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Coupled modelling of the solidification process predicting temperatures, stresses and microstructures

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Abstract

A coupled modelling of various phenomena which characterize the solidification of castings is presented. Thermal and mechanical calculations are linked by taking into account local and transient heat transfer coefficients at the casting mould interface dependent on the contact pressure or the air gap width. A new approach was developed to model this air gap-contact problem. A sophisticated microstructure model of dendritic solidification is introduced to determine the release of latent heat which influences the temperature evolution. Such a comprehensive simulation predicting temperatures, stresses and microstructure leads to a more accurate description of the casting process in order to optimize process parameters especially with regard to mechanical properties of the cast part.

Keywords: Casting process; Coupled modelling; Temperature, stress and microstructure simulation

1. Introduction

Numerical modelling of casting processes is a very useful and common tool to predict the final state of cast parts. By variation of single process parameters, i.e., the initial temperature or the position and shape of the feeding system the simulation allows an easy and quick assessment of optimization properties. However, the solidification of castings is characterized by the mutual influences of the predominant thermal, metallurgical and mechanical conditions, which are depicted in Fig. 1. Due to limited computational power it was frequently assumed that these complicated interactions within a casting system can be neglected. Nowadays, the increasing computational capacity enables a coupled simulation. The present work is focused on such a coupled modelling.

2. Method of simulation

The described simulations were performed by using the Foundry-Institute's three-dimensional finite element program CASTS (Computer Aided Solidification TechnologieS). Detailed information concerning this simulation code can be found in Refs. [1–3]. In order to perform a coupled analysis the code CASTS was extended to a new approach with the aim of modelling local and time dependent air gaps or contact pressure, respectively, between casting and mould. Furthermore, a model determining dendritic microstructure of castings was implemented. Both recent developments will be explained briefly.

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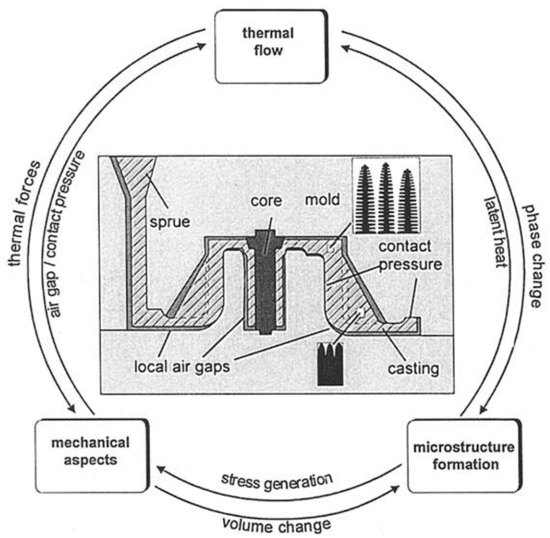

Fig. 1. Various aspects of a coupled modelling of a casting process.

2.1. Modelling the air gap-contact problem

Classical approaches to consider the air gap-contact problem at the casting-mould interface like the penalty method or the use of Lagrange multipliers lead very often to numerical problems due to a bad mathematical conditioning. Therefore, a new approach that is mathematically easy to handle, was developed. This approach is not restricted to non-deformable moulds. It is specially adapted to casting processes assuming negligible friction between casting and mould during cooling and a small shifting of neighbouring nodes at the casting-mould interface. Just a brief explanation is given in this paper. More details can be found elsewhere [4].

The casting-mould interface consists of elements that have no volumetric extension. Their element stiffness K_e is zero (Fig. 2a). This initial condition correlates physically to a gap at each node between casting and mould. Constraining a local contact between the node j (casting) and the node i (mould) at the interface can be achieved by reducing the rank of the finite element equation system of the strain stress calculation setting:

$$\delta_i = d_j = \delta_{ij}^* \text{ and } R_i + R_j = R_{ij}^* \tag{1}$$

with δ as incremental displacement and R as thermal force, see Fig. 2b. An algorithm controls closing and release of the interface nodes during the cooling dependent on, e.g., a local shrinkage of the casting on a core.

This described procedure increases the necessary computation time up to max. 35% depending on the complexity of the geometry, but various investigations have shown that this approach works without any convergence problems even for large geometries. Comparisons concerning the strain-stress calculation between geometries enmeshed without interface elements and with interface elements, for which steady contact was constrained, showed that the error made by the described procedure was negligible (less than 0.3% difference between compared deformations at significant nodes) even for geometries with more than 20000 elements.

By means of this approach it is possible to simulate effectively the mechanical interaction between

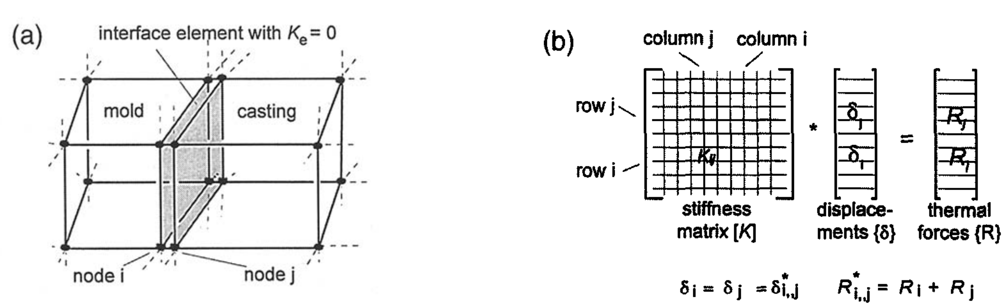

Fig. 2. (a) Schematic enmeshment of the casting mould interface. The interface element has the dimension zero and its element stiffness K_e is equal to zero. This correlates to a gap between casting and mould. (b) Finite element equation system for the strain calculation. In case of a local contact between the nodes i (mould) and j (casting) the rank of the matrix $\mathbf{K}$ is reduced by setting the incremental displacement δ_i equal to δ_j and superposing the thermal forces R_i and R_j.

casting and mould owing to the local opening or closing of gaps dependent on the transient thermo-mechanical condition. The calculated local air gap width or the local contact pressure, respectively, enables a precise coupled thermo-mechanical calculation by determining a local heat transfer coefficient between each node of the casting mould interface.

2.2. Determination of the heat transfer coefficient

The heat flux across the interface is controlled by an overall heat transfer coefficient, h_{eff}. The evaluation of a local heat transfer coefficient used in our simulation distinguishes between two cases:

2.2.1. Air gap between casting and mould

Due to the fact that in casting processes the thickness of an air gap is very small, the heat flow caused by convection can be neglected [5]. The heat transfer coefficient can be expressed as the sum of heat flux due to radiation and air conduction:

$$h_{eff} = h_{rad.} + h_{air\,cond.} = \sigma \cdot \left[\Theta_c^2 - \Theta_m^2\right]\left[\theta_c - \theta_m\right] \frac{1}{\frac{1}{\epsilon_c} + \frac{1}{\epsilon_m} - 1} + \frac{\lambda_{air}}{\delta_{air\,gap}} \quad (2)$$

where λ_{air}, ϵ, Θ, σ are the heat conduction of air, the emission coefficient and interface temperature (c: casting, m: mould), and the Boltzman-constant. $\delta_{air\,gap}$ stands for the calculated width of the air gap.

2.2.2. Pressure contact between casting and mould

The literature offers various sophisticated models, describing the heat transfer coefficient as a function of, e.g., contact pressure, surface roughness, hardness and further material parameters [6–8]. Because of lacking physical data for different material combinations used in casting processes a simplified relation was chosen, where the heat transfer depends only on the contact pressure between casting and mould considering a mean hardness of casting and mould:

$$h_{eff} = h_{contact\,cond.} = \gamma_1 \left[\frac{p_{int}}{H_e}\right]^{\gamma_2} \quad (3)$$

with γ_1, γ_2 as material parameters, H_e as Vickers Hardness and p_{int} as contact pressure at the interface.

2.3. Prediction of microstructure

The approach implemented in CASTS is based on a model developed by Roosz and co-workers [9–11]. This model was adapted to our demands in order to enable CASTS to predict the global microstructure formation of binary or ternary alloys during dendritic solidification of castings. It considers the main kinetic and thermodynamic effects that influence microsegregation, like solid state back diffusion, secondary dendrite arm coarsening, primary tip undercooling [12]. It offers a high capability owing to a thermodynamically formulated phase diagram, generated by means of the commercial code ChemApp™. Output data for each node of the enmeshed geometry are local primary and secondary dendrite arm spacings as well as the fraction solid as a function of the solidification path. The fraction solid, which is calculated stepwise during the solid–liquid interval, can be used as input data for the macroscopic temperature evaluation to control the release of latent heat.

3. Results

The simulation of the production process of single crystal turbine blades by the Bridgman-process has already reached a level of maturity. Nevertheless, the simulation can be improved considering, i.e., the evolution of local air gaps. Fig. 3 shows the calculated development of a local air gap arising during the directional solidification of a turbine blade. The geometry of the casting system has approximately 16000 nodes, including the furnace. The casting mould interface used for the coupled thermo-mechanical calculation consists of nearly 200 pentahedrons and 1200 hexahedrons. The importance of releasing single nodes at the interface is evident if the mould is not assumed to be rigid during the stress calculation.

The mechanical interaction between casting and mould is clearly depicted in Fig. 4. The deformed shape of a simple casting system in its symmetry plane, calculated with the described new air gap-con-

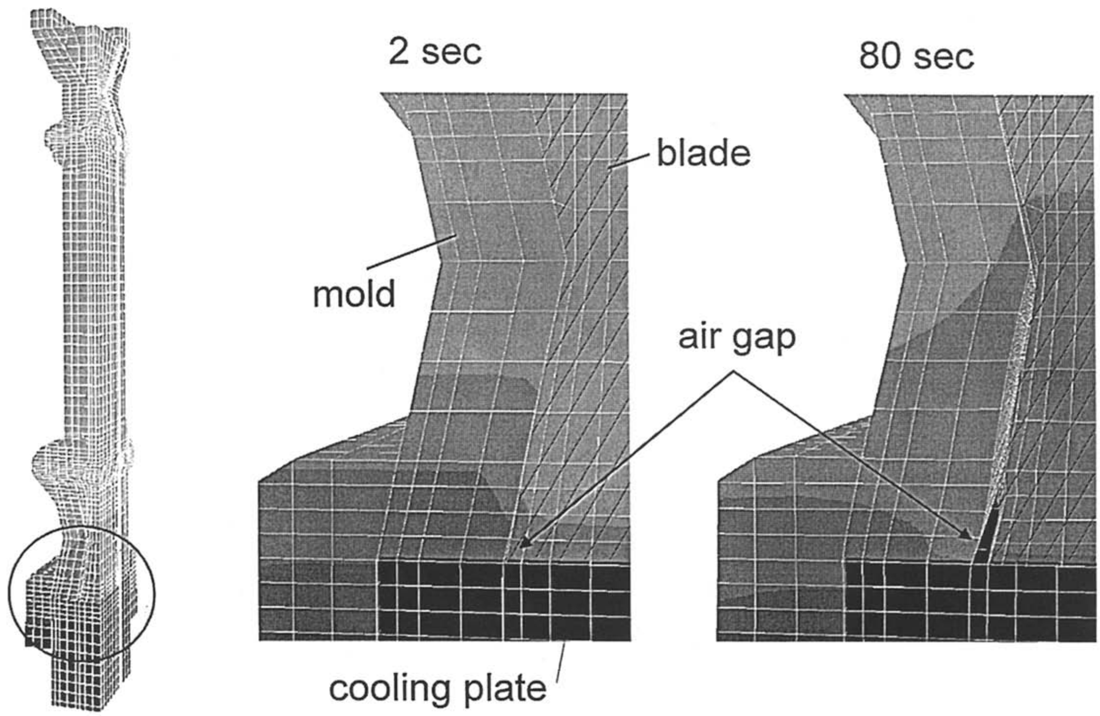

Fig. 3. Development of a local air gap of a complex cast part. The left figure shows a sectional view of an enmeshed turbine blade with cooling plate and ceramic mould. The figure on the right depicts the evolution of a local air gap during directional solidification of the blade. For reasons of clarity the deformations are magnified by 100 times.

tact model is shown. Clearly visible are the contact areas where the casting shrinks on the mould during the cooling. Air gaps arise where the shrinkage is not restricted. Due to the strong decrease of the local heat transfer, the appearance of air gaps changes the thermal history of the neighbouring regions remarkable.

Considering the effect of local air gaps on local cooling, the microstructure evolution of two similar alloys (Al–4.8 wt.% Si and Al–7.8 wt.% Si) under identical initial and cooling conditions was investigated. Fig. 5 shows the determined values of the primary (λ_1) and secondary (λ_2) dendrite arm spacing,, as well as for the amount of the (interdendritic) eutectic fraction, f_E, for both alloys [1]. As expected, for the alloy which concentration is closer to the eutectic composition compared to the more diluted alloy the average of λ_1 is smaller where as the average of f_E is higher. Due to the larger coarsening

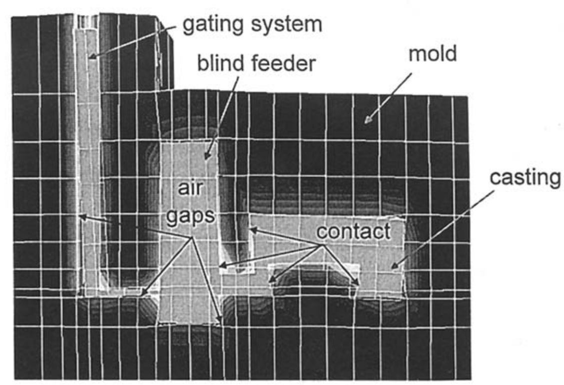

Fig. 4. Example showing the mechanical interaction between casting and mould. Zones with and without air gaps are clearly visible. To illustrate the distortion the displacements have been multiplied by a factor of 150.

[1] The simulation was performed for a principal die casting process. Due to the high cooling rates columnar dendritic solidification was assumed.

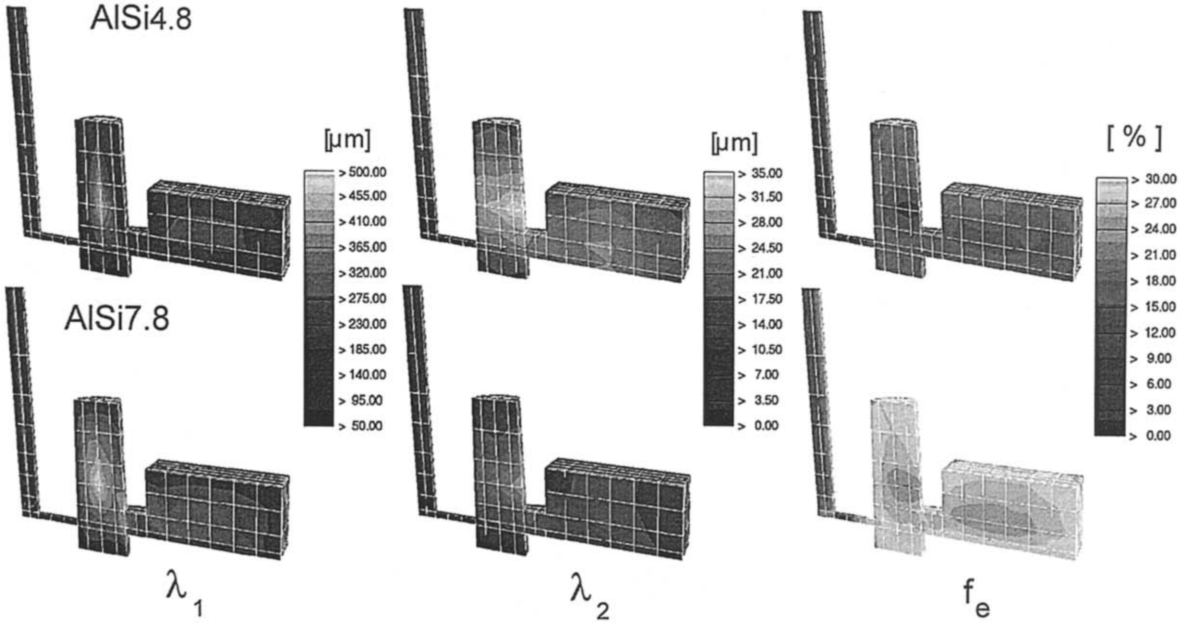

Fig. 5. Primary (λ_1), secondary (λ_2) dendrite arm spacing and fraction eutectic (f_e) for the alloys Al–4.8 wt.% Si and Al–7.8 wt.% Si under identical initial and cooling conditions. Notice, that in both cases the minimum in λ_1 does not correlate with the maximum in f_E.

time higher values for λ_2 are predicted. However, notice that in both cases the minimum in λ_1 does not correlate with the maximum in f_E, although regions with smaller λ_1 coincide with those of larger f_E. The explanation of this result is beyond the scope of this paper and thus will be given elsewhere [13]. The predicted microstructure formation may be used as a future guide to adjust required mechanical properties of a casting by varying cooling conditions.

4. Conclusions

Numerical results of a simulation of a casting process within a coupled treatment of stresses, temperatures and microstructure formations are presented. The appearance and the geometry of air gaps is effectively simulated. The dependence of the heat transfer coefficient on the contact pressure or the air gap width is taken into account. The simulation provides precise information about the temperatures, transient and residual stresses, including the deformed shape of the casting system. Primary and secondary dendrite arm spacing, as well as the amount of eutectic fraction are further results from the microstructure modelling.

This coupled modelling may improve the accuracy of the simulation of a casting process. The steady increase of computational power enables the development of new coupled algorithms to consider further complex phenomena, i.e., the generation of stresses during solid phase transformation. Experimental investigations are in progress to validate the shown simulation results.

Acknowledgements

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