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Combustion Simulation of Transportation Package Performance in Severe, Long Duration Fire – Update

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ABSTRACT

The Nuclear Waste Management Organization (NWMO) is responsible for designing and implementing Canada's plan for the safe, long-term management of Canada's used nuclear fuel. The plan, known as Adaptive Phased Management, requires used fuel to be contained and isolated in a deep geological repository. The transportation system is an important component of Canada's plan as it requires transporting used nuclear fuel from current interim storage facilities to a deep geological repository at a new centralized site.

Radioactive material must be transported in very robust packages. Transportation package robustness is demonstrated by satisfying stringent Canadian Nuclear Safety Commission (CNSC) and International Atomic Energy Agency (IAEA) regulations. The IAEA regulatory thermal test for Type B packages is designed to bound conditions in historic transportation fire accidents. The 30 minute, 800°C, fully engulfing regulatory fire test imposes an incredibly severe set of conditions on the test specimen. However, severity of this thermal test can often be difficult to communicate to the general public, especially in comparison to real-world transportation accidents involving long duration fires.

NWMO has developed an advanced computational fluid dynamics combustion model to simulate real-world long duration transportation accident fires. This fire simulation model will help study transportation package performance in hypothetical severe fires. Such a model and knowledge gained during development will help bridge the information gap between the 30-minute regulatory thermal test and real-world long duration transportation accident fires.

This paper describes the development and benchmarking of NWMO's combustion simulation model against real-world physical fire tests.

INTRODUCTION

The NWMO is developing in-house expertise in fire simulation modeling in support of future design, certification, and testing of Type B(U) radioactive material transportation packages. Accurate modeling or simulation of fires can be used to analyze package performance in regulatory fire tests and for possible accident scenarios.

Type B(U) packages are designed to meet IAEA regulations for the safe transport of radioactive material [1]. Certification under the IAEA regulations requires the assessment of package performance in Accident Conditions of Transport (ACT) tests. The ACT thermal test subjects a package to a fully engulfing, 800°C fire for 30 minutes [1]. This ACT thermal test presents very severe conditions that bound real-world accidents involving fires.

Many general purpose Finite Element Analysis (FEA) software codes can simulate the ACT thermal test conditions by applying heat transfer boundary conditions to a test specimen. The FEA approach can be tuned with conservative settings to produce bounding results for package certification. However, use of the FEA approach outside of package certification is limited as it does not capture the dynamic behaviour of a real fire. Simulating package performance in a real-world, dynamic fire scenario requires much more sophisticated tools.

NWMO is developing computer models to capture the dynamic nature of fires, and to simulate various transportation accident scenarios involving fires. A prototype of the Transportation Accident Fire Simulation (TAFS) model was presented at PATRAM 2016 [2]. This prototype model will henceforth be referred to as the *2016 TAFS Model*. This paper summarizes the progress-to-date of this model since PATRAM 2016 and discusses changes to the 2016 TAFS Model.

2016 TAFS MODEL

This section briefly summarizes the key elements of the 2016 TAFS Model presented at PATRAM 2016. Refer to the PATRAM 2016 paper for full details [2].

Modeling Approach

The 2016 TAFS Model is a coupled computational fluid dynamics (CFD) and Finite Element Analysis (FEA) model that can be used to simulate accident scenarios involving Type B packages in dynamic, transient fires. It was built in ANSYS. The solid test specimen (representative of a Type B package) was modeled using ANSYS Mechanical, a FEA code. The fire environment surrounding the test specimen was modeled using ANSYS Fluent, a CFD code. ANSYS Fluent and Mechanical were coupled together using Fluid Structure Interaction (FSI) so that the fire environment affects thermal state of the test specimen which, in turn, feeds back to and affects the fire environment.

Combustion Modeling

The fire environment was modeled using the Eddy Dissipation combustion model in Fluent. The Eddy Dissipation model is an infinitely fast chemistry submodel within the Species Transport model. The Species Transport model consolidates complex combustion chemical reaction steps into a simplified global reaction equation. The Species Transport model is a simple way to simulate interactions of reactants, formation of products, and release of heat energy. The Eddy Dissipation model couples the combustion reaction directly to turbulent flow and mixing. That is, the Eddy Dissipation model assumes that turbulent mixing of reactants (fuel and oxidizer) immediately produces products (carbon monoxide, carbon dioxide, water vapor, heat etc.) according to the global reaction equation for a particular fuel. Complete stoichiometric combustion is assumed at the mixing boundary. This idealized assumption simplifies chemistry modeling, should lead to maximum heat output, and should produce conservative results for the TAFS problem.

Fuel Source Modeling

The 2016 TAFS Model can theoretically model a fuel source as an arbitrarily shaped fuel pool. However, to keep the model simple, the fuel source was modeled as a fixed size circular fuel pool. The fuel pool was also assumed to be in a fixed location. That is, spilling and spreading of liquid fuel was not considered. Fuel was introduced into the simulation domain via a mass-flow-inlet boundary condition. The mass flow value was manually set constant at 0.054 kg/m^{2}s, the average kerosene burning rate estimated from experimental data for pool fires of similar size as those in the TAFS problem[1] [3]. It was noted that a constant mass flow boundary condition to simulate the vaporization of fuel from the fuel pool isn't quite representative of the real-world pool fires. In reality, fuel vaporization would vary across the fuel pool surface in response to fire conditions above the pool. However, complex fuel vaporization modeling was outside the scope of the PATRAM 2016 paper.

Heat transfer at the fuel pool surface was also not modeled. The fuel source inlet was manually given a black body temperature of 800°C in the radiation heat transfer calculations as a simplified representation for average flame temperatures.

Turbulence Modeling

Turbulence can be modeled using Reynolds Averaged Navier-Stokes (RANS) approaches, Large Eddy Simulation (LES) approaches, and Direct Numerical Simulation (DNS) approaches. RANS models are simple to use and carry relatively low computational cost while LES and DNS models carry prohibitively expensive computational cost. RANS models average turbulent effects over time and cannot model the real-time dynamic nature of fires. The computationally expensive LES and DNS models would not be practical for modeling long-duration fire scenarios. The 2016 TAFS Model used the Scale Adapted Simulation (SAS) turbulent model. SAS is a compromise between RANS models and LES models. SAS uses RANS models to simulate flow and heat transfer at boundaries, then switches to LES-like models to resolve larger eddies in the flow field away from boundaries. The SAS model allows the TAFS model to resolve real-time dynamic turbulent behaviour of fires, to accurately model heat transfer across fluid-solid boundaries, and to do so at a reasonable computational cost.

Radiation Heat Transfer Modeling

The 2016 TAFS Model used the Discrete Ordinates (DO) model for capturing radiation heat transfer. Relatedly, the kerosene-air mixture material in the TAFS had its Absorption Coefficient property set

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[1] Pool fire experiments show that the typical fuel level regression rate (an indication of fuel burning rate) is approximately 4mm/min for kerosene pool fires larger than 3m in diameter [3]. TAFS problems would involve fires in fuel pools approximately 7m in size. Assuming a kerosene density of 0.81g/cm^3, the mass flux value at the fuel pool boundary condition is estimated to be 0.054kg/m^{2}s.

to the Weighted Sum of Gray Gas Model (wsggm) so that Fluent can modify the absorptivity values of combustion products to account for radiative heat absorption/emission effects. The test specimen surface was assigned an emissivity value of 0.8 to represent a soot covered steel surface to conservatively maximize radiative heat input into the test specimen.

Soot Modeling

A large portion of heat flux from a hydrocarbon fuel fire is radiation from hot particles in the fire – soot. The 2016 TAFS Model modeled soot using Fluent's simplest built-in soot model: the one-step Khan and Greeves model.

Model Benchmarking

The 2016 TAFS Model was used to simulate conditions in a real-world fire test conducted at a Sandia National Laboratories [4]. The Sandia test subjected a large cylindrical calorimeter to a hydrocarbon fuel pool fire. The geometry and conditions of that Sandia test were modeled in the 2016 TAFS Model. The simulated temperature results were compared to the real-world fire test thermocouple measurements. The simulated temperature profiles did reveal non-uniform calorimeter temperature distributions, similar to the thermocouple measurement profiles. The 2016 TAFS Model did seem to capture the dynamic heat transfer characteristics of a real fire. However, the 2016 TAFS Model seemed to have underestimated heat input into the bottom of the calorimeter, underestimated the effect of wind on the leeward side of the calorimeter, and underestimated calorimeter temperature response in general. This suggested that the 2016 TAFS Model still required improvements.

Areas for Improvement

Factors that could have caused the discrepancy between the 2016 TAFS Model simulated results and the Sandia test thermocouple measurements were discussed. One factor could be the simplistic fuel inlet assumption. Modeling the fuel inlet with a uniform profile and constant mass flow rate is not quite representative of real-world pool fires. A potential area for improvement is in more realistic modeling of fuel vaporization across the fuel pool. Another factor could be the constant black body temperature assigned to the fuel pool boundary. The boundary may have acted as an artificial heat sink that drew heat away from the fire and from the bottom of the test specimen. Still another potential area for improvement is in better modeling of the fuel pool boundary. More sophisticated soot modeling was identified as another area for potential improvement. Finally, typical numerical simulation settings (such as mesh density and time-step size) could be tweaked to potentially improve model performance.

2019 TAFS MODEL UPDATE

This section describes changes to the 2016 TAFS Model since it was presented at PATRAM 2016. The latest model will be referred to as the *2019 TAFS Model*. Updated model benchmarking results are also presented in this section.

Modeling Approach

The 2016 TAFS Model separated the fluid domain from the solid domain to allow fine tuning of the mesh and the settings in each respective domain. Fluid Structure Interactions (FSI) link the two domains together so that they interact with each other and collectively influence the overall result. This FSI arrangement is typically used in problems where the fluid domain can deform the solid domain and the resultant deformation affects the fluid domain. For example, jet engine turbine blade design can be modeled in separate domains, a solid domain for the structural analysis of the blade, and a fluid domain for modeling airflow through the turbine. FSI then couples the two domains together so that pressures in the fluid domain bend the blade in the solid domain, and the resultant deformation of the blade affects airflow in the fluid domain. The TAFS problem however, does not involve large deformations. The fire environment does not impose significant fluid dynamics loads onto the solid test specimen, and the test specimen does not deform nor does it impose any dynamic effects on the fluid flow. Only heat is transferred between the fluid and solid domains. Fluent has the capability to model heat transfer in solid materials within a fluid domain. Therefore, the 2019 TAFS Model consolidates the TAFS problem into a CFD model, which is built completely in Fluent. That is, both the fire environment and the solid test specimen are modeled using CFD code. This change simplifies the model arrangement, removes the complexity of coupling together separate fluid and solid domain models, and reduces the computational cost associated with model complexity.

Combustion Modeling

The 2019 TAFS Model uses the same combustion modeling approach as the 2016 TAFS Model. The Eddy Dissipation model is still a practical model for simulating the chemical reactions within a fire.

Fuel Source Modeling

Modeling the fuel pool using a constant value mass flow inlet boundary condition in the 2016 TAFS Model had three problems: backflow, solver instability, and inaccurate representation of real fires. First, a mass flow inlet allows backflow. Combustion near the fuel pool surface lead to high pressure areas that overwhelm the mass inflow from the fuel pool. This pushes mass (along with its heat energy) out of the analysis domain through the fuel pool boundary condition, which is unrealistic. Second, the constant fuel mass value was based on average fuel burning rate achieved by fully developed fires. Applying that average burning rate at the beginning of the analysis run, just as the fire is beginning to develop, lead to solver instability. The constant mass flow inlet flooded the analysis domain with too much fuel too early, combustion could not develop correctly, and the solver would often crash. And third, a constant mass flow inlet boundary condition is not an accurate representation of fuel vaporization profile across a hydrocarbon fuel pool. In reality, the fuel vaporization rate would vary across the fuel pool surface in response to the fire conditions above. It is difficult to measure actual fuel vaporization rates at different points across the fuel pool during a fire. The closest approximation for fuel vaporization profile across the fuel surface is the flame temperature profile of the fire near the fuel surface. Large fires typically take on a conical shape. The hottest part of the fire is near the fire cone surface, where stoichiometric combustion occurs. As oxidizer (oxygen in the surrounding air) becomes consumed, the fire becomes progressively fuel rich towards the inner core. This fuel rich inner core burns cooler than the outer fire cone surface. This is reflected in flame temperature measurements of pool fires shown in Figure 1. In Figure 1, *R* is the radius of the fuel pool, and variables *r* and *z* refer to the measurement point radial location and height (above fuel surface) respectively. The *z/R=0.03* data series represents flame temperature measurements nearest to the fuel pool surface. That data series shows the flame temperature rising from the centre of the fuel pool towards the outer edge, peaking near 0.6 *r/R* ratio and falling off towards ambient temperature outside the fuel pool edge. This temperature profile should correlate to the fuel vaporization rate profile across the fuel pool as higher flame temperature would lead to higher fuel vaporization.

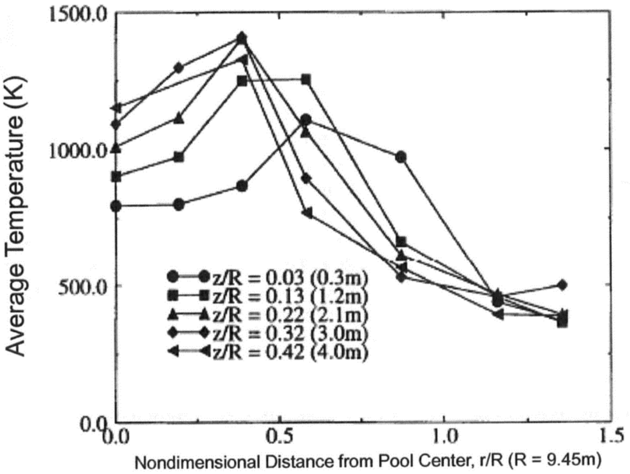

Figure 1: Average flame temperature profile at various flame heights [5]

The 2019 TAFS Model changed the fuel source modeling to address the aforementioned issues. The fuel pool is no longer represented by a mass flow inlet boundary condition. Instead, the fuel pool is modeled as a wall and given thermal material properties representative of a pool of liquid kerosene. This was done by copying values (such as density, specific heat, and thermal conductivity) from the Fluent built-in kerosene fluid material into a custom solid material, and applying that custom solid material to the fuel pool wall boundary condition. Changing the fuel pool from a mass flow inlet to a wall prevents unrealistic backflow of mass (and associated heat energy) out through the fuel pool boundary condition. Incidentally, this change also models more accurate heat transfer interactions between the fuel pool surface and the fire environment above. The fuel pool surface temperature can now rise in response to heat from the fire; and a hot fuel pool surface can radiate some of that heat to the bottom of the test specimen, representing what would happen in a real fire. Next, non-uniform fuel vaporization profiles were developed to better represent real fire behaviour. Four different profiles were developed, three to represent changing fuel vaporization during fire development, and one to represent steady burning of a fully developed fire in quiescent conditions. See Figure 2. The “Steady fire” profile was developed by manually tuning mass flux values until the profile is the same shape as the *z/R=0.03* data series in Figure 1 and the values result in an average mass flux of 0.054 kg/m^{2}s, matching average fuel burning rates from experiments [3]. The "Growing fire 1" through to "Growing fire 3" profiles adopt shapes that represent a fire that starts small at the centre of the fuel pool, then spreads out towards the pool edge, eventually developing into a steady burning fire with a fuel rich inner core, like a fully developed pool fire. The inflow of fuel vapors is modeled using mass source terms applied to a thin layer of cells at the fuel pool surface. Vaporization profiles in Figure 2 are encoded as a User Defined Function (UDF) and assigned to mass source terms in the fuel layer. For each cell, the UDF checks the position (r/R ratio) of the cell, and assigns the corresponding mass flux value to the cell mass source term.

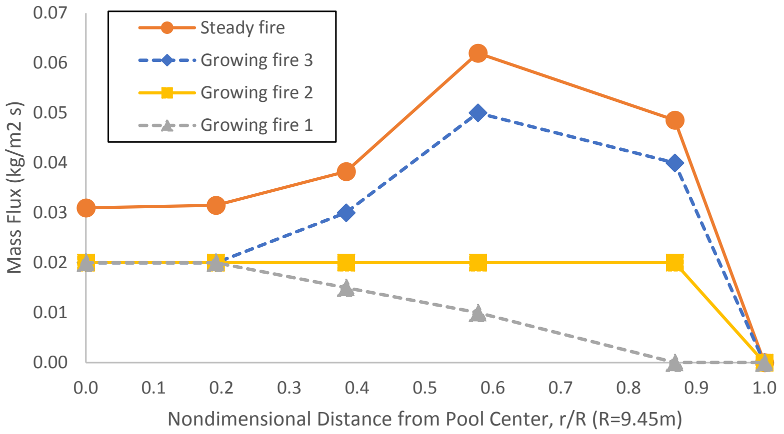

Figure 2: Mass flux profiles across the fuel pool at different stages of a fire

Ideally, fuel vaporization should be coupled with the fire conditions above the fuel pool surface. Typical large pool fires are pulsating phenomena. Flame temperatures within different parts of the fire continuously change. The state of the fire can also be affected by airflow around the fire. The fuel vaporization rate should be dynamically calculated based on heat flux or heat release rate from the ever-changing fire. This coupling can be implemented using User Defined Functions. Modeling fuel vaporization as a function of fire condition is reserved for future work.

Turbulence Modeling

The turbulence modeling developed in the 2016 TAFS Model is still appropriate for the TAFS problem. The SAS turbulence model accurately models heat transfer across test specimen boundaries and resolves eddies away from the boundaries to capture a fire's characteristic turbulent swirling behaviour. The 2019 TAFS Model continues to use the SAS turbulence model.

Radiation Heat Transfer Modeling

The 2019 TAFS Model continues to use Discrete Ordinates (DO) model to model radiative heat transfer.

Soot Modeling

Soot modeling in the 2019 TAFS Model was changed to the Moss-Brookes model per recommendation in the ANSYS theory manual [6]. More sophisticated models or approaches such as simulating particles using discrete phase modeling will be explored in the future.

Environmental Condition Modeling

Wind is one environmental condition that has significant impact on pool fires. Wind can change oxygen availability, can shift the shape and location of a fire plume, and can affect heat transfer within and around the fire. The 2019 TAFS Model can simulate wind conditions. The rectangular analysis domain easily represents cardinal directions. Setting any domain boundary as a velocity-inlet boundary condition turns that domain boundary into a wind source. More dynamic wind conditions can be modeled using a UDF. For example, a simple UDF script can be written to vary the inlet boundary velocity as a function of time to simulate changing wind conditions during the analysis. UDF is a specific ANSYS Fluent function, but other sophisticated CFD software should have similar functionality for specifying dynamic boundary conditions.

Model Benchmarking

The Sandia National Laboratories large scale fire test continues to serve as the real-world test data for benchmarking the TAFS model [4]. The geometry and conditions of the Sandia test were modeled in the 2019 TAFS Model. The simulated results were compared to the real-world fire test thermocouple readings. The comparison is shown in Figure 3 through Figure 6.

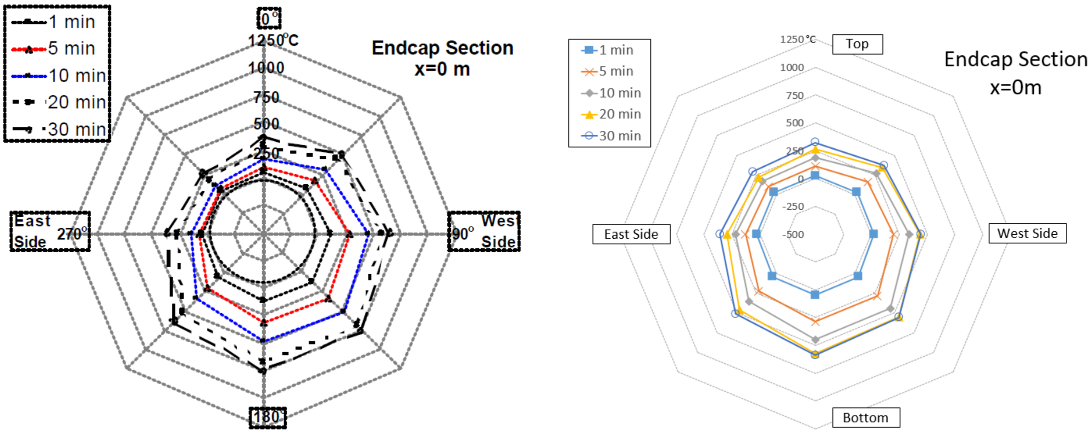

Figure 3: Comparing Sandia test thermocouple readings (left) to 2019 TAFS Model results (right), endcap section

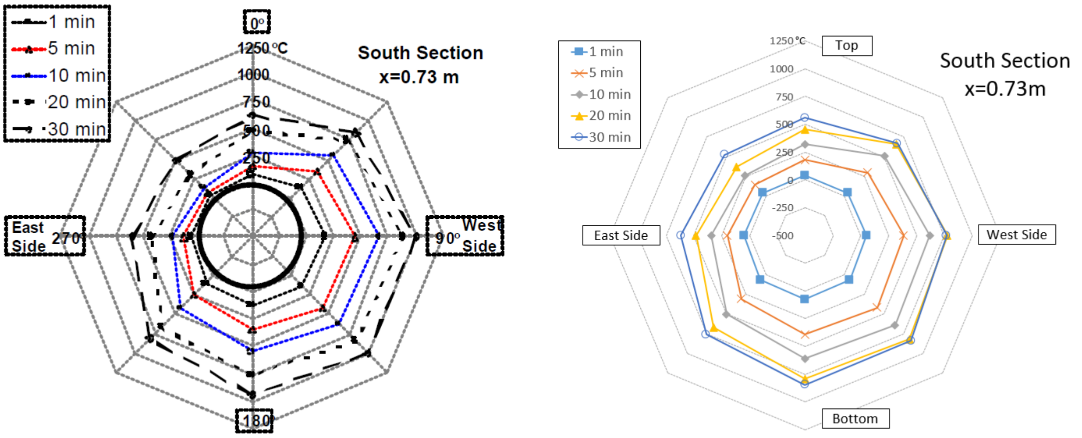

Figure 4: Comparing Sandia test thermocouple readings (left) to 2019 TAFS Model results (right), south section

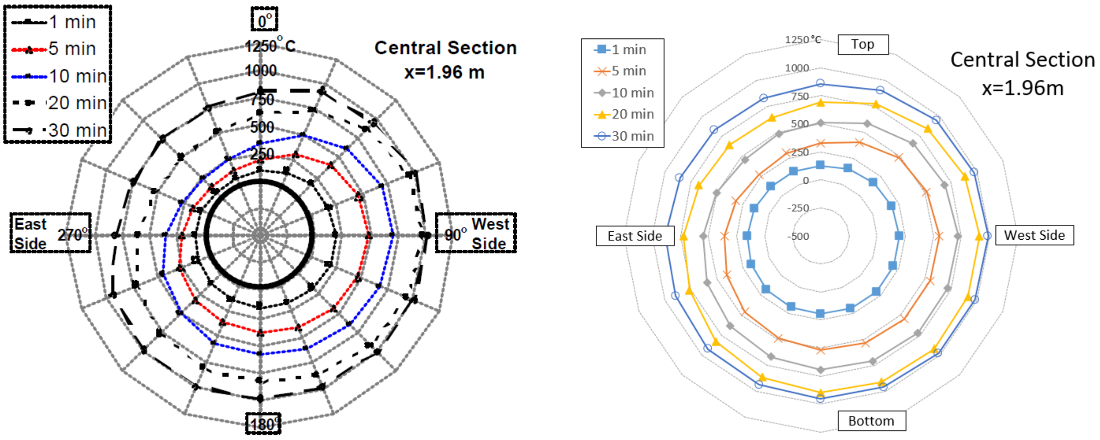

Figure 5: Comparing Sandia test thermocouple readings (left) to 2019 TAFS Model results (right), central section

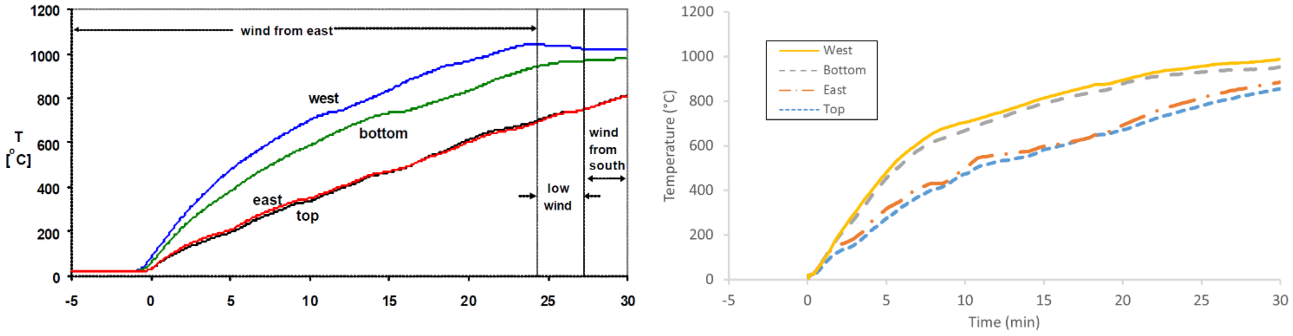

Figure 6: Comparing Sandia test thermocouple readings (left) to 2019 TAFS Model results (right), central section temperatures vs. time

Figure 3 through Figure 5 compare thermocouple measurements from the calorimeter in the real fire test to the simulated temperatures at corresponding thermocouple locations. Calorimeter temperature distributions were non-uniform in both the real fire test and the TAFS model simulated results. The 2019 TAFS Model captured the dynamic heat transfer characteristics of a real fire. The simulated temperature profiles had similar shapes as those of the real fire test, and temperature values also reached those measured in the real fire test. Figure 6 shows that the TAFS model replicated the temperature difference between east and west sides of the calorimeter. That is, the TAFS model successfully captured the effect of an easterly wind pushing the fire plume towards the west.

Limitations

Due to dynamic nature of real fires and the simulated dynamic nature of the TAFS model, individual thermocouple readings in a fire test cannot be directly compared to corresponding probe readings in the simulation results. It is only meaningful to compare general temperature distribution formed by multiple probe readings to the real fire test. In other words, the TAFS model results can only be meaningfully assessed qualitatively. A major limitation of the TAFS model is that it cannot be quantitatively validated.

The intent of this TAFS model is to replicate real fire scenarios. Its models and settings are tuned to accurately represent real-world fire conditions. Therefore, there are no margins for conservatism. It is not intended to be a design tool.

Due to these two limitations, the TAFS model shall not be used as the sole basis for design or for safety analyses of transportation packages. It may be used to support more conservative design analyses. The TAFS model can also be used for simulating hypothetical accident scenarios in support of public outreach and education.

CONCLUSION

A computational fluid dynamics (CFD) model was developed to simulate the response of large steel test specimen to large, dynamic pool fires. Development of the so-called Transportation Accident Fire Simulation (TAFS) model was discussed. The TAFS model was benchmarked against a real-world pool fire test. The TAFS model does capture the dynamic behaviour of fires and simulates test specimen temperature response in general agreement with real fire test data. However, the TAFS model can only be meaningfully assessed qualitatively and it does not have margin for conservatism. Therefore, the TAFS shall not be used as the sole basis for design or for safety assessment analyses of transportation packages. It may be used to support more conservative design analyses. The TAFS model can also be used for simulating hypothetical accident scenarios in support of public outreach and education.

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