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Combustion Simulation of Transportation Package Performance in Severe, Long Duration Fire Using Computational Fluid Dynamics Tools

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Abstract

The IAEA regulatory thermal test is designed to bound conditions in historic transportation fire accidents. The regulatory thermal test is a 30 minute, fully engulfing fire at 800°C. The severity of this thermal test is difficult to communicate to the general public, especially in comparison to recent real-world transportation accidents involving long duration fires. This paper describes NWMO's program to enhance staff skills and modelling techniques in simulating real-world long duration transportation accident fires. The fire modelling and simulation development program is designed to bridge the information gap between the 30 minute regulatory thermal test and real world long duration transportation accident fires.

Any established finite element analysis software can model heat transfer boundary conditions to simulate the regulatory thermal test. Modelling the highly dynamic nature of transportation accident fires requires sophisticated computational fluid dynamics analysis tools. Tools such as ANSYS Fluent model the chemical combustion reactions and their interactions with dynamic fluid flow. With Fluent, dynamics of a real-world fire can be modelled and compared to the severity of the regulatory thermal test. NWMO is building an understanding of dynamic nature of hydrocarbon fuel fires and their transient effects on large transportation packages by simulating the interaction between combustion and dynamic fluid flow.

Introduction

The Nuclear Waste Management Organization (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 in possible accident scenarios.

Type B(U) packages are designed to meet International Atomic Energy Agency (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 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. This paper summarizes the progress-to-date of this model development work.

Model development

Modeling approach

Physical testing of Type B(U) packages are typically done in pool fires. Type B(U) packages are usually quite large and require a large fire for testing. Those large fires can be sensitive to environmental factors such as wind and oxygen availability. Maintaining a large fire that fully engulfs a large package for 30 minutes is difficult. In addition, temperature distribution within a fire is non-uniform. Many factors contribute to a fire's dynamic behaviour. This work aims to explore those factors and develop a transient computational fluid dynamics (CFD) model to simulate dynamic fires. This Transportation Accident Fire Simulation (TAFS) model will be used to simulate transportation package response to hypothetical fires.

ANSYS Fluent and ANSYS Mechanical are the software tools used for this work but the principles apply to other, similarly capable Multiphysics simulation tools.

General CFD considerations

A number of typical CFD considerations and best practices apply to the TAFS problem. The TAFS problem is an external flow CFD problem. Therefore, its analysis domain is many times larger than the fire zone immediately surrounding the test specimen. This ensures that ambient conditions outside of the fire zone are simulated correctly. For this particular TAFS problem, the analysis domain is also rectangular in shape. Each one of its vertical sides correspond to a cardinal direction and can be mapped with a velocity boundary condition to simulate wind effects.

Typical CFD analysis domains should ideally be meshed with hexahedron elements that align with the fluid flow being studied. However, the TAFS problem is expected to involve highly turbulent and oscillating flow over potentially complex geometry. Therefore, the TAFS problem can be modeled appropriately using tetrahedron elements. Numerical diffusion, a major drawback with tetrahedron elements, will not get a chance to develop in a highly turbulent flow. The use of tetrahedron elements do not adversely affect solution accuracy in the regions of interest. Tetrahedron elements are also much more flexible for meshing complex geometry.

The fire zone is meshed with small elements to capture fine details of turbulent flow and geometry in

that area of interest. Inflation layers grow from the test specimen surface to correctly capture flow boundary layer and heat transfer on those surfaces. Mesh elements grow in size in the ambient surroundings away from the fire zone area of interest to minimize total element count.

The turbulence model used in the TAFS model works optimally with Courant Number close to 1 [2]. That is, the transient time step should be short enough that flow in the area of interest passes through one element in each time step. This results in time step size in fractions of a second. Discretizing a long duration fire (possibly lasting hours) with such small time steps could lead to impractical computation cost. Future work will explore balancing solution accuracy with computational cost.

Combustion modeling

A number of combustion models are available in Fluent. They are broadly divided into two categories: finite rate chemistry models and infinitely fast chemistry models. Finite rate models are appropriate for problems where flow characteristics change very quickly, within the same time scale as the combustion chemical reaction rate; or for problems where the analyst is interested in microscopic effects of turbulence on the combustion process. In finite rate chemistry problems, the combustion process can be limited/controlled by either turbulent fluid mixing or by chemical reaction rates. In contrast, fast chemistry models are appropriate for problems where turbulent flow characteristics do not change fast enough to disrupt the chemical reaction on the molecular level. The choice in appropriate model category (finite rate chemistry or fast chemistry) is guided by the Damkohler number (Da). The Damkohler number, in simplest terms, is the ratio of flow mixing time scale versus chemical reaction time scale. For $Da>>1$, chemical reactions proceed at much faster time scale compared to flow time scale. For $Da\sim1$, the flow and chemical reaction time scales are comparable. Transportation accident fuel spill fires likely involve hydrocarbon fuels such as gasoline, diesel, kerosene etc., which are designed to be fast burning. Fuel spill fires are also likely to proceed in relatively quiescent ambient conditions; the air flow involved would change at much slower time scale than the chemical reaction rate time scale. The analyst is also interested mostly in the macroscopic effect of turbulent flow on the combustion process, such as total heat output of a fire. Therefore, the TAFS problem has a Damkohler number much greater than 1 and is most appropriately modeled using fast chemistry combustion models.

Fast chemistry models are further divided into premixed, partially premixed, and non-premixed models. The TAFS problem is a non-premixed combustion problem as fuel is introduced into the analysis domain independently from the oxidizer. Two models remain for modeling non-premixed combustion problems: Species Transport model and Non-Premixed model. The Species Transport model is the simplest to implement and a good starting point for the TAFS problem. The Non-Premixed model will be explored in future work.

Combustion is a highly complex phenomenon in which fuel interact with oxidizer molecules through many chemical reaction steps to produce combustion products and heat. Fortunately, the overall

behaviour of a typical set of combustion reactions can be summarized and simplified into a global reaction equation. The Species Transport model models this global reaction equation and simulates interactions of reactants, formation of products, and release of heat energy. A number of sub-models are available within the Species Transport model category, from which, Eddy Dissipation model is the only fast chemistry model. The Eddy Dissipation model couples combustion reaction directly to turbulent flow. That is, Eddy Dissipation model assumes turbulent mixing of reactants (fuel and oxidizer) immediately produce products (carbon monoxide, carbon dioxide, water vapor, heat etc.) according to the global reaction equation for that particular fuel. Complete stoichiometric combustion is assumed at the mixing boundary. This idealized assumption should lead to maximum heat output in this simplified model, producing conservative results for the TAFS problem.

Fuel source modeling

Transportation accident fuel spills typically spread over large areas and continue to flow around the terrain as the fire progresses. A realistic simulation of transportation accident fires should account for dynamic flow of liquid fuel around the accident site, in combination with vaporization, in combination with fuel combustion. Unfortunately, interactions between liquid fuel flow, vaporization, and combustion of that fuel vapor are very difficult to model together. The current approach de-couples the liquid fuel spread (and vaporization) modeling from the combustion modeling. This work assumes a fixed location for a fuel pool and focus only on the combustion modeling. Simulation of liquid fuel spread is outside the scope of this paper and reserved for future work.

The TAFS model assumes a fuel pool of constant shape and size. The fuel level is also assumed to remain constant. Fuel is introduced into the domain via a mass-flow-inlet boundary condition. Mass flux at that fuel pool boundary condition is set to 0.054 kg/m^2s, the average kerosene burning rate estimated from pool fire experimental data [3]. A constant mass flux boundary condition assumes that fuel vaporization is uniform across the entire fuel pool surface. In reality, fuel vaporization would vary across the fuel pool surface in response to fire conditions above the pool. However, complex fuel vaporization modeling is outside the scope of this paper and reserved for future work.

Heat transfer at the fuel pool surface is an added modeling complication. The fuel pool surface acts as a wall that both absorbs and reflects radiation heat flux back into the fire and at the test specimen. Complex fuel pool modeling is reserved for future work. Currently, the fuel pool is simplified to behave like a wall at average fire temperature with respect to radiation heat transfer.

Turbulence modeling

Turbulence is a highly complex phenomenon that is very difficult to model. Accurate modeling of turbulence using CFD tools is a wide and deep field of study. Currently accepted turbulence models span a wide range between simple Reynolds Averaged Navier-Stokes (RANS) approach and Direct Numerical Simulation (DNS) approach. RANS models are simple to use and carry relatively low computational cost while the DNS approach is prohibitively expensive. In reality, the range of

practical turbulence models end with the Large Eddy Simulation (LES) model. And practicality of LES model is limited mostly to academia or to very simple problems over very short durations.

Scale Adapted Simulation (SAS), a hybrid between the RANS models and LES models, is a compromise between solution resolution and computational cost. In principle, SAS uses the SST-kω RANS models to simulate boundary flow then resolve larger eddies in the flow field away from boundaries. SAS has more forgiving requirements and lower computational cost compared to LES models. Detailed description of the SAS model can be found in the ANSYS documentation and in the ANSYS SAS turbulence modeling guide [2] [4]. The SST-kω model used near walls is the appropriate model for capturing heat transfer between fluid and solid interfaces [2]. SAS is the preferred approached for the TAFS problem because it can resolve the dynamic turbulent behaviour or fires and can accurately model heat transfer across the fluid-solid boundary layer, all at a reasonable computation cost.

Radiation heat transfer modeling

The dominant mode of heat transfer in hydrocarbon fires is typically radiation heat transfer. ANSYS documentation recommends the Discrete Ordinates (DO) model for combustion problems [2]. The DO radiation model discretizes space around each grid point into a finite number of solid angles or directions. Radiation properties are then calculated in each discretized slice. The resolution of the DO radiation model discretization is set with four parameters: theta divisions, phi divisions, theta pixels, and phi pixels. Higher resolution lead to higher accuracy solution but carries higher computational cost. The ANSYS documentation provide great detail on use of the DO radiation model and provides guidance on balancing discretization resolution with solution accuracy [2].

Activating radiation modeling in a combustion analysis has implications on material properties. In particular, the built-in kerosene-air mixture material must have its Absorption Coefficient property set to the Weighted Sum of Gray Gas Model (wsggm). The wsggm setting modifies absorptivity values of combustion products to account for radiative heat absorption/emission effects.

A second implication of activating radiation modeling is that surfaces participating in radiation heat transfer require specification of their emissivity properties. The surface of interest in this TAFS problem is the steel surface of the test specimen. Steel can have a wide range of emissivity values depending on surface finish. In addition, soot deposition in a fire can drastically change the surface finish of a test specimen. For simplicity, the test specimen may be assumed to be fully covered in soot throughout the analysis duration, giving it a constant emissivity between 0.8 and 0.9. These conservative emissivity values are supported by the accident conditions of transport thermal test requirements in the IAEA regulations [1].

Soot modeling

A large portion of heat flux from a hydrocarbon fuel fire is radiation off of hot particles in the fire –

soot. Fluent's built-in soot models calculate soot formation and adjusts the flow's absorptivity coefficient accordingly so that the radiation model can calculate the heat flux from soot. The simplest Fluent built-in soot model, the one-step Khan and Greeves model, is sufficient in this stage of model development [2]. More sophisticated models or approaches such as simulating particles using discrete phase modeling will be explored in the future.

Model validation

General purpose CFD analysis tools such as Fluent are extremely powerful and capable of simulating a wide variety of problems. This power and flexibility can very easily lead to good looking models that don't actually represent reality. The validation of simulation models against real-world test data is therefore very important for CFD analysis.

Fortunately, there is great interest in thermal analysis of Type B packages in severe fires. Transportation package designers around the world are diligent in designing packages that meet or exceed regulatory requirements, going so far as to physically fire test their designs at great expense. One experiment, conducted at Sandia National Laboratories by Kramer et al., is particularly suitable for validating the TAFS model [5]. The Kramer experiment subjected a large cylindrical calorimeter to a hydrocarbon pool fire to simulate Type B package testing under regulatory fire conditions. The pool fire in this experiment was fueled by JP-8, a kerosene-based hydrocarbon fuel. A number of thermocouples installed inside the calorimeter captured its response to the pool fire.

The simple geometry and conditions of the Kramer experiment were modeled in the TAFS model. Computational cost of this simulation was expected to be high. In the interest of minimizing analysis run time at this developmental stage, the mesh density and time step size requirements were relaxed. Despite computational cost reduction efforts, the analysis still took more than 6 days to complete on a powerful, business grade analysis workstation.

Figure 1 compares the simulated flame temperature distribution to photos taken during the experimental pool fire test [5]. Temperature distribution is not a definitive representation of flame shape but is a close approximation. Despite this imperfect representation, the simulated fire does take on the general shape of the real pool fire. The varied temperature distribution of the simulated fire shows that the TAFS model is capturing the dynamic turbulent nature of real fires.

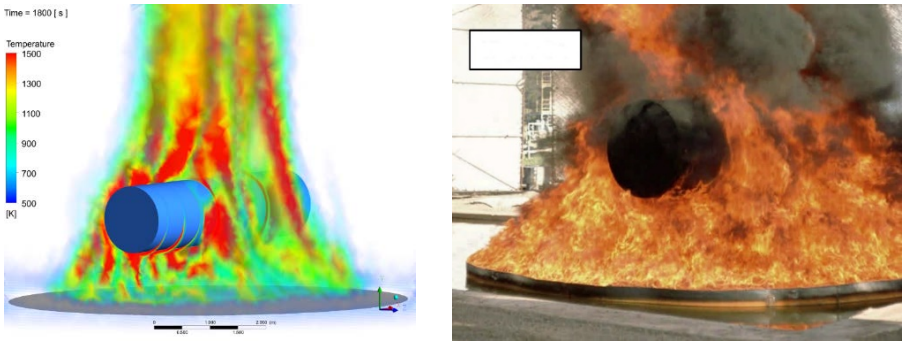

Figure 1: Comparison of simulated pool fire (left) with experimental pool fire (right) [5]

Thermocouple readings throughout the calorimeter during the pool fire test are summarized in Figure 2. Corresponding probe readings from the TAFS model are shown in Figure 3.

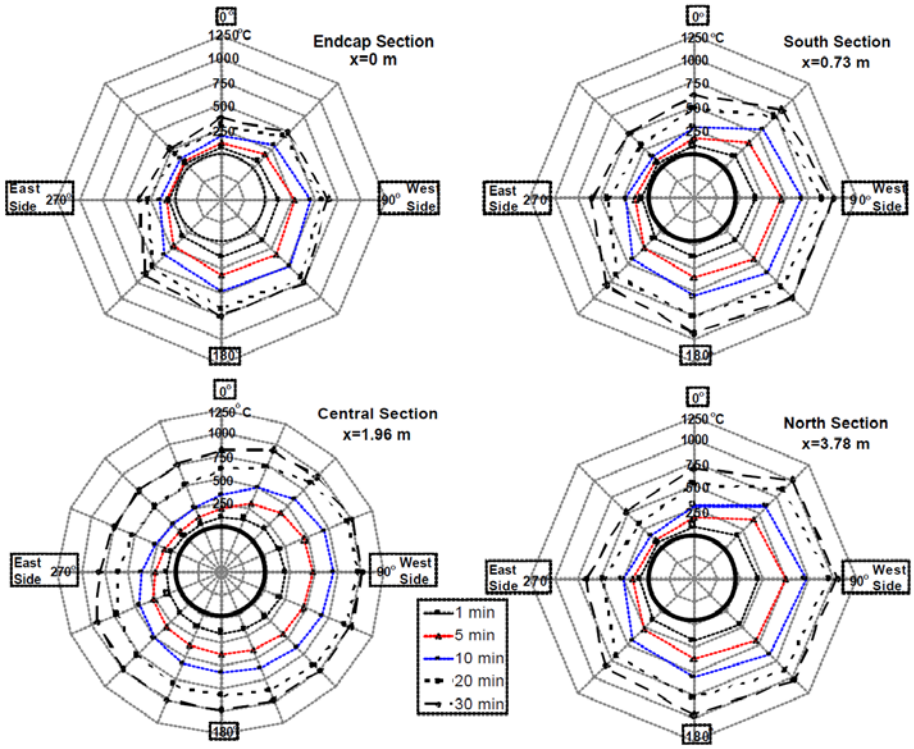

Figure 2: Thermocouple readings at various locations in the pool fire calorimeter [5]

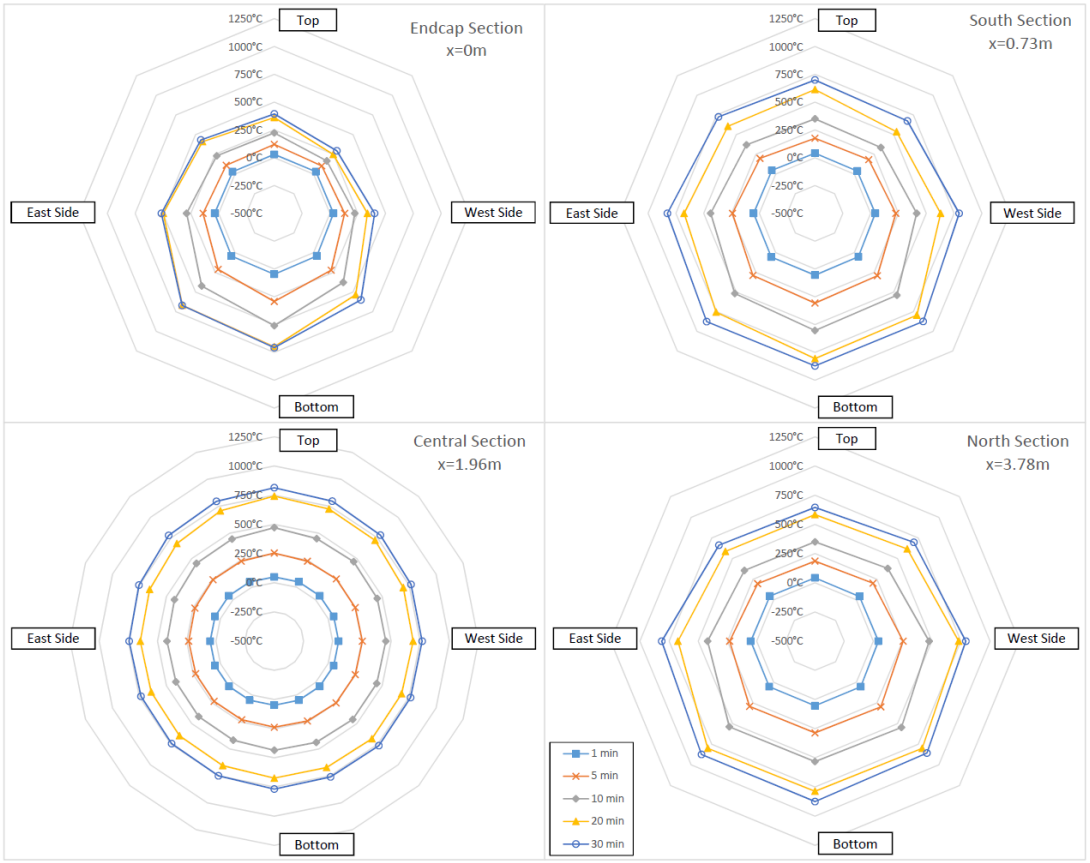

Figure 3: Corresponding temperature readings in simulated fire test specimen

Due to dynamic nature of the real fire and the simulated dynamic nature in the TAFS model, individual thermocouple readings in the 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. Such a comparison, shown in Figure 2 and Figure 3, reveal non-uniform calorimeter temperature distribution both in the real fire test and in the TAFS model. This suggests that the TAFS model is capturing dynamic heat transfer characteristic of a real fire. The simulated temperature profiles do look similar to those of the real fire test. However, TAFS model is underestimating the temperature distribution within the calorimeter. The temperature discrepancy varies across the calorimeter, with the largest discrepancy near the bottom and on the West side of the calorimeter. The TAFS seems to be underestimating heat input into the bottom of the calorimeter and underestimating the effect of wind on the leeward side of the calorimeter. This suggests that the TAFS model is not yet fully validated.

A factor that could have contributed to the TAFS model deficiency is the simplistic fuel inlet assumption. Modeling the fuel inlet with a uniform profile is not completely accurate. Fuel vaporization rate near the centre of the fuel pool should be lower than average while vaporization rate towards the pool edge should be higher than average. The centre of the fuel pool is a low oxygen and low combustion environment so input of fuel vapor at the average rate could have led to unrealistic accumulation of fuel. A large fuel rich zone at the centre of the fire would cool the overall temperature of the fire and therefore reduce overall heat input into the test specimen. Relatedly, limiting fuel flow at an average value near the pool edge could be underestimating the fuel vaporization rate (and combustion intensity) in those hotter areas. Future work will explore the accurate modeling of the complex fuel vaporization phenomenon.

The simple fuel inlet assumption could have further contributed to TAFS model deficiency by inaccurately modeling radiation heat transfer at the fuel pool boundary. The fuel pool boundary condition may have inappropriately acted as a heat sink for radiation heat flux, artificially cooling the base of the fire and the bottom of the calorimeter. The interaction between the fuel pool surface with the fire and any test specimen within the fire is not fully understood at this point. Future work will explore the accurate modeling of heat transfer interactions across fuel pool surface in fires.

The simple one step soot model used may have contributed to the underestimation of radiative heat flux off of soot particles. Future work will explore more sophisticated soot models or more sophisticated approaches such as simulating soot particles using Discrete Phase Modeling.

Finally, a common cause for simulation model deficiency is inadequate mesh density. Element sizes in the fire zone may be too large to capture small turbulent swirls and eddies in the fire that would have contributed to more thorough mixing of fuel and oxidizer. Eddy Dissipation Model simulates the combustion process based on turbulence. If turbulence is not captured in sufficient detail due to poor mesh density, then the model will underestimate combustion, leading to reduced heat input into the test specimen. In addition, the inflation layer mesh on the test specimen may be too thick. During

the validation run, y+ values at the calorimeter surface averaged around 3, which is still quite good. However, y+ values closer to 1 should improve heat transfer calculation accuracy. Future analysis will run on more refined mesh.

Related to mesh coarseness is time step coarseness. A coarse time step size could lead to the turbulence model missing flow details. A relatively large time step size was used for the validation simulation run to minimize run time. The resulting Courant Number turned out to be between 2 and 3. The SAS turbulence model is more accurate when Courant Number is closer to 1. Future analysis runs will use smaller time steps to ensure the turbulence model fully captures flow characteristics.

Conclusion

A coupled CFD-FEA 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, in its current state, was compared against a real-world pool fire validation 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 underestimates temperature response in some areas. The TAFS, in its current stage of development, is not yet fully validated. Some possible explanations for the discrepancy were discussed and future work planned for the continual development of the TAFS model.

Once fully validated, the TAFS model can aid the design of a physical fire tests for testing design to regulatory standards; and help study package performance in possible real-world accident scenarios involving severe, long duration fires.

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