

APPLICATION OF COMPUTATIONAL FLUID DYNAMICS TO THE DESIGN OF A WASTE VITRIFICATION FACILITY

J. Berkoe, C. Rayner, C. Barringer
Bechtel National, Inc.

ABSTRACT

The Hanford Waste Treatment Plant (WTP) -- the largest of its kind anywhere -- received full construction authorization from DOE in April 2003. In a waste vitrification facility, radioactive waste is combined with glass formers, heated to approximately 1200°C, and poured into stainless steel containers. The heat contained in the hot glass must be removed from the containers, and this must be accomplished within the production schedule constraints of the plant operation. In the Hanford Waste Treatment Plant, the glass is cooled in a small room, called the pour cave, in a concrete building. The room includes insulation to protect the concrete, along with ventilation and water-cooled cooling panels to facilitate heat transfer.

Since earlier vitrification facilities had processed waste at a lower rate and in larger rooms, there was no readily available data on the heat release rate from vitrified glass. This paper explains why the available information on the cooling rate of the glass was of little use in predicting heat load. The container heat release rate depends on the thermal properties of the glass, which will vary as the glass recipe changes. This rate also depends on the local environment, which includes other hot containers. The cooling process is strongly coupled, and is driven by the combined mechanisms of radiation, convection, and conduction heat transfer.

Computational fluid dynamics, CFD, was used to predict the heat load to the ventilation system, the cooling panels and to the insulated concrete walls for a variety of operating conditions, providing the data needed for the design of these systems. This paper describes the special techniques that were developed to simulate the pour cave operations and localized effects, presents the results of the simulations, and compares them with subsequent tests performed on containers in a similar environment.

INTRODUCTION

Overview of Waste Processing

The Hanford Waste Treatment Plant (WTP) — the largest of its kind anywhere — received full DOE authorization in April 2003 to begin construction. The huge waste treatment complex will be located on a 26-hectare site 40 kilometers north of Richland, Washington. Once completed, tested, and operational, WTP will immobilize all of the highly radioactive waste and a large portion of the low-activity radioactive waste stored in 177 aging steel and concrete underground tanks at the former nuclear weapons production facility.

201 million liters of radioactive and chemical waste — the legacy of 45 years of plutonium production — are stored at the site. The WTP will separate the high-level and low-level waste and use a process called vitrification to blend each waste stream with glass to produce an environmentally safe and stable product. Approximately 90 percent of the radioactivity will be contained in the high-level waste — 10 percent of the total volume.

An overview of the WTP waste vitrification process is described as follows –

- Storage Tanks - Liquid waste is pumped from the underground holding tanks (located on tank “farms”) to the WTP waste pretreatment facility.
- Pretreatment - Once in the pretreatment facility, waste is separated into high-level (HLW) and low-activity (LAW) radioactive waste through the use of filters and ion exchange columns.
- Separation – Low-activity waste is pumped to the LAW vitrification facility, while high-level waste goes to the HLW vitrification facility.
- Vitrification – In the vitrification facilities, the waste is mixed with silica and other glass-forming materials to form a slurry mixture. The mixture is then fed into high-temperature melters, where it is heated with electrical current for several days to form molten glass.
- Containers – The molten material is poured into stainless steel containers and cooled for several hours, after which each container is lidded, and decontaminated. The glass pouring temperature is approximately 1150°C. The time required to fill one LAW container is about 10 hours. The time required to fill one HLW container is about 24 hours.
- Transport and Storage – Containers from the LAW building are trucked to a storage site at Hanford, where they are buried in concrete-lined trenches. Containers from the HLW facility will be stored at Hanford in a special building until a national repository for high-level nuclear waste is ready.

Pour Cave Issues

The glass pouring and initial cooling process takes place in “pour caves.” The LAW pour caves consist of four shielded enclosures, each housing an elevator to accommodate moving a container to the pour position under the melter pour spout. The pour caves also contain a carousel to move containers to the cooling position and transfer position (where a full container is removed from the pour cave and an empty container is placed for indexing to the elevator position). Each cave is ventilated with about 2000 L/s of infiltration air at 45°C through the open transfer tunnel shield door, and about 200 L/s at 12.8°C entering from a duct in the north wall of the cave and an exhaust duct in the north wall. The south wall and viewing room wall are 50 cm thick concrete with 6-inches (15cm) of high temperature insulation (microporous silica insulation) and a stainless steel liner on the cave face. The floor is concrete, 1.5 m thick, with a stainless steel liner covering 6-inches (15cm) of cellular glass insulation on the cave floor. The ceiling and north wall are 8 cm thick steel plate with 6-inches (15cm) of microporous silica insulation. The top head enclosure surrounding the melter pour spout is stainless steel with 15cm of insulation and a stainless steel liner.

The HLW vitrification facility differs from the Low Activity Waste facility in several important features, as listed in Table I. Figure 1 shows a CAD model of two adjacent pour caves in the LAW facility and an overview of the HLW pour tunnel.

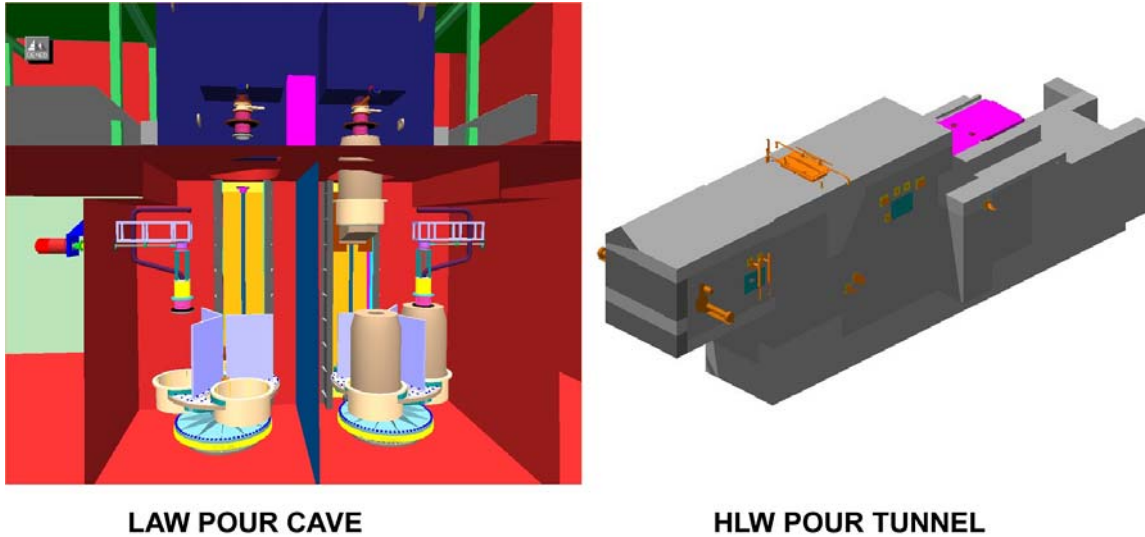


Fig. 1 CAD model of LAW pour caves, and HLW pour tunnel

Table I Comparison of LAW and HLW Facilities

Feature	LAW	HLW
Container Shape	1.22 m diameter by 2.286 m tall	0.61 m diameter by 4.42 m tall
Container Capacity	6000 kg	3300 kg
Fill time	10 hours	24 hours
Support during fill and initial cooling	Water Cooled Turntable	Uncooled Rail Supported Trolley (Bogie)
Pour Cave Dimensions (approximate)	5.18 m wide 7.62 m high 7.62 m long	3.35 m wide 7.62 m high 24.38 m+ long
Pour Cave Capacity	2 or 3 containers	1 or 2 containers
Pour Cave Cooling	Water Cooled Panels and Air Cooling (door inlet with outlet neat top)	Air Cooling (door inlet with outlet on the floor)

The HLW container contains less glass and is filled over a longer time so the heat transfer rate is lower. This is partially offset by the container shape, since the smaller diameter container cools faster.

The pour cave heat transfer problem is bounded by the following three Basic Design Requirements:

- **Concrete Wall Temperature:** Structural concrete shall be below 65.6°C during operating conditions, and 176.6°C during accident conditions.
- **Metal Surfaces (Equipment and walls):** Metal surfaces external to LAW pour caves shall be less than 34.4°C.
- **Pour Cave Air Temperature:**
 - The pour cave leaving air temperature shall not exceed 65.6°C during normal operations.
 - Ambient air within the pour cave should be less than 93.3°C.

Preliminary calculations revealed the heat loads in the LAW pour cave released by the glass containers could not be accommodated by HVAC ventilation airflow alone - additional means of removing the heat would be required in order to satisfy the above basic requirements. Thus the addition of water-cooled panels was proposed as a design solution for the LAW facility.

Task Objective

The design of the LAW pour cave requires accurate modeling of the HVAC airflow and heat transfer to predict the temperature conditions within the pour cave, the surrounding walls, ceiling, and below the floor. The specific objective of this project was to use computational fluid dynamics to:

- Analyze heat transfer within the pour cave: An analysis was performed on the heat transfer from the containers (which create the heat load into the cave) to the surrounding walls, floor, and HVAC cooling air (which remove the heat). The analysis focused on:
 - Predict surface temperatures and heat rejection rates from the containers over the pour cave's entire normal operation cycle
 - Predict temperature profiles of the concrete walls during peak heat load conditions over the pour cave's entire normal operation cycle
 - Predict surface temperatures and heat transfer to and from the containers, wall, ceiling, and floors, when insulation and/or cooling panels are utilized
- Develop recommendations for cooling equipment and insulation to permit the facility to operate at the required conditions. The recommendations focused on:
 - Cooling panel design requirements and location,
 - Insulation thicknesses where needed,
 - Other heat removal equipment to be installed in the vitrification facility pour caves
- Determine concrete temperature profiles during peak heat load conditions (with insulated walls and floors) during a design basis seismic event resulting in loss of power to the cooling panels and exhaust fans (considered as a worst-case off-normal event scenario).

MODELING APPROACH

Physical Effects

For the pour cave thermal analysis, the types of physical phenomena being modeled include fluid flow, convective heat transfer, conduction heat transfer, and radiative heat transfer. The types of input parameters include material properties for the glass waste, air, steel, insulation, concrete (specific heat, thermal conductivity, density), HVAC boundary conditions (e.g., flow rate and temperature), surface properties (e.g., emissivity), and detailed geometry data (typically obtained from CAD models). Since the glass waste is poured into the LAW and HLW containers at temperatures in the range of 1150°C-1200°C, the calculation of radiation heat transfer to the walls and conduction heat transfer in the glass is particularly important.

The heat transfer from the containers is highly coupled to the glass pour rate and glass thermo-physical properties, in particular its high thermal capacitance. Specification and initialization of the container surface and internal temperatures during the pour cycle is thus very challenging due to the high variability in heat output. To effectively simulate the heat transfer from the containers, transient calculations must be used to accurately predict the time-varying heat release to the surrounding environment. Additionally, inside the containers radiation heat transfer must be modeled to account for the high heat fluxes

transferred from the glass to the container walls during the pour. This is critical for capturing the heat losses inside the pour container to the wall above the glass level.

Computational fluid dynamics (CFD) is the method of solving the governing mass, momentum, scalar and energy equations on a computational grid representing the domain in question. CFD allows for the construction of realistic full-scale computer models, which simulate the airflow patterns inside the pour cave and all modes of heat transfer. The CFD model is based on the actual physical geometry of the pour cave and applies fundamental physical principles to compute the temperatures, velocities, and pressures.

Program Description

The scope of the CFD simulation consisted of three-dimensional transient and steady state calculations using commercial CFD analysis software. The software used in this analysis consisted of:

- Fluent Versions 5.5 and 6.0 (Fluent, Inc.) for the CFD analysis. Fluent uses the Finite Volume method and can handle unstructured grids for flexibility in quickly creating large detailed models.
- ICEM-CFD Hexa (ANSYS, Inc.) for the grid generation, which provided the discretization of the domain and model surface geometry.
- Fieldview Version 7 (Intelligent Light, Inc.) and Tecplot Version 9 (Amtec, Inc.) for post-processing of the results. Fieldview and Tecplot can process results from many CFD codes, including Fluent.

The Fluent incompressible flow solver has the following modeling capabilities, which were either employed or considered for this analysis:

- Flows in 3D geometries using unstructured solution-adaptive, quadrilateral/hexahedral grids - used for model discretization (i.e., meshing).
- Turbulent flow, including standard k-epsilon model (with standard wall functions) used in this calculation.
- Buoyancy-driven convection (i.e., gravitational effects) based on the incompressible ideal gas equation. This directly couples the momentum equation to the energy equation at every location in the air domain to explicitly account for the effects of temperature change on the air density. Buoyancy was considered a secondary effect due to the forced convection-type ventilation system employed for the LAW pour cave, and thus not included. Buoyancy was included in the calculation for the HLW pour cave since air cooling plays a more significant role and since the HVAC design was subjected to flow stagnation near the ceiling.
- Radiation heat transfer - The discrete ordinates method available in Fluent is substantially more accurate than other techniques such as surface-to-surface. This higher level of accuracy is essential for modeling the LAW pour cave conditions due to the high temperatures, surface shadowing effects, and degree of accuracy required.
- Coupled conduction/convective/radiation heat transfer

The three dimensional CFD simulations were primarily performed on Compaq XP1000 and ES40 667 MHz (Tru-64 Alpha Unix) workstations, and a multi-node Linux system running Windows 2000 in parallel. The typical time required to reach a converged transient solution for was approximately 4-6 days. The simulation run times were mostly driven by the radiation computation (using the cpu-intensive discrete ordinates mode), the pouring/transfer process, and the large thermal inertia in the thick concrete walls. It was critical that a "repetitive" thermal cycling condition be reached in the wall temperatures before the runs could be stopped.

MODEL SETUP

Model Geometry

The CFD model geometry was derived from the CAD model of the pour cave. Many features of the detailed design were simplified to accommodate a computational mesh of reasonable size. The mesh was generated using hexahedral cells, and included the following regions –

- Air inside the pour cave
- Inside region of each container (glass) bounded by zero-thickness steel liner
- Concrete walls (concrete) lined with zero-thickness layer of insulation resistance
- Zero-thickness cooling panels (with steel thickness resistance)
- Steel wall thickness for the elevator, turntable, and other non-concrete wall sections
- Pour cave window thickness (glass)

The HVAC airflow inlets were modeled as pressure inlets to allow for the calculation of the variable flow profile across the boundary, particularly important for the flow through the door. The HVAC exhaust was modeled with a constant velocity. The outside surfaces of the model were specified as convective boundaries using a typical ambient heat transfer coefficient to the surrounding areas. The cooling panels were typically modeled using a high heat (film) coefficient - typical for water-cooled systems – to a constant temperature heat sink.

Pour Schedule

Within the LAW facility, two melters fill containers enclosed within four pour caves. Each melter has two pour spouts that discharge glass. (Note: each spout supplies glass to one of two adjacent pour caves) The melter will alternate filling containers in each pour cave. After a container is filled in one pour cave, the melter will begin filling the next container in the adjacent pour cave.

Each pour cave holds three containers located at three stations on the turntable: the container fill station, the container cooling/venting station, and the container transfer station.

At the container fill station, molten glass is poured into the container. After filling, the container is moved to the cooling/venting station. At the transfer station, the cooled containers are moved out of the pour cave and into the transfer tunnel, and a new empty container is brought into the pour cave.

The glass pours into the containers were simulated as separate instantaneous patches of temperature (at the glass melting temperature) into each successive section of the container at the fill station. For the LAW analysis the pour container is filled in four patches. For the HLW analysis the container is filled in twelve patches. During the transient, the glass region to be poured is initialized in Fluent using the patching technique. The pours are 2.8 hours apart, with the container residing at the pour station for 10 hours. The last pour occurs 1.6 hours before the end of the fill station residence time. The containers also reside at the other stations for 10 hours.

Container Handling

The containers are not moved in simulation. Instead, temperatures are patched into locations occupied by the containers. Once the filled container in the pour position was at the end of its pour cycle, its temperature data is input into the volume of the container in the cooling position, thereby simulating the container being moved to the cooling/venting station. Also, at the end of the pour cycle (hour 10 for the

LAW facility), the patching sequence is repeated on a new empty container at the fill station. This simulates the filling of a new container. At the same time the container at the cooling/venting station cools. For the LAW facility, at the end of the second pour cycle (hour 20), the temperature data on the cooling container is read into the volume of the container in the transfer position. The temperature of the container that is currently in the fill position is patched into the container in the cooling position. The patching sequence is repeated on a new empty container at the fill station. This simulates the filling of a new container. Cooling continues in the containers at the cooling/venting and transfer stations.

To accurately model the cooling of the containers in the cooling/venting and transfer stations, it is necessary to model the internal conditions of the glass. Due to the relatively low conductivity and high specific heat properties of the glass, there is a significant radial temperature variation.

To model this behavior, the radial temperature profile was obtained from each of the four quarter-height sections at the end of the intermediate calculation cycles. A fourth-order polynomial expression was then derived for each profile (of temperature vs. radial position) using regression analysis (in Microsoft Excel). The resulting temperature profile equations were input to Fluent as "custom-field" functions.

The pour container profile was applied to the "cool-down" container. The "cool-down" container profile was applied to the associated "transfer" container sections at the start of the pour cycle.

GLASS PROPERTIES

Background

Key parameters for estimating the heat load from cooling glass are the glass specific heat, C_p , thermal conductivity, k , and density ρ . These are often combined in a parameter known as thermal diffusivity which is defined as $k / (\rho C_p)$. Thermal diffusivity is a measure of how fast the glass cools and can be verified fairly easily during large-scale tests by plotting temperature profiles at various positions in the glass log.

All these parameters are highly temperature dependent. Although there is much literature on thermal diffusivity, there have been only limited measurements of the thermal conductivity and specific heat of the glasses used for vitrifying waste, and the few measurements that there were available showed high variability.

In order to size the HVAC system the most important parameter is specific heat. This and glass temperature determine how much heat must be removed from the glass. Since the glass recipe will vary according to the characteristics of the waste being vitrified, a method was required for estimating the specific heat of a worst-case glass. The range of ingredients was available, but the composition with the highest specific heat was unknown. To make this estimate we turned to a computer code developed originally for the metals industry, where it is used for estimating the composition and specific heat of slags.

HSC is a computer code developed for the metallurgical industry for chemical reactions and equilibria calculations. It uses a thermochemical database which contains enthalpy, entropy and heat capacity data for more than 7600 chemical compounds. If the user gives the raw materials, amounts and conditions of any chemical process the program will give the amounts of the products as the result.

HSC does not solve all chemical problems because it does not take into account the kinetics or rates of reactions. It assumes that all reactions proceed to equilibrium corresponding to the lowest energy level.

In the real world reactions do not always proceed to equilibrium. However the equilibrium state is the lowest energy state and represents the greatest heat release and the result conservative for our analysis.

Baseline Definition

Glass is a eutectic mixture of many complex compounds in equilibrium. HSC was used in three steps to estimate the worst-case specific heat.

1. Determine specific heat of a typical glass. HSC is used to list all the compounds containing the glass ingredients. Unlikely compounds are eliminated and HSC can be instructed to calculate the equilibrium composition of the remaining compounds at several temperatures over the temperature range. The enthalpies of these compounds are in the HSC database so the enthalpy of the mixture at temperature is known, or can be easily calculated. The difference in enthalpy over a temperature range is a measure of the average specific heat over that range.
2. Determine the effect of each ingredient. By adjusting the amount of each ingredient it was possible to determine whether a greater percentage of that ingredient would increase or decrease the specific heat. A conservative glass composition was selected by increasing the percentage of all ingredients tending to increase specific heat toward the top of the expected range, and reducing the percentage of all ingredients tending to reduce specific heat to the bottom of the intended range.
3. Determine worst-case specific heat. Using the worst-case composition the specific heat was calculated over the full temperature range up to the glass pouring temperature.

These specific heat values were used in the CFD calculations of cooling glass containers.

CFD SOLUTION

LAW Design Basis

Figure 2 shows the transient wall temperature profile of the LAW pour and cooling containers for a period of two pour cycles. Figure 3 shows the corresponding heat release profiles for the two containers over the same time period. Note the cyclic nature of the heat release from the pour container due to the patching of the four glass batches. Also note the variable ranges in magnitude of heat release from the pour cave between 80 kW near the start to around 180 kW at the beginning of the final pour. The heat release from the cooling can decrease steadily during the same time period from around 135 kW to around 65 kW. The net effect is that the combined heat release does not vary too much between the start of the pour and end of the pour.

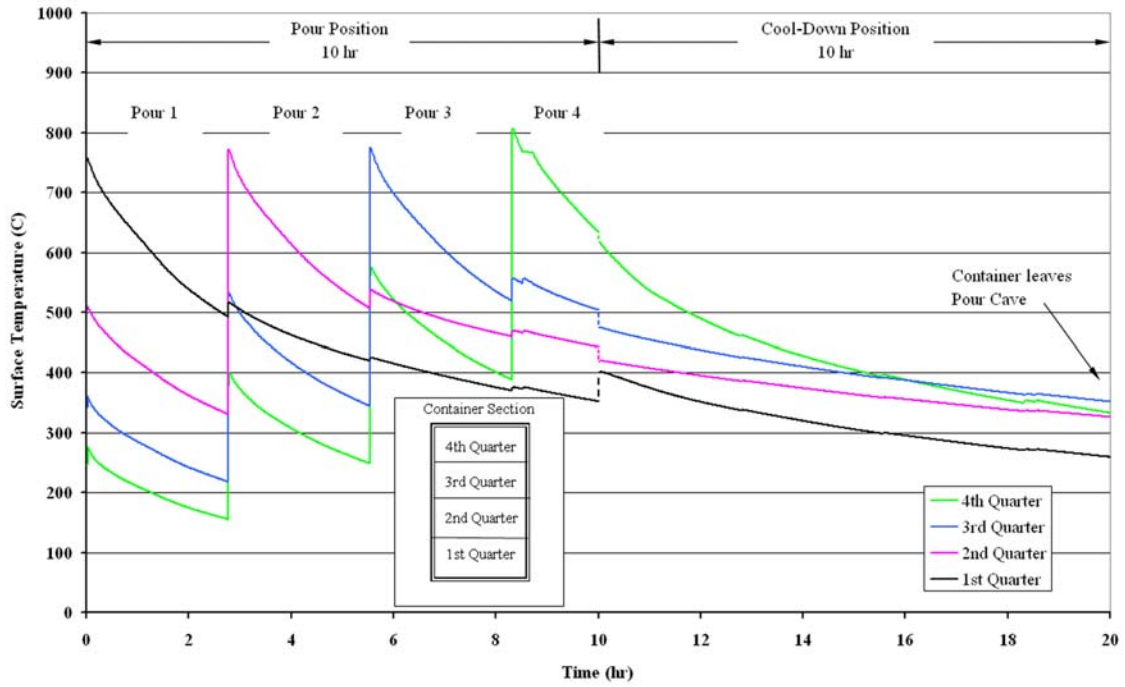


Fig. 2 Wall temperatures vs. time over two pour cycles, LAW containers

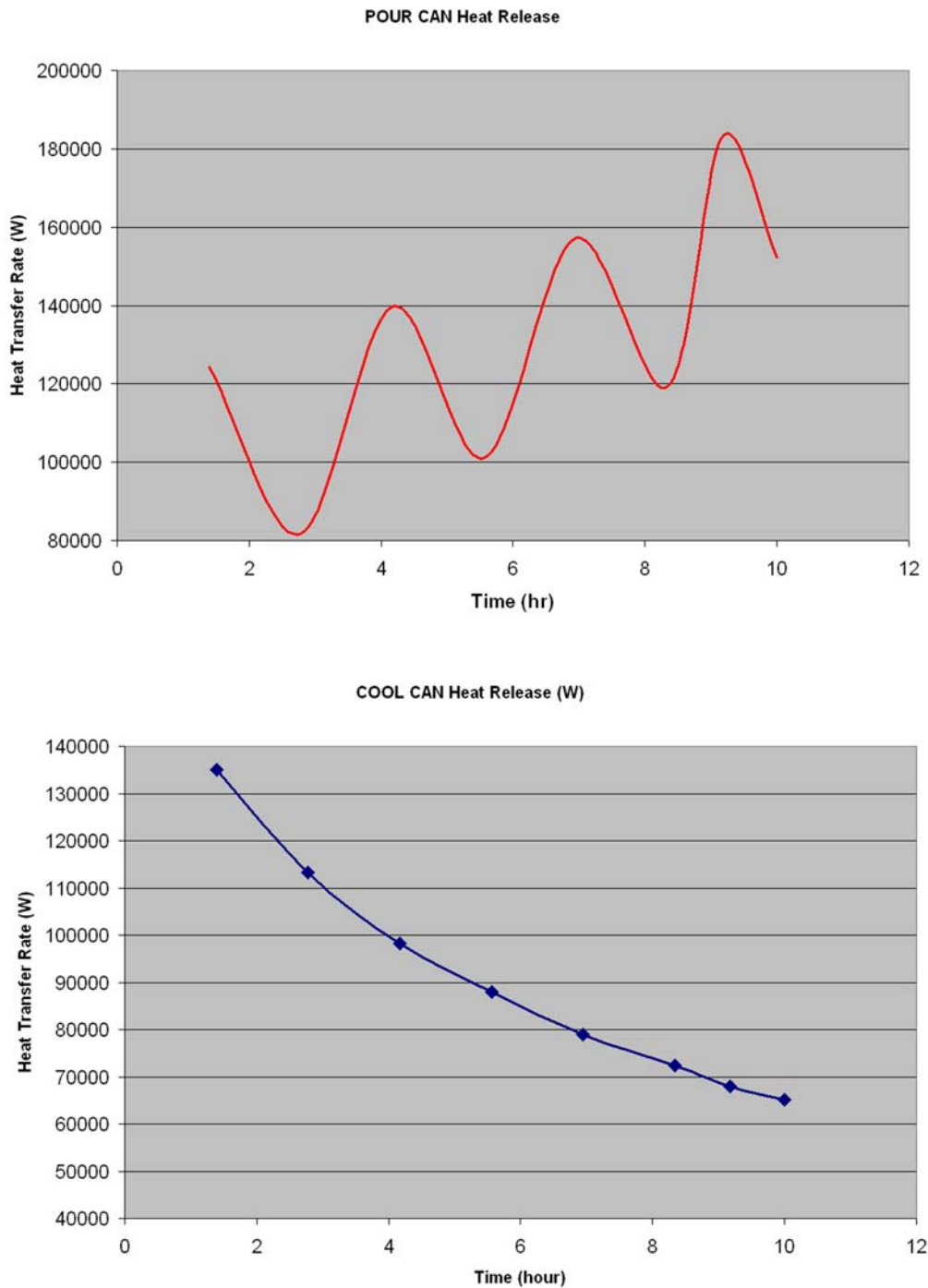


Fig. 3 Heat release vs. time of LAW pour and Ccooling containers.

Figure 4 shows the surface temperatures of the exposed walls in the LAW pour cave around the start of the final pour, which creates an area of relatively high temperature in the upper head region, and also shows the internal glass temperatures at the end of a pour cycle for LAW pour can and cooling can. Note the very high internal temperatures even after two pour cycles, resulting primarily from the high thermal capacitance combined with low conductivity of the LAW glass.

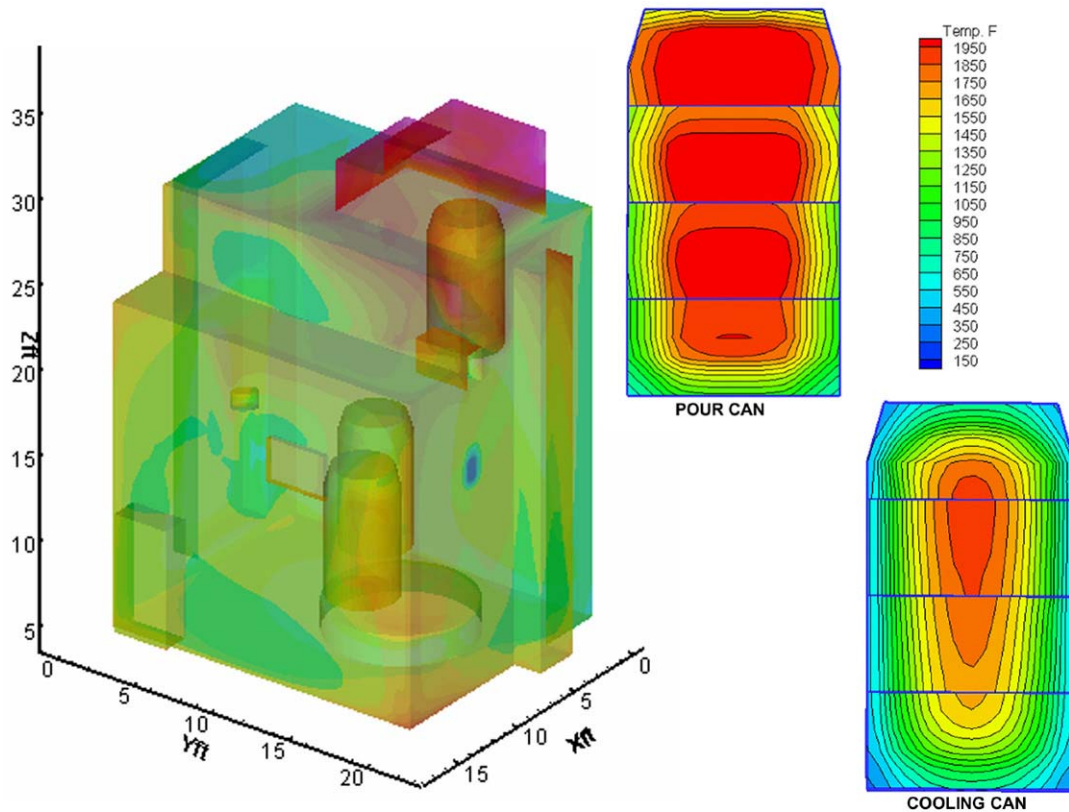


Fig. 4 Contours of LAW surface temperatures and internal glass temperature contours.

LAW Loss of Power Event

The objective of this task was to estimate concrete temperature profiles during peak heat load conditions during an eight-hour loss of power event. This event would shut down the cooling panels and exhaust fans, which could subject the pour caves to excessive thermal stress.

The results were compared to the Basic Design Requirements, including the requirement that the concrete surface temperature not exceed 176.7°C . The analysis also estimated what the leaving air temperature would be upon restart of the HVAC system.

This simulation was performed for a worst-case scenario. The simulated power loss occurred at a point in the cycle (hour 30) when the heat removed by the cooling panels and exhaust fans would be at a maximum.

The simulation predicted that the concrete temperatures would not exceed the 176°C accident period limit. The results also indicated that the pour cave ambient temperature would exceed the Basic Design Requirement's 93.3°C limit, which is allowable during short periods of time such as an off-normal event.

HLW Design Basis

As with LAW, the most significant constraint is the requirement that the concrete temperature stay below 65.6°C during normal operation. Other factors are the protection of the bogie axles, the bogie rails and

the bogie rail supports. Differential thermal expansion of the rails and rail supports can cause excessive loads and increased wear on the bogie wheels and rails.

Because there are no cooling panels on the walls, floor and ceiling, they must be protected with insulation. For the center mounted bogey rail support columns, a partial height sleeve provides protection from direct thermal radiation and allows convective cooling by buoyancy-induced airflow between the sleeve and the columns. CFD was used to determine the wall insulation requirements, and to show the effect of the sleeves on the support column temperatures.

HLW Spill Accident

The accident considered in the accident scenario is an accidental pour from the melter when a container is not in position to receive it. Catch cans are permanently positioned under the container, with sufficient capacity to handle the highest spill capacity.

The scenario considers the filling of a catch can at double the normal fill rate. CFD was used to plot the wall temperature as a function of time after the spill. Because of the large thermal capacity of the concrete walls the wall temperature continues to rise long after the glass and air temperatures start falling. CFD showed that the concrete temperature did not increase above that allowed during an accident condition.

Container Handling Effects

The cooling rate of the LAW container is required to determine when the container can be safely handled. The LAW containers are supported from below while being filled, and during initial cooling by the LAW elevator. After the initial cooling period, the containers are transferred out of the pour cave using devices that lift them by the top flange

The LAW container can be shipped from the LAW facility as soon as 40 hours after filling. At this stage the center of the container may still be extremely hot. CFD analysis demonstrated that there is little that can be done to control either the heat release rate vs. time for the LAW canisters, or the centerline temperature as a function of time. The insulating layers of cold glass at the perimeter of the container control these parameters.

CONCLUSIONS

CFD modeling realistically analyzes the effects of all modes of heat transfer and provides local details for identifying "hot spots". Several techniques were developed to combine a high level of detail and meet required schedule constraints. These techniques were developed to simulate glass pouring schedules, transient thermal properties, radiation heat transfer, and transfer of pour canister position. Advanced meshing techniques were employed to accurately represent the complex pour cave geometry details. These models were used to optimize insulation requirements, specify cooling panel design requirements, and confirm allowance during safety-related events such as loss of power or inadvertent glass spill.

It was determined that the specific heat and conductivity of the glass significantly affect the heat release transients, and therefore the heat load to the pour cave, and thus this represents an area of uncertainty due to the lack of available data. CFD analysis was also to evaluate options for increasing the cooling rate of the glass. This is an important issue as portions of the glass were predicted to remain extremely hot long after the containers have left the pour cave. CFD analysis indicated that the time to solidify could not be significantly accelerated due to the low conductivity of the glass.