61.0 CASTING MODELING AND QUALITY OF METALLIC ALLOYS

Nadira Surghani (Mines)
Faculty: Amy Clarke and Kester Clarke (Mines)
Industrial Mentor: Joe McKeown (LLNL)

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61.1 Project Overview and Industrial Relevance

US casting research programs aim to improve part quality, decrease rejection rate, and cut manufacturing costs to stay competitive in the global economy. Modeling is integral to casting research as it can be useful in improving mold designs and reducing product cycle time and cost [61.1]. There is a particular focus on modeling castings of high-density metallic alloys used for nuclear energy and defense applications. Casting modeling replaces trail-and-error experiments and minimizes nuclear waste, which is a vital consideration when working with nuclear materials. Lawrence Livermore National Laboratory (LLNL) has a need for process modeling at the part scale to support casting programs. Computer modeling programs using finite element analysis (FEA) lead the way in three-dimensional modeling of industrial mold filling and solidification problems. These programs couple convective fluid flow and heat transfer during mold filling to calculate the temperature gradient in the casting [61.2]. Accurately modeling thermal gradients can predict solidification behavior and determine the expected quality and microstructure of the final cast part. Ultimately, model predictions can inform future mold designs and casting processes to optimize manufacturing. Additionally, casting modeling is critical skill that is currently lacking across the U.S. DOE Complex. This project aims to address these needs though university collaboration, by developing a future work force with background and experience in casting modeling.

This project will use FLOW-3D®, a computational fluid dynamics (CFD) software, to develop a hemispherical uranium casting model of interest to LLNL. The casting predictions will be compared to publicly available instrumented casting data [61.3]. FLOW-3D® will be used to model other mold geometries, such as cylinders, and processing variations on other high-density metals, such as Sn-Pb alloys, to validate parameters and investigate solidification behavior. These models will be compared to other industrially relevant casting FEA modeling software, such as ProCAST®, to determine the advantages of each software/approach for modeling key attributes of nuclear part castings. Finally, small-scale casting experiments of high-density metallic surrogate materials, such as Sn-Pb alloys, will be pursued to compare model predictions to experimental outcomes.

61.2 Previous Work

61.2.1 Instrumented Uranium Hemispherical Casting

Using a multi-coil three-zone vacuum induction melting (VIM) furnace, an instrumented uranium casting experiment was conducted at Los Alamos National Laboratory (LANL) [61.3]. The casting is a hemisphere with an inner radius of 75 mm and wall thickness of 10 mm with a cylindrical sprue. The cast part is featured in **Figure 61.1**. The mold was an yttrium-oxide (yttria) coated 2020 grade graphite mold with 3 parts: a funnel, an outer mold case, and an inner mold core. The mold stack is presented in **Figure 61.2**. The mold stack was placed on a 2020 graphite base and pedestal to facilitate slow heating due to the large thermal mass. 2020 graphite is a fine-grained isostatically molded graphite commonly used for nuclear applications such as uranium castings and high-temperature gas-cooled reactor (HTGR) components [61.4]. The bottom-pour type 2020 graphite crucible was charged with 9200 g of 8 mm thick rolled depleted uranium (DU) strips which were cleaned of oxides. The instrumentation included the following: 15 interface contact probes, 3 thermocouples in the insulation skirt, 7 type-K thermocouples in the casting cavity, and 22 type-C thermocouples embedded in the mold. The positions of thermocouples and contact pins are provided in **Figure 61.2**. These thermocouples collected an extensive thermal history of the mold heating, mold filling, metal solidification, and mold cooling. Thermal data was used to calculate the mold-metal interfacial heat transfer coefficient as a function of time. Following casting, the part was sectioned for metallography and chemical analysis.

61.3 Recent Progress

61.3.1 Uranium and Graphite Thermophysical Property Databases

To model a uranium casting, a thermophysical database of uranium was needed. The FLOW-3D® metals database did not include uranium, therefore properties had to be sourced from literature. The temperature dependent properties required to run FLOW-3D® simulations include density, specific heat, thermal conductivity, surface tension coefficient, and viscosity. The temperature dependent properties are plotted in **Figure 61.3**. Additional required thermophysical properties include thermal expansion coefficient, latent heat of vaporization, liquidus temperature, solidus temperature, and latent heat of fusion; these are listed in **Table 61.1**. Some properties had to be approximated due to limited data, and such approximations are based on values of other materials readily available in the database and are subject to change in future iterations of the model. Solidification drag coefficient was set to 100 s^{-1} based on FLOW-3D® materials but can be up to 250 s^{-1} for gravity die castings [61.5]. Fraction of solid at coherency point and critical fraction of solid was set to 0.15 and 0.67, respectively. These approximations were set based on the readily available data for aluminum alloy A201. It is common practice to source these values from the pre-existing values in the database [61.6]. These approximated values were tested at minimum and maximum values to determine its effect on the overall simulation. Altering these values saw little to no effect. Although, it should be noted that any approximated values should be rigorously tested throughout iterations of the model to maintain minimal effect on the overall simulation.

The solids database did not include 2020 graphite to simulate the mold, and therefore properties had to be sourced from literature. The temperature dependent properties required for the mold include density*specific heat and thermal conductivity. Literature values provided radial and axial values of thermal conductivity; therefore, the average was utilized in the model. To calculate density*specific heat, a density of 1780 kg/m^3 was used [61.4]. The thermophysical properties of 2020 graphite used to run the model are depicted graphically in **Figure 61.4**.

61.3.2 Cylindrical Uranium Model

To test the thermophysical properties and better understand model set-up in the software, a simplified cylindrical geometry was modeled. Results from the cylindrical model were compared to a uranium casting in a graphite rod mold (casting number: 16C-791,792,795) conducted by LANL [61.6]. In this casting, thermal data for mold heating and filling was collected with 5 thermocouples placed in the mold cavity. **Figure 61.5** shows the rod mold with thermocouple locations. Thermal data from castings 16C-791 and 16C-795 were used to compare to the model. Casting 16C-792 had only 2 data points during filling and was excluded.

In the model, the cylinder has a height of 250 mm and radius of 80 mm. Thermocouple probes were placed in the mold and mold cavity to collect thermal data similar to the experimental rod mold. **Figure 61.6** shows the thermocouple locations and mesh resolution. The results of the thermocouples in the mold cavity and mold during filling and solidification are depicted in **Figure 61.7**. Time at 0 seconds is defined as the pouring time or when the stopper is removed from the crucible. Currently, the models only simulate filling and solidification, therefore thermocouple data during mold filling was compared to experimental filling data (**Figure 61.8**). The cylindrical model is highly simplified and does not consider the vacuum environment or the same boundary conditions in the experimental set up. Its purpose was to examine and verify the thermophysical properties of uranium and graphite. The cylindrical model is larger than the experimental rod, thus the fill times are different. In general, the thermocouples embedded in the walls are expected to increase once in contact with the metal and plateau during filling. During solidification, the temperature is expected to gradually decrease. The model sees a large jump when in contact with the metal unlike the experimental data because the model was not pre-heated. Based on the thermocouple data, the behavior was deemed reasonable to continue onto the hemispherical mold.

61.3.3 Hemispherical Uranium Model

Of the 11 process workspaces in FLOW-3D ® CAST, the gravity die casting workspace was selected for this model. This workspace was selected for this application due to its ability to place vacuum pointers and thermocouple probes, locally heat die parts, predict defects during solidification, and compute full heat transfer. Currently, only filling and solidification models have been built. As to geometry, the model currently includes the funnel, outer mold case, and inner mold core based on the experimental casting (**Figure 61.9**). The thermocouple locations (**Figure 61.10.a**) and mesh resolution (**Figure 61.10.b**) are featured in **Figure 61.10**. Two meshes were used: pour mesh with a cell size of 3 mm and a mold mesh with a cell size of 2 mm. A slightly lower resolution is sufficient for the pour because less detail is required for this region. Separate meshes also reduce simulation time. A gas pointer (see yellow probe in **Figure 61.10.a**) was used to define the vacuum condition in the mold cavity and was set at 50 Pa. The universal gas condition was also set to 50 Pa. Time dependent pressure data will be added in future iterations of the model. Thermocouple locations are meant to mimic those in the experimental casting and the labeling is reflective of the thermocouples in **Figure 61.2.** The current boundary conditions for this model are listed in **Table 61.2**. It should be noted that these are preliminary boundary conditions and are subject to change, such as boundaries set to 'Symmetry' which have no thermal characteristics. Without the insulation skirt or graphite base, z-min was altered to mimic these insulation conditions, such as a wall with a temperature of 500°C. The metal input conditions are sourced from the given time-dependent mass flow rate (kg/s) from the load cell data in the experiment. The crucible outlet was stated to have a 19 mm diameter and set to this value. **Figure 6.11-13** depicts the thermocouple data during filling (near pour time) and solidification and compares the models with experimental data. Time at 0 seconds is defined as the pouring time or when the stopper is removed from the crucible. Thermocouples in the casting cavity are observed to jump up and down from the pouring temperature (1300°C) to the ambient temperature (25°C) due to molten metal splashing onto the probes during pouring, consistent with experimental behavior. As thermocouples become fully immersed with metal, the readings become relatively constant followed by a gradual cooling during solidification. At the melting temperature of uranium (1135°C), the thermocouples remain at a constant temperature indicating the latent heat of fusion is being modeled. The experimental fill time was approximately 160 seconds while the modeled time was 202 seconds. Fill time is often used to evaluate accuracy of the pour thereby indicating further adjustments are needed. While this is the current state of the model, additional elements, such as the insulation skirt and graphite base (which serves as a heat sink) will be added in the future which will ultimately facilitate more accurate solidification behavior.

61.4 Plans for Next Reporting Period

- Add remaining experimental elements to hemispherical uranium model (i.e., graphite base, insulation skirt, additional thermocouples).
- Add mold heating and cooling simulations and verify with experimental data.
- Further refine mold filling and solidification simulations and verify with experimental data (thermal arrests during phase transformations, solidification time, thermal gradients, heat transfer coefficients).
- Finalize surrogate material (most likely a Sn-Pb alloy) and geometry for small casting validation experiments and prepare samples .

61.5 References

[61.1] A.B. Shapiro, W.J.I. Comfort, LLNL casting technology, 1994. https://doi.org/10.2172/10133336.

[61.2] J.F. Hetu, F. Ilinca, A finite element method for casting simulations, Numerical Heat Transfer. Part A, Applications. 36 (1999). https://www.osti.gov/biblio/20005609-finite-element-method-casting-simulations (accessed March 27, 2022).

[61.3] R.M.Jr. Aikin, An Instrumented Uranium Hemispherical Casting, 2019. https://doi.org/10.2172/1492626.

[61.4] F.H. Ho, Graphite design handbook, 1988. https://doi.org/10.2172/714896.

[61.5] N.T. Niane, S. Mascetti, Discovering optimal parameters for excellent casting simulations through, (2013). https://www.iosotech.com/files/application/xcengineering_euc2013_vIOSO.pdf.

[61.6] FLOW-3D®, Flow Science, Inc., Santa Fe, NM, 2021. https://www.flow3d.com.

[61.7] M.L.S. Zappulla, S.D. Imhoff, Sigma Casting Report - 16C-791,792,795, Los Alamos National Laboratory, 2022.

[61.8] S.D. Imhoff, Uranium Density, Thermal Conductivity, Specific Heat, and Thermal Diffusivity, 2021.

[61.9] J.A. Cahill, A.D. Kirshenbaum, The surface tension of liquid uranium from its melting point, 1406°K to 1850°K, Journal of Inorganic and Nuclear Chemistry. 27 (1965) 73–76. https://doi.org/10.1016/0022-1902(65)80192-0.

[61.10] P. Turchi, Viscosity and Surface Tension of Metals, 2018. https://doi.org/10.2172/1438687.

[61.11] P.E.A. Turchi, Thermodynamic, Diffusion, and Physical Properties of Nb-Ti-U-Zr Alloys, 2018. https://doi.org/10.2172/1459146.

61.6 Figures and Tables

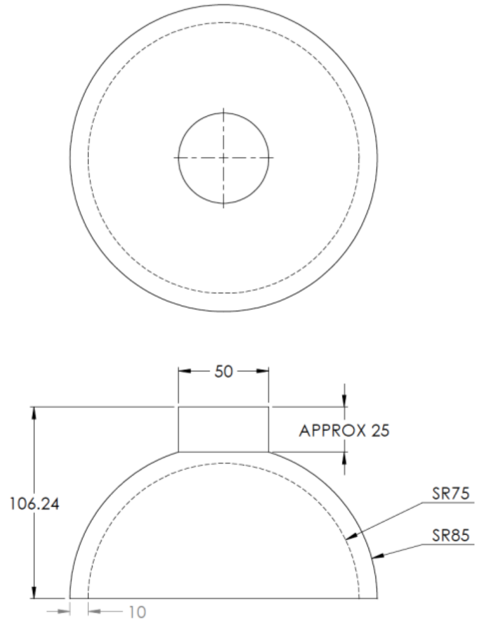


Figure 61.1: Final cast part from experiment and used for computational model. Dimensions in mm.

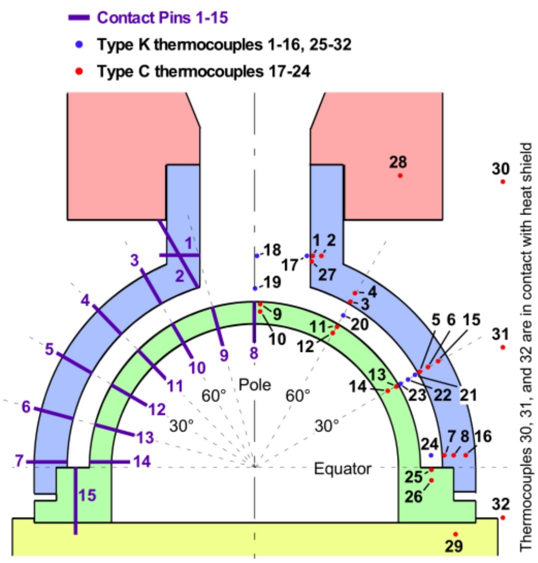


Figure 61.2: Thermocouple and contact pin locations in the mold stack (red: funnel, blue: case, green: core, yellow: base). Sourced from: [61.3].

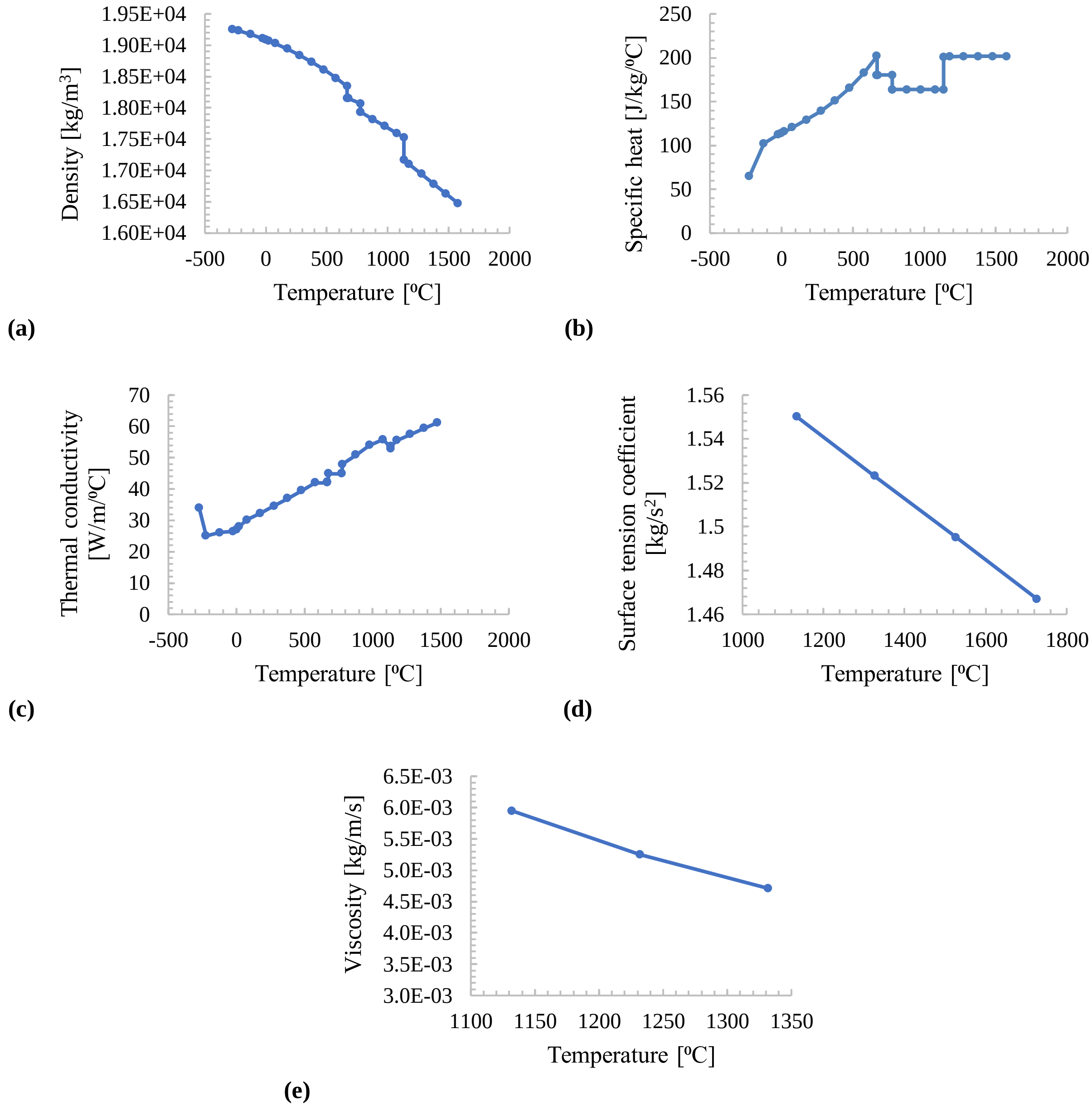
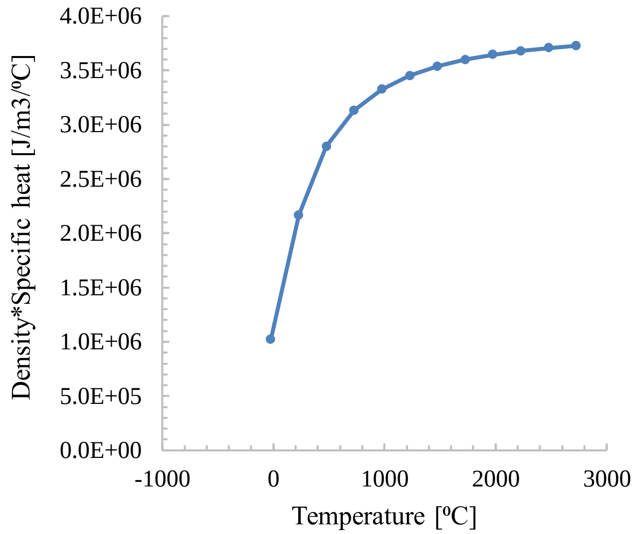


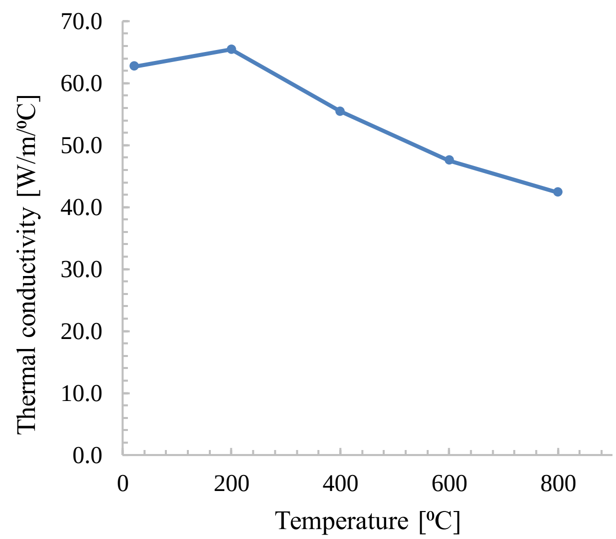
Figure 61.3: Temperature-dependent thermophysical properties used for uranium in FLOW-3D® simulations including **(a)** density, **(b)** specific heat, **(c)** thermal conductivity [61.5], **(d)** surface tension coefficient [61.6], and **(e)** viscosity [61.7].

Table 61.1: Thermophysical properties used for uranium FLOW-3D® simulations.

Property	Value	Source
Thermal expansion coefficient	3.428 1/K	[61.7]
Solidus temperature	1408 K	
Liquidus temperature	1408 K	
Latent heat of vaporization	38400 J/kg	[61.10]
Latent heat of fusion	1750000 J/kg	



(a)



(b)

Figure 61.4: Temperature-dependent thermophysical properties used for 2020 graphite in FLOW-3D® simulations including **(a)** density*specific heat and **(b)** thermal conductivity [61.4].

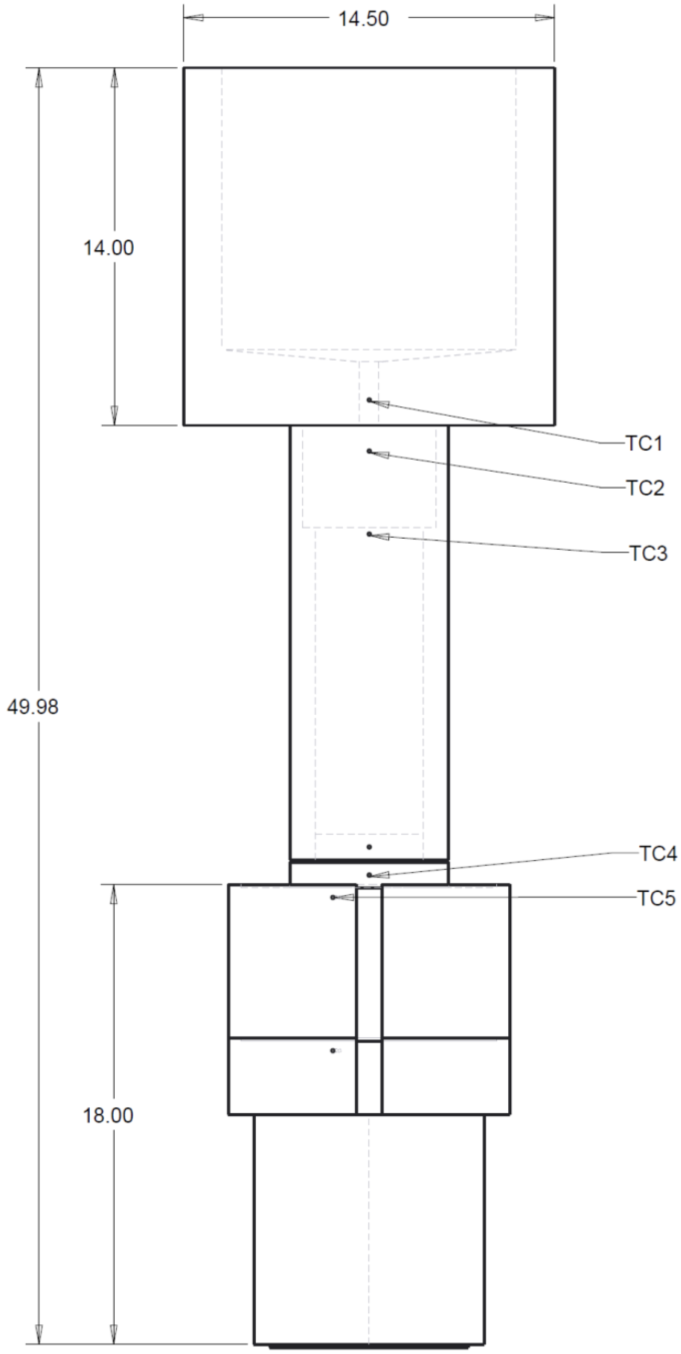


Figure 61.5: Plane of the uranium rod casting (casting number: 16C-791,792,795) with thermocouple locations. All units in inches. Sourced from: [61.6].

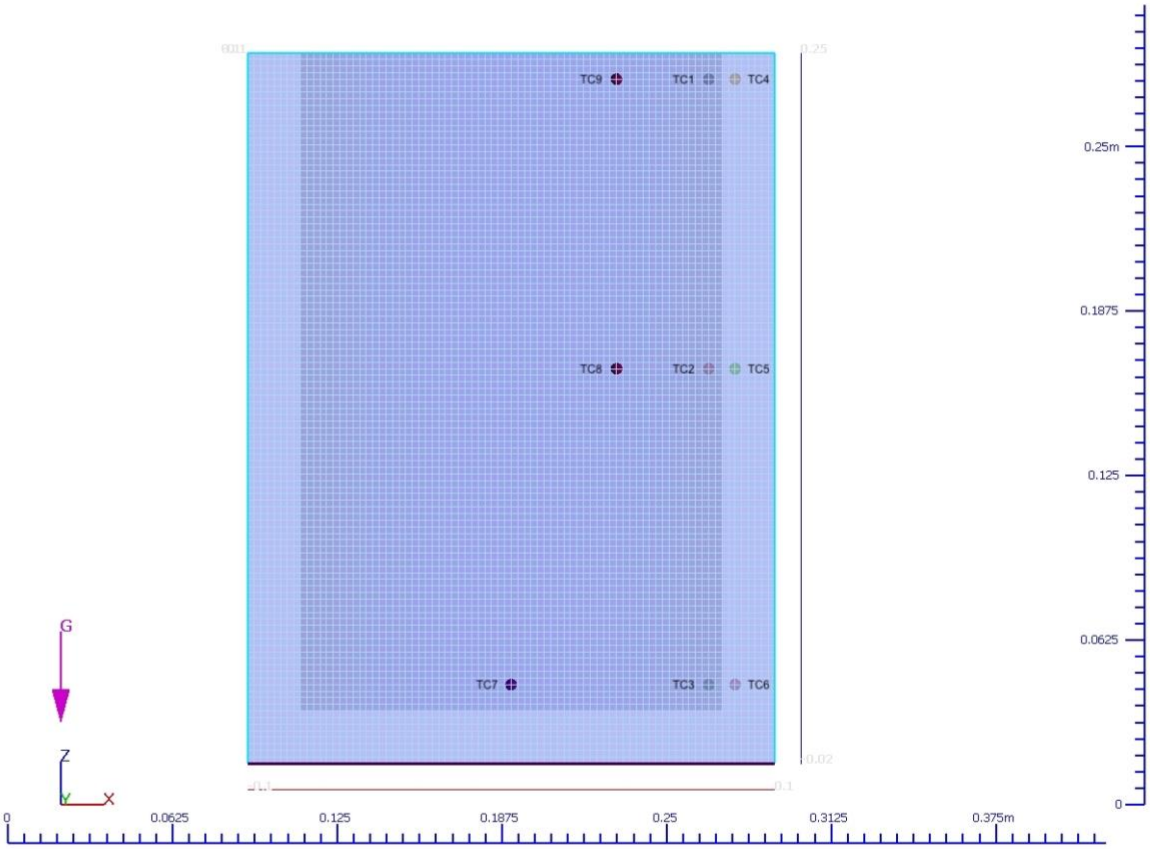
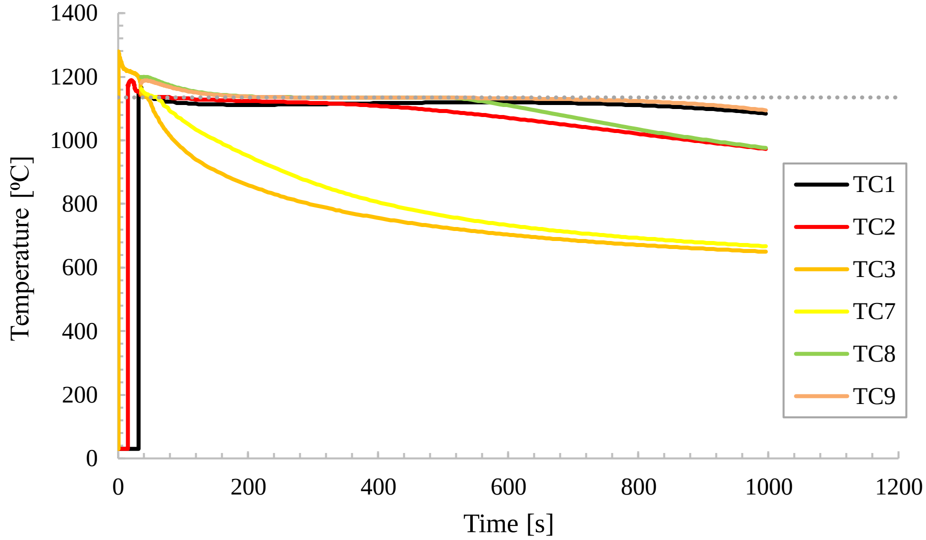
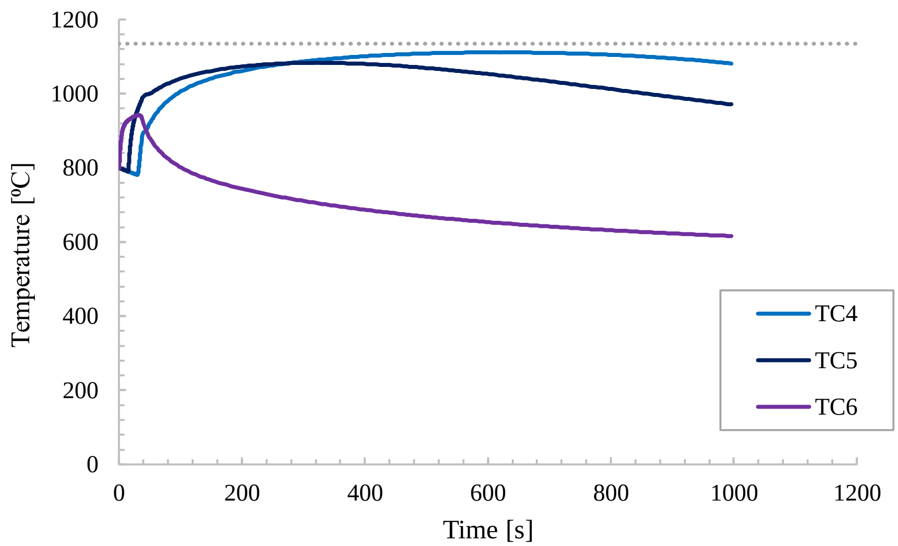


Figure 61.6: Z-X plane of the cylindrical uranium casting (H-250 mm x R-80 mm) FLOW-3D® model with thermocouple locations (TC1-6 used during filling and TC1-9 used during solidification) and mesh (cell size: 2.5 mm).



(a)



(b)

Figure 61.7: Temperature in the **(a)** mold cavity and **(b)** mold during metal solidification for the cylindrical uranium model in FLOW-3D®. The melting point of uranium is shown as a dashed line for reference. Filling is complete at ~36 seconds.

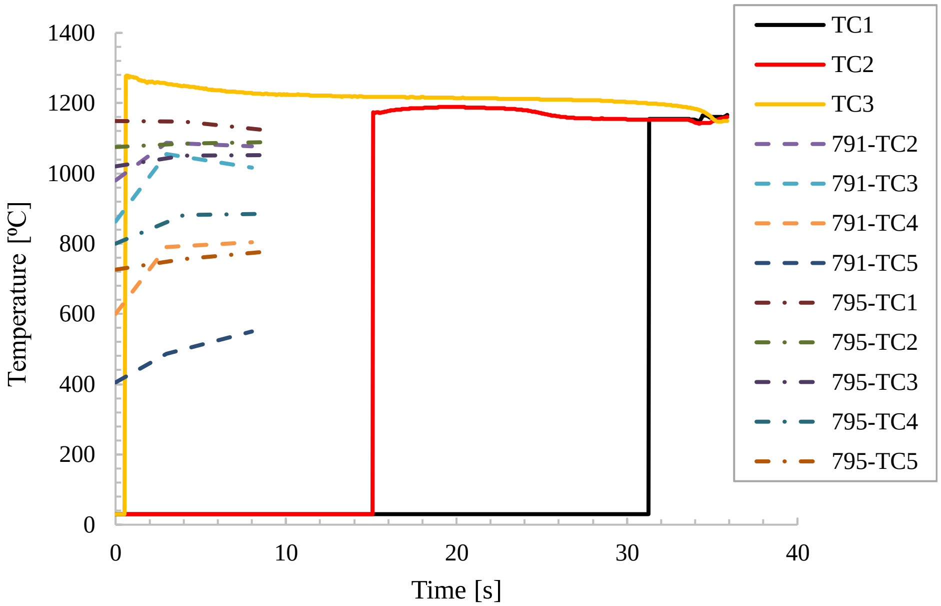


Figure 61.8: Comparison simulated (solid lines) and experimental (dashed lines, 16C-791,795) temperature in the mold cavity during mold filling. TC1 for casting 16C-791 was disconnected during mold heating [61.7].

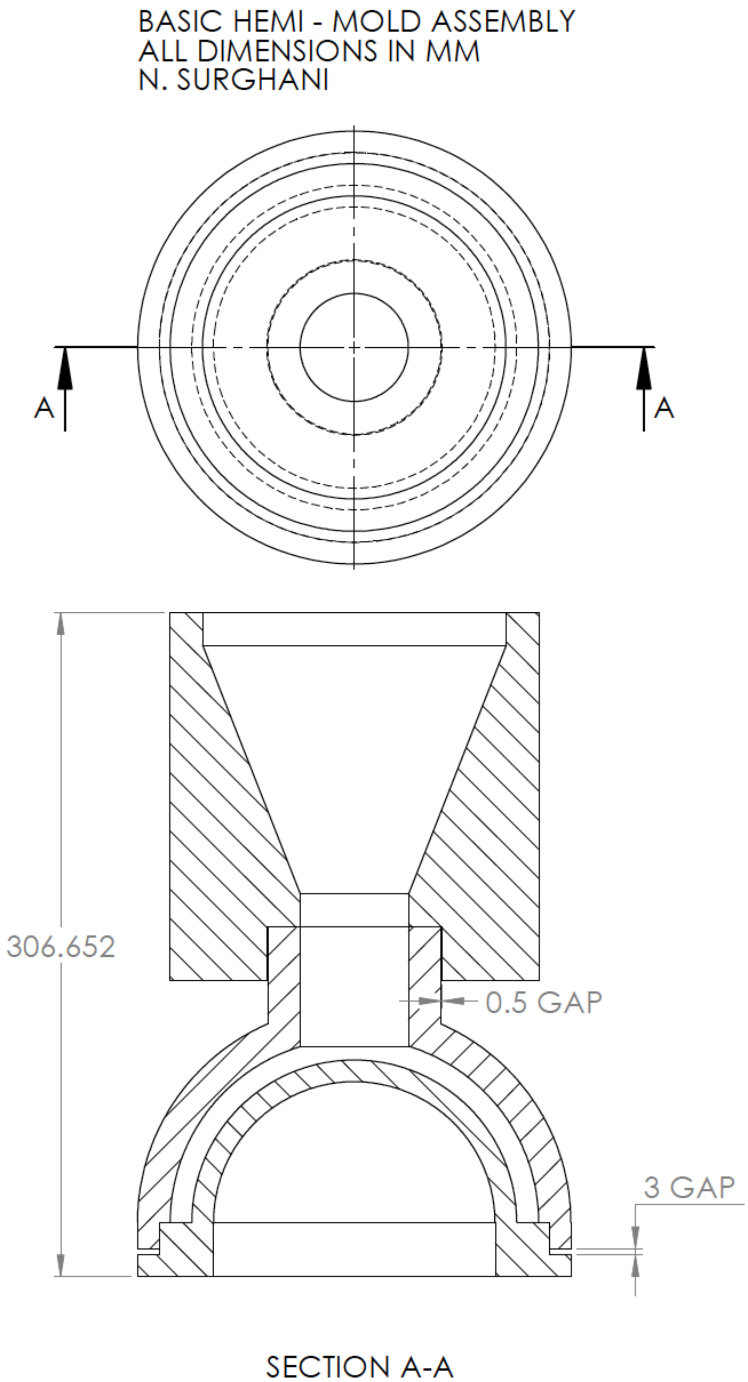


Figure 61.9: Mold stack design used in for the hemispherical uranium model in FLOW-3D®. Dimensions in mm.

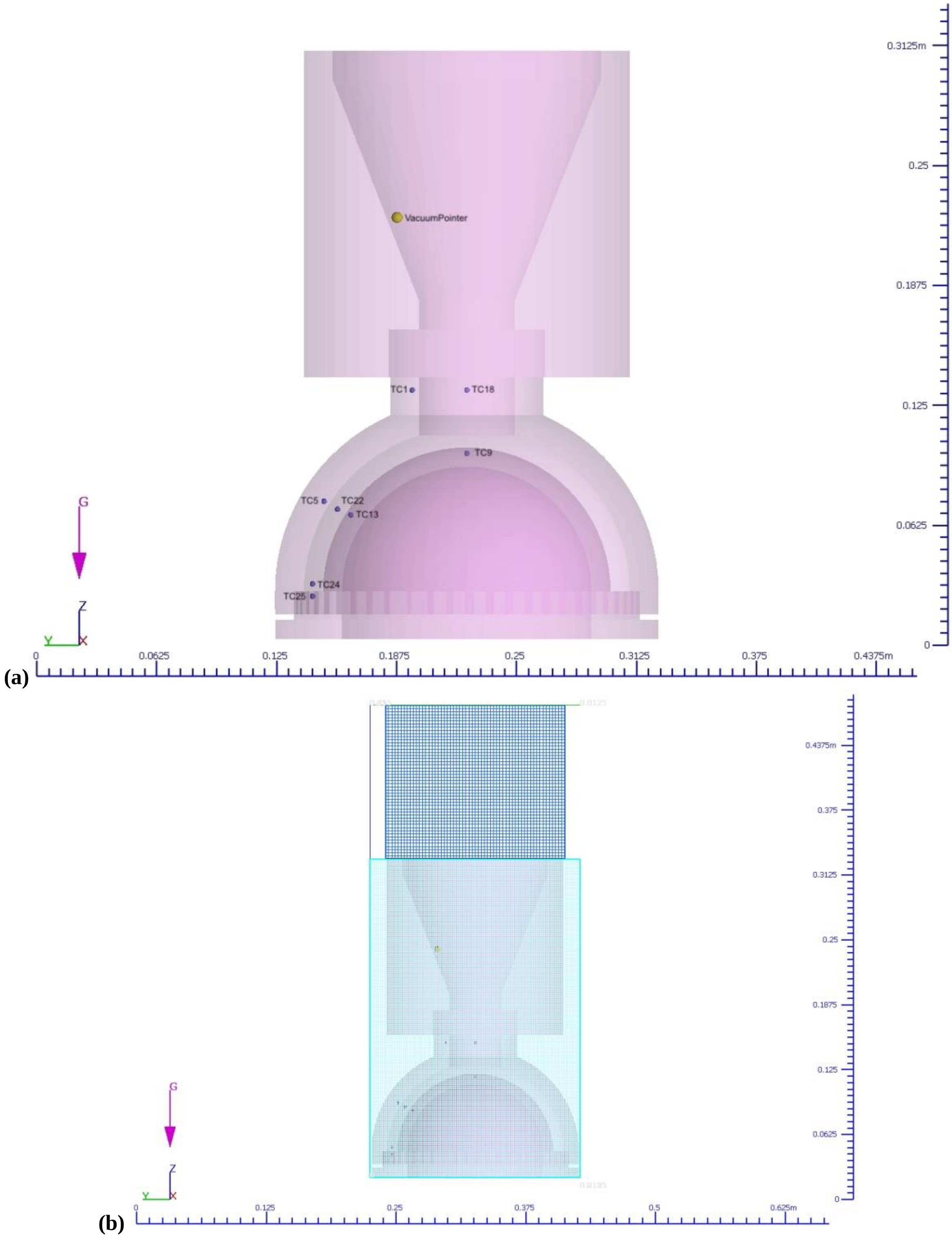


Figure 61.10: Z-X plane of the hemispherical uranium casting model with **(a)** thermocouple locations and **(b)** meshes (pour mesh in dark blue and mold mesh in light blue). The yellow pointer in **(a)** is used to define the vacuum in the mold cavity.

Table 61.2: Boundary conditions for the meshes in the hemispherical uranium model in FLOW-3D®.

Boundary	Type	
	Mold Mesh	**Pour Mesh**
X Min	Symmetry	Symmetry
X Max	Symmetry	Symmetry
Y Min	Symmetry	Symmetry
Y Max	Symmetry	Symmetry
Z Min	Wall T=500ºC	Symmetry
Z Max	Symmetry	Pressure: Gas T=25ºC P=50 Pa

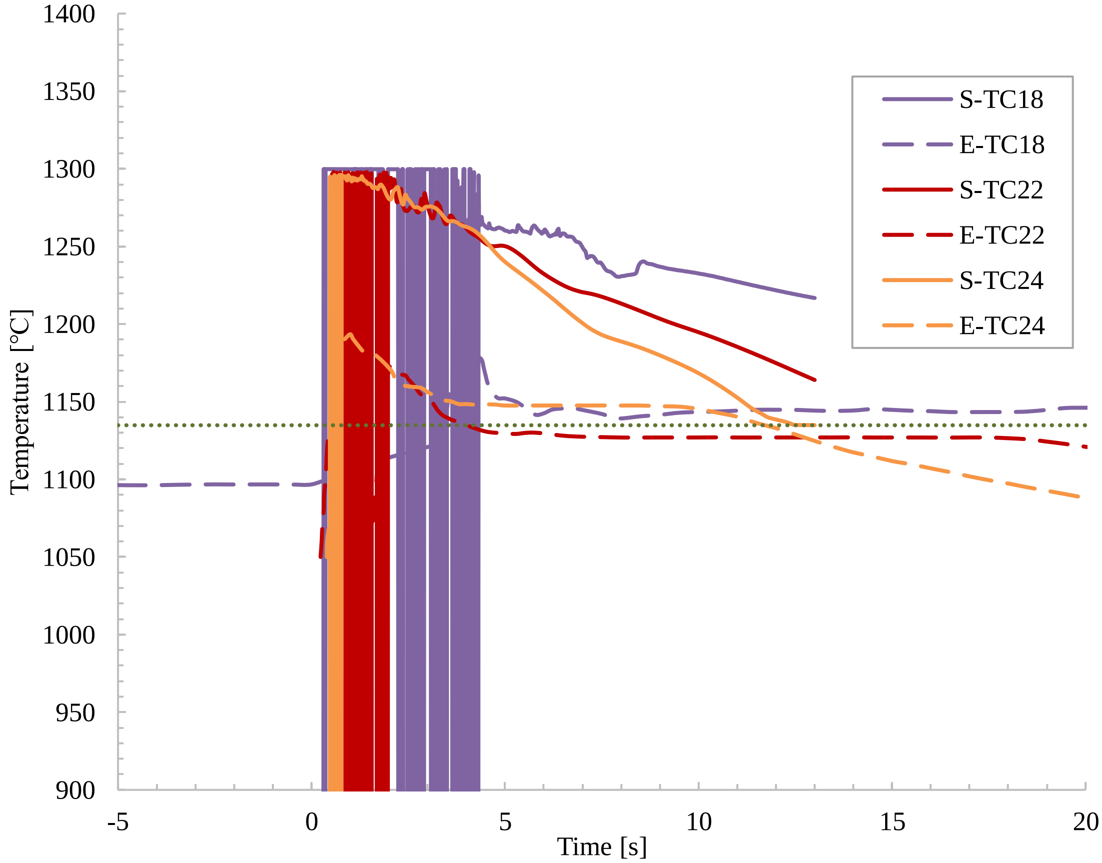


Figure 61.11: Comparison of experimental (denoted with E and dashed lines) and simulated (denoted with S and solid lines) temperature in the mold cavity as a function of time near pour time. The melting point of uranium is shown as a dotted line for reference.

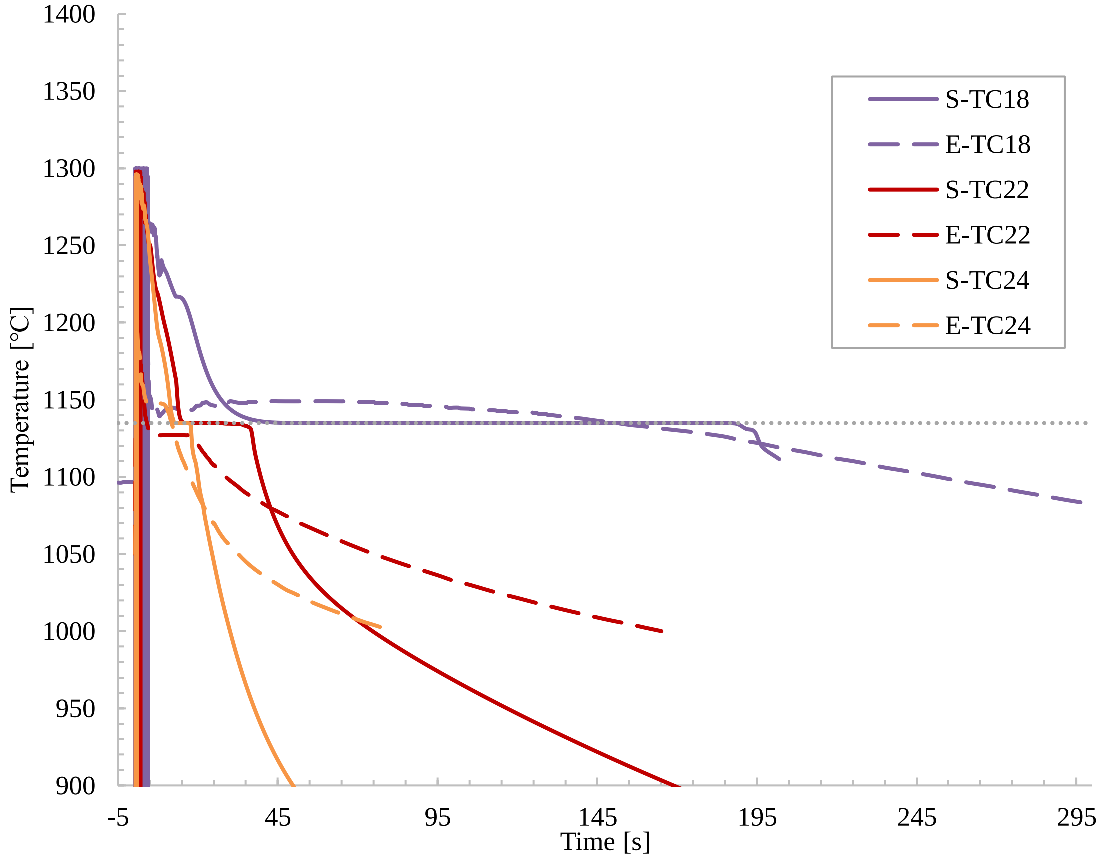


Figure 61.12: Comparison of experimental (dashed lines) and simulated (solid lines) temperature in the mold cavity as a function of time during metal solidification. Filling is complete at ~13 seconds.

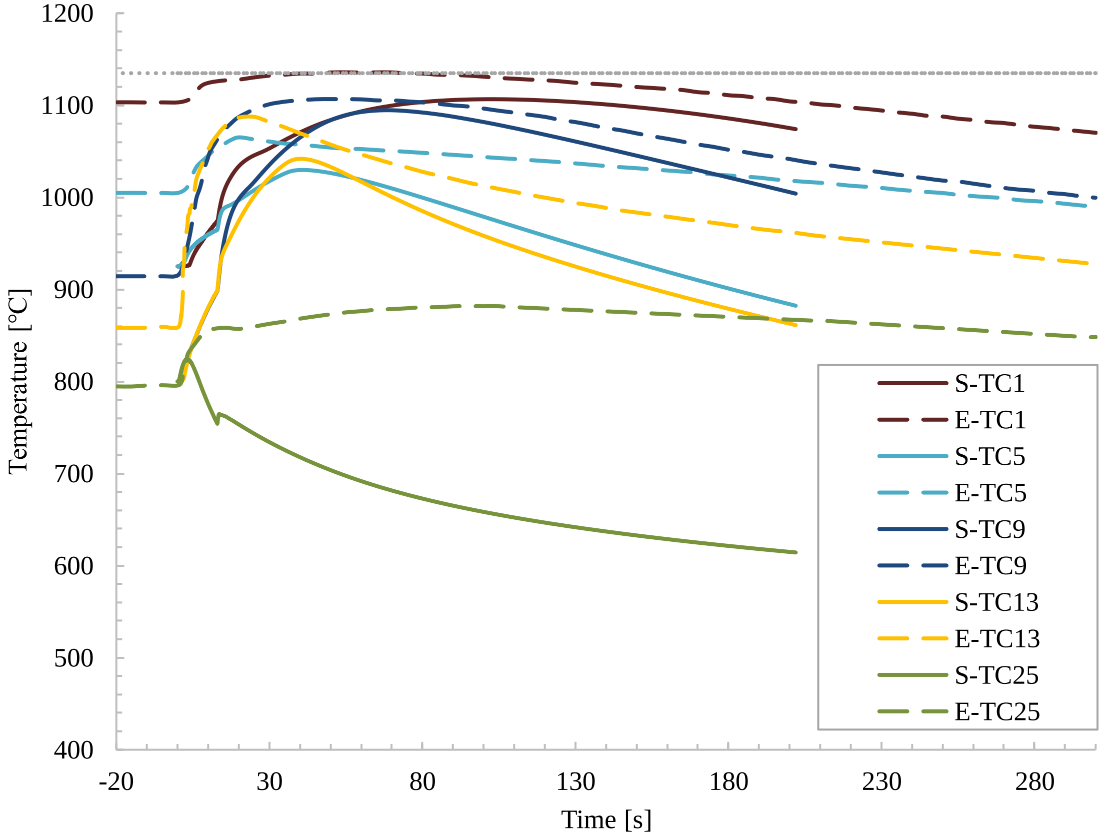


Figure 61.13: Comparison of experimental (dashed lines) and simulated (solid lines) temperature in the mold case and core as a function of time during metal solidification. Filling is complete at ~13 seconds.