Modeling of Hot Tearing and Other Defects in Casting Processes

Brian G. Thomas

1 Department of Mechanical Science & Engineering, University of Illinois (UIUC), 1206 West Green St., Urbana, Illinois, USA, 60801. bgthomas@uiuc.edu

1 Introduction

As computational models mature, their practical benefit to improving casting processes is growing. Accurate calculation of fluid velocities, temperature, microstructure, and stress evolution is just the first step. Achieving tangible improvements to casting processes requires the accurate prediction of actual casting defects and product properties. Defects that form during solidification are important not just to the casting engineer, because they are responsible for many of the defects in final manufactured products, and failures in service. They originate from inclusion entrapment, segregation, shrinkage cavities, porosity, mold-wall interactions, cracks, and many other sources that are process-specific. Casting defects can be modeled by extending the results of casting simulations through post processing, and/or by solving further coupled equations that govern these phenomena. The prediction of defect formation is made difficult by the staggering complexity of the phenomena that arise during commercial casting processes. This chapter introduces some of the concepts involved in modeling some of these solidification defects, and focuses in more detail on hot tearing.

A. Inclusions

Inclusions are responsible for many serious surface defects and internal quality problems in cast products. They arise from foreign particles, such as eroded sand particles, and impurities remaining in the liquid metal after upstream refining.[1] Nonmetallic inclusion particles act as sites of stress concentration and hydrogen gas nucleation, leading to lower fatigue life, hydrogen embrittlement, surface defects, and other problems in the final product. Predicting their damage requires knowledge of the number, size distribution, composition, and morphology of the inclusions coming from upstream processing prior to casting. Obtaining this knowledge ideally involves modeling the multiphase fluid flow, turbulent mixing and diffusion, species transport, chemical reactions, and particle interactions that create the inclusions in upstream processes.

Considerable modeling of these phenomena has been addressed in previous simulations of vacuum degassers, R-H degassers, ladles, tundishes, and other refining vessels and transfer operations used in metallurgical processing.[2] These models solve the multiphase Navier-Stokes equations for turbulent fluid flow, using software such as FLUENT,[3] and provide the flow field for subsequent simulation of inclusion particle transport. The first challenge is to properly incorporate the phenomena that drive the flow, which usually include the buoyancy of injected gas bubbles,[4] which depends on the shape of the bubbles, ranging from spherical caps to spheres. Other effects important to accurately computing the flow field may include natural convection, which requires a coupled heat transport solution for the temperature field, or electromagnetic forces, which requires modeling the applied magnetic field. Another challenge is to incorporate the effects of turbulence. Computationally-efficient choices include simple “mixing length” models, the two-equation models such as $k-\varepsilon$ to simulate the time-average flow pattern. Large eddy...
simulation (LES) models can simulate the details of the time-evolving turbulent vorticies, but at great computational expense. These methods have been compared with each other and with measurements of fluid flow in continuous casting.[5-7]

Modeling the thermodynamics and kinetics of particle formation, transport, collisions and removal or entrapment in the molten metal during upstream refining processes is the next crucial step. Thermodynamic reactions to quantify the precipitates that form in these multicomponent alloy systems can be predicted by simultaneous solution of chemical equilibrium equations, where the biggest challenge is to find accurate activity coefficients. Equilibrium compositions can also be found by comparing free-energy functions, such as used in Thermo-Calc,[8] FACT-Sage,[9] MTDATA,[10], Gemini[11] and other thermodynamic modeling software. The kinetics of non-metallic inclusion formation is generally controlled by species transport in the liquid, and at reaction interfaces, such as the slag-metal surface, where droplets of the different liquid phases, solid particles, and gas bubbles all interact. The physical entrainment of slag particles into the molten metal is another important source of inclusions,[12] which requires transient multiphase modeling of the free surface considering its breakup into droplets, and surface tension effects, and pushes the capabilities of current modeling capabilities to their limit.

Another important source of inclusions is re-oxidation of the molten metal by exposure to air. Oxygen absorbs rapidly from the atmosphere into any exposed molten metal, and combines to form precipitates, which has been predicted in molten steel from the alloy content.[13] Predictions are limited by understanding of the entrainment of oxygen from the atmosphere, the turbulent flow of the liquid steel during pouring, which determines the gas-metal interface shape, and the internal transport and reactions of chemical species in the molten metal.

The transport of particles through the flowing metal is the next crucial step to determine the inclusion distribution in the final product, and can be modeled in several ways.[14] Although the effect of bubbles on the flow pattern can be modeled effectively using Eulerian-Eulerian multiphase models, the fate of inclusion distributions is best modeled via Langrangian particle tracking. In this method, the trajectories of many particles are integrated from the local velocity field based on previous solution of the fluid velocities of a mold filling simulation. The effect of turbulence on the chaotic particle paths is very important, and is best modeled with the transient turbulent velocity field, using Large Eddy Simulation.[15] In more computationally-efficient time-averaged simulations of the turbulent flow field, the effect of turbulence on particle motion can be approximated using methods such as “Random Walk”, where the velocity at each time increment is given a randomly-generated component with magnitude proportional to the local turbulence level.[3] This method has been applied successfully to simulate particle motion in continuous casting molds.[16]

Inclusion particle size distributions evolve during transport due to collisions with each other and by their attachment to the surface of bubbles. Collisions can be modeled by tracking the evolution in the number distribution of particles in each size range, including the local effects of Brownian motion, turbulence, and diffusion, which is aided by size-grouping models to cover the large range of particle sizes.[17] Attachment and removal by bubbles can be modeled by computing the attachment rates of different particle sizes to different bubble sizes and shapes in computational models of these micro-scale phenomena.[16, 18] These attachment rates can then be incorporated into the macro-scale models of fluid and particle trajectories.[16, 18] In the extreme, inclusions may agglomerate into large clogs, which can restrict the flow of molten metal, cause detrimental changes in the downstream flow pattern, and can lead to catastrophic defects in the final product. Modeling and analysis of clogging is a complex subject, which has been reviewed elsewhere.[19]

Particle capture into the solidification front is a critical step during the modeling of inclusion transport. Small particles flow between the dendrites, so can be modeled as entrapped when they touch a domain wall. Larger particles may be pushed by the interface, or engulfed by a fast-moving planar front.[20]
More often, they are entrapped when they are suspended in front of the solidification front long enough for the dendrites to surround them. Entrapment is greatly lessened by tangential flow across the solidification front. A criterion for entrapment has been developed based on balancing the many forces which act on a particle suspended at the interface. Particles which never touch the interface, or escape capture, eventually may be removed if the flow pattern transports them to the casting boundaries, such as the top surface of some processes, where they can enter the slag layer.

The final step is to predict the property changes caused by the entrapped inclusions, which is a challenging modeling task, and depends on downstream processing, such as rolling, and heat treatment. Even with simply cooling to ambient, precipitation continues in the solid state, where the inclusion distribution is greatly affected by kinetic delays due to nucleation and solid-state diffusion. This is further complicated by preferential precipitation at grain boundaries and compatible existing inclusions, and is affected by strains, local microsegmentation, and many other phenomena. Clearly, the modeling of inclusions is a challenging task.

B. Segregation

Segregation is caused by the partitioning of alloys between the liquid and solid phases during solidification. Because species diffusion in the solid is very slow, this phenomenon is usually manifested by small-scale composition differences, called microsegregation, which explains how the spaces between dendrites are enriched in alloy relative to the dendrite centers. Although it contributes greatly to macrosegregation, porosity, inclusions, and other defects, microsegregation alone is not usually considered a defect, and it can be removed by homogenization heat treatment. When fluid flow is present, however, large-scale species transport leads to macrosegregation, where the composition differences arise over large distances, such as between the center and surface of a casting. This serious defect cannot be removed. It is extremely difficult to predict, because it involves so many different coupled phenomena, and at vastly different length and time scales. In addition to predicting fluid flow, species transport, and solidification, segregation requires prediction of the dendrite morphology and microstructure, and the complete stress state, including deformation of the spongy mushy zone and mechanical bulging and bending of the casting surface. Moreover, the fluid flow must be accurately characterized at both the microscopic scale between dendrite arms, and at the macroscopic scale of the entire casting. Each of these modeling tasks is a large discipline that has received significant effort over several decades.

Segregation is the main phenomenon responsible for many different kinds of special defects which only affect particular casting processes. For example, “freckle” defects can arise during the directional solidification of turbine blades when buoyancy-driven flow allows winding vertical channels to penetrate between dendrites and become filled with segregated liquid near the end of solidification. Inverse segregation or “surface exudation” in Direct-Chill continuous casting of aluminum ingots arises during the initial stages of solidification when thermal stress pushes out droplets of enriched interdendritic liquid through pores in the spongy mushy zone where it extends to the ingot surface. A comprehensive summary of the modeling of this important class of defects is beyond the scope of this chapter, and reviews of various aspects of this complex subject can be found elsewhere.

C. Shrinkage Cavities, Gas Porosity, and Casting Shape

Shrinkage cavities are voids in a casting which form due to the thermal contraction of liquid pockets after they become surrounded by solid which prevents the feeding of additional liquid. Porosity is the name for small voids that form due to the evolution and entrapment of gas bubbles. These two important classes of defects are related. They both involve the entrapment of liquid pockets, a criterion for the nucleation of gas bubbles, and depend on the overall shrinkage of the casting, which requires a complete thermo-mechanical stress calculation, in addition to accurate prediction of fluid flow and solidification. A rough estimate of shrinkage cavity potential is possible from post-processing analysis of the results of a simple
solidification heat transfer analysis, looking for regions where solid surrounds the liquid. This simple analysis can be automated by tracking parameters which represent shrinkage potential, such as the Niyama criterion.[30, 31] More accurate prediction of shrinkage requires complete modeling of fluid flow, heat transfer, and thermal-stress analysis. The fluid flow analysis is further complicated by the need for accurate characterization of the permeability of the porous dendritic network, which also depends on the microstructure, and alloy segregation. The stress analysis depends on the evolving strength of the solid, in addition to the mushy zone, interaction with the mold, and other phenomena which are discussed further in the section on hot tearing.

In addition to the phenomena which govern shrinkage cavity formation, gas porosity prediction also requires modeling the transport of dissolved gases, the nucleation of bubbles or gas pockets, and their possible transport after they form. This modeling also involves the same complications discussed in the prediction of inclusions, including non-equilibrium thermodynamics, chemical reactions, nucleation, precipitate formation and growth kinetics. Indeed, precipitation reactions are alternative ways for the dissolved gases to be consumed. Finally, gas bubbles that float during solidification can collide and coalesce, depending on surface tension. When combined with improper venting, this can lead to the creation of a defect found at the top of foundry castings known as a surface blow-hole.

Shrinkage and porosity defects are related to the final shape of the casting. When the solid metal shell is strong enough to resist shrinkage and retain its external dimensions, internal shrinkage and porosity might be more problematic. In contrast, practices which lessen shrinkage and porosity might involve more external shrinkage of the exterior. Inaccurate final dimensions is another casting defect. Inaccurate final dimensions is another casting defect. Because comprehensive modeling of these defects requires the simultaneous solution of so many different equation systems, with so many uncertain fundamental properties, this class of defects is difficult to predict and is the subject of intense ongoing research. The art of modeling these defects involves how to make simplifying assumptions with the least loss of accuracy. Further details on the current state of the art in modeling of this important class of defects is given elsewhere[28, 32, 33] and in Chapter ? [Peter Lee]

D. Mold Wall Erosion

Feeding molten metal into the casting cavity is a critical operation where defects may arise. Excessive turbulence and velocity impingement of the molten metal can erode the surface of the mold wall, especially near the in-gate. In sand molds, this can dislodge sand particles to act as another source of inclusions in the final casting. Even with permanent metal molds such as used in pressure die casting, excessive velocity against the metal walls can locally erode the metal, enlarging the casting cavity, and creating surface defects.

Erosion rate has been related to the metal velocity and other parameters in a few previous studies, based mainly on empirical correlations.[34] For example in die casting, erosion strength has been characterized by integrating the instantaneous velocity over the time of the injection cycle, for each local portion of the mold wall surface.[35] The resulting contours over the mold surface can be correlated with erosion damage.

Erosion of the mold wall due to fluid flow also may remove protective surface coatings and allow chemical reactions between the mold and the exposed mold metal. Thus, the mechanical erosion may be accompanied by chemical erosion and/or metallurgical corrosion, which often act together to wear away the mold surface. Analysis of the chemical component requires consideration of the thermodynamic reactions, and their kinetics. The interdiffusion of elements in the molten metal to contaminate the mold walls can lower the local melting temperature. This is responsible for the problem of soldering in aluminum die casting in steel molds.[36, 37]
E. Mold Wall Cracks

Cracks in the mold wall are another source of defects in the casting, in addition to lowering the lifetime of permanent molds. Mold cracks decrease the local heat transfer rate, allowing local concentration in the adjacent solidifying metal, and causing hot-tear cracks at the casting surface that mirror those in the mold. In water-cooled molds, mold cracks also pose a safety hazard, from the chance of molten metal contacting the cooling water. Mold cracks, or “heat checks” are caused by repeated rapid and severe fluctuations in the mold surface temperature. They can be predicted from the results of a transient thermal stress analysis of the mold itself, by combining the calculated inelastic strain (due to plasticity and creep) with measurements of cycles to failure from a thermal fatigue experiments. For example, surface cracks in copper molds used from continuous casting were predicted by comparing the results of transient 3-D finite element analysis of the copper mold and its support structure during cyclic loading with measured fatigue cycle-to-failure data.\cite{38} In addition to adopting practices to lower the maximum surface temperature, the mold lifetime was predicted to increase by lessening constraint of the mold by loosening bolts.\cite{38, 39} Often, the prediction of mold cracks requires consideration of the chemical interaction of the liquid metal with the mold, such as formation of brass in copper molds by the preferential absorption of zinc from the molten metal.

E. Other Defects

Many other casting defects arise due to problems specific to individual processes. Grain defects, such as unwanted grain boundaries, are important in directional solidification processes, such as the casting of single-crystal turbine blades, where high-temperature creep resistance is the most important property. In the Czochralski process, where single crystals are slowly pulled from doped melts to cast rods for making semiconductor wafers, even dislocations are serious defects that must be minimized. Examples in foundry “sand” casting include cold shut, blow holes, liquid metal penetration into the sand grains, and other surface defects. Some insight into these defects can found from analysis of the results of a solidification heat-transfer analysis. For example, problems related to cold shut can be estimated from a simulation if the molten metal freezes before the casting cavity is completely filled, leaving voids, or seams at the junction where two streams met. Crystal defects depend on the temperature gradient across the solidification front. Further insight can be gained from direct modeling of the microstructure\cite{40} and molecular dynamics or quantum-mechanics models of dislocations and other phenomena at the atomic scale.\cite{41} Many important process-specific defects have received little attention by the modeling community.

A final category of defects might be termed “goof-ups” because their cause is so obvious, and the solution involves at most only basic calculations. For example, a “short pour” occurs when the volume of metal poured is less than the volume of the casting cavity. Unsightly “mismatch” seams arise when the two halves of the foundry casting mold are not aligned, due to poor maintenance of the hinges and pins. Although obvious, avoiding such defects requires careful and diligent operations. Here, expert-system type software might help, aided in these examples by embedding simple volume calculations, and tracking of maintenance schedules. The rest of this chapter focuses on the important defect of hot-tear crack formation.

2 Hot tear Cracks

Crack formation is caused by a combination of tensile stress and metallurgical embrittlement. Although solidifying metal is subject to embrittlement due to a number of different mechanisms at different temperature ranges, hot-tear cracks form near the solidus temperature. Embrittlement is so severe near this temperature that hot-tear cracks form at strains on the order of only one percent, making them responsible for most of the cracks observed in cast products. Hot tear cracks form because thin liquid films between the dendrites at grain boundaries are susceptible to strain concentration, causing separation of the dendrites and
intergranular cracks. The prediction of these cracks presents a formidable challenge to modellers, owing to the many complex, interacting phenomena which govern stress and embrittlement, some of which are not yet fully understood:

- Predicting temperature, strain and stress during solidification requires calculation of the history of the cast product and its environment over huge temperature intervals. Characterizing the heat transfer coefficients at the boundaries and interfaces is one of many difficulties.

- The mechanical problem is highly non-linear, involving liquid-solid interaction and complex constitutive equations. Stress arises primarily from the mismatch of strains caused by large temperature gradients, and depends on the time- and microstructure-dependent inelastic flow of the material. Even identifying the numerous metallurgical parameters involved in these relations is a daunting task.

- The coupling between the thermal and the mechanical problems is an additional difficulty. This coupling comes from the mechanical interaction between the casting and the mold components, through gap formation or the build-up of contact pressure, modifying locally the heat exchange.

- Accounting for the mold and its interaction with the casting makes the problem multidomain, usually involving numerous deformable components with coupled interactions, and contact analysis.

- Cast parts usually have very complex three-dimensional shapes, which puts great demands on the interface between CAD design and the mechanical solvers, and on computational resources.

- The main cause of embrittlement is the segregation of solute impurities and alloying elements to the interdendritic liquid between primary grains, which lowers the solidus temperature locally. Segregation is most severe, and thus most important, at the grain boundaries, owing to the greater local interdenritic spacing locally, which allows the liquid to persist longer between grain boundaries.

- Larger primary grain size increases strain concentration and embrittlement, so must also be predicted. Because the grain size evolves with time, the grain size in the final cooled microstructure differs from the primary grain size, so grain size measurements for model validation should be inferred from analysis of the microsegregation pattern.

- Stress on the liquid films depend on the ability of liquid to flow through the dendritic structure to feed the volumetric shrinkage, relative to the strength of the surrounding dendritic skeleton. Thus, accurate permeability models are required for the mushy zone, which in turn require accurate prediction of the microstructure, including the dendrite arm shapes, especially at the grain boundaries.

- Crack prediction requires modeling the distribution of supersaturated dissolved gas, and its nucleation into pores or crack surfaces.

- The formation of solid precipitates tend to pin the primary grain boundaries, enhancing strain concentration. The interfering precipitates also act as nucleation sites for both gas bubbles and voids, both of which increase embrittlement. Modeling precipitation is difficult, owing to the multicomponent nature of commercial alloys, and the importance of kinetic delays.

- The subsequent refilling of hot tears with segregated liquid alloy can cause internal defects that are just as serious as exposed surface cracks, which oxidize. This again requires accurate prediction of both interdendritic and intergranular solute flow.

- The most important parameters to hot tearing: the stress tensor field which acts to concentrate tensile strain in liquid regions of the mushy zone, and the fluid velocity vector field which acts to fill the voids, are both three-dimensional time-varying quantities, which depend greatly on the orientation and shape of the microstructure. Thus, even empirical criteria to predict hot tears depend on conducting experiments with the proper load orientation, rates, and microstructures.
• The important length scales range from microns (dendrite arm shapes) to tens of meters (metallurgical length of a continuous caster), with a similar huge order-of-magnitude range in time scales.

A. Heat Transfer Modeling

Accurate calculation of the evolving temperature distribution during the casting process is the first and most important step in the analysis of hot tears. In addition to solving the transient heat-transport equation with phase change, this critical task usually requires coupling with turbulent fluid flow during mold filling, and interaction with the mold walls, with particular attention to the interfacial gap.

Heat transfer across the mold-casting interface depends on the size of the gap, (if open) or the contact pressure (if closed), so coupling with results from a mechanical analysis is often needed. Figure 1 shows the changes in interfacial heat transfer for these two cases. When a gap opens between the casting and the mold, due to their relative deformation, the heat transfer drops in proportion to the size of the gap. Heat flows across the interface, \( q_{\text{gap}} \), by conduction through the gas within the gap and by radiation between the two parallel surfaces, such as follows:

\[
q_{\text{gap}} = \frac{k_{\text{gas}}}{g} (T_c - T_m) + \frac{\sigma (T_c^4 - T_m^4)}{1 + \frac{1}{\varepsilon_c} - 1}
\]  

where \( k_{\text{gas}}(T) \) is thermal conductivity of the gap; \( g \) is gap thickness; \( T_c \) and \( T_m \) are local surface temperature of the casting and mold; \( \varepsilon_c \) and \( \varepsilon_m \) are emissivities; and \( \sigma \) is the Stefan-Boltzmann constant.

To avoid numerical problems at small gap sizes, this function should be truncated to a finite value, \( h_g \), which corresponds to the “closed-gap” case, and depends on the average roughness. More sophisticated functions can be applied to account for mold coating layers, different material layers, radiation-conduction, contact resistances to incorporate surface roughness, and other phenomena. Specific examples of these gap heat transfer laws are provided elsewhere for continuous casting with oil lubrication,\(^{[42]}\) and mold flux.\(^{[43]}\)

When contact between the mold and casting is good, the interfacial heat flux increases with contact pressure according to a power law\(^{[44]}\) such as:

\[
q_{\text{contact}} = (h_0 + A p_c^B)(T_c - T_m)
\]  

where \( p_c \) is contact pressure; \( A \) and \( B \) are fitting parameters which depend on the materials, lubricants, roughnesses, and temperature. After removal from the mold, heat transfer is given by uncoupled surface convection coefficients. Accurate characterization of the surface heat flux for all of these conditions requires careful calibration and validation with experimental measurements, and is a critical step in modeling.
B. Thermal-mechanical Modeling

Prediction of the displacements, strains, and stresses during the casting process is the next step in predicting residual stress, the distorted shape, and crack defects, including hot tears. As previously mentioned, stress analysis is also important in the prediction of porosity and segregation. The modeling of mechanical behavior requires solution of 1) the equilibrium or momentum equations, relating force and stress; 2) compatibility equations, relating strain and displacement and 3) the constitutive equations, relating stress and strain. This is because the boundary conditions specify either force or displacement at different regions of the domain boundaries.

B.1 Governing Equations

The conservation of force (steady-state equilibrium) or momentum (transient conditions) can be expressed by:

$$ \rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = \nabla \cdot \mathbf{\sigma} + \rho \mathbf{g} $$

(3)

where $\mathbf{\sigma}$ is the stress tensor, $\rho$ is the density, $\mathbf{g}$ is gravitational acceleration, $\mathbf{v}$ is the velocity field, $\cdot$ is dot product, $\nabla$ is the gradient operator, and matrices (vectors and tensors) are denoted in bold. Once solidified, the velocity terms which comprise the left side of Eq. (3) can be neglected.

The strains which dominate thermo-mechanical behavior during solidification are on the order of only a few percent, prior to crack formation. With small gradients of spatial displacement, $\nabla \mathbf{u} = \partial \mathbf{u} / \partial \mathbf{x}$, and the compatibility equations simplify to the following:\n
$$ \varepsilon = \frac{1}{2} \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) $$

(4)

where $\varepsilon$ is the strain tensor, $\mathbf{u}$ is the displacement vector, and $^T$ denotes transpose. This small-strain assumption simplifies the analysis considerably. The compatibility equations can also be expressed as a rate formulation, where strains become strain rates, and displacements become velocities. This formulation is more convenient for a transient computation with time integration involving fluid flow and/or large deformation.
Choosing constitutive models to relate stress and strain is a very challenging aspect of stress analysis of solidification, because it depends on accurately capturing the highly nonlinear evolution of the material microstructure with numerical parameters. Traditionally, this is accomplished with a family of elastic-plastic stress-strain curves at the appropriate temperatures and strain rate(s), and perhaps by adding a separate strain-rate function of temperature, stress and time to account for the time-dependent softening effects of creep.

However, the state variables of strain and time are not enough to quantify the strength of the material, especially during loading reversals. Furthermore, the effects of plastic strain and creep-strain rate are not independent. Thus, unified models have been developed which combine the different microstructural mechanisms together in terms of state variables which relate more closely to fundamental microstructural parameters such as dislocation density. Many models of different complexity can be found in the literature.\[^{46, 47}\] In their simplest form, these constitutive equations for metals are often expressed in terms of the state variables of temperature and inelastic strain, such as follows:

\[
\dot{\varepsilon} = \varepsilon^{el} + \varepsilon^{in} + \varepsilon^{th} \\
\varepsilon^{el} = \frac{1 + \nu}{E} \sigma - \frac{\nu}{E} \text{tr}(\sigma)I + \dot{T} \frac{\partial}{\partial T} \left( \frac{1 + \nu}{E} \right) \sigma - \dot{T} \frac{\partial}{\partial T} \left( \frac{\nu}{E} \right) \text{tr}(\sigma)I \\
\varepsilon^{in} = f(\sigma, T, \text{structure}) \\
\varepsilon^{th} = \left[ \frac{\rho(T_h)}{\rho} - 1 \right] I
\]

These tensor equations are expressed in terms of rates, where \(\dot{\cdot}\) is time derivative, \(\text{tr}\) is trace of a matrix, \(I\) is the identity tensor, and every variable should depend on temperature, \(T\). The strain rate tensor \(\dot{\varepsilon}\) is split into an elastic component, an inelastic (non-reversible) component, and a thermal component. Equation 6 is the hypoelastic Hooke’s law, where \(E\) is Young’s modulus, \(\nu\) the Poisson’s coefficient, and \(\sigma\) is time derivative of the stress tensor \(\sigma\). Equation 7 gives a framework for evolving the inelastic strain tensor, \(\varepsilon^{in}\), which is often used as the only parameter to characterize material structure. The thermal strains, Eq 8, include the solidification shrinkage and are based on the temperature field solved with the heat transfer model. Care should be taken in choosing a consistent reference temperature, \(T_h\), and in differentiating to extract the thermal strain rate, which can be accomplished numerically. Finding suitable constitutive equations to characterize the material mechanical response for the wide range of conditions experienced during solidification is a formidable task, which requires both careful experiments under different loading conditions, a reasonable form for the theoretical model, and advanced fitting procedures to extract the model coefficients.

B.2 Solution Strategies

Thermomechanical analysis of casting processes poses special difficulties due to the simultaneous presence of liquid, mushy and solid regions which move with time as solidification progresses, the highly nonlinear constitutive equations, complex three-dimensional geometries, coupling with the thermal analysis, interaction with the mold, and many other reasons. Several different strategies have been developed, according to the process and model objectives.

- A first strategy is to perform a small-strain thermo-mechanical analysis on just the solidified portion of the casting domain, extracted from the thermal analysis results. This strategy is convenient when the solidification front is stationary, such as the continuous casting of aluminum,\[^{48}\] and steel\[^{42, 49}\].
For transient problems, such as the prediction of residual stress and shape (butt-curl) during startup of the direct chill and electromagnetic continuous casting processes for aluminum ingots, the domain can be extended in time by adding layers.\cite{48}

- A second popular strategy considers the entire casting as a continuum, modifying the parameters in the constitutive equations for the liquid, mushy and solid regions according to the temperature and phase fraction. For example, liquid can be treated by setting the strains to zero when the temperature is above the solidus temperature. The primary unknowns are the displacements, or displacement increments. To facilitate the tracking of state variables, a “Lagrangian” formulation is adopted, where the domain follows the material. This popular approach can be used with structural finite element codes, such as MARC\cite{50} or ABAQUS\cite{51} and with commercial solidification codes or special-purpose software, such as ALSIM\cite{52} / ALSPEN,\cite{53} CASTS,\cite{54} CON2D,\cite{55, 56} Magmasoft,\cite{57} and Procast\cite{58, 59}. It has been applied successfully to simulate deformation and residual stress in shape castings,\cite{46, 61} DC casting of aluminum,\cite{48, 52, 53, 66, 62, 63} and continuous casting of steel\cite{55, 64}. Time integration of the highly nonlinear constitutive equations can benefit from special local-global integration numerical methods,\cite{56} or recent explicit methods.\cite{65} Assuming small strain and avoiding Poisson's ratio close to 0.5 for stability reasons\cite{66, 67} means that the liquid phase is not modeled accurately. Thus, some phenomena must be incorporated from other models, such as heat transfer from impinging liquid jets,\cite{68} and fluid feeding into the mushy zone.\cite{55}

- A third strategy simulates the entire casting, treating the mass and momentum equations of the liquid and mushy regions with a mixed velocity-pressure formulation. The primary unknowns are the velocity (time derivative of displacement) and pressure fields, which makes it easier to impose the incompressibility constraints, and to handle hydrostatic pressure loading. Indeed, the velocity-pressure formulation is also applied to the equilibrium of the solid regions, in order to provide a single continuum framework for the global numerical solution. This strategy has been implemented into codes dedicated to casting analysis such as THERCAST,\cite{64, 69, 70} and VULCAN.\cite{71} If stress prediction is not important so that elastic strains can be ignored, then this formulation simplifies to a standard fluid flow analysis, which is useful in the prediction of bulging and shape in large-strain processes. For problems involving large strain, such as squeeze-casting, this strategy is suited to an “arbitrary Lagrangian Eulerian” (ALE) formulation. In an Eulerian formulation, material moves through the computational grid, which remains stationary in the “laboratory” frame of reference, and requires careful updating of the state variables. In ALE, mesh updating is partially independent of the material velocity to maintain the quality of the computational grid. Further details are provided elsewhere.\cite{69, 72}

### C. Hot tearing criteria

The next step is to quantify embrittlement, and to incorporate it with the thermal-stress analysis to predict hot tear cracks. Hot tearing phenomena are too complex, too small-scale, and insufficiently understood to model in detail as part of the macro-scale thermal-mechanical analysis. Thus, several different criteria and approaches have been developed to predict hot tears from the results of such analyses. This topic is the focus of many ongoing research efforts, and although many of these criteria reproduce observed trends, much more work is needed before quantitative predictions are reliable.

Different approaches are needed for different microstructures and metals, according to the most important phenomena which govern crack formation. Hot tear cracks forming within large networks of mushy equiaxed grains require accurate constitutive models to quantify the rheology of the mushy region. Cracks between columnar grains require models which incorporate the balance between liquid feeding
between dendrites and tensile deformation perpendicular to the direction of dendrite growth. The hot tearing of aluminum alloys additionally depends on the critical stress to nucleate a gas bubble. In steel, dissolved gas contents are usually low, so hot tears usually refill with segregated liquid without opening into cracks. This macrosegregation is very damaging, so becomes a very important phenomenon to model accurately. Every criterion depends on experimental measurements and how best to incorporate them.

C.1 Thermal-analysis-based Criteria

The results of the solidification heat-transfer analysis alone can provide some important insights into hot tearing. As illustrated in Figure 2, the location of hot tear cracks observed in a casting can be related to their time of formation. Cracks tend to initiate near the casting surface ($x_1$) and propagate towards the center of casting, ($x_2$) as solidification progresses. Figure 2b) shows the progress of the mushy zone and important isotherms with time, based on the results of a solidification heat-transfer model. In the case of continuous casting, the time axis also corresponds to distance in the casting direction, so the figure depicts the actual shape of the solidification fronts in the real caster.

![Figure 2](image)

Figure 2 Relating the location of hot-tear crack formation to results of a transient thermal simulation

Casting conditions that produce faster solidification and alloys with wider freezing ranges are more prone to hot tears. Thus, many criteria to indicate hot-tear cracking susceptibility (HCS) are solely based on thermal analysis. One [73] simply compares the local time spent between two critical solid fractions $g_{s1}$ and $g_{s2}$ (typically 0.9 and 0.99, respectively), with the total local solidification time (or a reference solidification time), such as:

$$HCS_{C_{brane}} = \frac{t_{0.99} - t_{0.99}}{t_{0.90} - t_{0.40}}$$

(9)

C.2 Mechanical-analysis-based criteria

Many different criteria have been developed to predict hot tear cracks from the results of a mechanical analysis. Regardless of the model formulation, developing an accurate criterion function to predict hot tears relies on measurements, such as the submerged split-chill tensile test [74-76]. This experiment applies and measures a tensile load on the solidifying shell, perpendicular to the growth direction, so it matches the conditions present in hot tearing between columnar grains. Other experiments, such as the Gleeble, apply a tensile load to remelted metal which is held in place by surface tension. Care must be taken in the interpretation of such measurements because the load is generally applied in the same direction as
solidification front growth. Proper interpretation of any hot-tearing experiment requires detailed modelling of the experiment itself, because conditions are never constant and at best only raw data such as temperature, displacement and force can be measured. The parameters of greatest interest must be extracted using models.

Criteria based on classical mechanics often assume cracks will form when a critical stress is exceeded, and they are popular for predicting cracks at lower temperatures\cite{77-80}. Tensile stress is also a requirement for hot tear formation.\cite{81} This critical stress depends greatly on the local temperature and strain rate. The maximum tensile stress occurs just before formation of a critical flaw.\cite{82}

Measurements often correlate hot tear formation with the accumulation of a critical level of mechanical strain while applying tensile loading within a critical solid fraction where liquid feeding is difficult. This has formed the basis for many hot-tearing criteria. One such model\cite{81} accumulates inelastic deformation over a brittleness temperature range, which is defined, for example as $g_\text{s} \in [0.85, 0.99]$ for a Fe-0.15wt%C steel grade. The local condition for fracture initiation is then:

$$\sum_{g_{s1}}^{g_{s2}} \Delta e^m \geq \varepsilon_{cr}$$  \hspace{1cm} (10)

in which the critical strain $\varepsilon_{cr}$ is 1.6% at a typical strain rate of $3 \times 10^{-4}$ $s^{-1}$. Careful measurements during bending of solidifying steel ingots have revealed critical strains ranging from 1 to 3.8%.\cite{81, 83} The lowest values were found at high strain rate and in crack-sensitive grades (e.g. high-sulfur peritectic steel).\cite{81} In aluminum rich Al-Cu alloys, critical strains were reported from 0.09 to 1.6% and were relatively independent of strain rate.\cite{82}

The critical strain decreases with increasing strain rate, presumably because less time is available for liquid feeding, and also decreases for alloys with wider freezing ranges. The following empirical equation for the critical strain in steel, $\varepsilon_{cr}$, was based on fitting measurements from many bend tests\cite{84}:

$$\varepsilon_{cr} = \frac{0.02821}{\varepsilon^{0.3131} \Delta T_B^{0.8638}}$$  \hspace{1cm} (11)

where $\dot{\varepsilon}$ is the strain rate ($s^{-1}$), and $\Delta T_B$ is the brittle temperature range, ($^\circ$C) defined between the temperatures corresponding to solid fractions of 0.9 and 0.99.

An elegant analytical criterion-model has been derived to predict hot tearing, based on when the local liquid feeding rate along the interdendritic spaces between the primary columnar dendrites is insufficient to balance the rate of tensile strain increase in the perpendicular direction across the mushy zone.\cite{85, 86} Specifically, gas pores cavitate to separate the residual liquid film between the dendrites when the tensile strain rate exceeds a critical value:

$$\dot{\varepsilon} \geq \frac{1}{R} \left[ \frac{180 \mu_t}{\lambda_2} \left\| \nabla T \right\| \frac{\rho_L}{\rho_S} \left( p_m - p_c \right) - v_T \rho_S - \rho_L H \right]$$  \hspace{1cm} (12)

in which $\mu_t$ is the dynamic liquid viscosity, $\lambda_2$ is the secondary dendrite arm spacing, $p_m$ is the local pressure in the liquid ahead of the mushy zone, $p_c$ is the cavitation pressure, $v_T$ is the velocity of the solidification front, and $\left\| \nabla T \right\|$ is the magnitude of the temperature gradient across the mushy zone. The quantities $R$ and $H$ depend on the solidification path of the alloy:

$$R = \int_{T_2}^{T_1} \frac{g_i^2 F(T)}{g_i^3} dT \hspace{1cm} H = \int_{T_2}^{T_1} \frac{g_i^2}{g_i^3} dT \hspace{1cm} F(T) = \frac{1}{\left\| \nabla T \right\|} \int_{T_2}^{T_1} g_i dT$$  \hspace{1cm} (13)
where the integration limits are calibration parameters. The upper limit $T_1$ may be the liquidus or the coherency temperature, while the lower limit $T_2$ typically is within the solid fraction range of 0.95-0.99. This criterion model has been applied to hot tearing of aluminum microstructures.

For hot tearing within large mushy regions, typically equiaxed microstructures, constitutive behavior of the mushy zone to predict the local fluid flow and deformation of the dendritic network presents an important additional challenge. Other criterion models, which focus more on this aspect of hot tearing have recently been developed. Further details on hot tearing of aluminum alloys are reviewed elsewhere.

### C.3 Micro-scale model-based criteria

Detailed computational models can be developed of temperature, fluid flow, stress and strain in the mushy zone during solidification. For example, a finite-element model of an equiaxed mushy zone of aluminum has been applied to investigate constitutive behavior and to quantify strain concentration in the liquid films for a few specific sets of conditions. Once such models are more mature, their results can be incorporated into better criteria for hot tearing. A final difficult task is extracting results from the macro-scale model results to compare with the criterion models, owing to the sensitivity of numerical estimates of parameters such as strain rate to numerical oscillations and mesh refinement effects. Thus, coupling difficulties between the macro- and micro-scale models is another reason that hot tear crack prediction an ongoing challenge.

### D. Microsegregation Modeling

Quantifying the relation between temperature and phase fractions is an essential part of each model involved in the prediction of hot tearing, including the heat transfer, the mechanical, and the hot-tear criterion models. This relation determines how latent heat is evolved in the heat transfer model, and how to switch between constitutive models in the mechanical model. Although simple linear, lever-rule, or Scheil-based relations are usually sufficient for these macro-scale models, microsegregation is an essential aspect of embrittlement and greatly affects the phase-fraction temperature relation involved in any hot tearing criterion. Better relations use the results of microsegregation models which consider partial diffusion of multiple solute elements in the solid phase, using simple analytical solutions, or one-dimensional models of a single secondary dendrite arm. More advanced models couple this calculation together with the macro-scale models, and allow the relation to evolve to incorporate nucleation undercooling and other phenomena. Ideally, the relations applied between dendrites and at grain boundaries should be different, and they should vary with location in the casting, to account for macrosegregation and other phenomena. An important concept, which is often overlooked, is that the same (or very close) relation must be used in each model of the analysis. Inconsistency between microsegregation models is one of the main reasons why different researchers have proposed different critical temperatures in their hot tear criteria. Experiments conducted to quantify the parameters in hot tearing models should fully report both the raw data, and the models used to extract hot tearing parameters, including the microsegregation model.

### 3 Model Validation

Model validation is a crucial step in any computational analysis. Analytical solutions are needed to prove internal consistency of the model and to control discretization errors. Comparison with experiments is needed to prove the model assumptions, property data, and boundary conditions. Weiner and Boley derived an analytical solution for unidirectional solidification of an unconstrained plate, which serves as an ideal benchmark problem to validate thermal and mechanical models. The plate is subjected to sudden...
surface quench from a uniform initial temperature to a constant mold temperature, with a unique solidification temperature, an elastic-perfectly-plastic constitutive law and constant properties.

This benchmark problem can be solved with a simple mesh of one row of elements, extending from the casting surface into the liquid as shown in Figure 3. Numerical predictions should match with acceptable precision using the same element type, mesh refinement and time steps planned for the real problem. For example, the solidification stress analysis code, CON2D [55] and the commercial code ABAQUS [51] were applied for typical conditions of steel casting. [56]

Figure 3. One-dimensional slice-domain for modeling solidifying plate.

Figure 4 and Figure 5 compare the temperature and stress profiles in the plate at two times. The temperature profile through the solidifying shell is almost linear. Because the interior cools relative to the fixed surface temperature, its shrinkage generates internal tensile stress, which induces compressive stress at the surface. With no applied external pressure, the average stress through the thickness must naturally equal zero, and stress must decrease to zero in the liquid. Stresses and strains in both transverse directions are equal for this symmetrical problem. The close agreement demonstrates that the computational model is numerically consistent and has an acceptable mesh resolution. Such studies reveal that a relatively fine mesh is needed to achieve reasonable accuracy, and that results from many thermal-mechanical models reported in previous literature had insufficient mesh refinement. Comparison with experimental measurements is also required, to validate that the modeling assumptions and input data are reasonable.
Figure 4. Temperatures through solidifying plate at different times comparing analytical solution and numerical predictions.

![Figure 4](image.png)

Figure 5. Transverse (Y and Z) stress through solidifying plate at different times comparing analytical solution and numerical predictions.

![Figure 5](image.png)

4 Case Study: Billet Casting Speed Optimization

A Lagrangian model of temperature, distortion, strain, stress, hot tearing has been applied to predict the maximum speed for continuous-casting of steel billets without forming off-corner internal hot-tear cracks. The two-dimensional transient finite-element thermal-mechanical model, CON2D\[55, 56\] has been used to track a transverse slice through the solidifying steel strand as it moves downwards at the casting speed to reveal the entire 3-D stress state. The 2-D assumption produces reasonable temperature predictions because axial (z-direction) conduction is negligible relative to axial advection.\[43\] In-plane mechanical predictions are also reasonable because bulging effects are small and the undiscretized casting direction is modeled with the appropriate condition of generalized plain strain. Other applications with this model include the prediction of ideal taper of the mold walls,\[96\] and quantifying the effect of steel grade on oscillation mark severity during level fluctuations.\[97\]

The model domain is an L-shaped region of a 2-D transverse section, shown in Figure 6. Removing the central liquid region saves computation and lessens stability problems related to element “locking”. Physically, this “trick” is important in two-dimensional domains because it allows the liquid volume to change without generating stress, which mimics the effect of fluid flow into and out of the domain that occurs in the actual open-topped casting process. Simulations start at the meniscus, 100 mm below the mold top, and extend through the 800-mm long mold and below, for a caster with no sub-mould support. The instantaneous heat flux, given in Eq. (14), was based on plant measurements.\[98\] It was assumed to be uniform around the perimeter of the billet surface in order to simulate ideal taper and perfect contact between the shell and mold. Below the mold, the billet surface temperature was kept constant at its circumferential profile at mold exit. This eliminates the effect of spray cooling practice imperfections on sub-mold reheating or cooling and the associated complication for the stress/strain development. A typical plain carbon steel was studied (0.27%c, 1.52%Mn, 0.34%Si) with 1500.7 °C liquidus temperature, and 1411.8 °C solidus temperature.
Different constitutive models were used for each phase of the solidifying steel. The following elastic-visco-plastic constitutive equation was developed for the austenite phase as a function of percent carbon content (%C) by fitting constant strain-rate tensile tests and constant-load creep tests to the form in Eq 5 and Eq 7.

\[
\dot{\varepsilon}_{eq} = f_{\text{eqC}} \left( \sigma_{eq} - \sigma_0 \right)^{1/m} \exp \left( -\frac{4.465 \times 10^4}{T} \right)
\]

where

\[
f_{\text{eqC}} = 4.655 \times 10^4 + 7.14 \times 10^4 (%C) + 1.2 \times 10^4 (%C)^2
\]

\[
\sigma_0 = (130.5 - 5.128 \times 10^{-3} T) \varepsilon_{eq} f_2
\]

\[
f_2 = -0.6289 + 1.114 \times 10^{-3} T
\]

\[
1/m = 8.132 - 1.54 \times 10^{-3} T
\]

with \(T[\text{K}], \sigma_{eq}, \sigma_0[\text{MPa}]\)

Further equations, such as the associated flow rule, are needed to transform this scalar equation into tensor form, and to account for reversals in loading conditions. Equation 15, and a similar one for delta-ferrite, have been implemented into the finite-element codes CON2D and THERCAST and applied to investigate several problems involving mechanical behavior during continuous casting.

Elastic modulus is a crucial property that decreases with increasing temperature. It is difficult to measure at the high temperatures important to casting, owing to the susceptibility of the material to creep and thermal strain during a standard tensile test, which results in excessively low values. Higher values are obtained from high-strain-rate tests, such as ultrasonic measurements. Elastic modulus measurements in steels near the solidus temperature range from \(\sim 1\ \text{GPa}\) to \(44\ \text{GPa}\) with typical modulus values \(\sim 10\ \text{GPa}\) near the solidus.
The density needed to compute thermal strain in Eq. 8 can be found from a weighted average of the values of the different solid and liquid phases, based on the local phase fractions. For the example of plain low carbon steel, the following equations were compiled\[55] based on the phase fractions of alpha-ferrite ($f_\alpha$), austenite ($f_\gamma$), delta-ferrite ($f_\delta$)\[109,110] and liquid ($f_l$) measurements.\[111]

\[
\rho(kg/m^3) = \rho_\alpha f_\alpha + \rho_\gamma f_\gamma + \rho_\delta f_\delta + \rho_l f_l
\]

\[
\rho_\alpha = 7881 - 0.324T(^\circ C) - 3 \times 10^{-3}T(^\circ C)^2
\]

\[
\rho_\gamma = \frac{100[8106 - 0.517T(^\circ C)]}{[100-(^\circ C)][1+0.008(^\circ C)]^3}
\]

\[
\rho_\delta = \frac{100[8011 - 0.47T(^\circ C)]}{[100-(^\circ C)][1+0.013(^\circ C)]^3}
\]

\[
\rho_l = 7100 - 73(^\circ C) - [0.8 - 0.09(^\circ C)][T(^\circ C) - 1550]
\]

Sample results are presented here for one-quarter of a 120 mm square billet cast at speeds of 2.0 and 5.0 m/min. The latter is the critical speed at which hot-tear crack failure of the shell is just predicted to occur. The temperature and axial (z) stress distributions in a typical section through the wideface of the steel shell cast at 2.0 m/min are shown in Figure 7 and Figure 8 at four different times during cooling in the mold. Unlike the analytical solution in Figure 4, the surface temperature drops as time progresses. The corresponding stress distributions are qualitatively similar to the analytical solution (Figure 5). The stresses increase with time, however, as solidification progresses. The realistic constitutive equations produce a large region of tension near the solidification front. The magnitude of these stresses (and the corresponding strains) are not predicted to be enough to cause hot tearing in the mold, however. The results from two different codes reasonably match, demonstrating that the formulations are accurately implemented, convergence has been achieved, and that the mesh and time-step refinement are sufficient.

Figure 7. Temperature distribution along the solidifying slice in continuous casting mold.
Figure 8. Lateral (y and z) stress distribution along the solidifying slice in continuous casting mold.

Figure 9(a) shows the distorted temperature contours near the strand corner at 200 mm below the mold exit, for a casting speed of 5.0 m/min. The corner region is coldest, owing to two-dimensional cooling. The shell becomes hotter and thinner with increasing casting speed, owing to less time in the mold. This weakens the shell, allowing it to bulge more under the ferrostatic pressure below the mold.

Figure 9(b) shows contours of “hoop” stress constructed by taking the stress component acting perpendicular to the dendrite growth direction, which simplifies to $\sigma_x$ in the lower right portion of the domain and $\sigma_y$ in the upper left portion. High values appear at the off-corner sub-surface region, due to a hinging effect that the ferrostatic pressure over the entire face exerts around the corner. This bends the shell around the corner and generates high subsurface tensile stress at the weak solidification front in the off-corner subsurface location. This tensile stress peak increases slightly and moves towards the surface at higher casting speed. Stress concentration is less and the surface hoop stress is compressive at the lower casting speed. This indicates no possibility of surface cracking. However, tensile surface hoop stress is generated below the mold at high speed in Figure 9(b) at the face center due to excessive bulging. This tensile stress, and the accompanying hot-tear strain, might contribute to longitudinal cracks which penetrate the surface.
Hot tearing was predicted using the criterion in Eq. (10) with the critical strain given in Eq. (11). Inelastic strain was accumulated for the component oriented normal to the dendrite growth direction, because that is the weakest direction and corresponds to the measurements used to obtain Eq. (11). Figure 9(c) shows contours of hot-tear strain in the hoop direction. The highest values appear at the off-corner subsurface region in the hoop direction. Moreover, significantly higher values are found at higher casting speeds. For this particular example, hot-tear strain exceeds the threshold at 12 nodes, all located near the off-corner subsurface region. This is caused by the hinging mechanism around the corner. No nodes fail at the center surface, in spite of the high tensile stress there. The predicted hot-tearing region matches the location of off-corner longitudinal cracks observed in sections through real solidifying shells, such as the one pictured in Figure 10. The bulged shape is also similar.

Results from many computations were used to find the critical speed to avoid hot tear cracks as a function of section size and working mold length, presented in Figure 11. These predictions slightly exceed plant practice, which is generally chosen by empirical trial and error. This suggests that plant conditions such as mold taper are less than ideal, that other factors limit casting speed, or those speeds in practice could be increased. The qualitative trends are the same.

This quantitative model of hot tearing provides many useful insights into the continuous casting process. Larger section sizes are more susceptible to bending around the corner, so have a lower critical speed, resulting in less productivity increase than expected. The trend towards longer molds over the past
three decades enables a higher casting speed without cracks by producing a thicker, stronger shell at mold exit.

Figure 11. Comparison of critical casting speeds, based on hot-tear criterion, and typical plant practice.\cite{112}

5 Conclusions

The prediction of defects represents the culmination of solidification modeling. It enables models to make practical contributions to real commercial processes, but it requires incorporating together and augmenting the models of almost every other aspect of casting simulation. Hot-tear crack prediction requires accurate thermal and mechanical analysis, combined with criteria for embrittlement. As computing power and software tools for computational mechanics advance, it is becoming increasingly possible to perform useful analysis of fluid flow, temperature, deformation, strain, and stress, and related phenomena in real casting processes. Computations are still hampered by the limits of mesh resolution and computational speed, especially for realistic three-dimensional geometries and defect analysis. The modeling of defects such as hot tears is still in its infancy, and there is much work to be done.

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References


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