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Validating the Thermal Stress Evolution Model

Gandharv Kashinath and Melissa Carter
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Flow Science, Inc.

I. Introduction

Thermal stresses develop during the solidification of a casting due to non-uniform cooling of the casting part. These stresses are driven by thermal gradients, expansion and contraction of metal and its interaction with the mold. Engineers are interested in studying thermally induced stresses and the resulting deformations to gain insights in to the integrity of the part. The Thermal Stress Evolution (TSE) model in ***FLOW-3D*** is one such tool that allows casting engineers to study this phenomenon.

In this paper, the stresses predicted by the TSE model are validated with experimental results. Several key aspects of the modeling process are discussed to demonstrate the capabilities while also accounting for the limitations of the model.

II. Experiment Setup

Pokorny *et al.* studied stresses developed during cooling of a binary Magnesium-Aluminum alloy and compared simulations results with measurements from experiments. In the current study, stresses measured for Mg-9 wt. pct. Al alloy without hot tear published by Pokorny et al (1) were compared to the stresses obtained using ***FLOW-3D***.

In the reference paper, measurements from specially designed experiments were extracted for the evolution of temperature and contraction forces during solidification and cooling of a restrained rod-shaped casting in a steel mold. These experiments were carried out for several initial mold temperatures. For this study, results for the mold temperature of T_{mold} = 773K (500°C) were used for comparisons. The absence of hot tear made this an ideal candidate for evaluation of the TSE model in ***FLOW-3D***.

Hot tearing is not modeled in ***FLOW-3D*** due to the lack of a fracture model for the mush during the solidification phase. This is also true for the simulation results presented in the reference paper and consequently the stresses were over-predicted compared to the experimental measurements. The coupling of the stress model with the feeding flow and macrosegregation calculations is also important in accurately predicting stresses in the presence of hot tear (1).

Figure 1 shows a schematic of the experimental test setup. Detailed description of the dimensions and measurement procedures can be found in the reference paper (1). The casting consists of a long horizontal rod with a vertical sprue on one end through which the molten metal is poured. The horizontal rod tapers from the sprue-rod junction to the tip where a steel rod is inserted into the casting which is connected to a load sensor. The load sensor measures the contraction force on the horizontal rod. In order to view the measured experimental forces in terms of stresses, the forces were divided by the cross-section area of the rod at the sprue-rod junction. The thermal contraction of the rod is constrained on one end by the sprue and the other end by the rigid steel rod. TC1 is a thermocouple placed inside the casting at the sprue-rod junction.

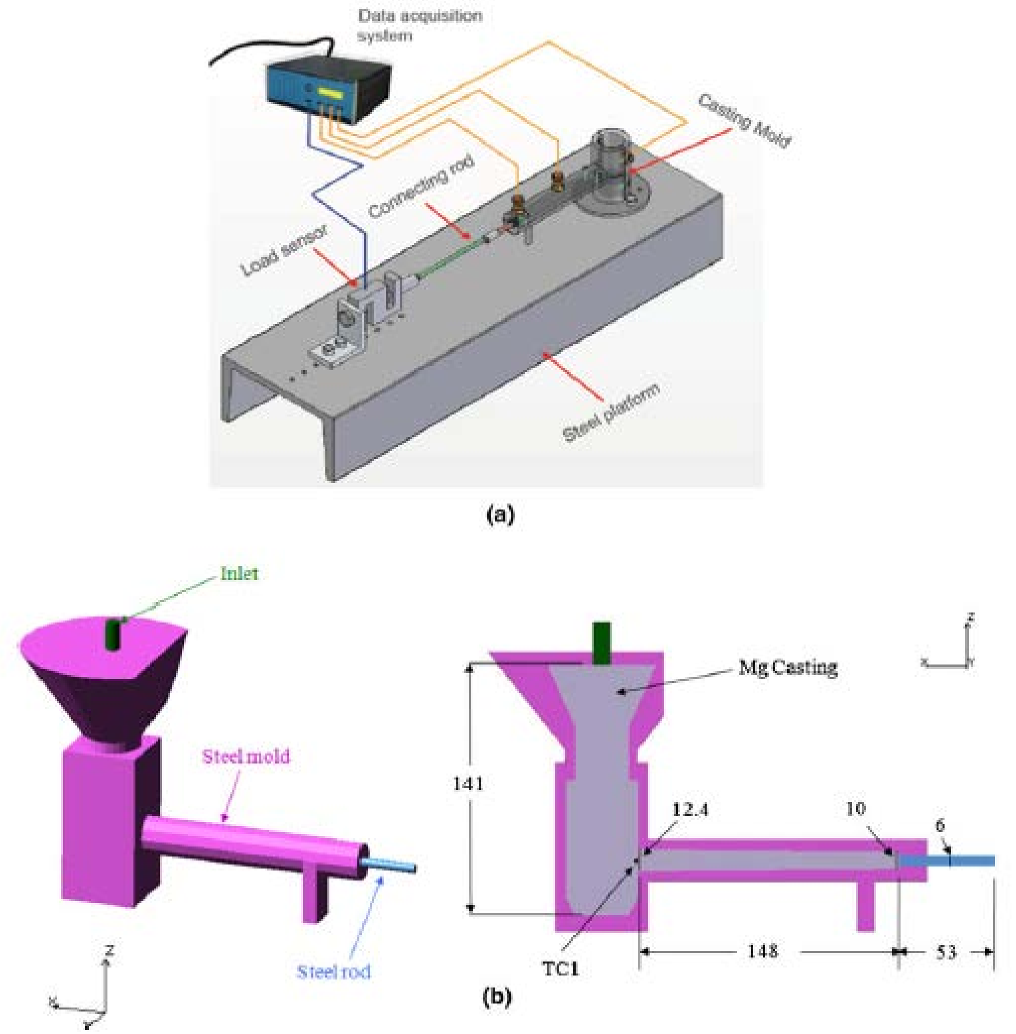


Figure 1: Experimental test setup: a) overall view and b) geometry of the casting and the mold as used in the simulations (all dimensions are in millimeters).

III. Thermal Simulation Properties for *FLOW-3D*

The necessary thermophysical properties, such as thermal conductivity, viscosity, density and specific heat, were obtained as a function of temperature from JMatPro (2). The liquidus temperature and the eutectic temperature for the Mg-9 wt. pct. Al alloy was 877K and 710K, respectively. As mentioned in the reference paper, the interfacial heat transfer (IHTC) coefficient between the mold and the metal as a function of temperature is a critical parameter in obtaining the correct cooling curve which in turn defines the stress evolution in the solidified metal, as discussed in section V below.

In the reference paper, the IHTC variation was determined by a trial-and-error process where IHTC was varied until good agreement between the simulation and measured temperatures at the spruce-rod junction was obtained. This specified IHTC variation is unclear due to the ad-hoc "cubic function" reference in the definition. Hence an “optimization” like algorithm was used in this study to replicate the trial-and-error process to obtain a suitable IHTC variation for ***FLOW-3D***. The “optimization” algorithm entailed constructing a suite of simulations where the value of IHTC was adjusted until the error between the experimental and simulation temperature curve was sufficiently reduced. This procedure was automated using a basic minimization approach in Python (3). An initial guess matching the values suggested in the paper was used to start the optimization program. Results from this IHTC variation study and its impact on the stress results are discussed in section V.

IV. Thermal Stress Evolution (TSE) Model in *FLOW-3D*

The TSE model in ***FLOW-3D*** uses the finite-element method to simulate stresses and deformations within solidified fluid regions. ***FLOW-3D*** employs a fully coupled solid dynamics and fluid flow solver to model TSE. A detailed discussion of the governing equations and the discretizations can be found in the Theory section of the ***FLOW-3D*** manual (4).

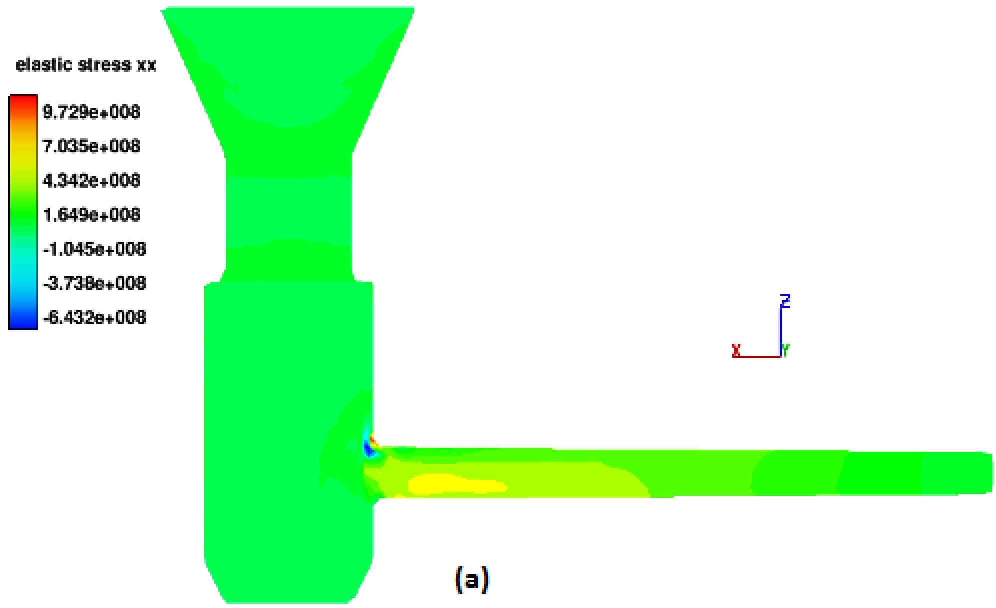
Unlike in the reference paper, where the thermal and stress simulations were performed sequentially, in ***FLOW-3D*** the stress calculations were coupled with thermal calculations. The TSE model in ***FLOW-3D*** provides several controls to realistically model the stresses in the solidified fluid region. One such control is the activation of the stress calculation (FSTSE) based on the local solid fraction. In accordance with the reference paper, the stress calculations were initiated when the solid fraction reached the critical value of FSCR = FSTSE = 0.84. The coherency point was set at FSCO = 0.5 (1).

The mechanical properties like the Young’s modulus, yield stress as a function of temperature and Poisson ratio required for the stress calculations were extracted from the data provided in the reference paper. It must be noted that most of these properties are from other sources except for the yield stress which was obtained iteratively until a good match of the measured stresses was achieved (1). For this study, the yield stress curve reported in the reference paper, σ_0 was extracted and used without any modifications. This is a potential parameter that can be tuned to further improve the results as discussed in section V.

The measurements were conducted until the temperature in the thermocouple at the sprue-rod junction reached 573K (300°C). This was replicated in the ***FLOW-3D*** simulations by defining a probe at the sprue-rod junction and then using the Active Simulation Control feature in ***FLOW-3D*** to terminate the simulation when the temperature of 573K was reached at the probe.

V. Results & Discussions

FLOW-3D results for stress, strain and displacements for the case of Mg-9 wt. pct. Al at T_{mold}=773K (500°C) are shown in Figure 2, at the time when the probe temperature at sprue-rod junction reached 573K (300°C). The results are comparable to those presented in the reference paper, where the high stresses are mostly confined to the rod section of the casting. The forces are tensile in nature (positive), relatively uniform and in the direction along the rod axis. Negative, compressive stresses are present near the upper corner of the sprue-rod junction where the metal is pressed against the mold.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7.035e+008
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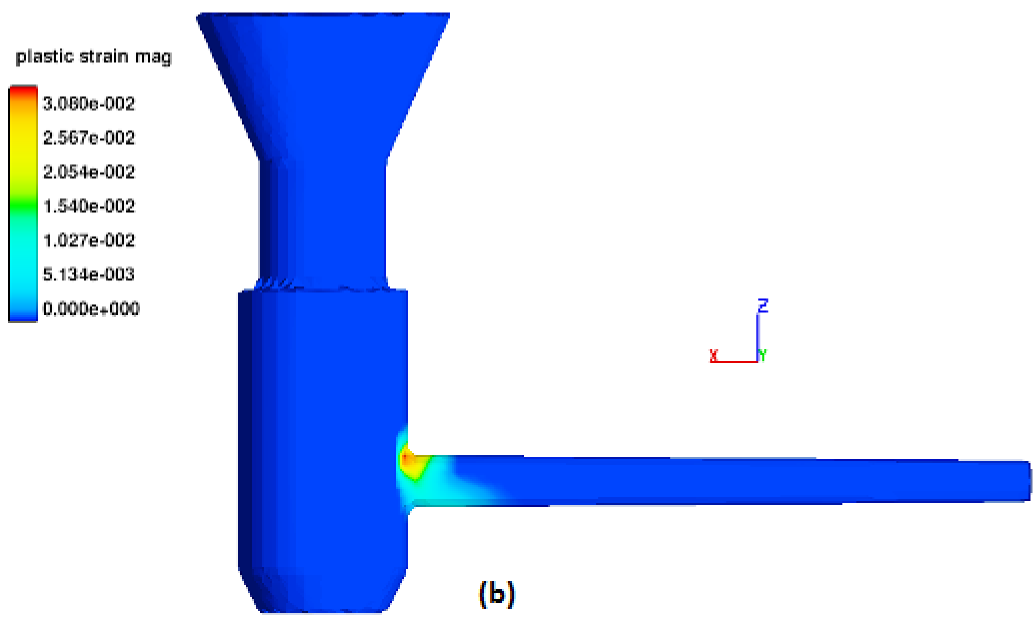
Z
X
Y

(a)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2.567e-002
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Z
X
Y

(b)

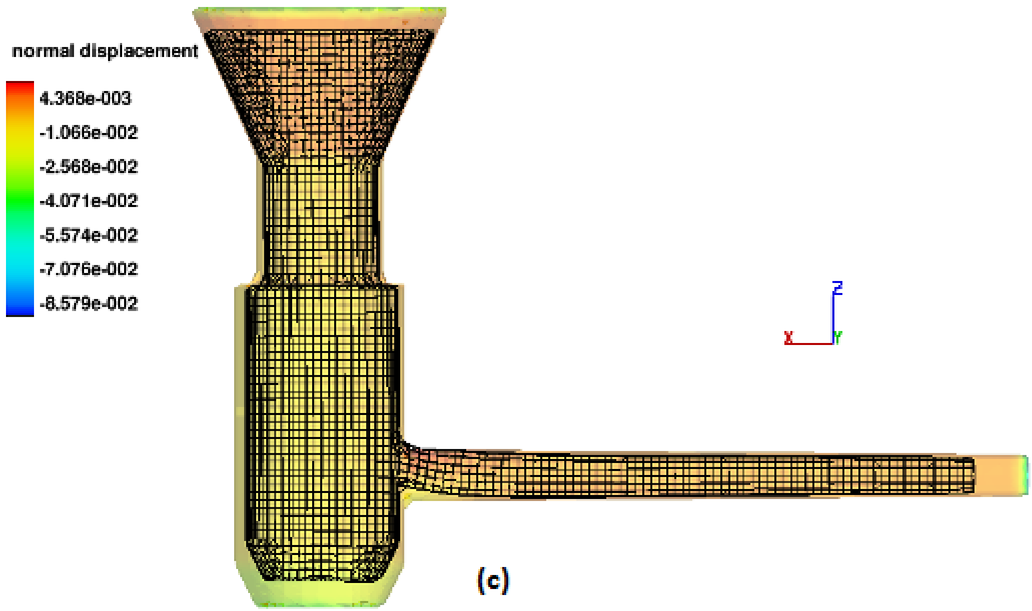

Figure 2: Predicted stress, strain and normal displacement at the end of solidification the Mg-9 wt. pct. Al, T_{mold} = 773K (500°C): a) x-direction stress, b) plastic effective strain, and c) normal displacement (magnified 20 times).

The calculated stress is influenced by the cooling curve. The cooling curve is dictated by the interfacial heat transfer (IHTC) coefficient between the mold and the metal (HOBS1 in ***FLOW-3D***). The following plot shows the final IHTC variation with temperature obtained using the automated "optimization" algorithm. The initial guesses for this algorithm marked in red were obtained from the values prescribed in the reference paper. Effects of varying the IHTC value are studied further at the end of this section.

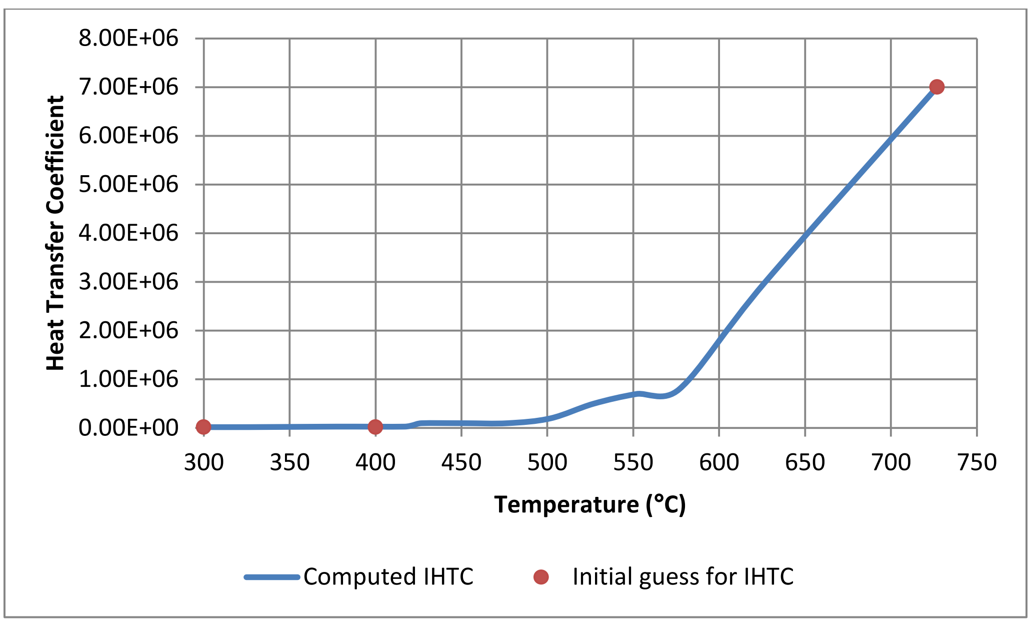

Figure 3: Computed interfacial heat transfer coefficient (IHTC) used for the *FLOW-3D* simulation.

The resulting cooling curve is compared to the experiment in Figure 4. T_{sol} is the temperature at which the sprue-rod junction completely solidifies and $T_{cut\text{-}off}$ is when the sprue-rod junction reaches 300°C.

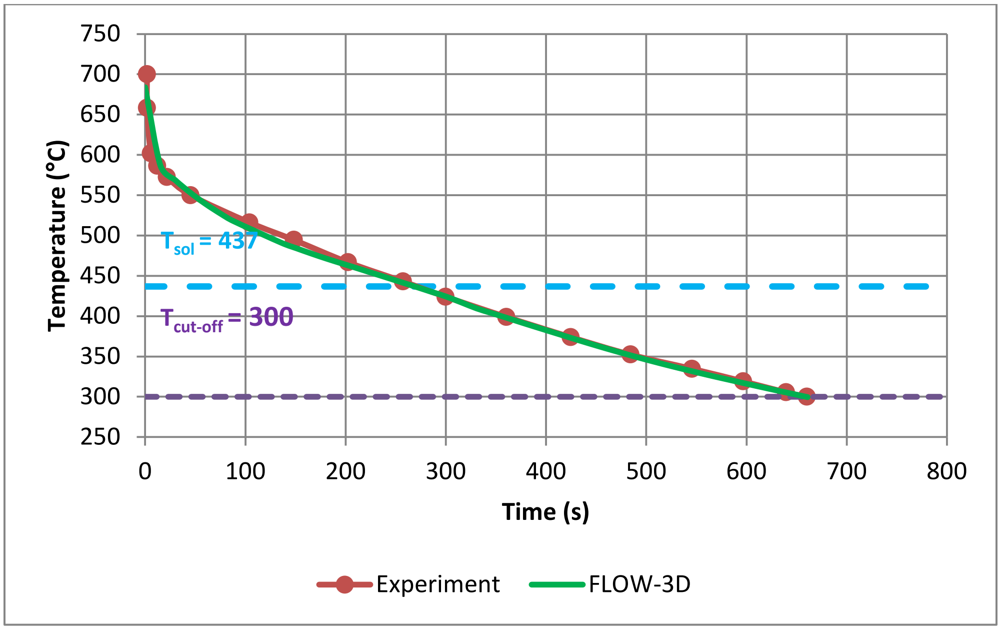

Figure 4: Evolution of temperature at the sprue-rod junction.

The reference paper specifies that the total stress at the sprue-rod junction was computed by averaging the stresses in the elements that constitute the junction. In order to compare ***FLOW-3D*** results with the reference experiment, a similar approach was designed to output the average stress at the sprue-rod junction. Presented below is a comparison of the ***FLOW-3D*** output with the results from experiment.

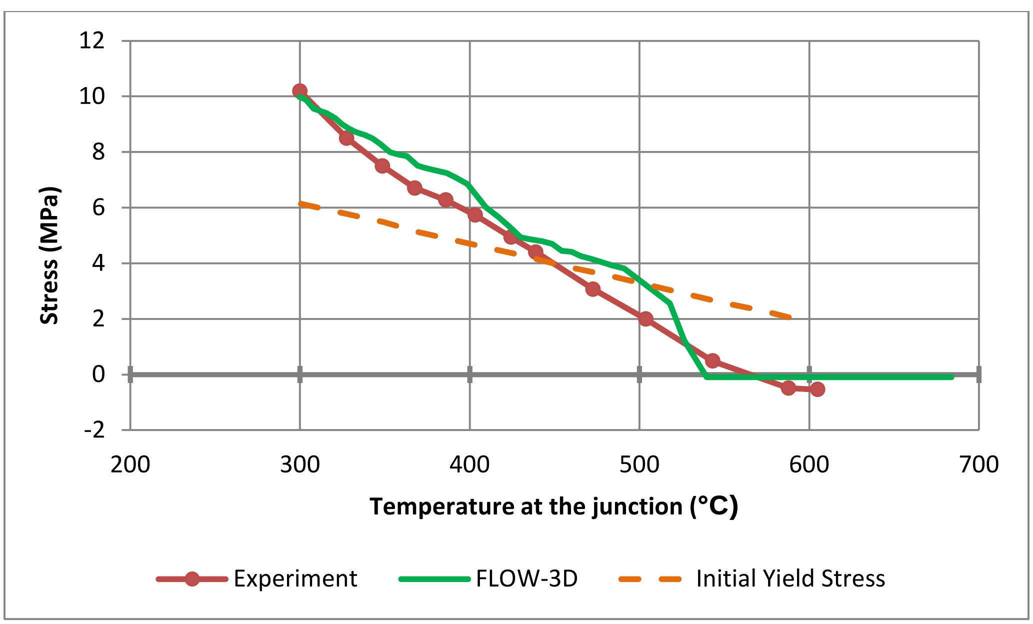

Figure 5: Average stress at the sprue-rod junction.

The experiment is in good agreement over the entire temperature range. The maximum stress at the junction reported as 10 MPa matches well the experiment at 573K (300°C). The maximum differences occur between 425°C and 525°C. This could be attributed to the transition from the mushy to fully solidified state and to the uncertainties in the behavior of the yield stress in this temperature range. The yield stress relieves the stresses through plastic deformations. The error between the experiment and the simulation could be further reduced by tuning the initial yield stress, σ_0. Figure 6 shows improvements in the predicted stress values going from a constant yield stress value to the yield stress as a function of temperature taken from the reference paper. This indicates that having a high quality time-dependent yield stress is important in getting accurate results.

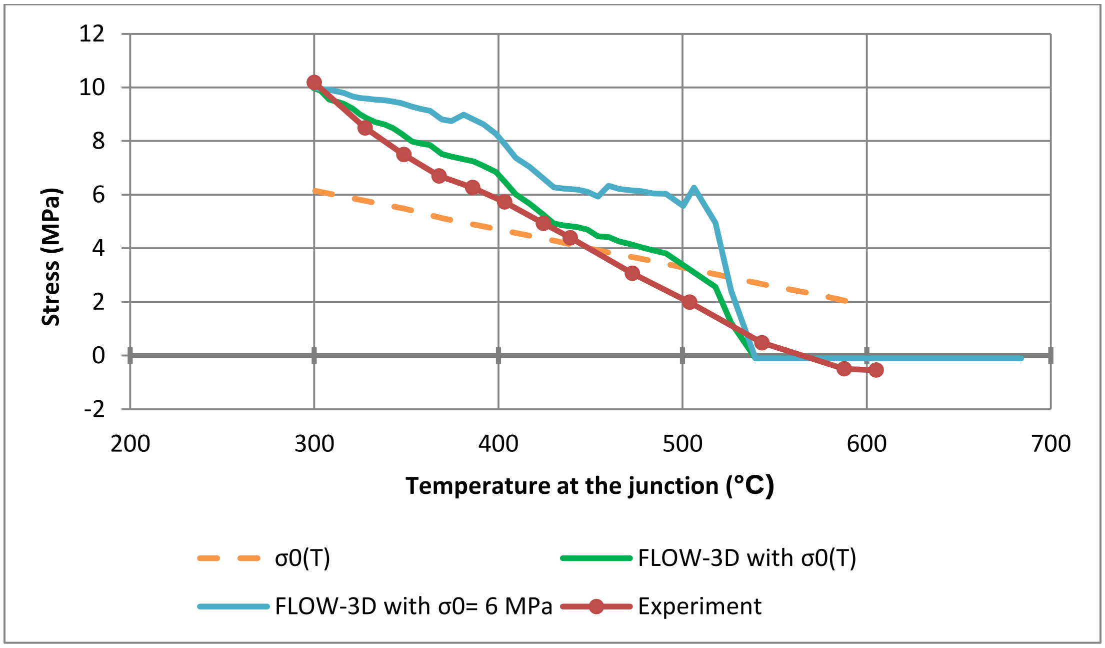

Figure 6: Stress evolution at the sprue-rod junction with varying initial yield stress, σ_0.

As mentioned previously the interfacial heat transfer coefficient is another important parameter that affects the stress results. Presented below is a plot showing the variation in the stress values at the sprue-rod junction with varying IHTC. Specifically, results from a constant IHTC = 7000 W/m^2 K are compared to IHTC (T) as a function of temperature from the reference paper. The constant IHTC results in a steeper cooling curve which results in an earlier onset of stresses at the sprue-rod junction. This can be seen in Figure 7 where the stresses begin to develop at 544°C unlike in the IHTC (T) case where it begins at 526°C. For both cases the yield stress was varied with temperature according to the reference paper.

Although the general trend in the stress evolution is similar, the maximum stress developed at the end of the simulation is only 7.76 MPa for constant IHTC as opposed to 10 MPa from the experiment and the IHTC (T) case. This can be attributed to the yield stress function used from the reference paper. Due to the rapid decrease in temperature, the yield stress function needs to be accurately defined to obtain the desired 10 MPa.

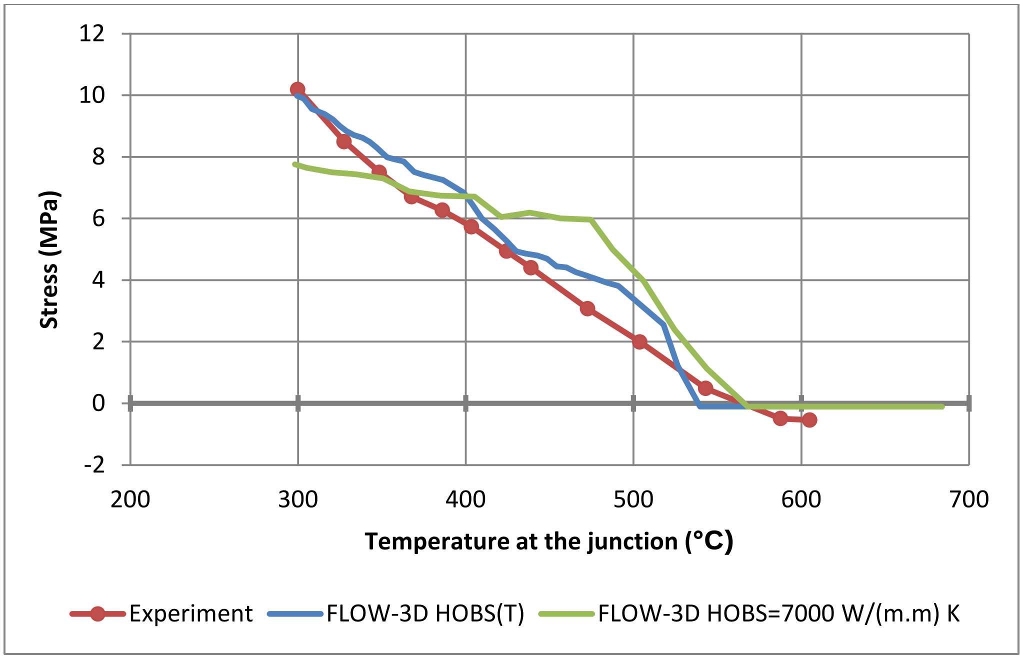

Figure 7: Stress evolution at the sprue-rod junction with varying interfacial heat transfer coefficient, IHTC.

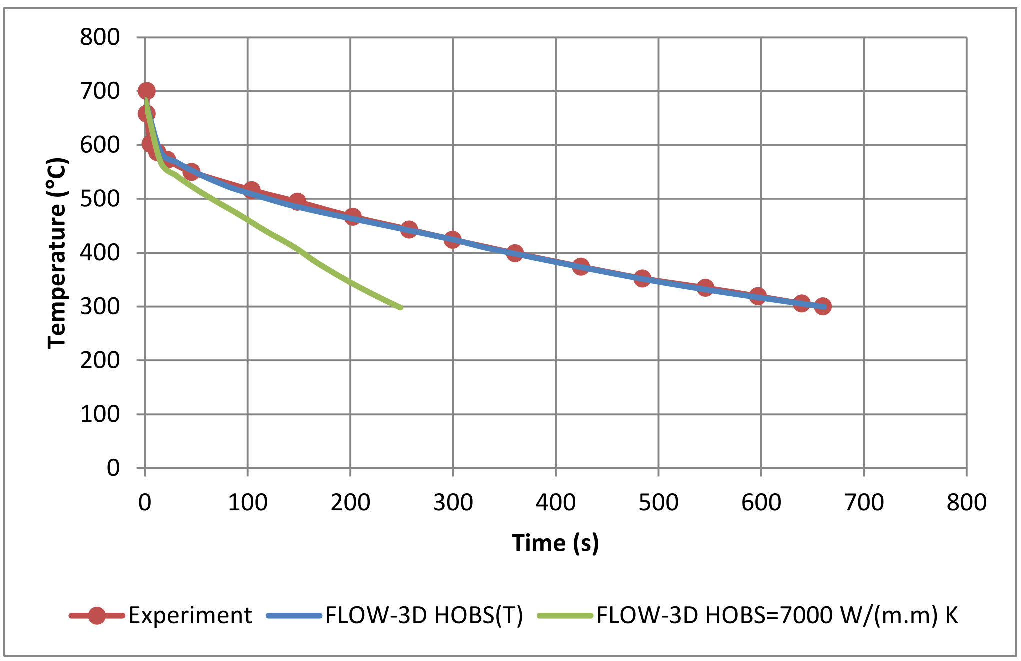

Figure 8: Evolution of temperature at the sprue-rod junction with constant and varying interfacial heat transfer coefficient, IHTC.

VI. Conclusions

In this paper, the Thermal Stress Evolution (TSE) model in ***FLOW-3D*** was successfully validated with experimental results for Mg-9 wt. pct. Al alloy casting. The stress value computed at the sprue-rod junction during the solidification and cooling of the casting part compared well with the experimental data. The results were sensitive to the definition yield stress and interfacial heat transfer coefficient as functions of temperature. Hence it is critical to provide accurate data for these two parameters to obtain high quality results. The experimental results published also provide data for hot tearing and strain hardening. Future development efforts for the TSE model should be directed towards including these two aspects of the solidification process.

VII. References

1. *Simulation of Stresses during Casting of Binary Magnesium-Aluminum Alloys.* **Pokorny, M.G., et al., et al.** 2010, The Minerals, Metals & Materials Society and ASM Internatonal.

2. **Sente Software Ltd.** *JMatPro v4.0.* Surrey, United Kingdon : Sente Software Ltd.

3. **The SciPy Community.** *Optimization and root finding (scipy.optimize).* 2008-2014. http://docs.scipy.org/doc/scipy/reference/optimize.html#module-scipy.optimize.

4. **Flow Science Inc.** FLOW-3D v11.1.0 User Manual. Santa Fe, NM, USA : s.n., 2015.