On the prediction of shrinkage defects by thermal criterion functions

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Abstract. The indirect prediction of shrinkage induced solidification defects is considered in this study. The previously suggested criterion function methods, in particular the Pellini and Niyama criteria are analyzed in details, and their shortcomings are shown as a result of our analysis (e.g. the scale/shape-dependency of critical values and the inability to distinguish between cold- and hot-spots). To moderate limitations related to criterion function methods, a new method is introduced to predict the location of centerline shrinkage in metal castings. Unlike the alternative methods which are derived more empirically based on the result of experimental observations, the suggested method in this study is derived theoretically based on a heuristic two-scale, macro-meso-scale, approach. The application of the suggested method is limited to low freezing range alloys. The feasibility of the presented method is studied by comparing numerical results against the available experimental data.

Keywords. criterion function, defect prediction, macroshrinkage prediction, multiscale analysis, Niyama criterion, two-scale approach.

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1 Introducation. Porosity is one of the major defects in castings which results in a deterioration of mechanical properties, in particular fatigue and a reduction in ultimate tensile strengths. It is induced by two mechanisms, solidification shrinkage and gas segregation, both of which occur concomitantly but with different intensities [1].

The goal of this study is two folds. First to analyze available thermal criterion function methods for the prediction of shrinkage defects in castings. Second, to introduce a new thermal criterion function which annihilate some limitations related to alternative criterion function methods. In practice, the formation of shrinkage defects has a close relation to gaseous defects. Consequently, as they are difficult to distinguish, in particular from the viewpoint of defect nucleation, we shall attend to the mechanism of gas porosity formation to explore validity conditions for our criterion.

2 Spatial length scales involving the casting process. Alloy solidification is a multiscale phenomenon in nature. It includes multiple spatial scales such as macro, meso, micro, atomic and sub-atomic (electronic) scales. In the case of metal casting, it is possible to consider a three-scale situation with respect to space (see the sketch in Figure 1); i.e., there exist

- macroscale: a length $\Sigma \approx 1-10^{-2}$ m, in which the whole process takes place;
- microscale: length scale $\varepsilon \approx 10^{-4}-10^{-6}$ m related to typical dendrite tip radii;
- mesoscale: a length $\xi$, $\varepsilon \ll \xi \ll \Sigma$, which marks the finest resolution for the description that is of practical importance in porosity formation. Since porosities mainly form as a result of crystal interactions, the typical primary dendritic arm spacing or grain size is a feasible choice for this length scale, i.e. $\xi \approx 10^{-2}-10^{-4}$ m;

It is common to classify shrinkage defects in the casting process based on their physical appearance and spatial scales. Porosity in castings can be classified by the size of the pores as macroporosity and microporosity or dispersed porosity (see Figure 2). Macroporosity defects can be divided into three categories: pipe shrinkage, centerline shrinkage and surface sink (also called external shrinkage porosity).

The spatial scales of macroporosity and microporosity are formally matched with the above mentioned macro and meso scales, respectively. Due to the limitation of available computational
resource, it is almost impossible to simulate a practical casting process at the mesoscale. Consequently, we have to perform a macroscale solidification analysis to predict solidification induced defects. Therefore, only a fraction of defects can actually be resolved by such a macroscale simulation. This spatial filter usually covers the macro porosities and hopefully the upper-range of micro porosities.

From a mesoscale viewpoint, in a typical casting process the solid/liquid interface is non-planar as a result of unstable solidification due to the melt supercooling in the vicinity of the solidifying front and/or the constitutional supercooling in the case of alloy solidification. However, from a macroscopic point of view, it is possible to consider the solid/liquid interface as a sharp and planar interface when we have a narrow mushy region. In this case the mushy zone usually includes almost parallel short columnar. Some authors (e.g. [2, 3]) assumed the flow of melt is governed by a very simple form of Darcy-law and then used it to predict the susceptibility of cease of flow and so formation of meso-scale solidification defects. However, we believe that this is a blind assumption which ignores couple of important physics behind such a meso-scale fluid flow and defect formation. Later in this paper we illustrate our criticisms in this regard.

In the case of wide freezing range alloys, in particular when the thermal diffusivity of melt is large and the thermal conductivity of the mold is small, the entire casting would quickly fill with a mixture of solid dendrites and liquid, the remaining volume being filled by the mushy material until the end of solidification. In this solidification mode, it is not possible to distinguish between solid and liquid phases from a macroscopic viewpoint. In this case it is reasonable to consider the
dendritic skeleton as a randomized porous media like [4]. Later, we shall argue that using thermal
criterion functions are not feasible for such cases.

Prior to closing this section, let us to define some quantities which are used throughout this
paper. The total freezing time of casting, local freezing time, local cooling rate at the freezing
time, local velocity of the solidus isotherm and feeding gradient are denoted by \( t_s, t_f, R, v_s \) and \( G \), respectively. The feeding gradient referred to here is the component of the temperature gradient in
the feeding direction, i.e.

\[
G = \nabla \theta_c \cdot \hat{n}
\]

where \( \theta_c \) denotes the temperature field inside the cast region and \( \hat{n} \) is the unit normal of the
solid/liquid interface directed toward the liquid region. Since the iso-contours of the local freezing
time field represent the position of the solid/liquid interface at a specific time, \( \hat{n} \) satisfies the relation
\( \hat{n} = \nabla t_f / ||\nabla t_f|| \). An upwind-like method was suggested by Niyama et al. [5] to compute the feeding
gradient on a structured grid; specifically, to compute \( G \) on a cell \( c \), we calculate

\[
G = \max_{i \in nb} \frac{\theta_i - \theta_c}{||x_i - x_c||_2}.
\]

where \( nb \) denotes the liquid neighborhood of the desired cell. In the case of two dimensions, this
neighborhood is limited to those cells among the 8 nearest neighbors in which the temperature is
larger than the solidus temperature (see Figure 3). In three spatial dimensions, this neighborhood
has 26 members. Knowing the local freezing time field as a result of the solidification analysis, \( v_s \)
satisfies \( v_s = (\nabla t_f \cdot \hat{n})^{-1} \). It can be computed in the same way as described above for \( G \).
Since the feeding capacity of the liquid metal ceases when the volume fraction of the solid phase is larger than a critical value, some authors suggest to evaluate the solidification parameters at a temperature $\theta_{s}^+$ slightly higher than the solidus temperature. For example Carlson et al. [6] suggested to take $\theta_{s}^+$ equal to the solidus temperature plus 10 percent of the interval between the solidus and liquidus temperatures, i.e., $\theta_{s}^+ = \theta_s + 0.1(\theta_l - \theta_s)$, where $\theta_l$ and $\theta_s$ denote the liquidus and solidus temperatures, respectively. In the present study every parameter which is computed at $\theta_{s}^+$ is denoted by a plus superscript, $\Box^+$.

3 Related work. During the past two decades several computational methods have been developed to predict shrinkage defects in castings [7, 8]. Early approaches include the numerical solution of the energy equation and evaluation of a local criterion function to predict shrinkage defect susceptibility. The applied criterion was usually a function of $G$, $R$ and $v_s$. These methods are known as criterion function methods. More advanced approaches, e.g. [9, 10, 11], include the solution of energy and momentum equations coupled with a suitable mesoscale pore nucleation and growth model. Although these methods include more physics and are more accurate, none of them could be considered as a direct numerical simulation of mesoscale effects. For example, based on the authors knowledge, none of these works considered the interaction of floated porosity with dendrites. Furthermore, the mechanism of porosity nucleation, in particular when regarding high quality melts, is still in question which increases difficulties of mesoscale direct numerical simulation (see, for example, chapter 7 of [1]). Since the focus of this paper is on criterion function methods, it is worth to review these methods in details.

Early work by Pellini [12] on introducing a thermal criteria to evaluate the feeding ability reported
that $G$ should be greater than a critical value, $G_{cr}$, to avoid centerline shrinkage in plate and bar castings. Niyama et al. [5] also examined a number of commercial castings and confirmed that the feeding gradient could be used to predict the formation of shrinkage porosity. These researchers detected that, $G_{cr}$ depends on both shape and size of a particular casting and could not be predicted in advance. Later, Niyama et al. [2] discovered that both the scale of porosity and the dendritic structure varied in proportion to the size of the casting. As a result, they discovered that $G_{cr}$ is proportional to $1/\sqrt{t_s}$. Therefore, their criterion function can be expressed as $G\sqrt{t_s}$. Finally, they have approximated $t_s$ by $(\theta_l - \theta_s)/R$ and presented $GR^{-1/2}$ as their criterion function. The critical value of this criterion was proven to be independent of the casting size, first by Niyama et al. [2], and later by other researchers on some simple-shaped castings.

It is worth noting that replacing $\sqrt{t_s}$ by $1/\sqrt{R}$ stems from an asymptotic analysis by Niyama et al. [2] to justify their measure theoretically. This analysis includes the solution of a one-dimensional quasi steady-state Darcy flow within the mushy zone to compute the pressure drop due to the friction of dendritic structure. The current authors believe that this analysis not only does not support the validity of the Niyama criterion but is also misleading about the ability of this measure to predict microporosity formation. In particular, the computation of the Niyama criterion in the form of $GR^{-1/2}$ does not always give reasonable results and it is recommended to use $G\sqrt{t_s}$ instead [6, 13, 14, 15].† We shall address this issue in more detail in section 4.

On the other hand, the Niyama criterion is commonly used in real-world designs, in particular in the case of steel castings. Consequently, almost all commercial casting simulation packages have the ability to use this measure. In research, the Niyama criterion has recently also been used extensively by Carlson, Beckermann and coworkers to develop new feeding-distance rules for low alloy [6, 13] and high alloy [14, 15] steels.

Although the Niyama criterion is more universal than the Pellini criterion and resolves the size dependence problem, the shape dependency of the critical value seems to be an unresolved issue. The problem is due to this fact that (based on Pellini’s observation) the minimum temperature gradient required to feed a bar is about 5–10 times greater than what is needed to feed a plate. As mentioned in [16], the Niyama criterion fails to solve the shape-dependency problem. Hansen

†The commercial package MAGMASOFT also uses $G\sqrt{t_f}$ as the Niyama criterion
and Sahm \cite{16} did a series of numerical simulations for bar and plate geometries with different scales, i.e., multiplying all dimensions by a scaling factor $N$. They showed that when the casting dimensions are scaled by factor $N$, the temperature gradient, cooling rate and feeding flow velocity are scaled by factors $N^{-1}$, $N^{-2}$ and $N^{-1}$, respectively. The feeding flow velocity, $U$, was computed based on the solution of mesoscale fluid flow governed by Darcy’s law. Based on these results, they try to remove the scale-dependency from criterion functions that depend on $G$, $R$ and $U$ using a power scaling; this leads to the criterion $GR^{-1/4}U^{-1/2}$. Although their analysis just confirms that this criterion could be scale-independent, they claimed the shape independency of this measure too, i.e., the critical values of this criterion for plate and bar geometries are the same. However, this claim is only supported by their numerical experiment on plate and bar castings of Pellini. To the best of the authors’ knowledge, no further experimental or numerical work supports this assertion. Consequently, we believe that the analysis is not sufficient to justify the shape-independency of this measure. In fact, we shall argue in section 4 that this measure cannot be shape-independent as the shape dependency has a global nature which cannot be summarized into local parameters such as $G$, $R$ and $U$. The source of the shape-dependency of the Niyama criterion will be discussed in section 4 as well. Since we have to solve the flow equations coupled with energy equation to evaluate Hansen and Sahm’s criterion, it is computationally inefficient in contrast to the Niyama criterion. It is worth noting that the Niyama criterion is also scale-independent (for more details see \cite{17,8}).

Sigworth and Wang \cite{18} also considered the formation of centerline shrinkage in plate castings. They have proposed a geometric model in which $G_{cr}$ is a function of the angle of the inner feeding channel inside the casting, $\Theta_c$. Their criterion has the following generic form: $G_x\sqrt{t_s} > c \tan \Theta_c$, where $G_x$ is the temperature gradient along the major axis of the plate and $c$ is a constant. These authors estimate a critical angle for steel plates between 2 and 5 degree. In contrast to the previously mentioned works which are constructed based on experimental observations, this criterion resulted from a theoretical analysis. Therefore, its limitation can be predicted based on the considered assumptions. For example, it is obvious that this measure is not universal and its application is limited to plate-like castings. Further, applying this measure does not seems to be feasible in the case of long freezing range alloys. The most important conclusion, however, is that this alternative derivation results in the same functional dependence between the temperature gradient and the solidification time as that found experimentally by Niyama et al. \cite{2}. It turns out that the critical
value of the Niyama criterion should have a shape dependent component which confirms the shape-dependency of this measure.

Recently, a dimensionless version of the Niyama criterion is recently suggested by Carlson and Beckermann [3]. In this work it was claimed that their criterion function could predict position and quantity of defects without using a-priori known threshold value. This claim is recently rejected in [19] (see also response letter [20]). We believe that our analysis in this paper partly support the discussion of Sigworth [19] and hopefully resolve this challenge by more rigorous reasoning.

Regarding long freezing range alloys, a criterion function of the form $\frac{Gt_f^{2/3}}{v_s^{-1}}$ was suggested by Lee et al. [21]. This criterion is supported by combining theoretical analysis and experimental observations. Following the scale-dependency study suggested in [16, 8], it is obvious that this criterion is neither scale- nor shape-independent. According to [7, 8] criterion function methods have so far had little success in predicting porosity formation in the case of long freezing range alloys.

Prior to closing this section we would like to point out to an elegant discussion on the shortcomings of the Niyama criterion by Spittle et al. [22] which is partly in agreement with our discussion.

4 Analysis of criterion function methods. In this section we will analyze criterion function methods, in particular regarding their limitations. To this end, let $\Omega = \Omega_c \cup \Omega_m$ be the spatial domain, where $\Omega_c \subset \mathbb{R}^d$ ($d = 2$ or $3$) is a portion of $\Omega$ which includes the casting and $\Omega_m \subset \mathbb{R}^d$ denotes the mold region. The interface between the two is denoted by $\Gamma_{c-m} = \overline{\Omega_c} \cap \overline{\Omega_m}$. From a macroscopic point of view, if the effect of melt flow during solidification is neglected, solidification is governed by heat conduction [23, 24]:

$$\rho_c c_c \frac{\partial \theta_c}{\partial t} = \nabla \cdot (k_c \nabla \theta_c) + \rho_c L \frac{\partial f_s}{\partial t} \quad \text{in } Q_c = \Omega_c \times [0, T]$$

(3)

where $\rho_c$ is the cast density, $c_c$ is the cast specific heat, $\theta_c$ is the temperature field in the casting region, $t$ is the time variable, $k_c$ is the cast thermal conductivity, $L$ is the fusion latent heat, $f_s$ is the solid fraction field, and $[0, T]$ denotes the temporal domain. The initial condition is $\theta_c = \theta_c^0$ in $\Omega_c \times \{t = 0\}$, where $\theta_c^0$ is the pouring temperature. In the mold region we have:

$$\rho_m c_m \frac{\partial \theta_m}{\partial t} = \nabla \cdot (k_m \nabla \theta_m) \quad \text{in } Q_m = \Omega_m \times [0, T]$$

(4)
where \( \rho_m, c_m, \theta_m, k_m \) are mold analogues of the variables defined above. The initial condition in the mold region is \( \theta_m = \theta_\infty \) in \( \Omega_m \times \{ t = 0 \} \), where \( \theta_\infty \) is the ambient temperature. Natural boundary conditions are applied at the mold-air interface, i.e., \( k_m \frac{\partial \theta_m}{\partial n_m} = h_\infty (\theta_\infty - \theta_m) \) on \( \Gamma_{m-a} \times [0, T] \), where \( h_\infty \) denotes the mold-air convective heat transfer coefficient, \( \Gamma_{m-a} \) is the mold-air interface and \( n_{m-a} \) is the unit normal vector directed toward the environment. The cast-mold interface is modeled by the interfacial heat transfer coefficient method \([25, 26]\), i.e., \( -k_c \frac{\partial \theta_c}{\partial n_i} = k_m \frac{\partial \theta_m}{\partial n_i} = h_i (\theta_c - \theta_m) \) on \( \Gamma_{c-m} \times [0, T] \), where \( n_i \) is the unit normal vector directed toward the mold and \( h_i \) is the local heat transfer coefficient of the cast-mold interface.

From a macroscopic point of view, if the effect of gravity on the distribution of porosities is neglected, shrinkage porosities will be located at the last solidified points, i.e., hot spots. In particular, this holds for centerline shrinkages. Consequently, we need to look for hot spots in a casting to predict the locations of the centerline shrinkages. If we assume that the temperature field is sufficiently smooth, the hot spots are a subset of the critical points of the temperature field \([27]\). Since shrinkage defects form near the freezing time, it is sufficient to only consider critical points at \( t = t_f \) or \( \theta = \theta_s \), i.e. we only consider the admissible set

\[
A_{ad} = \{ x \in \Omega_c \mid |\nabla \theta(x, t = t_f)| = 0 \},
\]

or a suitable numerical approximation of it. Note that this set contains not only hot spots, but also cold spots and saddle points. A sufficient condition for \( x^* \in A_{ad} \) to be a hot spot is if the Hessian matrix of the temperature field, \( H_\theta(x) = \nabla^2 \theta(x, t = t_f) \), is negative definite at \( x^* \), i.e., for all vectors \( d \in \mathbb{R}^d, d \neq 0 \),

\[
d^T H_\theta(x^*) d < 0. \quad (5)
\]

An equivalent condition is if all eigenvalues of the Hessian are negative. Later, we shall present a physical counterpart of this sufficient condition.

As already mentioned in section 3, Niyama et al. \([5]\) observed that the scaling factor \( 1/\sqrt{t_s} \) resolves the size-dependency problem of the Pellini criterion. The authors justified their criterion through one-dimensional quasi steady-state fluid flow within the dendritic structure governed by the Darcy law. Their analysis showed that the pressure drop due to the friction of dendritic structure is inversely proportional to factor \( GR^{-1/2} \) and they introduce their measure as \( GR^{-1/2} \) instead of \( G\sqrt{t_s} \).
On the other hand, to the authors’s knowledge, neither Niyama et al. nor other researchers provided experimental support for the criterion $GR^{-1/2}$ as an interdendritic microshrinkage predictor measure in a purely unidirectional solidifications. In fact, all experimental support for the Niyama criterion are actually related to multi-directional solidifications, a concern already mentioned in [18, 22]. In particular, Spittle et al. [22] emphasized that available supportive experimental data for the Niyama criterion are more related to simple-shaped castings. Furthermore, in the case of unidirectional solidification, the formation of shrinkage porosity is depends on gravity [28], a factor not covered by Niyama’s analysis. Detailed discussion on this effect can be found in [29].

Moreover, it is important to note that the Darcy-law based assumption of flow which is used in [5, 3] does not cover the whole physics behind the defect formation. For example formation of defect in the either form of void shrinkage or gas bubble needs defect nucleation which is very important in small scales (cf. [1, 29]). The nucleation phase is so important that it can completely change the distribution of defects. Due to importance of this issue we briefly notify this effect here (more details can be found in [29]).

In general formation of void in a clean melt is very difficult as tensile strength of liquid metals is very large (cf. [ch. 7 of 1]). According to [ch. 7 of 1], homogeneous nucleation of void region is almost impossible. And formation of void regions are aided either by formation of gas porosity or nucleation (in fact initiation) on the pre-existing bubbles in the melt (which are not available for high quality melts). In the case of clean melts, if shape of casting be appropriate (e.g. plate-like castings), shrinkage can be compensated by surface sink and no internal shrinkage (cf. Figure 7.4 of [1]). This theory is also supported by experimental works in [30, 31, 29]. In the appendix section of this paper we briefly recall results of our experimental works in this regard.

Moreover, to study Darcy law based micro-defect formation, it is required to consider a two-phase flow in porous structure formed by dendrites (gas or void as dissolved and/or distinct phase in addition to the melt). Moreover, the gravity has an important effect on the flow which is easily ignored by the mentioned authors. To see effect of gravity, interested peoples are refereed to the following experimental works [32, 33, 34, 35].

After this brief discussion, we believe that the Niyama’s criterion gives its feasibility according to a macro-scale analysis. Here we justify it using the Chvorinov’s rule instead of the simplified Darcy
law. According to [4], the following relation can be obtained by a unidirectional analysis of metal solidification in a low conductivity mold:

\[ M_c = \frac{V_c}{A_c} = \frac{2}{\sqrt{\pi}} \left( \frac{\theta_M - \theta_\infty}{\rho_c L} \right) \sqrt{k_m \rho_m c_m \sqrt{t_s}}, \]  

(6)

where \( M_c \) is the geometrical modulus of the casting, \( V_c \) the casting volume and \( A_c \) the casting surface area through which heat is lost, and \( \theta_M \) the melting point. Chvorinov’s rule is usually expressed as

\[ M_c = C \sqrt{t_s} \]  

(7)

with a constant \( C > 0 \). According to Chvorinov’s rule the square root of the freezing time is proportional to the casting size. So it is possible to remove the size effect from the Pellini’s critical feeding gradient using term \( \sqrt{t_s} \). This leads to measure \( G \sqrt{t_s} \) which is identical to Niyama et. al. observations, but this time with a fairly feasible macro-scale heat transfer analysis.

However, Chvorinov’s rule is derived based on a unidirectional solidification analysis, and consequently can not predict the total solidification time of an arbitrary geometry. For example, in the case of bar casting, the solidification condition coincides with Chvorinov’s assumptions in the early stage of solidification, but later the mode of solidification change from unidirectional to multidimensional and the cooling rate is considerably increased [36, 37]. According to Flemings [4], the generalized counterpart of Equation 6 for cylindrical and spherical geometries has the following form

\[ M_c = \frac{V_c}{A_c} = \frac{\theta_M - \theta_\infty}{\rho_c L} \left( \frac{2}{\sqrt{\pi}} \sqrt{k_m \rho_m c_m \sqrt{t_s}} + \frac{n k_m t_s}{2r} \right), \]  

(8)

where \( n = 0, 1 \) and 2 for plate, cylinder and sphere, respectively, and \( r \) is the radius of the casting. Consequently, a generalized Chvorinov’s rule has the following form

\[ M_c = C \left( \sqrt{t_s} + \frac{\sqrt{\pi} \alpha_m n}{4 r} t_s \right) \]  

(9)

where \( \alpha_m = k_m / \rho_m c_m \) is the mold thermal diffusivity. Comparing Equation 7 with Equation 9, it is clear that the simple Chvorinov and Niyama approximations are valid if the mold thermal diffusivity or the overall mean curvature of the casting, \( n/r \), are small. This suggests that a generalized Niyama criterion would have the form

\[ G \left( \sqrt{t_s} + \frac{\sqrt{\pi} \alpha_m n}{4 r} t_s \right) > \mathcal{B} \]  

(10)

with a constant \( \mathcal{B} \) that depends on the physical properties of mold and metal as well as the ambient temperature. To determine \( n \) and \( r \) in Equation 10, some geometric reasoning procedures are
required. Of course, this formula appears to be in conflict with Niyama et al. [5] as that work was on cylindrical geometries not plate-like ones. The discrepancy is easily resolved by computing the relation of the two terms in parentheses of Equation 10 for the cases given in Niyama et al. [5]: using physical properties and casting conditions given in [5], the relative size of the second term is smaller than 0.01 for the all test cases.

According to the above discussion, we would like to accept the Niyama criterion as a macroscopic shrinkage prediction measure as it only detect regions around hot centers. We are hopeful that our theoretical justification remove a-priori made miss-leading about which is due to Niyama analysis based on micro fluid flow within mushy zone. Therefore, we can not confirm the claim of [20] which is already mentioned in this paper. Moreover, our analysis show that the shallow thermal gradient regions, the Niyama criterion detects are not essentially hot spots. But they can be also cold spots or saddle points. Such points usually happen in complicated castings not simple plate-like ones examined in literature. To cope this limitation, it is possible to check for second order derivative of the temperature field. It is worth to mention that almost all of the experimental support for the Niyama criterion are related to simple shaped castings and detected defects regions are related to nothing else regions around hot-spots (as complement of discussion here see also appendix).

Moreover, it is reasonable to consider the thermal criterion function as macroscopic defect prediction measures (in fact they detects nothing else hot-spots). Therefore, regarding to long freezing range alloys for which defects are not concentrated at hot centers, we are unable to simply use thermal criteria. Therefore, the focus of this study is on the short freezing range solidifications in which the solid/liquid interface can be considered as a macroscopically planar interface. As it is experimentally shown in [31], increasing the concentration of dissolved gas in the melt changes the distribution of defects from concentrated macro-shrinkages to distributed micro-porosities. This is due to ease of defect (in connection to gas porosity) nucleation near solid/liquid interface during solidification (cf. alos Figure 7.26 of [1]). Therefore, we also have to limit application of thermal criteria to high quality melts which are sufficiently degassed too.

As a final remark in this section we note that the generalized Niyama criterion introduced here is expected to be less dependent on the shape of a casting. This is due to the contribution of the extra term that models the casting’s overall mean curvature, $\kappa = \frac{\mathbf{\nabla} \cdot \mathbf{r}}{r}$. However, the overall mean curvature
is a poor measure in the case of complicated geometries. Instead, one may use a criterion that considers $\kappa$ to be a local quantity $\kappa(x)$ that depends on $x$: it would denote an effective curvature at a point $x$ by only considering the geometry within a neighborhood of diameter $\mathcal{R}$ around $x$, where $\mathcal{R}$ is smaller than the diameter of the casting but larger than the maximum distance of points in the cast from the mold in the neighborhood of the desired point. We will not directly pursue this line of thought further, however, and leave it for future research. However, we shall consider the role of local mean curvature in section 5 where we introduce our criterion function.

5 New thermal criterion function. The number, size and distribution of shrinkage defects depend on the physical properties of the melt and mold, quality of the melt and the geometry of casting. If the effect of gravity on the distribution of shrinkage defects is neglected, the last solidification points are located at the spatial position of local hot spots. Therefore, to predict the location of macroscopic shrinkages, it is sufficient to determine the position of local hot spots (see section 4). As shown schematically in Figure 4, mesoscale shrinkages are usually formed during the evolution of a solidifying front to form a macroscopic shrinkage. In fact, an elongated liquid pool usually leaves some dispersed mesoscale shrinkages along its major axis. It is obvious that the width of the mushy zone or sizes of dendrites affect on the distribution and morphology of these mesoscale shrinkages. We have exaggerated this effect in the figure for the purpose of exposition.

Figure 4: Formation of a centerline shrinkage and some dispersed mesoscopic shrinkages along its major axis.

In order to construct an indicator function for the formation of centerline shrinkages and related dispersed mesoscale shrinkage around their wakes the (signed) local mean curvature $\kappa = -\nabla \cdot \hat{n}$ of the macroscopic solid/liquid interface, is a good measure to predict the closeness of the solid/liquid interface. We use a critical value, $\kappa_{cr}$, to predict the formation of shrinkage defects. Obviously, the magnitude of $\kappa_{cr}$ should decrease as the width of the mushy zone increases; it will also depend on the size and distribution of crystals as well as local solidification conditions cf.
Figure 5: Effect of the macroscopic interface curvature on the formation of shrinkage defects: Increasing interface curvature from a to d; a and b show negative curvature (concave interface) c and d show positive curvature (convex interface). Circles show underlying macroscopic curvature.

Figure 4.18] and other physical parameters. Notice that when the local mean curvature of the solid/liquid interface is positive, i.e., when the interface is convex, the danger of shrinkage formation is minimal (see Figure 5). We therefore only consider the case $\kappa_{cr} < 0$, and assume the following for our macroscopic criterion function:

$$\mathcal{F}_\Sigma(\kappa) = a + b\kappa > \kappa_{cr}(M, G, R, v_s),$$

(11)

where $\mathcal{F}_\Sigma$ denotes the macroscopic defect predictor measure, $a, b$ are constants and $M$ denotes the contribution of materials properties on $\kappa_{cr}$. Models including higher powers of $\kappa$ are obvious extensions. Let us note that the sign of the local curvature of the temperature field $\kappa$ corresponds to the local convexity of the temperature Hessian [40]: when the local curvature is positive the Hessian matrix is locally positive definite and vice versa. In other words, the critical interface curvature criterion above covers the required sufficient and necessary conditions mentioned in section 4. On the other hand, criteria like the one above can not predict the size of macroshrinkages. However, we are hopeful to predict the spatial extent of macroshrinkages by predicting the dispersed meso-scale defects in the vicinity of each macroshrinkage (such dispersed defects are also causes this miss-leading that thermal criteria are micro-shrinkage prediction measures).

Now, let us to extend Equation 11 by incorporating the dependency of the critical value to the field solution. For this purpose, we add meso-scale information to the suggested macroscopic measure:

**Model I: Using the mushy zone width.** The width $L$ of the mushy zone can be estimated by

$$L \approx \frac{\theta_l - \theta_s}{G}.$$ 

(12)
Since with increasing the mushy zone width the absolute value of $\kappa_{cr}$ in Equation 11 should decrease, the following measure can be introduced:

$$F_{\Sigma \xi}(\kappa, G) = (a + b\kappa)L^c > \kappa_{cr} = \kappa_{cr}(M),$$

(13)

where $F_{\Sigma \xi}$ denotes the macroscopic criterion which is enriched with mesoscale information, and $c$ is a constant. For our numerical studies below, we will choose $a = 0$ and all of the other constants equal to one, yielding

$$F_{\Sigma \xi}^I(\kappa, G) = \kappa G^{-1} > \kappa_{cr} = \kappa_{cr}(M)$$

(14)

Model II: Using the primary dendritic arm spacing. According to Kurz and Fisher [39], the primary dendritic arm spacing, $D$, or crystal size, can be approximated by the following relation,

$$D \approx K v_s^{-1/4} G^{-1/2},$$

(15)

where $K$ denotes a material constant. We expect the absolute value of $\kappa_{cr}$ to decrease with increasing dendritic arm spacing, resulting in

$$F_{\Sigma \xi}(\kappa, D) = (a + b\kappa)D^c > \kappa_{cr} = \kappa_{cr}(M).$$

(16)

With the same choice of constants, we get

$$F_{\Sigma \xi}^I(\kappa, v_s, G) = \kappa v_s^{-1/4} G^{-1/2} > \kappa_{cr} = \kappa_{cr}(M)$$

(17)

Model III: A heuristic reasoning. It is clear that by increasing speed of solid/liquid interface the time for the mass diffusion is decreased. Moreover, for a constant front speed, feeding ability is increased by increasing temperature gradient in the vicinity of interface. As a result parameter $v_s^c G^d$ could shows difficulty of melt feeding. Assuming constants $c$ and $d$ are equal to one, the following heuristic criterion can be introduced

$$F_{\Sigma \xi}^{II}(\kappa, v_s, G) = \kappa v_s G^{-1} > \kappa_{cr} = \kappa_{cr}(M)$$

(18)

Model IV: Generalized model. The above results suggest that realistic criterion functions should depend on $\kappa$, $v_s$ and $G$. A criterion generalizing all of the above relationships could then have the following form:

$$F_{\Sigma \xi}^{IV}(\kappa, v_s, G) = (a + b\kappa)v_s^c G^d > \kappa_{cr} = \kappa_{cr}(M)$$

(19)
Determining the unknown constants $a, b, c, d$ for a specific alloy and casting conditions, quantitative experimental data are obviously required. They can then be computed using parameter estimation procedures such as the least-squares method [41].

6 Results and discussion. In this section will evaluate the presented method on some known test cases for which experimental results are available. The energy equation is solved by the classical explicit finite difference method and the effect of phase change is incorporated into the heat equation using the effective heat capacity method [42]. A personal computer with an AMD Athlon 2.41 Ghz CPU and 3GB RAM was used as the computing platform in this study.

6.1 Pellini’s plate and bar casting. In this section the, we consider sand mold casting of plain carbon steel. We choose two rectangular geometries with $W/T = 1$ (bar) and $W/T = 3$ (plate), respectively; in each case, $L/T = 9$, where $T$, $W$ and $L$ denote the casting thickness, width and length. Following Pellini’s experimental data [12], the casting thickness is taken to be equal to 2 and 4 inches (approximately 5 and 10 cm) for both geometries. Physical properties and initial and boundary conditions used here presented in Table 1. According to Pellini [12], in 2-inch-thick plates, shrinkage porosity occurred in an area where the feeding gradient ($G^+$ in this case) was less than $20–40 \, ^\circ C/cm$. Regarding to 4-inch bars a higher feeding gradient is required to prevent the centerline shrinkage: $120–240 \, ^\circ C/cm$. We discretize the domain by a three-dimensional uniform Cartesian grid with mesh size $T/30$ in this study.

Table 1: Physical properties, initial and boundary conditions used in Pellini’s plate and bar casting test cases. Units are in SI, except for the temperature which is expressed in $^\circ C$.

|       | $k$   | $\rho$ | $c$  | $L$   | $\theta_0$ | $\theta_1$ | $\theta_s$ | $h_i$ | $h_\infty$ |
|-------|-------|--------|------|-------|-------------|-------------|------------|-------|------------|
| metal | 33.5  | 7200   | 627  | $2.7 \times 10^5$ | 1594        | 1490        | 1440       | 418   | -          |
| sand  | 0.7   | 1500   | 1130 | -     | 20          | -           | -          | 75    | -          |

Figure 6 and Figure 7 show the results of this numerical experiment, in which contour plots of the local freezing time, curvature map, $F^{I}_{\Sigma \xi}$, $F^{II}_{\Sigma \xi}$, $F^{III}_{\Sigma \xi}$ and the Niyama criterion are included. The plots show that regions with a large negative curvature coincide with centerline shrinkage. Therefore, the curvature value can be used (at least) as a qualitative defect indicator measure. Further, the
suggested criteria in this study provide a sharp contrast between the centerline shrinkage and the healthy parts of the castings. However, the contrast provided by the third suggested measure, $F_{III}$, is superior to the others.

Figure 6: Results of simulations for Pellini’s plate casting, 2D cross section at T/2: a) Local freezing time in seconds, b) Interface curvature map in cm, c) $F_{II}$ in $\text{deg}^{-1}$, d) $F_{II}$ in $\text{deg}^{-1/2} \text{min}^{1/4} \text{cm}^{-3/4}$, e) Niyama criterion in $\text{deg}^{1/2} \text{min}^{1/2} \text{cm}^{-1}$, f) $F_{III}$ in $\text{deg}^{-1} \text{min}^{-1} \text{cm}$.

Figure 8 shows the variation of $F_{III}$ along lines parallel to either the width or length of the castings and through the center of the castings. The plots show the desired sharp contrast of the criterion value in the vicinity of the centerline shrinkage. This property makes the selection of appropriate threshold values for this criterion much simpler as the region where shrinkage is predicted to occur becomes largely insensitive to the choice of threshold value. To select a useful threshold, various iso-contours of $F_{III}$ in conjunction with the corresponding critical feeding gradient (based on Pellini’s measurements) and the critical Niyama value are plotted in Figure 9 and Figure 10 for plate and bar geometries, respectively. The plots show that the iso-contours $F_{III} = -0.5$ to $-10.0 \text{deg}^{-1} \text{min}^{-1} \text{cm}$ seems to be a good range for a critical value. Note that we do not want to make a sharp decision on the critical value as we are still believed to the mentioned shape-dependency problem (though our measure introduced to moderate it). Moreover, our results show that critical iso-contours of Niyama and Pellini criterion are not identical to each other. But they are more qualitatively matched.
6.2 Niyama’s cylinders casting. Niyama et al. [2] presented experimental results for cast vertical cylinders of different diameters (3, 6 and 9 cm) with a top riser and mold made from furan-banded silica sand. They had five different steels ranging from low alloy to high alloy steels. They showed that the critical temperature gradient, $G_{cr}$, which is required to avoid shrinkage porosity is about 24, 12 and 8 deg cm$^{-1}$ for 3, 6 and 9 cm diameter cylinders, respectively. Further, they showed that the critical value for Niyama’s criterion is about 1 deg$^{1/2}$ min$^{1/2}$ cm$^{-1}$ independent from the casting size. Simulation parameters used in our computations are given in Table 2. Niyama’s cylinders are discretized by a uniform three-dimensional Cartesian grid with mesh size $D/30$, where $D$ denotes the cylinder diameter.

Table 2: Physical properties, initial and boundary conditions used in Niyama’s cylinders casting test cases. Units are in SI, except for the temperature which is expressed in °C.

|        | $k$  | $\rho$ | $c$  | $L$   | $\theta^0$ | $\theta_1$ | $\theta_s$ | $h_i$ | $h_\infty$ |
|--------|------|--------|------|-------|-------------|-------------|------------|-------|------------|
| metal  | 33.5 | 7200   | 712  | $2.7 \times 10^5$ | 1610         | 1520        | 1485       | infinite | -          |
| sand   | 0.84 | 1500   | 1130 | -     | 20          | -           | -          | -     | 21         |

Figure 11 shows the results of this numerical experiment, in which the contour plot of the local freezing time, curvature map, the three criteria introduced in this study and the Niyama criterion are
Figure 8: Results of simulations for Pellini’s test cases. Left: Variation of $F_{III}^{Σξ}$ along a horizontal line through the casting center. Right: Variation along a vertical line through the casting center. Top: Plate. Bottom: Bar.

included. The validity of the curvature map as a qualitative defect indicator measure is also obvious in this numerical experiment. Further, the sharp contrast of the suggested criteria to identify the centerline shrinkage, in particular of $F_{III}^{Σξ}$ is obvious.

Figure 12 shows the variation of $F_{III}^{Σξ}$ along scan lines which are parallel to either the diameter or height of the cylinders and through the centers of the cylindrical parts of the geometry. This plot again shows the sharp contrast of $F_{III}^{Σξ}$ in the vicinity of defects, making the choice of a threshold value a simple one. To do so, various iso-contours together with the corresponding critical feeding gradient (based on Niyama’s results) and the critical Niyama value are plotted in Figure 13 for Niyama’s cylinders. Again, the iso-contour $F_{III}^{Σξ} = -0.75_{to} - 10.0 \, \text{deg}\, \text{min}^{-1} \, \text{cm}$ appears to be a good range for critical values. However, we should emphasis that due to provided high contrast of the suggested measure there is more freedom for selection of a critical value (though in general there is no universal critical value as measure is not essentially shape-independent).
These results indicate that the suggested criterion and the Niyama or Pellini criteria predict different shapes for the defect region, as shown by the presence or absence of the ring-like shape around the riser in the vicinity of riser-cast connection. We believe that this discrepancy results from the fact that the latter criteria only use the sufficient condition mentioned in section 4 and violate the necessary condition, whereas our criterion properly takes it into account. In fact, the presence of the sharp re-entering edge at the connection of the riser to the casting increases the cooling rate, and consequently leads to a cold spot-like region. Note that in original specimens of Niyama, this a conical connection is considered (not with a sudden cross section), and as a result such ring-like regions were not detected in their analysis.
Figure 10: Results of simulations for Pellini’s bar casting: Iso-contours of the critical feeding gradient ($G^+$) and critical Niyama value in conjunction with various iso-contours of $\mathcal{F}_{\Sigma \xi}$. 
Figure 11: Results of simulations for Niyama’s cylinder casting, 2D cross section at D/2: a) Local freezing time in seconds, b) Interface curvature map in cm, c) $F_{II}$ in deg$^{-1}$ d) $F_{III}$ in deg$^{-1/2}$ min$^{1/4}$ cm$^{-3/4}$, e) Niyama criterion in deg$^{1/2}$ min$^{1/2}$ cm$^{-1}$, f) $F_{III}$ in deg$^{-1}$ min$^{-1}$ cm. Top: $D = 3$ cm. Middle: $D = 6$ cm. Bottom: $D = 9$ cm.
Figure 12: Results of simulations for Niyama’s cylinders casting. Left: Variation of $\mathcal{F}^{III}$ along the objects centerline. Right: Variation along a horizontal line through the cylinder’s center. Top: $D = 3$ cm. Middle: $D = 6$ cm. Bottom: $D = 9$ cm.
Figure 13: Results of simulations for Niyama’s cylinders casting: iso-contours of the critical feeding gradient ($G$) and critical Niyama value ($Ni$) in conjunction with various iso-contours of $\mathcal{F}^{III}_{\Sigma I}$. 

$G = 24 \text{ deg cm}^{-1}$  
$Ni = 1.0 \text{ deg}^{3/2} \text{ min}^{-1/2} \text{ cm}^{-1}$  
$\mathcal{F}^{III}_{\Sigma I} = -0.5 \text{ deg}^{-1} \text{ min}^{-1}$  
$\mathcal{F}^{III}_{\Sigma I} = -0.75 \text{ deg}^{-1} \text{ min}^{-1}$  
$\mathcal{F}^{III}_{\Sigma I} = -1.0 \text{ deg}^{-1} \text{ min}^{-1}$  
$\mathcal{F}^{III}_{\Sigma I} = -10.0 \text{ deg}^{-1} \text{ min}^{-1}$

$G = 12 \text{ deg cm}^{-1}$  
$Ni = 1.0 \text{ deg}^{3/2} \text{ min}^{-1/2} \text{ cm}^{-1}$  
$\mathcal{F}^{III}_{\Sigma I} = -0.5 \text{ deg}^{-1} \text{ min}^{-1}$  
$\mathcal{F}^{III}_{\Sigma I} = -0.75 \text{ deg}^{-1} \text{ min}^{-1}$  
$\mathcal{F}^{III}_{\Sigma I} = -1.0 \text{ deg}^{-1} \text{ min}^{-1}$  
$\mathcal{F}^{III}_{\Sigma I} = -10.0 \text{ deg}^{-1} \text{ min}^{-1}$

$G = 8 \text{ deg cm}^{-1}$  
$Ni = 1.0 \text{ deg}^{3/2} \text{ min}^{-1/2} \text{ cm}^{-1}$  
$\mathcal{F}^{III}_{\Sigma I} = -0.5 \text{ deg}^{-1} \text{ min}^{-1}$  
$\mathcal{F}^{III}_{\Sigma I} = -0.75 \text{ deg}^{-1} \text{ min}^{-1}$  
$\mathcal{F}^{III}_{\Sigma I} = -1.0 \text{ deg}^{-1} \text{ min}^{-1}$  
$\mathcal{F}^{III}_{\Sigma I} = -10.0 \text{ deg}^{-1} \text{ min}^{-1}$
6.3 Industrial hammer casting. As a more realistic example, we consider the solidification of a steel hammer casting used for the 1988 TMS-AIME conference as a benchmark [43]. Detailed information about geometries, physical properties and casting conditions can be found in [43, 26]. The hammer’s mold-box is discretized into a uniform Cartesian grid with mesh size 3 mm, using the Spen Source software package CartGen [44], resulting in about 6 millions grid points.

Figure 14 shows the results of this numerical experiment, including local freezing time contours, and iso-contours at critical value for the Niyama criterion and $F_{\Sigma \Sigma}^{H} = -1.0 \, \text{deg}^{-1} \, \text{min}^{-1} \, \text{cm}$. The plot shows that both methods predict the correct location of the major hot spot below the riser as well as four separated hot spots around the hammer’s core. However, the defect contrast and extent of predicted macroshrinkage provided by the suggested measure in this study is better than by the Niyama criterion. It is obvious that the Niyama criterion hardly detects the macroshrinkage which is formed in the pouring basin due to the formation of an isolated liquid pool at the early stage of the solidification there while the criterion proposed herein detects this defect well. Finally, Niyama’s criterion predicts some fictitious defect regions due to the violation of the necessary condition mentioned in section 4.

\[\text{CartGen: http://mehr.sharif.ir/~tav/cartgen.htm}\]
Figure 14: Results of simulations for industrial hammer casting: a) Local freezing time contours at a selected section (in seconds), b) Iso-contour of the critical value $N_i = 1.0 \text{ deg}^{1/2} \text{ min}^{1/2} \text{ cm}^{-1}$ of the Niyama criterion, c) Iso-contour of $F_{3/2}^{III} = -1.0 \text{ deg}^{-1} \text{ min}^{-1} \text{ cm}$. 
7 Closing remarks. The prediction of the centerline shrinkage in metal castings using thermal criteria is a practically very important problem. In this contribution, we have briefly reviewed existing methods and analyzed their important limitations. Our analysis results that thermal criteria are in fact macro-shrinkage prediction measure not unlike available miss-leadings in literature which introduce them as micro-shrinkage prediction measures. Moreover, application of these measures are limited to short freezing range alloys and when the quality of melt is good. Our analysis also suggests that that critical values for thermal criteria functions are essentially shape-dependent and these measures should be more considered as qualitative measures than quantitative ones.

Based on a heuristic two-scale analysis, a new thermal criterion function is introduced. Our main motivation was moderating the shape-dependency problem of the critical values for thermal criteria functions, in light provided by our analysis. The feasibility of the suggested measure is shown using available experimental data. Our results show that the measure $\kappa v_s G^{-1}$ with a threshold values around -0.5 to -10.0 deg$^{-1}$ min$^{-1}$ cm is success in predicting the formation of centerline shrinkages in steel castings. This measure can be generalized to the the form $(a + b\kappa)v_s G^d$. Obviously, experiments are required to determine the unknown coefficients $a$, $b$, $c$ and $d$ as well as corresponding critical thresholds for specific alloy and casting conditions.

Appendix: Formation of shrinkage in plate-like castings. In this section we provide some experimental data which support our a part of our argument in this study. Our experiments are related to casting of $40 \times 20 \times 4$ cm plate-like CK45 carbon steel. We cast our sample without any feeding and just design gating system such that it (hopefully) compensates liquid-state shrinkage of melt. Couple of samples are cast under two conditions: 1) not sufficiently de-gassed melt and well de-gassed melt (with 0.1 weight percent aluminium). Figure 15 show cross section of these castings. As plots show, for melt with dissolved gas shrinkages are combined with gas porosity and are distributed within cast. It should be noted that regions near mold walls are free of defects in this case. According to plot, there is no sign of shrinkage within cast for the case of well de-gased melt. Instead, the shrinkage is compensated by surface sink in this case. We partly connect this observation to the difficulty of defect nucleation in a clean melt and possibility of casting surface deformation for plate-like castings. A part of this observation can be connected to effect of gravity too.
Figure 15: Cross section of CK45 plate-like (40×20×4 cm) steel castings incompletely de-gassed melt (left) and well de-gassed melt (right).

By this experiment, we want to conclude that formation of central shrinkage in plate-like castings are very difficult if the quality of melt be high. And if shrinkages are observed in central regions they are more like dispersed shrinkages which nucleate with the aid of pre-existing bubble and/or supersaturation of melt with dissolved gases. To justify this prediction, we show X-ray photograph of Pellini for his plate- and bar-like samples in Figure 16. Plot clearly show that shrinkage appeared enterally for bar-like sample while it has appearance of dispersed micro-porosities for the case of plate-like sample which is a sign for low quality melt.

With the same reasoning, we want to make doubt on validity experimental works reported in [6, 13] as they used plat-like (also bar-like which is not in question) samples and only used X-ray photography to detect defect regions. They did not report any photograph from cross-section of their castings which determines type of their defects (dispersed microporosity due to melt preparing procedure or actual concentrated center-line shrinkages). In particular their casting are performed by couple of industrial foundations which increase susceptibility of careless melt preparation.

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Figure 16: X-ray photographs related to figure 11 (bottom) and figure 17 (top) of Pellini [12] paper which are related to plate and bar castings respectively.

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