Modelling of Thermal Gap Conductance in Casting using Finite Element Analysis

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Abstract

This paper presents a case study for modelling a thermal gap conductance in a finite element analysis (FEA) of a casting process. A theoretical model of the thermal gap conductance and its implementation into FEA is described. The thermal gap conductance model is used to simulate the heat transfer between the cast and mould interfaces of the casting process. Mould filling and solidification aspects of the casting process are simulated using a thermal FEA. The gap formation between the cast and mould, cast shrinkage, mould expansion and shrinkage and residual stresses are simulated in a fully coupled thermo-mechanical FEA. The effect of the thermal gap conductance model is described. The results showed that the thermal gap conductance plays an important role in predicting the temperature distribution in the cast and the mould.

Keywords: thermal gap conductance, finite element analysis, casting

1. Introduction

Casting is a process where the material is heated to its melting temperature or above, poured or injected into a mould with a specific geometry and cooled to room temperature. During cooling, the cast shrinks and allows a gap to be created between the cast and the mould. This gap has a different clearance along the cast/mould interface and affects the heat transfer between the cast and the mould. Typically, heat may pass through the interface via three paths: conduction through the contact spots, conduction through the gas present in the gap and radiation across the gap [1].

Cooper et al. [2] have studied the resistance to the heat flow between two thick solid bodies in contact in a vacuum. Existing analyses of single idealised contacts have been summarised and compared, and then applied, together with results of recent electrolytic analogue tests, to predict the conductance of multiple contacts. Madhusudana [3] has investigated the heat flow across a joint formed by two concentric cylinders, which depends not only on the geometrical, thermo-physical and surface properties of the cylinders but on the heat flux and maximum operating temperatures. An analysis has been presented in which it has been shown that, depending on the heat flow direction, the contact may be reinforced or completely relaxed during operation. Lee et al. [4] have investigated an indirect squeeze casting process experimentally and numerically. A two-dimensional FEA for fully coupled heat transfer and deformation analysis has been used to simulate the cooling curves obtained from the experiments. Thermal contraction of the material during solidification creates an air gap between the mould and the cooling material. The experimental and predicted results have been discussed in conjunction with the relationships between the cooling rate, microstructure, die geometry and applied pressure. Singhal et al. [5] have developed a predictive model for estimating thermal contact conductance between two nominally flat metallic rough surfaces,
which has been experimentally validated. The predictive model consists of two complementary parts, the first of which is a surface deformation analysis to calculate the actual area of contact for each contact spot, while the second accounts for the effects of constriction resistance and gas gap conductance between the contacting surfaces.

Despite the current research developments in heat transfer between two interfaces, there are a limited number of publications where theoretical thermal gap conductance models are considered in the FEA analysis of casting. Usually, the thermal gap conductance is simulated in the FEA by applying constant or temperature dependent heat transfer coefficients between two interfaces in contact. The main objective of this study is to develop a thermal gap conductance model, which takes into account the radiation, and conductance between the cast and mould interfaces. Also, temperature dependent thermal and physical properties of the gas, cast and mould interface materials are considered. Another objective is to implement the developed thermal gap conductance model into FEA and demonstrate a FE technique for simulation of casting processes.

2. Thermal contact

To simulate a casting process a considerable attention must be paid to the thermal contact between the mould and cast interfaces. Generally, the thermal contact can be treated as either contact between two interfaces touching each other (perfect contact) or interfaces with a gap between them. In the FE modelling, the contact can be defined between a node from the slave surface and a projection of this node to the nearest element face from the master surface. Using the FE method, the gap conductance coefficient needs to be specified for achieving the heat transfer between two interfaces in a contact.

2.1. Theoretical model of thermal gap conductance

Figure 1 shows a contact between two interfaces represented by nodes 1 and 2 with temperatures $T_1$ and $T_2$ and clearance $d$ between them. A gap between two solid interfaces exists when $d>0$. Typically, the gap is filled with air or another gas.

![Figure 1: Thermal contact between two interfaces](image)

The gap heat transfer can be defined by the summation of the gas conductance heat transfer and the radiation heat transfer between the two interfaces.

$$q_g = q_c + q_r$$

(1)

where $q_g$ is the gap heat transfer, $q_c$ is the gas conductance heat transfer and $q_r$ is the radiation heat transfer. The gas conductance heat transfer can be given by [1].

$$q_c = \frac{k_g(T_1 - T_2)}{d}$$

(2)
where \( k_g \) is the conductance coefficient of the gas, \( T_1 \) and \( T_2 \) are the temperatures at nodes 1 and 2, and \( d \) is the gap clearance. Taking into account the roughness of the surfaces and the temperature jump distances from the kinetic theory, Equation (2) can be given by:

\[
q_c = \frac{k_g (T_1 - T_2)}{d + d_r + g_1 + g_2}
\]  

(3)

where \( d_r \) is related to the roughness of the two contacting surfaces and \( g_1 \) and \( g_2 \) are the temperature jump distances for nodes 1 and 2 of the contacting pair, which are given by Kennard [6]:

\[
g_1 = \frac{k_g (2-a_1)}{P_g a_1} \left( \frac{2\pi T_1}{R} \right)^{1/2} \left( \frac{\gamma_1 - 1}{\gamma_1 + 1} \right)
\]  

(4)

\[
g_2 = \frac{k_g (2-a_2)}{P_g a_2} \left( \frac{2\pi T_2}{R} \right)^{1/2} \left( \frac{\gamma_2 - 1}{\gamma_2 + 1} \right)
\]  

(5)

where \( P_g \) is the gas pressure, \( R = 8.3144 \) kJ is the universal gas constant, \( a \) is the accommodation coefficient for the corresponding interface material, \( \gamma \) is the specific heat ratio for the corresponding interface material. The accommodation coefficient is a fraction of heat transfer between the surface and the molecule. The radiation heat transfer between two nodes in contact is given by [1]:

\[
q_r = f\sigma(T_1^4 - T_2^4)
\]  

(6)

where \( f \) is the radiation factor, \( \sigma = 5.6697 \times 10^{-8} \) W/(m\(^2\)K\(^4\)) is the Stefan-Boltzmann constant, \( T_1 \) and \( T_2 \) are the temperatures in nodes 1 and 2 and they must have units in Kelvin. The radiation factor in a bisurface system is given by [1].

\[
f = \left( \frac{\rho_1}{\alpha_1} + \frac{1}{F_{1-2}} + \frac{A_1 \rho_2}{A_2 \alpha_2} \right)^{-1}
\]  

(7)

where \( \rho_1 \) and \( \rho_2 \) are the densities, \( \alpha_1 \) and \( \alpha_2 \) are the thermal diffusivities, \( A_1 \) and \( A_2 \) are the cross sectional areas for interface materials 1 and 2 and \( F_{1-2} \) is the view factor. The view factor \( F_{1-2} \) between parallel plates is equal to one. The two cross section areas are equal \( (A_1=A_2) \) for FE contact modelling between two nodes and the radiation factor can be given by [1]:

\[
f = \left( \frac{\rho_1}{\alpha_1} + \frac{\rho_2}{\alpha_2} \right)^{-1}
\]  

(8)

The radiation factor can be given as a function of the emissivity by [1]:

\[
f = \left( \frac{1}{\varepsilon_1} + \frac{1}{\varepsilon_2} - 1 \right)^{-1}
\]  

(9)

where \( \varepsilon_1 \) and \( \varepsilon_2 \) are the emissivity coefficients for interfaces 1 and 2.

2.2. Implementation of the thermal gap conductance model into FEA

The theoretical model of the thermal gap conductance is implemented into ABAQUS using the user-defined GAPCON subroutine. The heat transfer between contacting interfaces in ABAQUS is defined as [7]:

\[
q_c = \frac{k_g (T_1 - T_2)}{d + d_r + g_1 + g_2}
\]  

where \( d \) is the gap clearance, \( k_g \) is the conductance coefficient of the gas, and \( g_1 \) and \( g_2 \) are the temperature jump distances at nodes 1 and 2. Taking into account the roughness of the surfaces and the temperature jump distances from the kinetic theory, Equation (2) can be given by:

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q_c = \frac{k_g (T_1 - T_2)}{d + d_r + g_1 + g_2}
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where \( d_r \) is related to the roughness of the two contacting surfaces and \( g_1 \) and \( g_2 \) are the temperature jump distances for nodes 1 and 2 of the contacting pair, which are given by Kennard [6]:

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g_1 = \frac{k_g (2-a_1)}{P_g a_1} \left( \frac{2\pi T_1}{R} \right)^{1/2} \left( \frac{\gamma_1 - 1}{\gamma_1 + 1} \right)
\]  

(4)

\[
g_2 = \frac{k_g (2-a_2)}{P_g a_2} \left( \frac{2\pi T_2}{R} \right)^{1/2} \left( \frac{\gamma_2 - 1}{\gamma_2 + 1} \right)
\]  

(5)

where \( P_g \) is the gas pressure, \( R = 8.3144 \) kJ is the universal gas constant, \( a \) is the accommodation coefficient for the corresponding interface material, \( \gamma \) is the specific heat ratio for the corresponding interface material. The accommodation coefficient is a fraction of heat transfer between the surface and the molecule. The radiation heat transfer between two nodes in contact is given by [1]:

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q_r = f\sigma(T_1^4 - T_2^4)
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where \( f \) is the radiation factor, \( \sigma = 5.6697 \times 10^{-8} \) W/(m\(^2\)K\(^4\)) is the Stefan-Boltzmann constant, \( T_1 \) and \( T_2 \) are the temperatures in nodes 1 and 2 and they must have units in Kelvin. The radiation factor in a bisurface system is given by [1].

\[
f = \left( \frac{\rho_1}{\alpha_1} + \frac{1}{F_{1-2}} + \frac{A_1 \rho_2}{A_2 \alpha_2} \right)^{-1}
\]  

(7)

where \( \rho_1 \) and \( \rho_2 \) are the densities, \( \alpha_1 \) and \( \alpha_2 \) are the thermal diffusivities, \( A_1 \) and \( A_2 \) are the cross sectional areas for interface materials 1 and 2 and \( F_{1-2} \) is the view factor. The view factor \( F_{1-2} \) between parallel plates is equal to one. The two cross section areas are equal \( (A_1=A_2) \) for FE contact modelling between two nodes and the radiation factor can be given by [1]:

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The radiation factor can be given as a function of the emissivity by [1]:

\[
f = \left( \frac{1}{\varepsilon_1} + \frac{1}{\varepsilon_2} - 1 \right)^{-1}
\]  

(9)

where \( \varepsilon_1 \) and \( \varepsilon_2 \) are the emissivity coefficients for interfaces 1 and 2.
where $q$ is the heat transfer between corresponding nodes 1 and 2, $h$ is the coefficient of gap conductance. The heat transfer equilibrium equation according to the theoretical definition can be given by [1]:

$$q = q_g = q_r$$

or

$$h(T_1 - T_2) = \frac{k_g(T_1 - T_2)}{d + d_r + g_1 + g_2} + \left(\frac{1}{\epsilon_1} + \frac{1}{\epsilon_2} - 1\right)^{-1} \sigma (T_1^4 - T_2^4)$$

The gap conductance coefficient from Equation (13) is implemented into the user-defined GAPCON subroutine in ABAQUS. This subroutine is called for each time increment of the fully coupled thermo-mechanical analysis. When the GAPCON subroutine is called, it provides the following variables for solving Equation (13): Distance clearance $d$ and temperatures $T_1$ and $T_2$, for the contacting nodes 1 and 2. The known and the unknown variables from Equation (13) for defining the thermal gap conductance coefficient can be given by:
**Known variables:**
- Distance clearance \( d \)
- Temperatures \( T_1 \) and \( T_2 \) for nodes 1 and 2.
- Stefan-Boltzmann constant \( \sigma = 5.67 \times 10^{-8} \text{W(m}^2\text{K}^{-4}) \)

**Unknown variables:**
- Emissivity for interface 1 \( \varepsilon_1 \)
- Emissivity for interface 2 \( \varepsilon_2 \)
- Gas conductance coefficient \( k_g \)

**Variables to be defined:**
- Gap conductance coefficient \( h \)

The gas temperature \( T_g \) is calculated as:

\[
T_g = \frac{T_1 + T_2}{2}
\]  

(14)

A temperature dependant gas conductance coefficient is included in the GAPCON subroutine. After linear interpolation for the corresponding gas temperature, the gas conductance coefficient is obtained (see Figure 2).

![Air conductance coefficient versus temperature](image)

**Figure. 2: Air conductance coefficient versus temperature [1]**

Linear interpolation is also used to define the temperature dependent emissivity coefficients \( \varepsilon_1 \) and \( \varepsilon_2 \) for nodes 1 and 2. In perfect thermal contact \( (d=0) \), Equation (13) becomes indefinite \( (h=\infty) \). This means that a very large value must be assigned for \( h \). It must be taken into account that very large values for \( h \) can cause numerical problems in the FE solver. In high pressure die casting, for pressure applied to the liquid metal in range \( 10 – 100 \text{MPa} \) the \( h \) is known to be \( 50 – 100 \text{kw/m}^2\text{C}^\circ \) [8]. Therefore, a maximum value of \( 50 \text{kw/m}^2\text{C}^\circ \) is applied for \( h \) in this study, where the contact pressure is caused mainly by the gravity. This value is applied in perfect contact and when the gap separation is very small and the calculated \( h \) is higher than \( 50 \text{kw/m}^2\text{C}^\circ \).

**3. FE simulation of casting**

The casting FE simulation is carried out in two consecutive simulations in ABAQUS, thermal and fully coupled thermo-mechanical analyses. Figure 3 shows the sequence of the casting simulations. First, a thermal analysis is performed and the main goals are:

- Modelling of the mould filling.
- Performing a solidification criterion.
Figure 3: Sequence of casting simulation

The mould filling is performed by a contact pair activation technique. The defined contact between the cast and mould interfaces is initially defined as inactive. The cast is split in twelve layers and the contacts between the mould and cast layers are activated in separate steps. After the mould filling is completed, a solidification criterion is performed during the cooling process. The main reason for performing a solidification criterion is to define when the cast starts solidifying and separating from the mould. When this moment is detected, the temperature distribution for the thermal FE model is transferred to the fully coupled thermo-mechanical FE analysis where the gap formation, thermal gap conductance, cast shrinkage, mould expansion and shrinkage and the residual stresses are investigated. Detailed information regarding the mould filling and solidification detection techniques can be found in [9]. The fully coupled thermo-mechanical analysis is also performed in ABAQUS and the main goals are:

- Transferring the temperature distribution from the thermal analysis, where the solidification criterion is applied, as an initial condition.
- Implementing the gap conductance by the user-defined GAPCON subroutine.
- Cooling to room temperature and obtaining the distortions and residual stresses.

The model is generated in ABAQUS/CAE. Two assembled parts define the final geometry of the model. The part, which represents the mould, has a parallelepiped shape with an extruded cavity in the middle. The overall dimensions of the mould are: width = 200 mm; height = 140 mm; cavity width = 160 mm; cavity height = 120 mm and wall thickness = 20 mm. The second part which represents the cast has also a parallel piped geometry with dimensions: width = 160 mm and height = 120 mm. For both, the thermal and the fully coupled thermo-mechanical analyses, hexahedron elements with eight nodes are used (see Figure 4).

Heat transfer 3D linear elements DC3D8 are used for the thermal analysis and 3D coupled temperature-displacement elements with reduced integration and hour glass control C3D8RT are used for the temperature-displacement analysis from the ABAQUS library. The cast has 18,816 hexahedron elements, while the mould has 12,396 hexahedron elements. The ABAQUS automatic algorithm for determination of a suitable increment size for each
increment of the step is used. Very small initial time and linear elements are used to avoid spurious oscillations in the heat transfer analysis. Also, the time increment is additionally controlled by specifying a maximum allowable temperature change of 5°C in an increment for the thermo-mechanical analysis.

**Figure. 4: FE mesh**

### 3.1. Material properties

Temperature dependant material properties are used for the thermal and fully coupled thermo-mechanical analyses. The mould is modelled with steel P91 material properties, which can be found in [10]. The cast is modelled as an Inconel 718 nickel-based alloy. Thermo-physical temperature dependent material properties are used for the Inconel 718 alloy, such as thermal conductivity [11], specific heat capacity [11] and density [12, 13]. A latent heat of 145 kJ/kg, melting temperature of 1336°C and solidus temperature of 1260°C are used [14]. The expansion coefficient, elastic modulus, Poison’s ratio and the yield strength material properties can be found elsewhere [15-20]. The yield and the ultimate stresses at room temperature are 890 MPa and 1252 MPa respectively.

### 3.2. Boundary conditions

The boundary conditions are described separately for the thermal and fully coupled thermo-mechanical analyses. The following thermal boundary conditions are applied to the thermal analysis:

- Initial temperature of the cast (pouring temperature) = 1475°C.
- Initial temperature of the mould (mould preheating) = 1050°C.
- Contact between the cast and mould interfaces is applied as inactive at the beginning of the analysis and contact activation is performed during the mould filling.
- Gap conductance coefficient of 50,000 W/m²°C is applied between the contacting surfaces. This means that the contact is considered to be a perfect contact.
- Convection is applied to the outer surfaces of the mould and the top surface of the cast at the end of the mould filling process.

The following thermo-mechanical boundary conditions are applied into the fully coupled thermo-mechanical analysis:
Initial temperatures for the mould and the cast are imported from the thermal analysis after performing the mould filling and the solidification criterion.

The thermal gap conductance model from Equation (13) is implemented into the user-defined GAPCON subroutine.

Convection is applied to the outer surfaces of the mould and top surface of the cast.

The mould is constrained in the z direction at the bottom surface.

3.3. Results and discussion

After transferring the temperature distribution from the thermal analysis, a cooling to room temperature is performed in a fully coupled thermo-mechanical analysis. During cooling, the cast starts to shrink and a gap is formed between cast/mould interfaces where the gap is filled with air. Figure 5 shows the temperature distribution for time of 1000 seconds of the cooling.

![Figure 5: Temperature distribution during cooling for time of 1000 s](image)

It can be seen that the gap grows between the mould and cast interfaces due to shrinkage of the cast. The final cast shrinkage is achieved when the cast is cooled to room temperature. Two areas, A and B are enlarged in order to analyse the gap conductance influence on the temperature distribution. The gap clearance between the cast and mould and the temperature contours can be seen in the enlarged area A. A maximum temperature difference of 75 °C is observed between the mould and cast interfaces in this area (see Figure 6). This temperature difference is due to the thermal gap conductance model implemented in this study. Area B is also enlarged where a perfect contact is observed. It can be seen in Figure 7 that the cast and mould interfaces have similar temperatures. The residual stress distribution and the gap formation for the model are shown in Figures 8. Maximum Von Mises stresses of 830.6 MPa for the cast and 416.5 MPa for the mould are located in the centre of the edge.
Figure 6: Temperatures at area A at the cast and mould interfaces

Figure 7: Temperatures at area B at the cast and mould interfaces

Figure 8: Von Mises stresses at the end of the cooling
4. Conclusions

A thermal gap conductance model was studied and implemented into finite element simulation of a casting process. The model takes into account the gap formation and separation, temperature dependent thermo-physical properties for the cast and mould interface materials, radiation between two interfaces and gas conductance. The results showed that the thermal gap conductance model predicts the same temperatures for the cast and mould interfaces in perfect contact. It was also observed, when a gap is formed, that the temperatures at the cast and mould interfaces are different.

The finite element technique for casting process simulation was demonstrated. Thermal analysis was performed to simulate the mould filling. Fully coupled thermo-mechanical analysis was then carried out to simulate the cast shrinkage, gap formation, mould and cast distortions and residual stresses. The thermal gap conductance model was implemented into the fully coupled thermo-mechanical analysis to simulate the heat transfer between the mould and cast.

References


