New Computational Resources and Stress Model Validation

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Objectives

- A pioneer attempt to predict the coupled evolution of temperature, shape, stress and strain distribution in the solidifying shell in continuous casting mold by using commercial multipurpose finite element package

- The recent increase in computational speed and capabilities of commercial finite element software make this task feasible and desirable.

- Will validate the model with available analytical solution and then add more complexity to the model from real plant measurements and finally compare and benchmark the results with in-house code

- ABAQUS™ claims that it can solve the most challenging nonlinear problems. Will check this statement by applying Abaqus to our complex phenomena.

- Even Though ABAQUS offers the user a wide range of capabilities, it is relatively simple to use, it has imbedded pre and post processing tools, and a rich library of 2D and 3D elements. Other modelers in this field can largely benefit from this work, including our final customers – the steel industry
Basic Phenomena

- Initial solidification occurs at the meniscus and is responsible for the surface quality of the final product.

- The shell shrinks away from the mold due to thermal contraction and a gap is formed between the mold and the strand.

- At inner side of the strand shell the ferrostatic pressure linearly increasing with the height is present.

- The mold taper has the task to compensate the shell shrinkage yielding good contact between strand shell and mold wall.

- Many other phenomena are present due to complex interactions between thermal and mechanical stresses and microstructural effects. Some of them are still not fully understood.
Program Validation and Preliminary Results

1D Solidification Stress Problem

- Analytical Solution exists (Weiner & Boley 1963)
- 1D FE Domain used for validation
- Generalized plane strain both in y and z direction to give 3D stress/strain state
- Yield stress linearly drops with temp. from 20Mpa @ 1000C to 0.07Mpa @ Solidus Temp 1494.35C
- Tested both internal PLASTIC Abaqus procedure and a special high-creep function to emulate Elastic-Prefect Plastic material behavior
Governing Equations

Heat Transfer Equation:

\[ \rho \left( \frac{\partial H(T)}{\partial T} \right) \left( \frac{\partial T}{\partial t} \right) = \frac{\partial}{\partial x} \left( k(T) \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k(T) \frac{\partial T}{\partial y} \right) \]

Equilibrium Equations 2D:

\[ \frac{\partial \Delta \sigma_x}{\partial x} + \frac{\partial \Delta \tau_{xy}}{\partial y} = \Delta F_x \]
\[ \frac{\partial \Delta \sigma_y}{\partial y} + \frac{\partial \Delta \tau_{yx}}{\partial x} = \Delta F_y \]
\[ \int \Delta \sigma_z dA = \Delta F_z \]
\[ \int x \Delta \sigma_z dA = \Delta M_x \]
\[ \int y \Delta \sigma_z dA = \Delta M_y \]
More Equations:

Constitutive Equations:

\[
\{\Delta \sigma\} = [D]\{\Delta \varepsilon\} + [\Delta D]\{\varepsilon\}
\]

where,

\[
\{\sigma\} = \left\{\sigma_x, \sigma_y, \sigma_z, \tau_{xy}\right\}^T
\]

\[
\{\varepsilon\} = \left\{\varepsilon_x, \varepsilon_y, \varepsilon_z, \varepsilon_{xy}\right\}^T
\]

Generalized Plane Strain

\[
\Delta \varepsilon_x = \frac{\partial \Delta u_x}{\partial x}
\]

\[
\Delta \varepsilon_y = \frac{\partial \Delta u_y}{\partial y}
\]

\[
\Delta \varepsilon_{xy} = \frac{1}{2} \left( \frac{\partial \Delta u_y}{\partial x} + \frac{\partial \Delta u_x}{\partial y} \right)
\]

\[
\Delta \varepsilon_z = a + bx + cy
\]

Finite Elements Implementations

\[
[K]\{T\} + [C]\{\dot{T}\} = \{Q\}
\]

\[
[K]\{\Delta u\} = \{\Delta F_{ei}\} + \{\Delta F_{pl}\} + \{F_{fp}\} + \{F_{el}\}
\]

Incremental Total Strain

\[
\{\Delta \varepsilon\} = \{\Delta \varepsilon_e\} + \{\Delta \varepsilon_{th}\} + \{\Delta \varepsilon_{pl}\}
\]
Constants Used in B&W Analytical and Abaqus Numerical Solutions

- Conductivity [W/mK] 33.
- Specific Heat [J/kg/K] 661.
- Thermal Linear Exp. [1/k] 2.E-4
- Density [kg/m³] 7500.
- Poisson’s Ratio 0.3
- Liquidus Temp [°C] 1494.48
- Solidus Temp [°C] 1494.38
- Initial Temp [°C] 1495.
- Number of Elements 300.
- Uniform Element Length [mm] 0.1

Artificial and non-physical thermal BC from B&W (slab surface quenched to 1000C), replaced by a convective BC with h=220000 [W/m²K]

Simple calculation to get h, from surface energy balance at initial instant of time:

\[-k \frac{\partial T}{\partial x} = h(T - T_\infty)\]

and for finite values

\[33 \cdot \frac{495}{0.0001} = h \cdot 495\]
Temperature and Stress Distributions for 1D Solidification

Abaqus and Analytical (Weiner-Boley) Solutions

- The numerical representations from MATLAB and Abaqus produces almost identical results
- Model is numerically consistent and has acceptable mesh

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Add more complexity (physics) to the Abaqus model by means of user subroutines.

Applied instantaneous Heat Flux from a real plant measurements:

\[
q(\text{MW/m}^3) = \begin{cases} 
5 - 0.2444t \text{ (sec.)} & t \leq 1.0 \text{ sec.} \\
4.7556t \text{ (sec.)}^{-0.504} & t > 1.0 \text{ sec.}
\end{cases}
\]

Elastic modulus decreases as temperature increase:
The only difference between solid and liquid is a large creep rate in the liquid

\[
\dot{\varepsilon} = \begin{cases} 
10^{-11} (|\sigma| - \sigma_{\text{yield}})^2 & \text{if } |\sigma| > \sigma_{\text{yield}} \\
0 & \text{if } |\sigma| \leq \sigma_{\text{yield}} 
\end{cases}
\]

Elastic visco-plastic model of Kozlowski for solidifying plain-carbon steel as our constitutive model:

\[
\dot{\varepsilon}(1/\text{sec.}) = f(\%C) \left[ \sigma (MPa) - f_1(T(^\circ K)) \varepsilon \right] \exp \left( -\frac{4.655 \times 10^4 \left( ^\circ K \right)}{T \left( ^\circ K \right)} \right)
\]

where

\[
f_1(T(^\circ K)) = 130.5 - 5.128 \times 10^{-3} T \left( ^\circ K \right)
\]

\[
f_2(T(^\circ K)) = -0.6289 + 1.114 \times 10^{-3} T \left( ^\circ K \right)
\]

\[
f_3(T(^\circ K)) = 8.132 - 1.54 \times 10^{-3} T \left( ^\circ K \right)
\]

\[f(\%C) = 4.655 \times 10^4 + 7.14 \times 10^4\%C + 1.2 \times 10^5 (\%C)^2\]
Temperature and Stress Distribution
Elastic-visco-plastic model by Kozlowski

- Different residual stress values due to different creep rate function
- Lower temperatures due to real flux data

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Comparison of Abaqus and CON2D for previous complex model

<table>
<thead>
<tr>
<th></th>
<th>CON2D</th>
<th>ABAQUS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Element type</td>
<td>6 node triangular</td>
<td>4 node rectangular</td>
</tr>
<tr>
<td>Number of elements</td>
<td>400</td>
<td>300</td>
</tr>
<tr>
<td>Number of nodes</td>
<td>1803</td>
<td>603</td>
</tr>
<tr>
<td>Initial time step</td>
<td>1.E-4</td>
<td>1.E-11</td>
</tr>
<tr>
<td>RAM used</td>
<td>&lt;1Gb</td>
<td>6Gb</td>
</tr>
<tr>
<td>Wall clock normalized to 1Ghz</td>
<td>17 minutes</td>
<td>204 minutes</td>
</tr>
</tbody>
</table>

![Graph showing stress-strain comparison](chart.png)

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Conclusions and Future Work

- Nowadays, it is possible to perform numerical simulations of steel solidification process in the Continuous Casting Mold with multipurpose commercial finite element code-Abaqus.
- 12 times more CPU and 6 times more memory resources are needed with Abaqus compared to in-house code CON2D for identical problem due to superior CON2D robust implicit-explicit integration scheme.
- Quantitatively results are matching well, qualitative differences are under investigation.
- It is realistic to expect much better wall clocks both with CON2D and Abaqus on the newest NCSA High Performance Architectures (IBM Regatta, Linux IA-64 Clusters).
- If there are enough dofs, parallel Abaqus features can be applied (each increment solved in parallel).
- Move to 2D and perhaps 3D FE domains with Abaqus and to increase process understanding.
- More Complexity (Physics) to the model: Internal BC with Ferrostatic Pressure, contact and friction between mold and shell, input mold distortion data, effects of superheat...
- Replace Abaqus native integration model and apply robust implicit-explicit integration scheme form CON2D with another user defined subroutine UMAT.
NCSA Terascale Linux Clusters

- 1 TF IA-32 Cluster of Parallel PC-s
  - 512 1 GHz dual processor nodes
  - Myrinet 2000 interconnect between PC-s
  - 5 TB of RAID storage

- 1 TF IA-64 Cluster of Parallel Itanium PC-s
  - 164 800 MHz dual processor nodes
  - Myrinet 2000 interconnect between PC-s

- Can solve a million equations with million unknowns in less than a minute by performing $17 \times 10^9$ floating point operation per second

- Great Potential to solve large scale problems in computational fluid dynamics and computational solid mechanics!

NCSA machine room expansion
- capacity to 20 TF and expandable
- dedicated September 5, 2001

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New NCSA Capabilities: Coming Soon

- Shared memory systems IBM Regatta, Power 4
  - 2+ TF of clustered SMP
  - 32 SMP CPUs, 1.3 Ghz
  - Large, 256 GB memory
  - AIX IBM Unix OS

Perfect for engineering commercial software like:

- Abaqus, Ansys, Fluent, LS-Dyna, Marc, PRO/E

- Cluster expansion
  - 5 TF Pentium4 Linux cluster

- Secondary and tertiary storage
  - 500 TB secondary storage SAN
  - 3.4 PB tertiary storage

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Computing in 21\textsuperscript{st} Century, a story of TeraGrid

\textit{Computing Resources: Anytime, Anywhere}

\textbf{Qwest 40 Gb/s Backbone}

- Abilene
- Chicago
- Indianapolis
- Urbana
- Los Angeles
- San Diego

\textbf{TeraGrid Backbone}

\textbf{I-WIRE}

\textbf{StarLight}
International Optical Peering Point (see www.startap.net)

\textbf{Qwest 40 Gb/s Backbone}

- OC-48 (2.5 Gb/s, Abilene)
- Multiple 10 GbE (Qwest)
- Multiple 10 GbE (I-WIRE Dark Fiber)

\textbf{Starlight / NW Univ}
\textbf{Ill Inst of Tech}
\textbf{Univ of Chicago}
\textbf{NCSA/UIUC}

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\textbf{Univ of Chicago}
\textbf{NCSA/UIUC}

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