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Solidification Stress Modeling using ABAQUS

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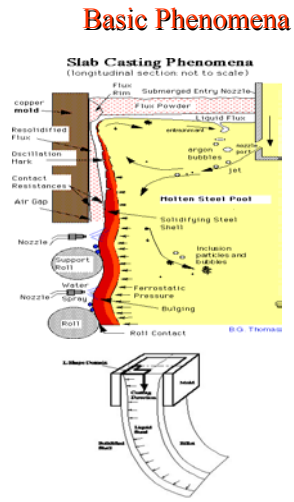
Objectives

- To predict the evolution of temperature, shape, stress and strain distribution in the solidifying shell in continuous casting mold by a nonlinear multipurpose commercial finite element package with an accurate approach.
- Validate the model with available analytical solution and benchmarks with in-house code CON2D specializing in accurate modeling of 2D continuous casting.
- To enable new model to be applied to the continuous casting problems by incorporating even more complete and realistic phenomena.
- To perform a unique realistic 3D thermal stress analysis of solidification of the shell of a thin slab caster that can accurately predict the 3D mechanical state in some critical regions important to crack formation.
- Apply FE results to predict the effects of casting speed on total strain evolution, to predict maximum casting speed to avoid bulging, to predict damage strains and transverse and longitudinal cracks, to find ideal taper and more.

Why ABAQUS?

- It has a good user interface, other modelers in this field can largely benefit from this work, including our final customers – the steel industry.
- Abaqus has imbedded pre and post processing tools supporting import of the major CAD formats. All major general purpose pre-processing packages like Patran and I-DEAS support Abaqus.
- Abaqus is using full Newton-Raphson scheme for solution of global nonlinear equilibrium equations and has its own contact algorithm.
- Abaqus has a variety of continuum elements: Generalized 2D elements, linear and quadratic tetrahedral and brick 3D elements and more.
- Abaqus has parallel implementation on High Performance Computing Platforms which can scale wall clock time significantly for large 2D and 3D problems.
- Abaqus can link with external user subroutines (in Fortran and C) linked with the main code than can be coded to increase the functionality and the efficiency of the main Abaqus code.

Basic Phenomena



- Once in the mold, the molten steel freezes against water-cooled walls of a copper mold to form a solid shell.
- Initial solidification occurs at the meniscus and is responsible for the surface quality of the final product. To lubricate the contact, oil or powder is added to the steel meniscus that flows into the gap between the mold and shell.
- Thermal strains arise due to volume changes caused by temp changes and phase transformations.
  Inelastic Strains develop due to both strain-rate independent plasticity and time dependant creep.
- At inner side of the strand shell the ferrostatic pressure linearly increasing with the height is present.
- Mold distortion and mold taper (slant of mold walls to compensate for shell shrinkage) affects mold shape and interfacial gap size.
- Many other phenomena are present due to complex interactions between thermal and mechanical stresses and micro structural effects. Some of them are still not fully understood.

Governing Equations

Heat 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 Equation (small strain assumption):

$$\nabla\cdot\boldsymbol{\sigma}(\mathbf{x})+\mathbf{b}_o=0$$

Rate Representation of Total Strain Decomposition:

$$\dot{\boldsymbol{\varepsilon}}=\dot{\boldsymbol{\varepsilon}}_{el}+\dot{\boldsymbol{\varepsilon}}_{ie}+\dot{\boldsymbol{\varepsilon}}_{th}$$

Constitutive Law (Rate Form, No large rotations):

$$\dot{\boldsymbol{\sigma}}=\underline{\underline{\mathbf{D}}}:(\dot{\boldsymbol{\varepsilon}}-\dot{\boldsymbol{\varepsilon}}_{ie}-\dot{\boldsymbol{\varepsilon}}_{th}) \qquad \underline{\underline{\mathbf{D}}}=2\mu\underline{\underline{\mathbf{I}}}+(k-\frac{2}{3})\mathbf{I}\otimes\mathbf{I}$$

Inelastic (visco-plastic) Strain Rate (strain rate independent plasticity + creep):

$$\dot{\bar{\varepsilon}}_{ie}=f(\bar{\sigma},\ T,\ \bar{\varepsilon}_{ie},\%C) \qquad \bar{\sigma}=\sqrt{\frac{3}{2}\mathbf{S}:\mathbf{S}}\ ,\ \mathbf{S}=\boldsymbol{\sigma}-\frac{1}{3}\text{trace}(\sigma)\mathbf{I}\ ,\ \dot{\bar{\varepsilon}}_{ie}=\sqrt{\frac{2}{3}\dot{\boldsymbol{\varepsilon}}_{ie}:\dot{\boldsymbol{\varepsilon}}_{ie}}$$

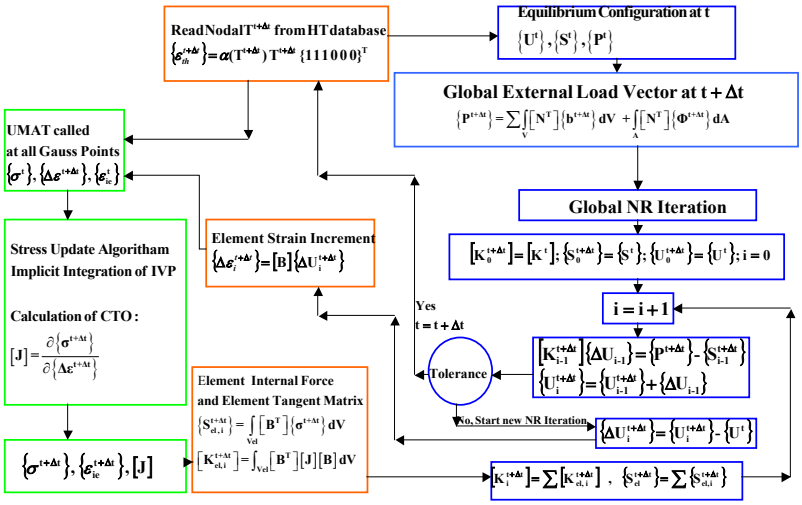
Thermal Strain:

$$\{\varepsilon_{th}\}=(\alpha(T)(T-T_{ref})-\alpha(T_i)(T_i-T_{ref}))[111000]^T$$

Computational Methods Used to Solve Governing Equations

- **Global Solution Methods** (solving global FE equations)
  - -Full Newton-Raphson used by Abaqus
  - -Operator-Splitting used by CON2D
- **Local Integration Methods** (on every material points integrating constitutive laws)
  - -Abaqus provided via CREEP subroutine, fully implicit followed by local NR
  - -Abaqus provided via CREEP subroutine, explicit
  - -Fully Implicit followed by local bounded NR
  - -Fully Implicit followed by Nemat-Nasser
  - -Radial Return Method for Rate Independent Plasticity, for liquid/mushy zone only

Big Picture: Materially Non-Linear FEM Solution Strategy in ABAQUS with UMAT



Big Picture 2: CON2D Solution Procedure Operator Splitting Technique (No global iterations, no CTO !)

Given: $\{\Delta\varepsilon\}^t, \{\sigma\}^t, \{\varepsilon_{ie}\}^t$ $\{\sigma^*\}^{t+\Delta t} = [D]^{t+\Delta t}\left(\{\varepsilon\}^t - \{\varepsilon_{ie}\}^t + \{\varepsilon_{th}^{t+\Delta t}\} + \{\Delta\varepsilon\}^t\right), \{S^*\}^{t+\Delta t} = \{\sigma^*\}^{t+\Delta t} - \{\sigma^*_{hyd}\}$

Calculate Trial Stress:

LOCAL STEP: Implicit Integration of constitutive law followed by 2 level local bounded NR.

Local Step Output: $\hat{\bar{\sigma}}^{t+\Delta t}, \hat{\bar{\varepsilon}}_{ie}^{t+\Delta t}$

Radial Return Factor: $\alpha = \dfrac{\hat{\bar{\sigma}}^{t+\Delta t}}{\bar{\sigma}^{*t+\Delta t}}$ **Stress Estimate Expansion:** $\{\hat{\sigma}\}^{t+\Delta t} = \alpha\{S^*\}^{t+\Delta t} + \{\sigma^*_{hyd}\}^{t+\Delta t}$

Inelastic Strain Rate Estimate: $\hat{\dot{\bar{\varepsilon}}}_{ie}^{t+\Delta t} = f\left(\hat{\bar{\sigma}}^{t+\Delta t}, \hat{\bar{\varepsilon}}_{ie}^{t+\Delta t}\right)$, **Flow Rule:** $\{\hat{\dot{\varepsilon}}_{ie}\}^{t+\Delta t} = \dfrac{3}{2}\dfrac{\{\hat{S}^{t+\Delta t}\}}{\hat{\bar{\sigma}}^{t+\Delta t}}\hat{\dot{\bar{\varepsilon}}}_{ie}^{t+\Delta t}$

GLOBAL STEP: Finite Element Solution of equilibrium equation.
Using constitutive law with initial strain.
Inelastic strain rate $\{\hat{\dot{\varepsilon}}_{ie}\}^{t+\Delta t}$ **based on estimate from Step1**
Solve linear global system for $\{\Delta d\}^{t+\Delta t}$ **only once for every time increment:**

$$\Sigma\int_{V_{el}}[B^T][D][B]dV\{\Delta d\}^{t+\Delta t} = \Sigma\int_{V_{el}}[B^T][D]\{\hat{\dot{\varepsilon}}_{ie}\}^{t+\Delta t}\Delta t dV + \Sigma\int_{V_{el}}[B^T][D]\{\Delta\varepsilon_{th}\}^{t+\Delta t}dV -$$

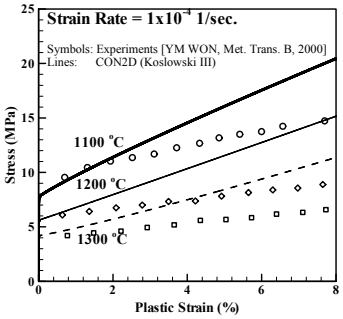
$$-\Sigma\int_{V_{el}}[B^T][D]\{\varepsilon_{el}\}^t dV + \Sigma\int_{V_{el}}[N^T]\{b\}^{t+\Delta t}dV + \Sigma\int_{S_\phi}[N^T]\{\phi\}^{t+\Delta t}dA$$

Update Values : $\{d\}^{t+\Delta t} = \{d\}^t + \{\Delta d\}^{t+\Delta t}, \{\Delta\varepsilon\}^{t+\Delta t} = [B]\{\Delta d\}^{t+\Delta t}, \{\Delta\varepsilon_{ie}\}^{t+\Delta t} = \{\hat{\dot{\varepsilon}}_{ie}\}^{t+\Delta t}\Delta t$

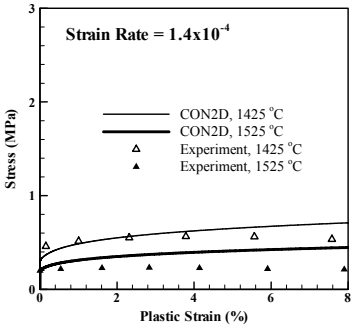
Update Stress: $\{\sigma\}^{t+\Delta t} = \{\sigma\}^t + [D]\left(\{\Delta\varepsilon\}^{t+\Delta t} - \{\Delta\varepsilon_{ie}\}^{t+\Delta t} - \{\Delta\varepsilon_{th}\}^{t+\Delta t}\right)$

Constitutive Models for Solid Steel (T<=Tsol)

Kozlowski Model for Austenite (Kozlowski 1991)



Modified Power Law for Delta-Ferrite (Parkman 2000)



Constitutive Models for Solid Steel (T<=Tsol)

Kozlowski Model for Austenite (Kozlowski 1991)

$$\dot{\varepsilon}(1/\sec.) = f(\%C)\left[\sigma(MPa) - f_1\left(T(^oK)\right)\varepsilon\left|\varepsilon\right|^{f_2\left(T(^oK)\right)-1}\right]^{f_3\left(T(^oK)\right)} \exp\left(-4.465\times10^4\,(^oK)/T(^oK)\right)$$

$$f_1\left(T(^oK)\right) = 130.5 - 5.128\times10^{-3}T(^oK)$$

$$f_2\left(T(^oK)\right) = -0.6289 + 1.114\times10^{-3}T(^oK)$$

$$f_3\left(T(^oK)\right) = 8.132 - 1.54\times10^{-3}T(^oK)$$

$$f(\%C) = 4.655\times10^4 + 7.14\times10^4\%C + 1.2\times10^5\,(\%C)^2$$

Modified Power Law for Delta-Ferrite (Parkman 2000)

$$\dot{\varepsilon}(1/\sec.) = 0.1\left|\sigma(MPa)/f(\%C)\left(T(^oK)/300\right)^{-5.52}(1+1000\varepsilon)^m\right|^n$$

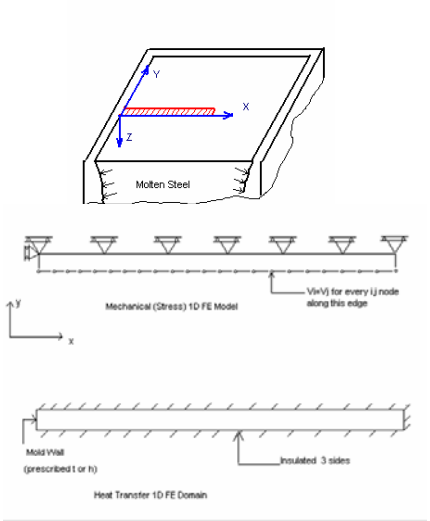
$$f(\%C) = 1.3678\times10^4\,(\%C)^{-5.56\times10^{-2}}$$

$$m = -9.4156\times10^{-5}T(^oK) + 0.3495$$

$$n = 1/1.617\times10^{-4}T(^oK) - 0.06166$$

1D Solidification Stress Problem for Program Validation

- Analytical Solution exists (Weiner & Boley 1963). Elastic in solid, Perfectly Plastic in liquid/mushy. No viscoplastic law for solid yet in this model.
- Provides an extremely useful validation test for integration methods, since stress update algorithm in liquid/mushy zone is a major challenge !
- Yield stress linearly drops with temp. from 20Mpa @ 1000C to 0.03Mpa @ Solidus Temp 1494.35C
- A strip of 2D elements used as a 1D FE Domain for validation
- Generalized plane strain both in y and z direction to give 3D stress/strain state
- Tested both of our methods to emulate Elastic-Perfectly Plastic material behavior plus both Abaqus native CREEP integration methods.



Constants Used in Abaqus Numerical Solution of WB Analytical Test Problem

Conductivity	[W/mK]	33.
Specific Heat	[J/kg/K]	661.
Elastic Modulus in Solid	[Gpa]	40.
Elastic Modulus in Liq.	[Gpa]	14.
Thermal Linear Exp.	[1/k]	2.E-5
Density	[kg/m^3]	7500.
Poisson's Ratio		0.3
Liquidus Temp	[^{o}C]	1494.48
Solidus Temp	[^{o}C]	1494.38
Initial Temp	[^{o}C]	1495.
Latent Heat	[J/kgK]	272000.
Number of Elements		300.
Uniform Element Length [mm]		0.1

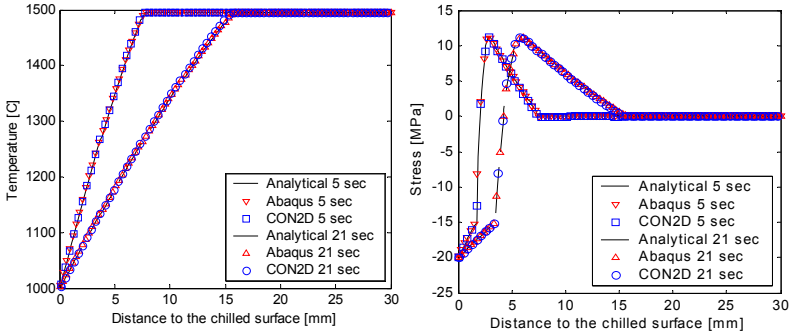
Artificial and non-physical thermal BC from VB (slab surface quenched to 1000C), replaced by a convective BC with h=220000 [W/m^{2}K]

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

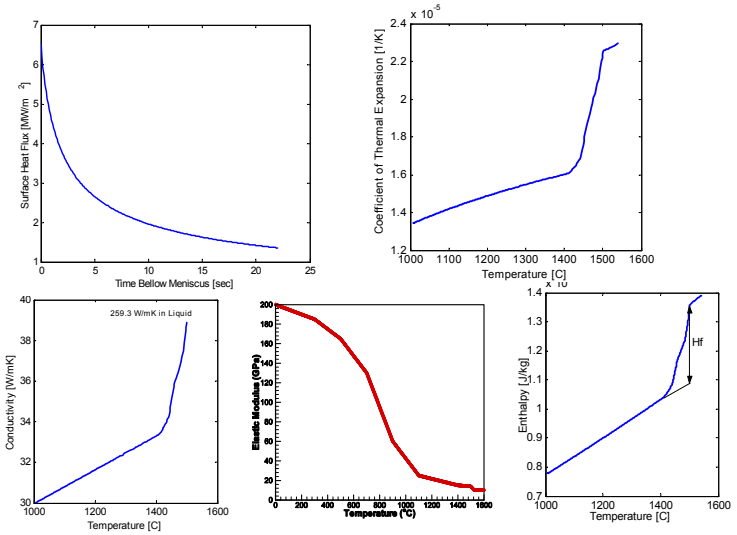
$$-k\frac{\partial T}{\partial x} = h(T - T_\infty) \quad \text{and for finite values} \quad 33\frac{495}{0.0001} = h\,495$$

Analytical, CON2D, and Abaqus Temperature and Stress Results (Weiner-Boley)

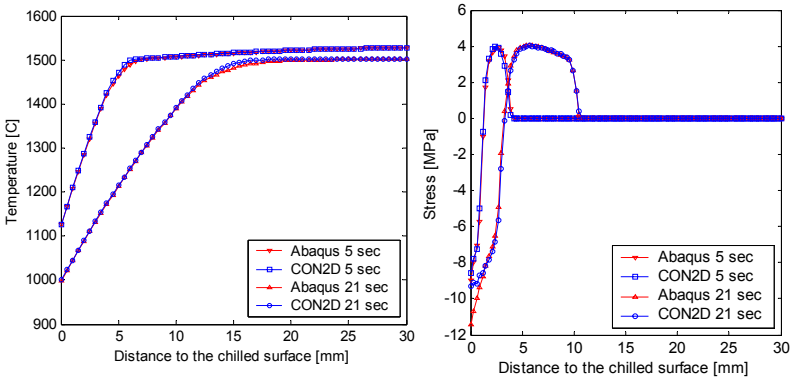
All different Stress Update Integration methods in Abaqus yield the same result, and are represented by a single Abaqus curve in bellow stress graph.



Solidifying Slice (0.27 %C) with Realistic Heat Flux and Temperature Dependant Material Properties



Abaqus and CON2D Temperature and Stress Results for Realistic Solidifying Slice in CC Mold



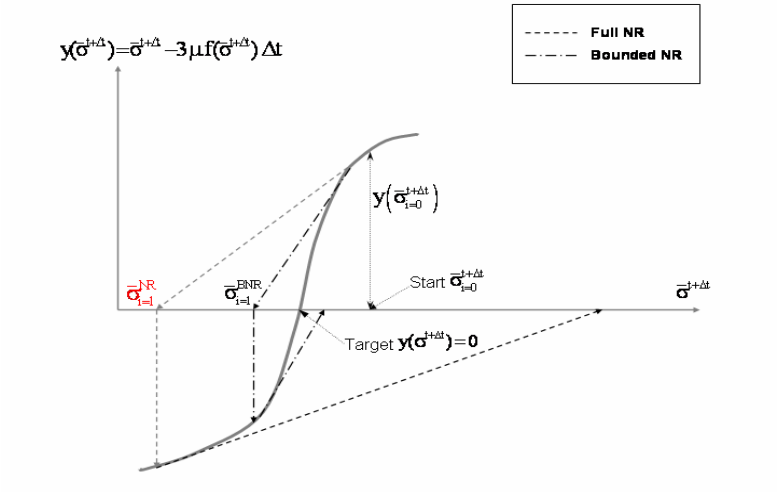
CPU Benchmarking Results

CODE	Global Method for Solving BVP	Local Integration Method	Treatment of Liq./Mushy zone	CPU time (Minutes)
Abaqus	Full NR	Implicit followed by local Bounded NR	Liquid Function	55
Abaqus	Full NR	Implicit followed by Nemat-Nasser	Liquid Function	53
Abaqus	Full NR	Implicit followed by local Bounded NR	Radial Return	5.6
Abaqus	Full NR	Implicit followed by loc. full NR (CREEP)	Radial Return or Liquid Function	Failed
Abaqus	Full NR	Explicit (CREEP)	Liquid Function	185
CON2D	Operator Splitting (Initial Strain)	Implicit followed by local Bounded NR	Liquid Function	6
CON2D	Operator Splitting (Initial Strain)	Implicit followed by Nemat-Nasser	Liquid Function	5.9

Conclusions

- The temperature and stress results are matching very well between two codes. A small discrepancy between the stress results in the coldest zone is under investigation.
- It took Abaqus in average 2-3 iterations with its global full NR methods to achieve convergence, while CON2D is using explicit operator splitting technique to solve global equilibrium equations without any iterations per increment which is CPU cost effective, but might be prone to some minor errors and oscillations.
- Local implicit integration followed by local bounded NR method turned out to be the most efficient and robust method for integrating our highly nonlinear constitutive laws.
- CPU time for Abaqus with our UMAT using local implicit rate independent plasticity algorithm (Radial Return) in liquid/mushy zone and fully implicit local integration method followed by local bounded NR in solid is totally comparable to CON2D, a clear sign that Abaqus with our UMAT is now ready to tackle large problems.

Local Bounded NR versus Local Full NR, a key fast convergence



Current & Future Work

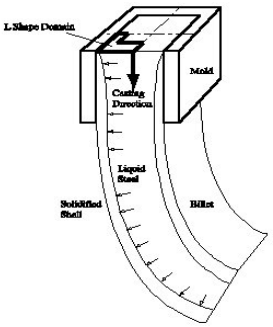
- Add more Phenomena (Physics) to the model in order to match real process condition: Internal BC with Ferrostatic Pressure, contact and friction between mold and shell, input mold distortion data.
- Program a consistent tangent operator with respect to temperature in our UMAT and perform incrementally-coupled 2D analysis with Abaqus (L-Shape FE Domain).
- Incorporate a realistic gap-size heat transfer coefficient that can produce a reasonable match with realistic heat flux from plant measurements.
- Perform a realistic 3D thermal stress analysis with adequate mesh refinement of solidification of shell of a thin slab caster that can accurately predict the 3D mechanical state in some critical zones important to crack formation. This would be the first of its kind ever performed. With enough dofs (3D), parallel Abaqus features will be applied (each time increment solved in parallel on NCSA's SMP machines). The UMAT presented here has been already coded for a 3D stress state.
- Add constitutive model for steels with delta-ferrite.

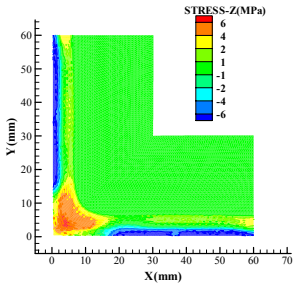
2D Application, Shell Behavior with strand corner

Predict the temperature, stress, and strain evaluation across a 2D section of the strand

Predict the distorted shape of the strand

Good for billet and corner portions of the slab



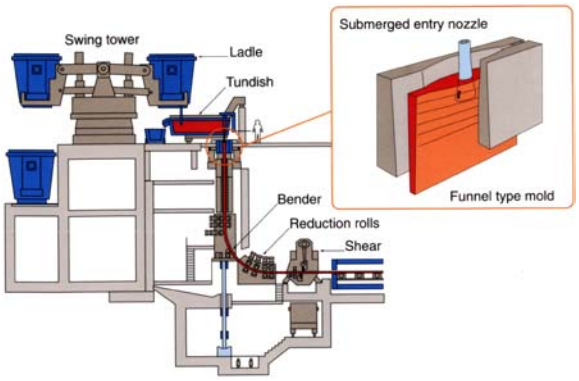


V=2.2 m/min V=4.4 m/min

Courtesy of Chungsheng Li, CON2D

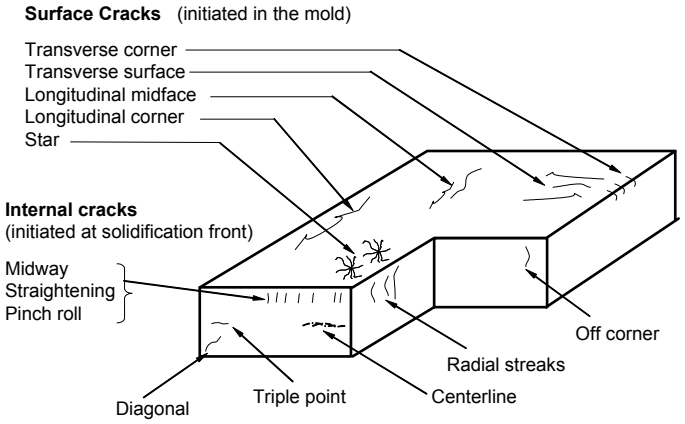
3D Application, Thin Slab Caster

Due to a funnel type mold, complex geometry in casting direction is causing an in-plane bending phenomena which was not modeled in 2D CON2D models. Only a 3D model can give the accurate stress distribution.



Crack defects in continuous cast slabs

Cracks form by combination of 1) tensile stress and
2) metallurgical embrittlement



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