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ISSUES IN THERMAL-MECHANICAL MODELING OF CASTING PROCESSES

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Synopsis

Mathematical modeling of stress generation in casting processes is a difficult, complex subject that is now receiving increased attention. This paper reviews the basic equations, solution methods and important phenomena associated with casting processes that require special numerical treatment. Stress modeling begins with a coupled, transient heat transfer analysis, including solidification, shrinkage-dependent interfacial heat transfer, and fluid flow effects. Further complicating phenomena include phase transformations, temperature, stress and structure-dependent plastic-creep, interaction between the casting and the mold, hydrostatic pressure from the liquid, the effects of fluid flow, and crack formation. Computational issues include numerical methods for handling these phenomena, mesh refinement, and two-dimensional stress state. Example applications are presented for the thermal-mechanical behavior of the solidifying steel shell in the mold region of a continuous slab caster, using a finite-element model, which accounts for many of these phenomena.

1. Introduction

Numerical calculation of the stresses and strains that arise during solidification processes is important for the prediction of surface shape and cracking problems. Many previous mathematical models have been applied to predict this behavior, which are summarized in part in a previous review.[1] Owing to the great computational complexity of the problem, many previous stress analyses have oversimplified several important aspects. These include the effects of anisotropic properties, phase transformations, interaction with the mold, fluid flow, temperature dependence of the elastic modulus, liquid properties, combined creep and plasticity, microstructural effects, mesh refinement, and two-dimensional stress state. As part of a larger project to develop comprehensive finite-element models of the continuous casting process, this paper explores the treatment of some of these issues.

2. Simple description of basic phenomena

Deformation and stress in a solidifying body develops differently than in a totally solid part undergoing the same thermal history. This is due to the nature of the liquid, which displaces without generating stress. Fig. 1 shows a simplified sequence of steps which lead to the typical stress and distortion profiles found in a solidifying shell.

Consider liquid metal suddenly contacting a chilled substrate (mold). An “outer” (lower) layer of liquid quickly solidifies into a thin shell and cools. If it does not stick to the substrate, then no significant stress is generated. This is because the thin layer is relatively free to shrink, and can displace some of the liquid above it. The next layer of liquid inside (above) the solid shell then solidifies. This layer, which comprises the inner surface of the shell, only balances the hydrostatic pressure, so again solidifies almost stress free. The result is a stress-free solid shell which is hot on its inside and cold on its outside. The final step of cooling and shrinking the inner layer then generates distortion and / or stress. Shrinkage of the inner layer tends to bend the shell inward, leading to thermal distortion if the shell is unconstrained. This sequence of steps is repeated as later layers solidify, so the length scale of this distortion may vary widely.

If the ends of the section of shell are constrained to remain vertical, then distortion is prevented and the shell remains flat. This induces the classic stress pattern of compression in the outside of the shell and tension just beneath the inside, which is quantified by the analytical solution[2] in Fig. 2. To maintain force equilibrium, the average stress through the shell thickness is zero. The generic subsurface tensile stress is responsible for hot tears, when accompanied by metallurgical embrittlement. Surface cracks may originate from deviations from this classic behavior which produce tension at the surface. These deviations can arise from changes in surface cooling rate, interaction with the mold, phase transformations, and multidimensional effects.

2. Governing Equations

Thermal-mechanical analysis involves solving the equilibrium equations, constitutive equations, and compatibility equations, which relate force to stress, stress to strain, and strain to displacement, respectively.[3] A rate formulation is required, as the previous discussion has revealed that stress generation during solidification is essentially a transient phenomenon. The total strain rate, $\dot{\boldsymbol{\varepsilon}}$, is split into 3 components:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^{e} + \dot{\boldsymbol{\varepsilon}}^{T} + \dot{\boldsymbol{\varepsilon}}^{p} . \tag{1}$$

where the elastic strain rate, $\dot{\boldsymbol{\varepsilon}}^{e}$, thermal strain rate, $\dot{\boldsymbol{\varepsilon}}^{T}$, and inelastic strain rate, $\dot{\boldsymbol{\varepsilon}}^{p}$, each involve phenomena and computational issues, discussed in later sections.

2.1. Elastic Strain

Elastic strain is directly responsible for stress. Differentiating the classical elastic tensor equations relating stress and strain components yields the following relation between stress rate, $\dot{\boldsymbol{\sigma}}$, and elastic strain rate, $\dot{\boldsymbol{\varepsilon}}^{e}$:

$$\dot{\boldsymbol{\sigma}} = \mathbf{D} : \dot{\boldsymbol{\varepsilon}}^{e} + \dot{T}\frac{\partial \mathbf{D}}{\partial T} : \dot{\boldsymbol{\varepsilon}}^{e} \tag{2}$$

where $\mathbf{D}$ is the tensor, with components: $\mathbf{D}_{ijkl}(T) = \lambda(T)\, \delta_{ij}\, \delta_{kl} + \mu(T)\, (\delta_{ik}\, \delta_{jl} + \delta_{il}\, \delta_{jk})$

The second term in this equation is often ignored. This introduces errors in a casting simulation because elastic modulus increases significantly with decreasing temperature.

Measurement of the elastic constants in **D** at high temperature is difficult and large discrepancies exist between the measurements of different researchers. For example, Hub[4] measured the elastic modulus of steel at 1200 ˚C to be about 90 GPa while Mizukami et al.[5] measured 15 GPa at the same temperature. These differences may have arisen from different amounts of creep strain in the sample due to testing at different strain rates, different steel compositions, different initial microstructures, or even small unaccounted strains in the testing machines.

Poisson’s ratio is also difficult to measure at elevated temperatures, due to creep. Since inelastic strains are incompressible, Poisson’s ratio approaches 0.5 as the amount of creep strain increases. Thus, experimental observations of increased Poisson’s ratio with temperature may be simply due to increasing amounts of creep during the test. If this is the case, a constant Poisson’s ratio should be used in the stress model, which treats inelastic strain separately.

2.2. Thermal Strain

Stresses are generated in a casting mainly by the few percent of thermal contraction (strain) that accompany the cooling of metal in the solid state. Although thermal strain does not cause stress directly, it creates a "mismatch" that generates elastic strain. It is found from the temperature history, T(t), given the thermal linear expansion, TLE, for the material:

$$\dot{\varepsilon}^T = \frac{(TLE(T_{t+\Delta t}) - TLE(T_t))}{\Delta t}\delta \qquad \text{where } TLE(T) = \sqrt[3]{\frac{\rho(T_0)}{\rho(T)}} - 1.0\ . \qquad (3)$$

Changes in density, ρ(T), occur due to both thermal contraction and phase transformations. The temperature history is found by solving the energy equation, including the effects of transient heat conduction, solidification, shrinkage-dependent interfacial heat transfer, and fluid flow. This is the subject of intense ongoing research, reviewed elsewhere.[6-8]

2.3. Inelastic Strain

Microstructural relaxation continually acts to reduce stress in a casting by replacing elastic strain with plastic strain and creep. This phenomenon is very complex, and depends on the stress and temperature histories in addition to the composition and microstructure of the material, which also evolves with time. It is difficult to quantify the behavior with experiments, let alone capture the effects mathematically.

Different testing methods reveal different aspects of the material behavior. Tensile testing records stress variation with strain at constant strain rate. Creep tests measure strain increase with time under constant stress. Stress relaxation tests measures stress decrease with time under constant strain. To be accurate for casting simulation, a valid constitutive equation should reproduce all of these behaviors. Furthermore, it should reproduce the behavior obtained when the conditions change during the test, such as during cyclic loading. Relatively little data is available in the literature regarding this mechanical behavior at the high temperatures, low strains, and low strain rates important to casting.

At lower temperatures, it is reasonable to measure plastic strain data and creep data from independent tests and incorporate these two types of inelastic strain into the stress model separately. This is because the tensile test is fast enough to avoid time dependent plasticity. At higher temperatures, creep is significant even during a tensile test and cannot be distinguished from plastic strain. Thus, the mechanical behavior is very sensitive to strain rate.

To address this issue, "unified" constitutive models have been developed, which treat inelastic strain rate, $\dot{\varepsilon}_p$, as a single function of the current stress, temperature, and structure. The structure is characterized by state variable(s) which also evolve with time. When the state variable is simply the time or the inelastic strain, the model is usually called a "creep" or "viscoplastic" model respectively. Simple constitutive equations of this type have recently been developed for plain-carbon austenite (steel) under continuous casting conditions.[9]

More sophisticated systems of unified constitutive equations, such as MATMOD, have been developed for pure Al, stainless steel, and other metals.[10] These equations can capture microstructural phenomena including strain hardening, the Bauschinger effect, static recovery, dynamic recovery, and solute drag. Implementing the MATMOD equations into an aluminum casting stress model produced differences in results, which were attributed to the kinematic hardening effects.[11] The equations should be modified to include the complexities of the mushy zone and to leave out phenomena that are not important to casting.

3. Complicating Phenomena

3.1. Anisotropic Mechanical Properties

Conventional stress calculations assume isotropic behavior, so scalar variables, such as the Von Mises effective stress, are combined with the Prandtl - Reuss equations[12] to define 3-D behavior from uniaxial property data. Anisotropic effects greatly complicate both the measurements and their mathematical description. This is necessary for stress analysis of some materials, such as composites. In the aligned columnar grains of most castings, anisotropic effects have received little attention. In cast iron solidification, different yielding behavior in tension and compression was found to be very important to stress development.[13]

3.2. Phase transformations

Solid-state phase transformation affects stress generation in two ways. Firstly, it generates large volumetric expansion or contraction, which can be treated as thermal strain in Eq. 3. For example, the 1 % volume expansion accompanying the decomposition of austenite during the solidification and cooling of large steel ingots has a huge effect on stress development, equivalent to a temperature change of over 150 ˚C.[14] This can be accounted for in the temperature-dependent density function by calculating a weighted average density based on the mass fractions of the phases present. This allows a separate microstructural model to find the phase fractions present at each time and position in the casting. For example, phase transformation kinetics for the decomposition of austenite in steel were incorporated from time - temperature transformation data to approximate the phases present for the different temperatures and cooling rates calculated during the simulation.[14]

Secondly, phase transformation is accompanied by significant changes in mechanical properties. The atomic rearrangement during phase transformation induces significant inelastic strain, in proportion to the existing stresses.[15]

3.3. Interaction with the mold

The mold greatly affects and complicates stress calculations in several different ways. Firstly, heat extraction through the mold affects temperature history of the casting, so usually needs to simulated as part of the analysis. More importantly, the thermal resistance of the gap that forms between the solidifying shell and the mold controls the heat transfer. Complete modeling of this effect requires coupling between the heat transfer and stress calculations.

Secondly, the mold can interact mechanically with the shell if contact occurs. Contact and friction against the mold is the source of many of the critical stresses in a casting. Mathematical penetration of the shell into the mold is a computational problem that must be addressed and prevented. Several different contact algorithms are available, including general-purpose “gap” elements,[16-18] and specialized algorithms to improve the speed of the calculations, when the behavior is partly known apriori.[19, 20] The nature of the mold material greatly influences the methods used for this calculation. Sand molds can deform to accommodate distortion of the casting.[13] Rigid mold materials, such as ceramics or metals, resist deformation and generate stresses in the casting.

Thermal distortion of the mold is important to the analysis, because it is usually similar in size to the shrinkage of the casting.[21] Thus, it must be accounted for to properly incorporate the thermal and mechanical interactions between the mold and the casting. A mold analysis is of practical importance in its own right because thermal strains and stress in the mold also affect mold life. The mechanical system supporting and constraining the mold is sometimes important to this calculation[21] and has been linked to quality problems in the cast product.[22]

Incorporating the mold is complicated further when there is relative motion between the casting and the mold, as occurs in continuous casting processes. Eulerian models, with their reference frame on the stationary mold, are complicated by the need to convect both heat and history-dependent variables such as strain through the domain. Lagrangian models, with their reference frame on the moving casting, have the advantage of reducing the 3-D problem to 2-D, when axial conduction is negligible. Mechanical friction between the casting and mold is an important phenomena to consider in either case.

3.4. Liquid and hydrostatic pressure

Incompressible liquid is subject to large shear deformation without generating stress. However, it can transmit hydrostatic pressure, which can be the dominant mechanical load, responsible for creep bulging in large castings. Several approaches can be taken to handle this in a stress model.

One method is to numerically “strip away” the liquid elements according to the results of the heat transfer calculation. Pressure boundary conditions are easily applied to the new surface of the domain. This has been applied successfully to steady continuous casting,[23] but has numerical disadvantages when the solidification front moves with time. In a fixed mesh analysis, hydrostatic pressure can be applied as an internal boundary condition to appropriate nodes.[20]

Alternatively, the mechanical properties can be altered with temperature, to avoid shear stress generation in the liquid without changing the mesh. A natural approach is to lower the elastic modulus by several orders of magnitude as temperature increases across the mushy zone. This leads to large elastic strains, which create unreasonable stresses after solidification, if all the terms in Eq. 2 are properly incorporated.[24] To further minimize troublesome stress in the liquid, thermal expansion can be prevented above the solidus temperature.

The preceeding methods are unable to simulate phenomena such as the large volume contraction of liquid in the mushy zone, which contributes to hot tearing cracks and porosity. One way to achieve this is to increase Poisson's ratio to 0.5,[25] which conserves liquid volume, as appropriate, but presents numerical difficulties.[24] Another method, based on a large inelastic deformation rate in the liquid, is being developed to simulate behavior of the mushy zone, while avoiding the numerical problems.[24]

3.5. Effect of fluid flow

One of the most difficult aspects of solving for the temperatures is the treatment of the convective heat transfer arising from fluid flow, both during and after mold filling. The conventional approach in stress models is to enhance thermal conductivity of the liquid by several times. When fluid flow effects are very important, however, the momentum and turbulence equations must be solved. It is extremely expensive and difficult to simulate all three phenomena (fluid flow, solidification heat conduction, and stress generation) simultaneously using a single model, although this approach is being pursued.[26] Alternatively, a decision must be made regarding where to make the split(s) between two or more models.

When the position of the solidifying interface in the domain is greatly affected by the fluid flow pattern, (such as during mold filling or in metal alloy castings with large freezing ranges and a high superheat), the logical choice is to solve the coupled fluid flow / solidification problem first and send the temperature results to a stress model. Unfortunately, this approach may require iteration between the stress and solidification models if the gap heat transfer is important.[23] Transferring files between large commercial packages can create significant computational overhead.

Alternatively, if the position of the solid / liquid interface is known a priori to have little effect on the fluid flow, (such as in the early stages of continuous casting low carbon steel) then the division between models may be made at the solid / liquid interface. The superheat transferred from the flowing liquid to the solidifying shell can then be calculated with a fluid flow model[27] and then applied as an internal heat source condition in a heat conduction model, coupled with a thermal stress model.[28]

4. Computational Issues

The phenomena governing stress generation are extremely complex and present a large number of computational challenges.

4.1. Integration of constitutive equations

The standard treatment available in most commercial programs, such as ABAQUS,[16] is to split the inelastic strain into a rate-independent plastic part and a rate-dependent creep part. The numerical methods for solving these equations are well-established,[29] but are inefficient and unstable when the rate-dependent effects are large, which occurs at the high temperatures important to casting. More efficient numerical methods are being developed to integrate arbitrary constitutive equations, including unified equations with severe nonlinearities, and is a topic of active current research.[10, 24] Of particular interest are the operator splitting techniques, which alternate between implicit and explicit forms of the total strain rate (on the global level) and inelastic strain rate (on the local level) during a two-step integration method.[30]

4.2. Mesh Refinement

It is very important to validate a numerical model before using it. Recent work has compared numerical results from an elastic-viscoplastic finite-element model with the analytical solution to a solidification stress problem[2] shown in Fig. 2. The results show that to achieve accuracy within 10% requires at least 8 quadratic elements across the shell.[24] The accuracy improves with smaller time step size, although an accuracy limit exists for a given mesh.[24]

4.3. Two-dimensional problems

Several different choices are available to simplify the actual 3-D casting problem into a 2-D stress analysis. These include axisymmetric, shell, plane stress, plane strain, and generalized plane strain. Castings that exhibit radial symmetry, such as continuous casting of round sections, are accurately modeled using axisymmetric equations.[11, 23] Casting sections with thin walls can be reasonably approximated using shell elements, only after they are fully solidified. To model sections through typical, unconstrained castings, the best approximation is usually generalized plane strain. The plane stress assumption ignores axial stress, although recent work shows it is a reasonable approximation for in-plane behavior. By constraining against axial thermal expansion, plane strain tends to overestimate axial stress, with accompanying changes to the in-plane behavior.[24]

5. Applications

There are many important uses for thermal-mechanical models of casting processes. Understanding the history of the shape and stress of a casting is important for process development and improvement. They can also assist in the design of mold shape, (to match shrinkage), and in the prediction of cracks and residual distortion. Two examples are discussed.

5.1. Shell growth in Continuous Slab Casting

A coupled finite-element thermal-stress model has been developed at the University of Illinois to simulate thermal and mechanical behavior of a horizontal section through the solidifying steel shell as it moves down through the continuous slab casting mold.[28] A new two-level algorithm[24] is used to integrate the elastic-viscoplastic constitutive equations developed by Kozlowski et al.[9] The equations reproduce both the tensile test data measured by Wray[31] and creep curves from Suzuki et al[32] for austenite. The model incorporates the effect of asymmetric fluid flow on superheat delievery using a data base of results from a 3-D turbulent flow model[27] using an internal heat source condition. The shape of the rigid boundary of the water-cooled copper mold is found from a separate 3-D calculation of mold distortion.[21] The interface heat flow parameters (including thickness profile of the solid and liquid mold flux layers) were calibrated using thermocouple measurements down the centerline of the wideface for typical conditions at LTV Steel.[28]

An example of the predicted temperature contours and distorted shape of a region near the corner are compared in Fig. 3 with measurements of a breakout shell.[28] Good agreement was expected and found in the region of good contact along the wideface, where calibration was done. Near the corner along the narrow face, steel shrinkage is seen to exceed the mold taper, so an air gap is predicted. This lowers heat extraction from the shell in the off-corner region, where heat flow is one-dimensional. When combined with high superheat delivery from the bifurcated nozzle directed at this location, the shell growth is locally reduced. Just below the mold, this thin region of the shell caused the breakout. Near the center of the narrow face, creep of the shell under ferrostatic pressure from the liquid is seen to maintain contact with the mold, so less thinning is observed. The surprisingly close match with measurements all around the mold perimeter tends to validate the other features and assumptions of the model. This model has been applied to predict ideal mold taper, to prevent breakouts such as the one discussed here[33] and to understand the cause of other problems such as off-corner surface depressions and longitudinal cracks in slabs.

5.2. Crack Prediction

Using a stress model to investigate crack formation requires a valid fracture criterion, linking the calculated mechanical behavior with the microstructural phenomena that control crack initiation and propagation. The task is difficult because crack formation depends on phenomena not included in the stress model, such as microstructure, grain size and segregation. Thus, experiments are needed to determine the fracture criteria empirically.

Many of the cracks that occur during solidification are hot tears. These cracks form between dendrites when tensile stress is imposed across barely-solidified grains while a thin film of liquid metal still coats them. Very small strains can start hot tears when the liquid film is not thick enough to permit feeding of surrounding liquid through the secondary dendrite arms to fill the gaps. Long, thin, columnar grains and alloys with a wide freezing range are naturally most susceptible. The phenomenon is worsened by microsegregation of impurities to the grain boundaries, which lowers the solidus temperature locally and complicates the calculations.

Because strain damage leading to cracks can accumulate over successive loading periods,[34] the entire mechanical history of the casting should be evaluated, rather than simply to search for a peak stress or strain. Criteria to predict hot tear cracks, are best characterized by a critical amount of inelastic strain accumulated over a critical range of liquid fraction, f_L, such as $0.01< f_L <0.1$ [35] or

$0.01 < f_L < 0.2$ [34] Careful strain measurements during bending of solidifying steel ingots has revealed critical strains ranging from 1.0 to 3.8%.[34, 36] The lowest values were found at high strain rate and in sensitive grades (e.g. high S peritectic steel).[34] In aluminum rich Al-Cu alloys, critical strains were reported from 0.09% to 1.6% and were relatively independent of strain rate.[37] Tensile stress also appears to be a requirement for hot tear formation.[34] The maximum tensile stress occurs just before formation of a critical flaw.[37] However, tension is usually unavoidable in the susceptible inner portion of the shell, as discussed earlier. The previous fracture criterion[34] combined with a finite-element simulation which accumulated strain throughout the entire process was able to predict internal hot-tear cracks in a continuously-cast steel slab.[38]

Cracks which form at lower temperatures are generally predicted using a maximum stress criterion. These cracks are also grade and strain-rate sensitive, but the fracture criteria have received less attention.

A numerical supplement to experimental measurements of fracture criteria is to model phenomena such as segregation, strain localization and failure on the microstructural level. This work is very computationally expensive and is still in the early stages, however.[39] The effect of local volume contraction of the liquid metal on fracture criteria has yet to be taken into account in a stress model. There is still much work to be done on fracture criteria, despite significant progress in recent years.

6. Conclusions

Mathematical modeling of stress generation in casting processes is a difficult, complex subject that is receiving increased attention. Despite huge gains in computing power, numerical algorithms, understanding, and modeling of the basic phenomena, which have been made in recent years, the ability to tackle and solve real problems is only beginning. Accurate measurement of the composition-sensitive mechanical properties and their mathematical representation in reliable constitutive equations remains one of the greatest obstacles to stress analysis. Incorporating microstructural effects and fracture criteria to predict cracks is a further challenge.

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Figures

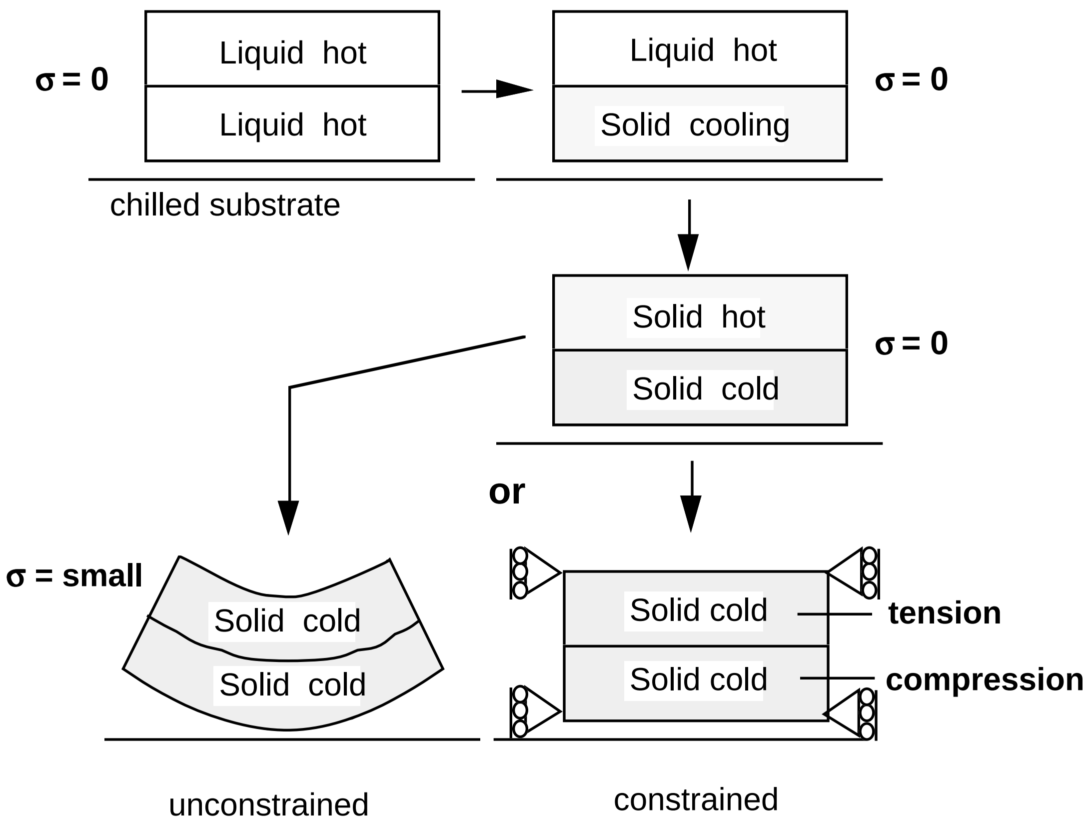

Fig. 1 Mechanical Behavior of a solidifying shell (without friction)

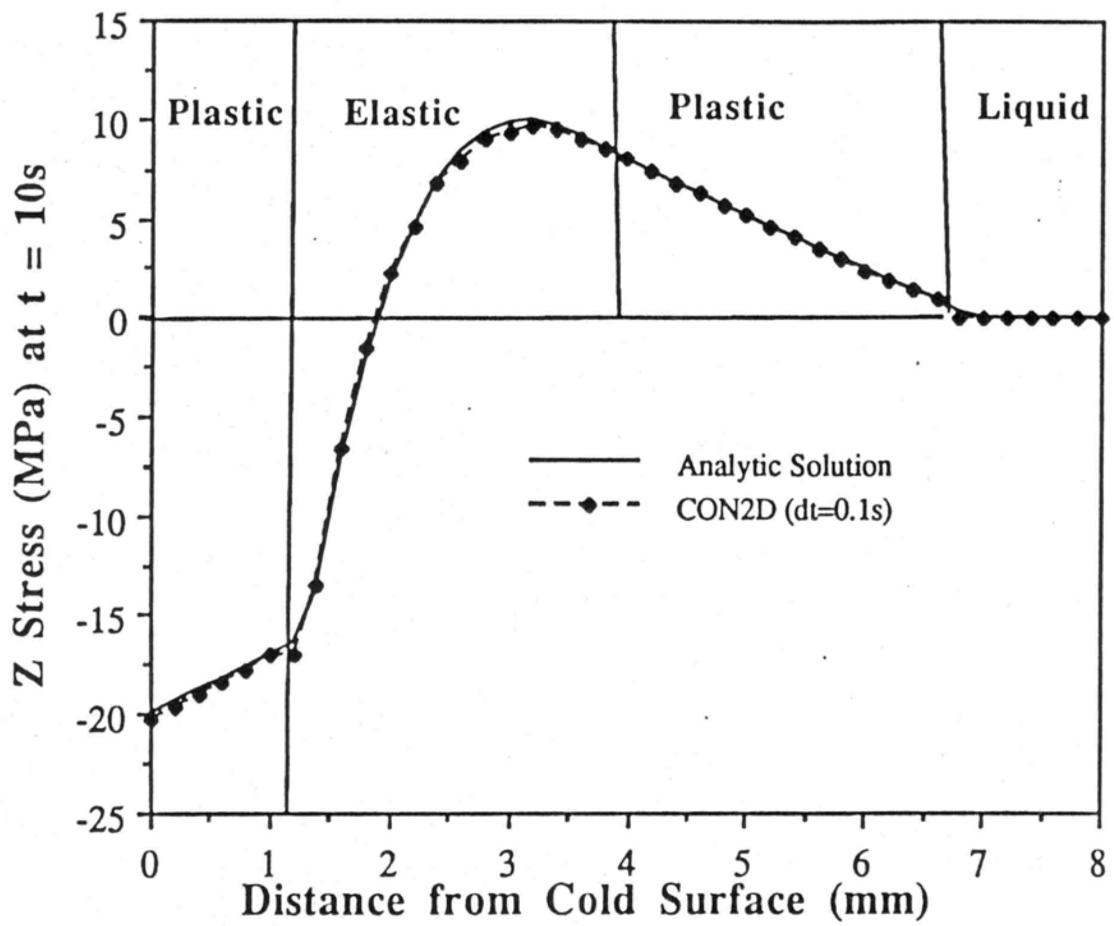

Fig. 2. Comparison of analytical and computed stress distribution through shell thickness.

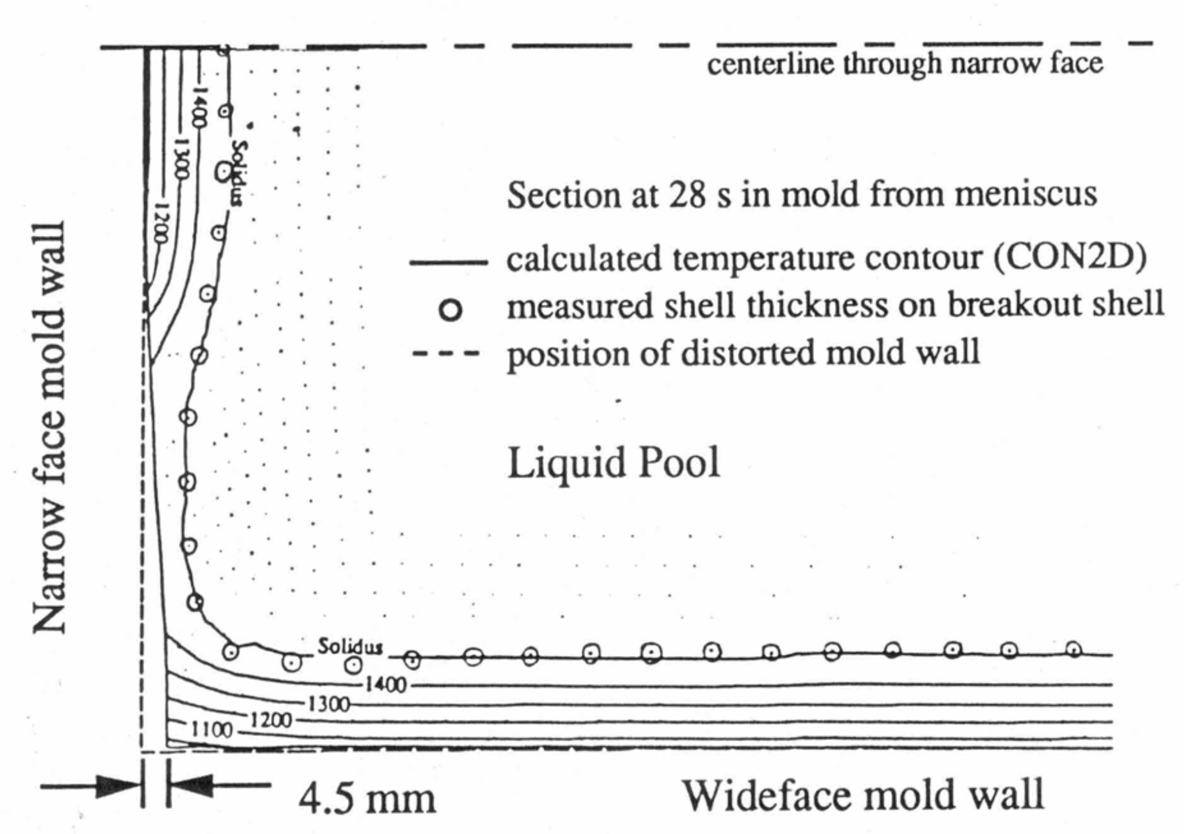

Fig. 3. Comparison between predicted and measured shell growth thickness in a transverse section through the corner of a continuous-cast steel breakout shell