Interfacial Heat Transfer Coefficient between Ti6Al4V Alloy Castings and Ceramic Shells in Investment Casting: Postprint

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Abstract

A one-dimensional inverse calculation model for the interfacial heat transfer coefficient (h) at the Ti6Al4V alloy casting/mold interface was established. The effects of shell thermophysical parameters and thermocouple positioning on h calculation were investigated from mathematical and numerical simulation perspectives, and the distinct characteristics of these parameter influences were analyzed. Based on this, the shell thermophysical parameters and thermocouple positions were corrected, improving the accuracy of the inverse calculation of h. The inverse calculation results after parameter correction show that under Ti6Al4V alloy investment casting conditions, the variation of h can be divided into four stages: (1) when the casting is liquid, h remains at approximately 440 $W/(m^2 \cdot K)$; (2) a complete solidified layer forms on the casting surface, during which h decreases by nearly 60%; (3) the solidified layer continuously thickens until the casting is fully solidified, during which h decreases to approximately 20% of the peak value; (4) after solidification, h decreases slowly with temperature. The inverse-calculated h was verified in a three-dimensional model, and the simulated temperatures obtained were in good agreement with the measured temperatures, indicating that the inverse-calculated h is relatively accurate and can be applied to numerical simulations of the Ti6Al4V alloy investment casting process.

Full Text

Research on the Interfacial Heat Transfer Coefficient Between Casting and Ceramic Shell in Investment Casting Process of Ti6Al4V Alloy

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Abstract

A one-dimensional inverse calculation model for the interfacial heat transfer coefficient (h) between Ti6Al4V alloy casting and ceramic shell in investment casting was established. The influence of shell thermophysical parameters and thermocouple positioning on the calculated h was investigated from mathematical and numerical simulation perspectives. The distinct characteristics of different parameter effects were analyzed, and corrections were applied to the shell thermophysical parameters and thermocouple positions, thereby improving the inverse calculation accuracy. The corrected results indicate that under investment casting conditions for Ti6Al4V alloy, the variation of h can be divided into four stages: (1) When the casting is liquid, h remains at approximately 440 $W/(m^2 \cdot K)$; (2) Upon formation of a complete solidified layer on the casting surface, h decreases by nearly 60%; (3) As the solidified layer continues to thicken until complete solidification, h decreases by approximately 20% of its peak value; (4) After solidification, h decreases slowly with temperature. The inverse-calculated h was validated using a three-dimensional model, and the simulated temperatures agreed well with measured values, demonstrating that the obtained h is accurate and applicable to numerical simulation of Ti6Al4V alloy investment casting.

Keywords: titanium alloy, investment casting, interfacial heat transfer coefficient

Introduction

Titanium alloys are widely used in aerospace, medical, and chemical industries due to their high specific strength, good heat resistance, excellent corrosion resistance, and biocompatibility. However, titanium alloy components often have complex geometries that are difficult to machine, necessitating the use of investment casting. Numerical simulation has become increasingly popular in investment casting process development because it can predict defect formation and reduce development time and costs [1~3].

The accuracy of numerical simulation is directly affected by the precision of relevant simulation parameters, such as thermophysical properties of casting and mold, and the interfacial heat transfer coefficient between casting and mold. Generally, the former can be obtained with reasonable accuracy from literature or experimental measurements, while the latter is often estimated and frequently treated as a constant [1,2], raising questions about its reliability and accuracy.

Therefore, dedicated research on the interfacial heat transfer coefficient between titanium alloy castings and molds under investment casting conditions is particularly necessary.

Recent studies on casting/mold interfacial heat transfer coefficients have covered various processes including die casting [4~8], investment casting [9~15], squeeze casting [16~18], sand casting [19,20], and continuous casting [21,22], involving aluminum alloys, magnesium alloys, superalloys, and steel, with promising results. Guo et al. [4~7] conducted extensive research on interfacial heat transfer behavior in aluminum alloy die casting, establishing a comprehensive numerical model and analyzing the effects of casting thickness, die casting pressure, mold temperature, and measurement location on the interfacial heat transfer coefficient. Konrad et al. [11] investigated interfacial heat transfer behavior in investment casting of IN738LC superalloy, measuring the specific heat capacity and thermal diffusivity of ceramic shell, studying the influence of shell preheating temperature and thickness on grain size and secondary dendrite arm spacing, and inverse-calculating the variation of interfacial heat transfer coefficient with casting temperature during solidification under different process parameters. Sun et al. [16] studied interfacial heat transfer behavior between AM60 magnesium alloy and metallic mold in squeeze casting, comparing polynomial fitting methods with inverse algorithms, with results showing higher accuracy of the inverse algorithm. Xu et al. [19] investigated the interfacial heat transfer coefficient between ZL104 alloy and mold in sand casting, presenting its variation with time. Wang et al. [22] measured steel surface temperatures at different distances from the meniscus in continuous casting, inverse-calculated the interfacial heat transfer coefficient during continuous casting, and predicted solidified shell thickness at different locations, with predictions matching well with measured results.

Titanium alloys have high melting points and high chemical reactivity, typically requiring investment casting with ceramic molds in vacuum furnaces [23,24], which significantly increases experimental design and data processing difficulty. Currently, few studies have examined the casting/mold interfacial heat transfer coefficient in titanium alloy casting processes, limiting production assistance. Therefore, this work employs inverse heat conduction calculation to determine the casting/shell interfacial heat transfer coefficient for Ti6Al4V alloy investment casting, aiming to provide accurate parameters for numerical simulation.

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1. Mathematical Model

1.1 Physical Model of Casting/Mold Interfacial Heat Transfer

This work employs a plate-shaped casting with temperature measurement at the central region of the plate. Considering that the casting height and width are much greater than its thickness, the temperature field in the central region of the plate shell can be approximated as a one-dimensional temperature field varying with distance from the casting/shell interface, as shown in [Figure 1: see original paper].

In the shell, the temperature distribution T satisfies: [MATH_1]. In [Figure 1: see original paper] and equations (1)~(3), T represents temperature at different positions and times in the shell, x is the distance from the casting/shell interface, τ is time, q_1 is the interfacial heat flux between casting and shell, and q_2 is the heat flux across the shell outer surface.

1.2 Mathematical Model for Mold Temperature Distribution

In the simplified one-dimensional heat transfer model, the temperature distribution within the mold satisfies the following conditions: [MATH_2]. In equations (4)~(7), , c, and λ represent the density, specific heat capacity, and thermal conductivity of shell material, respectively; T_0 is the initial temperature of the shell.

Experimental measurements of ceramic shell thermophysical properties indicate that both c and λ vary only slightly with temperature. Ignoring temperature effects on shell thermophysical properties and treating c and λ as constants, equation (4) can be simplified to: [MATH_3].

Assuming $q_2 = 0$ and considering only the influence of q_1 on T, we have: [MATH_4]. The T in equation (9) satisfies conditions (6), (8), (10), and (11).

Assuming for a specific heat flux q*, T* is the solution satisfying (6), (8), (10), and (11). Decomposing q* into two heat fluxes q_1* and q_2*, and assuming T_1* and T_2* are solutions when q* equals q_1* and q_2* respectively, satisfying (6), (8), (10), and (11), let T* = T_1* + T_2*. Then T* satisfies (6), while (13) and (14) are identical to (10) and (11), meaning T* is the solution when q* satisfies (6), (8), (10), and (11). By solution uniqueness, T* = T_1* + T_2*, indicating the effect of q* on the temperature field is equivalent to the superposition of effects from q_1* and q_2*.

Similarly, treating q* as the superposition of M heat fluxes (M being any positive integer), if T * is the solution when q* = q *, satisfying (6), (8), (10), and (11), then: [MATH_5]. This demonstrates that if q* is treated as the superposition of M heat fluxes, these heat fluxes affect the temperature field independently, with the total effect being the simple superposition of individual effects. Likewise, for q_1, if treated as the superposition of several heat fluxes, their effects on the temperature field also superimpose simply, and the effect of q_1 on the shell temperature field is equivalent to the simple superposition of effects from q_1 and q_2 on the temperature field.

1.3 Solution Method for Interfacial Heat Transfer Coefficient

The interfacial heat transfer coefficient is calculated using the nonlinear estimation method proposed by Beck et al. [25]. The fundamental principle is: at time t*, the interfacial heat transfer coefficient has been calculated (known); assuming *h remains constant at value h* for the next N time steps Ndt, the temperature field evolution during these N steps is calculated based on previous h values, temperature field, and current h*. The objective function is: [MATH_6].

In equation (18), q represents radiative heat flux: [MATH_7], where σ and are effective emissivity and blackbody radiation constant; T_{bg} is background temperature (vacuum furnace inner wall temperature). Equation (19) represents the difference between calculated and measured temperature fields when h remains h* after t. *A smaller f indicates the estimated h* is closer to reality. Therefore, the calculation aims to minimize f, and the h* at minimum f is the sought interfacial heat transfer coefficient at t*.

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2. Experimental Design

This work employed two symmetric plate-shaped castings to obtain more experimental data. The model and thermocouple arrangement are shown in [Figure 2: see original paper]. The plate dimensions were 170 mm × 170 mm × 25 mm. Different thermocouples were embedded in the casting or shell. Casting thermocouples, numbered TC_{casting} 1, 2, 3, and 4 from top to bottom, were located in the riser, plate center, ingate, and sprue, respectively. TC_{casting} 1, 2, and 4 used tungsten-rhenium thermocouples for casting temperature measurement, while TC_{casting} 3 was a K-type thermocouple for measuring metal arrival time. Shell thermocouples at the same horizontal level with 10 mm lateral spacing were placed near the plate center, with distances from the casting/shell interface of 3, 6, and 9 mm, numbered TC_{mold} 1, 2, and 3 (K-type). Due to symmetric casting geometry, identical thermocouples placed on the opposite side allowed obtaining two datasets from one pour.

Shell material thermophysical properties were measured experimentally. The specific heat capacity variation with temperature is shown in [Figure 3: see original paper], with an abrupt increase around 900 °C related to mullitization of kaolin components. Thermal conductivity was minimally temperature-dependent, remaining around 1.4 W/(m·K), and density was 2170 kg/m^3.

The Ti6Al4V alloy nominal composition (mass fraction) was Al 6%, V 4%, balance Ti. Its specific heat capacity and thermal conductivity variations with temperature are shown in [Figure 4: see original paper]. The abrupt changes in Ti6Al4V specific heat capacity and thermal conductivity at 1620~1650 °C correspond to melting/solidification, while those at 980~1000 °C correspond to solid-state phase transformation.

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3. Results and Discussion

3.1 Experimental Temperature Measurement and Inverse Calculation Results

[Figure 5: see original paper] shows measured temperatures from thermocouples on one side. Based on multiple measurements, unprotected thermocouples reached ~1700 °C within seconds after pouring, while protected ones heated slower, maintaining ~1570 °C for extended periods. The Ti6Al4V alloy two-phase region is 1620~1650 °C; using the median 1635 °C, the temperature measured by thermocouple 2 was estimated ~4% lower than actual. Shell thermocouples, sintered with the shell, had good contact, so measured temperatures were considered actual shell temperatures.

[Figure 6: see original paper] shows the h-t relationship inverse-calculated from TC_{casting} 2 and TC_{mold} 1~3 temperatures, with an inset detailing 0~200 s.

3.2 Error Analysis and Correction

3.2.1 Effects of Shell Material Specific Heat, Thermal Diffusivity, and Thermocouple Positioning In a one-dimensional heat transfer model, if the h variation is known, casting/mold thermophysical parameters are accurate, initial conditions are known, and thermocouple positions are exact with error-free temperature measurements, then temperature evolution at each thermocouple can be obtained through simulation. Using these simulated temperatures with accurate parameters and positions, h can be precisely inverse-calculated. However, actual shell thermophysical parameters and thermocouple positions are not always accurate, and O' Mahoney et al. [9] noted these errors significantly affect inverse calculation results, necessitating error assessment and minimization.

[Figure 7: see original paper]~[Figure 9: see original paper] show relationships between calculated h and preset h when shell material c, thermal diffusivity a, and actual thermocouple positions deviate from intended positions, plus temperature comparisons under conditions A, C, and E. Conditions A~F are: assumed c 20% low/high, assumed a 20% low/high, and actual thermocouple positions at 2.5, 5.5, 8.5 mm and 3.5, 6.5, 9.5 mm.

Comparison of [Figure 7: see original paper]~[Figure 9: see original paper] reveals distinct error characteristics: c error significantly affects casting temperature and temperature differences among shell points, causing large h calculation errors; a error has minimal effect on casting temperature but noticeably affects shell point temperature differences, with limited impact on h calculation accuracy; thermocouple positioning error affects casting temperature and h calculation accuracy primarily within ~50 s after pouring, with subsequent effects inherited from this initial period, while having negligible effect on temperature differences within the shell.

3.2.2 Error Assessment and Correction Based on measured shell material specific heat capacity and thermal conductivity, c was considered [MATH_8] J/(kg·K), $\lambda = 1.4$ W/(m·K), a = 5.0$×10^{-7}$ m^2/s. The average shell thickness was ~18 mm, the effective minimum distance between thermocouples and interface was 3.5 mm, and pouring temperature was ~1720 °C (considering Ti6Al4V alloy contact with mold in gating system before entering cavity and slow gravity pouring, the average temperature after entering cavity was considered ~1680 °C).

[Figure 10: see original paper] compares calculated and measured temperatures at thermocouples during 0~750 s h inverse calculation. The simulated maximum shell temperature was ~840 °C, suggesting minimal mullitization effect. Using original shell thermophysical parameters, calculated temperature differences among shell thermocouples were significantly smaller than measured differences, and casting temperature decrease rate was lower than actual. From previous assessment, the assumed shell a was higher than actual while c was lower. Additionally, the simulated time for casting temperature to begin decreasing was earlier than actual, indicating the minimum effective distance from thermocouples to interface was smaller than actual.

Addressing these issues, c was appropriately increased, a decreased, and the effective thermocouple-to-interface distance was fine-tuned to ensure inverse-calculated casting temperatures matched measurements and shell temperature differences matched measured differences. After multiple adjustments, when c = [MATH_9] J/(kg·K), a = 4.09$×10^{-7}$ m^2/s, and minimum effective thermocouple-to-interface distance was 3.6 mm, inverse-calculated casting and shell temperatures matched well with measurements. [Figure 11: see original paper] shows the corrected h and temperatures.

[Figure 11: see original paper] demonstrates good agreement between calculated and measured casting/shell temperatures after correcting shell thermophysical parameters and thermocouple positions. The inverse-calculated h shows dramatic changes within ~20 s after pouring, rising from 0 to ~440 W/(m^2·K) then quickly dropping to ~184 W/(m^2·K), corresponding to initial metal-mold contact and surface shell formation. Subsequently, h slowly decreased to ~110 W/(m^2·K) as solidification progressed. During this stage, contact conditions deteriorated with increasing shell thickness and casting contraction, with h decreasing by ~20% of its peak value. After complete solidification, h decreased with casting cooling at a slower rate than previous stages.

3.3 Relationship Between Interfacial Heat Transfer Coefficient and Casting State

3.3.1 h vs. Solidified Layer Thickness and Temperature As described above, after pouring the casting state progresses through: fully liquid, surface shell formation, increasing shell thickness, and complete solidification. Inverse calculation yields not only h variation with time but also casting internal temperature and solid fraction distribution. Before complete solidification, treating the region below Ti6Al4V liquidus temperature as solidified layer yields the solidified layer thickness δ variation with time.

Based on h and δ variations, their relationship is obtained, shown in [Figure 12: see original paper]. [Figure 12: see original paper] indicates h remains near its peak before solidified layer formation, but drops sharply once formed. When δ 0.8 mm, h decreases to ~184 $W/(m^2 \cdot K)$, then slowly decreases with increasing δ. When δ reaches 11 mm, h differs little from the fully solidified value.

Therefore, for simplicity, the relationship between h and solid fraction before complete solidification can be divided into three stages: [MATH_{10}], where Stage 1: metal is liquid with minor h fluctuations; Stage 2: shell forms on metal surface with mushy zone advancing inward—h decreases sharply by nearly 60% as complete shell forms and contact changes; Stage 3: complete surface shell forms with fixed contact condition—h decreases slowly by ~20% of peak value. Afterward, the casting is essentially solid and cools rapidly, with h depending mainly on interface temperatures and emissivity.

After solidification, based on h and casting surface temperature T variations, their relationship is obtained, shown in [Figure 13: see original paper]. [Figure 13: see original paper] shows that after solidification, h decreases with casting temperature, with minor fluctuations. The relationship can be simplified as: [MATH_{11}].

3.3.2 Validation of Interfacial Heat Transfer Coefficient Substituting equations (20) and (21) into the three-dimensional model shown in [Figure 2: see original paper], where h at each casting surface location is determined by local solidification state or surface temperature, with other thermophysical parameters identical to the 1D inverse model, yields temperature variations at three thermocouple locations in casting and mold. Comparing these calculated temperatures with measured values produces [Figure 14: see original paper].

[Figure 14: see original paper] shows calculated shell and casting temperatures based on inverse-calculated h match measured temperatures well, confirming good accuracy of the obtained h and validating the selected parameters. Some discrepancies remain, attributed to: (1) non-ideal 1D casting-mold system causing systematic errors; (2) imprecise shell/mold geometry and thermocouple effects on temperature field; (3) deviations in experimental parameters including thermophysical properties and thermocouple positions.

Conclusions

1. A one-dimensional heat transfer mathematical model for investment casting casting/shell heat transfer was established. The relationship between

mold internal temperature field and mold inner surface heat flux was discussed under constant thermal conductivity and specific heat capacity, mathematically analyzing the different effects of specific heat capacity, thermal diffusivity, thermocouple positioning, and temperature measurement errors on interfacial heat flux and interfacial heat transfer coefficient inverse calculation.

2. From numerical simulation perspective, the effects of specific heat capacity, thermal diffusivity, and thermocouple positioning errors on temperatures at various casting and mold locations were evaluated, and corrections were made based on preliminary inverse calculation results.
3. An accurate interfacial heat transfer coefficient was obtained, and its relationship with casting state (solidified layer thickness, temperature) was analyzed. Analysis shows: during solidified layer formation, h drops sharply by ~60%; during layer growth, h decreases slowly by ~20% of peak value; after solidification, h decreases with casting temperature at a much slower rate than previous stages.
4. This relationship was validated in a three-dimensional casting/mold model. Results demonstrate that corrected parameters are accurate and the inverse-calculated h relationship with casting state is reliable.

References

[1] Liu J, Yang Y, Lu D. Foundry, 2008; 57: 1155

[2] Atwood R C, Lee P D, Curtis R V, Maijer D M. Dent Mater, 2007; 23(1): 60

[3] Liang Z J, Xu Q Y, Li J T, Li S Q, Zhang J, Liu B C, Zhong Z Y. Rare Met Mater Eng, 2003; 32: 164

[4] Guo Z P, Xiong S M, Cho S H, Choi J K. Acta Metall Sin, 2007; 43: 1149

[5] Guo Z P, Xiong S M, Cho S H, Choi J K. Acta Metall Sin, 2007; 43: 1155

[6] Cao Y Y, Guo Z P, Xiong S M. China Foundry, 2014; 11: 314

[7] Guo Z P, Xiong S M, Liu B C, Mei L, Allison J. Int J Heat Mass Transfer, 2008; 51: 6032

[8] Long A, Thornhill D, Armstrong C, Watson D. Appl Therm Eng, 2011; 31: 3996

[9] O’ Mahoney D, Browne D J. Exp Therm Fluid Sci, 2000; 22: 111

[10] Yuan S, Bu K, Dong Y W. Foundry Technol, 2012; 33: 177

[11] Konrad C H, Brunner M, Kyrgyzbaev K, Völkl R, Glatzel U. J Mater Process Technol, 2011; 211: 181

[12] Zhang W H, Xie G N, Zhang D. Exp Therm Fluid Sci, 2010; 34:

[13] Dong Y W, Bu K, Dou Y Q, Zhang D H. J Mater Process Technol, 2011; 211: 2123

[14] Rafique M M A, Iqbal J. Int J Heat Mass Transfer, 2009; 52: 2132

[15] Jin H P, Li J R, Yu J, Liu S Z. Rare Met Mater Eng, 2010; 39: 767

[16] Sun Z Z, Hu H, Niu X P. J Mater Process Technol, 2011; 211:

[17] Ilkhchy A F, Jabbari M, Davami P. Int Commun Heat Mass Transfer, 2012; 39: 705
[18] Aweda J O, Adeyemi M B. J Mater Process Technol, 2009; 209:
[19] Xu H, Hou H, Zhao Y H, Chen Z. Chin J Nonferrous Met, 2003; 13: 881
[20] Palumbo G, Piglionico V, Piccininni A, Guglielmi P, Sorgente D, Tricarico L. Appl Therm Eng, 2015; 78: 682
[21] Chen L P, Wang Y X, Peng L M, Fu P H, Jiang H Y. Exp Therm Fluid Sci, 2014; 54: 196
[22] Wang Z F, Yao M, Wang X D, Zhang X B, Yang L S, Lu H Z, Wang X. J Mater Process Technol, 2014; 214: 44
[23] Watanabe K, Miyakawa O, Takada Y, Okuno O, Okabe T. Biomaterials, 2003; 24: 1737
[24] Liang Z J, Xu Q Y, Li J T, Li S Q, Zhang J, Liu B C, Zhong Z Y. Rare Met Mater Eng, 2002; 31: 353
[25] Beck J V, Blackwell B, St Clair C R. Inverse Heat Conduction: Ill-Posed Problems. New York: Wiley, 1985: 145

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