Simulation of ferro-alloy smelting in DC arc furnaces using Pyrosim and FactSage

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Chromite Smelting

• Production of ferro-alloys is important for steelmaking, and for the South African economy
• 2 GW of electrical power is used for ferro-alloy smelting in South Africa
• DC arc furnaces have been used industrially for chromite smelting since 1984. The first furnace was 12 MW.
Features of DC arc furnaces

- Operates with open arc, open bath
- **Can accept fine feed materials** (< 10 mm)
- Does not require coke
- Can achieve high temperatures (> 1500°C)
- Lower electrode consumption
- No arc repulsion (and resulting hot spots)
- DC furnaces carry higher currents per electrode (no ‘skin effect’)
- Energy supplied by open plasma arc, so less sensitive to electrical properties of slag
- Power supplied to furnace is independent of slag composition, so slag can be changed to one that allows higher Cr recovery
DC arc furnaces for chromite smelting in South Africa

- South Africa currently has the following DC arc furnaces for chromite smelting:
  - 2 x 60 MW
  - 1 x 30 MW
  - 1 x 10 MW
DC arc furnaces for chromite smelting in Kazakhstan

- Kazakhstan currently has the following DC arc furnaces for chromite smelting:
  - 4 x 72 MW
Chromite Smelting – highly simplified

FeO.Cr_2O_3 + 4C → Fe + 2Cr + 4CO

~1700°C

Chromite spinel: (Fe,Mg)O•(Cr,Al)_2O_3
Chromite ore compositions (mass %)

<table>
<thead>
<tr>
<th>Origin</th>
<th>Cr$_2$O$_3$</th>
<th>FeO</th>
<th>MgO</th>
<th>Al$_2$O$_3$</th>
<th>SiO$_2$</th>
<th>Cr/Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kazakhstan</td>
<td>51.2</td>
<td>11.9</td>
<td>19.8</td>
<td>6.5</td>
<td>6.9</td>
<td>3.8</td>
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<tr>
<td>Zimbabwe</td>
<td>50.8</td>
<td>13.3</td>
<td>17.9</td>
<td>12.7</td>
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<td>3.4</td>
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<tr>
<td>India A</td>
<td>53.5</td>
<td>16.9</td>
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<td>12.7</td>
<td>1.2</td>
<td>2.5</td>
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<tr>
<td>North America</td>
<td>44.0</td>
<td>18.2</td>
<td>12.8</td>
<td>12.5</td>
<td>5.9</td>
<td>2.1</td>
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<tr>
<td>South Africa LG</td>
<td>46.6</td>
<td>25.0</td>
<td>10.8</td>
<td>15.1</td>
<td>0.6</td>
<td>1.6</td>
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<tr>
<td>South Africa UG2</td>
<td>42.6</td>
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Typical slag and alloy compositions

<table>
<thead>
<tr>
<th></th>
<th>Al$_2$O$_3$</th>
<th>CaO</th>
<th>Cr$_2$O$_3$</th>
<th>FeO</th>
<th>MgO</th>
<th>SiO$_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slag</td>
<td>30-40</td>
<td>2-15</td>
<td>4-6</td>
<td>0.5-2</td>
<td>30-40</td>
<td>bal.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Cr</th>
<th>Fe</th>
<th>Si</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>HC FeCr</td>
<td>50-52</td>
<td>bal.</td>
<td>0.5-1.5</td>
<td>6-8</td>
</tr>
</tbody>
</table>
Pyrosim computer software

1985: Apple II (1 MHz)
1988: MS-DOS version
Historical background to Pyrosim

- Originally developed to simulate production of raw stainless steel
- Programming started in 1985, on a 64kb (1 MHz) Apple II computer
- Presented at APCOM 87 in 1987
- First used in industry in 1988
- 1500 fold increase in speed and storage capacity, from Apple II (typical simulation took one hour) to fast Pentium
- Basic - structured & compiled
  - PowerBASIC DLL compiler
- 95 installed sites in 22 countries on 6 continents
Pyrosim

• Equilibrium models - free-energy minimization using Gunnar Eriksson’s equations
• Ideal Mixing of Complex Components
• Empirical models
  – Calculate degrees of freedom from number of chemical elements in feed, and number of phases present
  – Specify content (mass %) of any species in any phase
  – Specify ratios between any pair of species in any phase
  – Direct solution of linear equations from an independent set
• Pyrobal: % Cr$_2$O$_3$, % FeO, % Si, % C,
  P slag / P metal, S slag / S metal
• Spreadsheet versions of empirical model
F*A*C*T and FactSage

- Facility for the Analysis of Chemical Thermodynamics was established in the late 1970s
- Mid 1980s – Remote access of McGill University computer system via Saponet satellite link
- Limited number of elements in equilibrium calculation
- 1990s – Personal computers
- Main strengths were assessed thermodynamic data, multi-component non-ideal solution models, and leading algorithm for free-energy minimization (Solgasmix)
Plant simulation methodology

1. Calculate metal composition [Pyrosim]
2. Calculate liquidus of metal [FactSage, SGTE]
3. Design slag to have liquidus 100-150°C above liquidus of metal [FactSage, FTOxid]
4. Adjust slag chemistry for viscosity [FactSage, Viscosity]
5. Adjust slag composition and reductant mixture for slag conductivity and compatibility with refractories
Metal liquidus temperature

Liquidus isotherms in °C at 8% C for a Fe-Cr-Si-C alloy

<table>
<thead>
<tr>
<th></th>
<th>Cr</th>
<th>Fe</th>
<th>C</th>
<th>Si</th>
<th>Liquidus (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HC FeCr from SA</td>
<td>50.0</td>
<td>40.5</td>
<td>8.0</td>
<td>1.5</td>
<td>1528 (SGTE)</td>
</tr>
<tr>
<td>operation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HC FeCr from</td>
<td>71.0</td>
<td>20.0</td>
<td>8.0</td>
<td>1.0</td>
<td>1644 (SGTE)</td>
</tr>
<tr>
<td>Kazakhstan</td>
<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
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Calculations using FactSage 7.0
Slag liquidus temperature

Bulk liquidus temperature of MgO-Al₂O₃-SiO₂-CaO, ignoring undissolved chromite spinel, 100 to 150°C above metal liquidus temperature

FactSage 7.0, FTOxid database
Slag liquidus temperature (Silica as flux)

- Kazakhstan, M/A = 3.05
- LG, M/A = 0.72
- UG2, M/A = 0.62
- MG, M/A = 0.56

Liquidus of metal HCFeCr in Kazakhstan
Liquidus of metal HCFeCr in South Africa

g SiO$_2$ added to 100 g ore (excluding CrO$_x$ and FeO$_x$)
Slag viscosity (CaO as flux)

Add CaO to lower viscosity, but don't increase liquidus T too much

FactSage 7.0, FTOxid database
Conclusions

• The past three decades have seen the introduction of an effective new smelting technology for ferro-alloys, as well as increasingly capable process simulation tools

• Flowsheet simulators based on chemical thermodynamic databases running on personal computers were introduced to the pyrometallurgical industry in the 1980s and have become rather ubiquitous since then

• There is a place for equilibrium calculations involving non-ideal slag and alloy solutions, as well as for empirical models that can be used in an operating plant environment
Mintek’s DC furnaces

http://www.mintek.co.za/Pyromet/