C) \ C_R^{-0.4835} & \text{for } C_C \leq 0.15 \\
   143.9 \ C_R^{-0.3616} \ C_C^{(0.5501-1.996C)} & \text{for } C_C > 0.15 
   \end{cases}
   \]

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

4. The effect of $C_R$ less than 100 °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 microsegregation 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 °C

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

<table>
<thead>
<tr>
<th>C (wt%)</th>
<th>0.003</th>
<th>0.044</th>
<th>0.1</th>
<th>0.18</th>
<th>0.3</th>
<th>0.44</th>
<th>0.6</th>
<th>0.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_f$ (sec)</td>
<td>0.303</td>
<td>0.350</td>
<td>0.437</td>
<td>0.575</td>
<td>0.846</td>
<td>1.268</td>
<td>1.862</td>
<td>2.862</td>
</tr>
<tr>
<td>$C_R$ (°C/sec)</td>
<td>73.5</td>
<td>96.6</td>
<td>114.1</td>
<td>120.5</td>
<td>113.0</td>
<td>97.8</td>
<td>82.5</td>
<td>65.1</td>
</tr>
<tr>
<td>$\lambda_{SDAS}$ (μm)</td>
<td>20.0</td>
<td>14.4</td>
<td>9.36</td>
<td>18.3</td>
<td>27.6</td>
<td>35.9</td>
<td>40.6</td>
<td>40.2</td>
</tr>
<tr>
<td>$T_{\text{liq}}$ (°C)</td>
<td>1524.8</td>
<td>1521.6</td>
<td>1517.2</td>
<td>1511.0</td>
<td>1501.6</td>
<td>1490.7</td>
<td>1478.2</td>
<td>1462.6</td>
</tr>
<tr>
<td>$T_{\text{sol}}$ (°C)</td>
<td>1502.5</td>
<td>1487.7</td>
<td>1467.3</td>
<td>1441.7</td>
<td>1406.0</td>
<td>1366.7</td>
<td>1324.5</td>
<td>1276.4</td>
</tr>
</tbody>
</table>
Prediction of Phase Fraction
(at 10 mm from surface)
Prediction of $t_f$, $C_R$ and $\lambda_{SDAS}$ Profiles
Predicted Effect of Carbon Content on $T_{\text{sol}}$ Variation through Shell Thickness at Mold Exit
Microsegregation Model Implemented into CON1D

new outputs: \( t_f, C_R, \lambda_{SDAS} \) 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