

COMPUTATIONAL FLUID DYNAMICS COMBUSTION SIMULATION OF TRANSPORTATION PACKAGE PERFORMANCE IN SEVERE, LONG DURATION FIRE

Y. Sui

Nuclear Waste Management Organization (NWMO), Toronto, Ontario, Canada

ysui@nwmo.ca

Abstract

The Nuclear Waste Management Organization (NWMO) is designing a new transportation package to meet international regulations for the safe transport of radioactive material. One requirement in the regulation is an accident condition thermal test involving a 30-minute, fully engulfing fire at 800°C. That regulatory test presents severe bounding conditions based on international experience and research. However, fresh on the minds of the public are examples of transportation accidents that have resulted in long duration fires. Therefore, the regulatory thermal test is not immediately relatable to the general public. Reconciling the 30-minute regulatory thermal test with long duration transportation accident fires lasting hours requires careful discussion and verbose explanation. NWMO wishes to add support to that discussion by building skills and expertise necessary to simulate hypothetical transportation accident scenarios involving NWMO's transportation packages and severe, long duration fires.

The regulatory thermal test is a set of well-defined conditions that are easily modeled in finite element analysis software using heat transfer boundary conditions. In contrast, modeling highly dynamic nature of transportation accident fires requires sophisticated, computational fluid dynamics analysis tools. This work explores the use of ANSYS Fluent for modeling severe, long duration fires. By simulating complex interactions between chemical combustion reactions with dynamic fluid flow, NWMO builds understanding of dynamic nature of fires and their transient effects on large transportation packages.

1. 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 used nuclear fuel transportation packages. Accurate modeling or simulation of fires can be used to analyze package performance in regulatory fire tests and in possible accident scenarios.

A package for transporting Canada's used nuclear fuel must be designated as a Type B(U) transportation package. 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. A package designed to survive the ACT thermal test will stay well within its performance envelope during any reasonably conceivable real-world accident involving fires.

However, severity of the ACT thermal test is difficult to appreciate. The most severe aspect of the ACT thermal test – the fully engulfing fire requirement – is easy to gloss over. Instead, the focus shifts to the test duration. 30 minutes does not feel long enough, especially to members of the public whose recent

memory contain instances of long duration fire transportation accidents. For example, severe traffic accidents involving petroleum carrying transport trucks can lead to fires lasting hours. A collision between a petroleum transport and a used fuel transport is possible but low in probability. Even in such an unlikely scenario, the resulting large scale oil spill fire will spread over a large area, and move within the affected area with changing fuel availability and fluctuating environmental conditions. The likelihood of a fire staying localized to a precise area to fully engulf a transportation package for 30 minutes is extremely low. Unfortunately, explanation of low probability of such a scenario and discussion of the dynamic nature of large scale fuel spill fires are not always convincing enough to reconcile the 30 minute ACT thermal test with real-world long duration fires. For this reason, NWMO is developing a computer model to capture the dynamic nature of fires, and to simulate various transportation accident scenarios involving fires.

2. Model development

2.1 Modeling approach

The regulatory ACT thermal test is designed in such a way that facilitates straightforward analysis. The fully engulfing and constant fire temperature conditions are easy to model with convection and radiation boundary conditions in a numerical thermal analysis. The fire duration is also easy to capture using transient analysis. Any commercial Finite Element Analysis (FEA) software with basic thermal analysis capability will be able to model conditions of the regulatory ACT thermal test. In contrast, physical recreation of the regulatory fire test conditions in the real-world is far more difficult. Type B(U) packages are typically tested in pool fires. Fires are dynamic and respond to environmental factors such as wind and oxygen availability. Type B(U) packages are typically quite large and therefore require a large fire for testing. Those large fires can be sensitive to environmental factors and can also create their own environmental condition, like wind. Maintaining a large fire that fully engulfs a large package for 30 minutes is difficult. In addition, temperature distribution within a fire is not uniform. Therefore, test specimen response to a real-life fire test cannot be captured using basic boundary conditions FEA thermal analysis.

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 model will be used to simulate transportation package response to hypothetical fires. ANSYS Fluent is the software tool used for this work but the principles apply to other, similarly capable CFD tools.

2.2 Analysis domain

CFD analysis problems can be roughly divided into two types: internal flow and external flow. In an internal flow problem, the domain (or extents of the analysis) is typically defined by the physical geometry. For example, the domain for a liquid flow within a pipe problem is bound by the pipe geometry. In contrast, transportation accident fire simulation is an external flow problem. The test specimen is burned in an open environment. The analysis domain therefore needs to be large enough to encompass both the fire zone immediately surrounding the specimen and the ambient air outside of the fire zone. The bottom of the domain is bound by solid ground but domain extents in all other directions must be sized large enough to simulate surrounding ambient conditions. There isn't any rigid rules for sizing the domain for external flow problems. Typical recommendations range between 5 times to 10 times the characteristic size of the area of interest. For the transportation accident fire simulation, the

area of interest is the fire zone, the characteristic size of which can be approximated by the fuel pool size.

The shape of the domain can be flexible. A cylinder is the simplest shape to model the domain but a square domain is more suitable for this application. Figure 1 shows an example of what the analysis domain could look like. The bottom horizontal face of the domain is a solid surface representing the ground. The remaining faces represent ambient conditions far away from the fire zone. The four vertical faces of the domain are each associated with a compass direction. Air flow boundary conditions can be easily mapped to those vertical faces to simulate windy conditions if desired. The fuel pool (and the fire zone above it) is located at the bottom centre of the domain. Test specimen geometry can be easily added to the domain above the fuel pool in whatever orientation the scenario-under-study calls for.

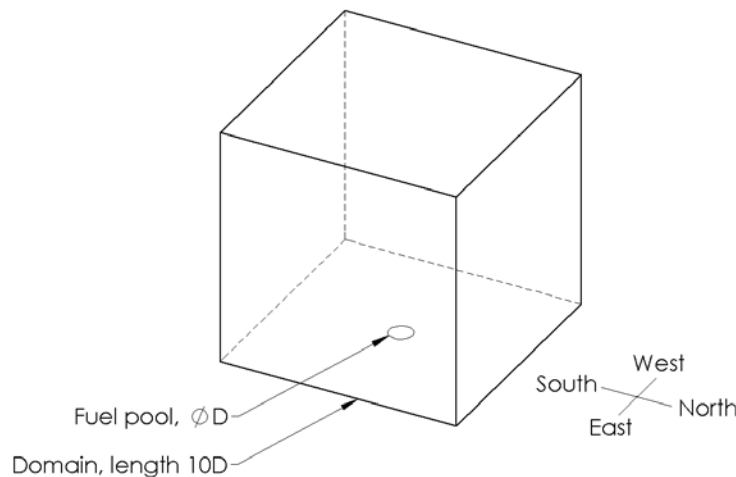


Figure 1 Analysis domain example

2.3 Meshing

Meshing is the discretization, or breaking up of the domain into small elements containing nodes (also called grid points) at which flow calculations are performed. Simulation quality depends greatly on quality meshing of the analysis domain.

Domain discretization or meshing for CFD analysis can be a large and complex topic. Fully detailed discussion of meshing is outside the scope of this paper. Only the most pertinent details are discussed.

A major factor contributing to simulation quality is mesh size. A fine mesh made of small elements is required to capture details in the fire zone. The test specimen also adds some geometry complexity to the analysis. A fine mesh is needed to conform to the test specimen geometry in sufficient detail to ensure air flow around the specimen is correctly simulated. Mesh fineness or density is a compromise with computational cost. The number of elements, grid points, and therefore analysis run time grow exponentially with increasingly dense mesh. For optimal balance of solution accuracy and computational cost, the mesh in non-critical areas is allowed to coarsen. In the example mesh shown in Figure 2, the fire zone (with a round test specimen) at the centre is densely meshed with small elements. That dense, fine mesh relaxes to larger elements further away from the fire zone. Ambient conditions outside the fire zone are expected to be near quiescent, with slow changes in air flow and thermal

characteristics. Therefore, coarse mesh in those non-critical areas away from the fire zone does not affect solution quality.

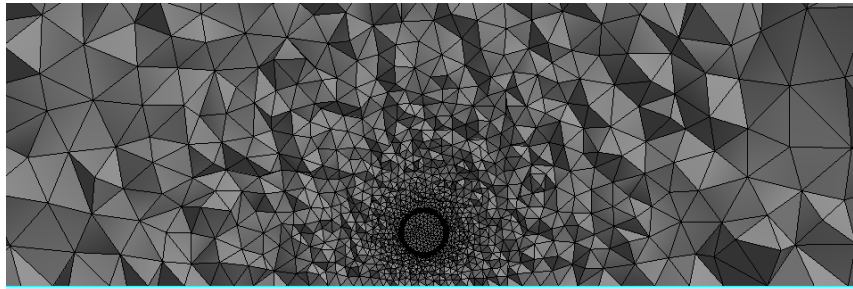


Figure 2 Example mesh

Another important factor contributing to simulation quality is appropriate boundary meshing. Fluid flow across boundaries is a complex phenomenon. Flow near a boundary must transition from its free stream velocity down to zero at the boundary surface. This so called velocity boundary layer is very thin and lie very close to the boundary surface. In the physical world, this boundary layer is described by the Law of the Wall, a well-established and experimentally verified fluid dynamics principle. The Law of the Wall is well documented and can be found in any fluid dynamics textbook. In the CFD world, capturing details of the very thin boundary layer requires an inflation layer mesh – many layers of small elements near the boundary surface. Inflation layers begin with a very thin first layer at the boundary surface, then grows in distance and element size away from the surface until its upper layer blends into the surrounding mesh. The example in Figure 3 shows an inflation layer mesh around a cylindrical test specimen. Tuning of the inflation layer to accurately resolve (or model) the flow velocity boundary layer is critical to solution quality. An appropriate inflation layer is especially important for problems involving heat transfer across fluid-solid interfaces, such as the transportation accident fire simulation problem. Adequacy of the inflation layer can be inferred from the y^+ metric. Y^+ is a non-dimensional variable used in the Law of the Wall principle. In the CFD simulation context, the y^+ metric indicates the location of the first grid point in the fluid boundary layer. The appropriate location of the first grid point depends on the turbulence model and wall models used in the analysis. The turbulence model used in this transportation accident fire simulation is the SAS model (justifications discussed in section 2.8), ideally requires a y^+ value between 1 and 3. To achieve y^+ value close to 1, the first grid point must be very close to the wall. The inflation layer mesh is often tuned with an iterative approach, where the analyst adjusts inflation layer thickness based on y^+ values from multiple analysis test runs.

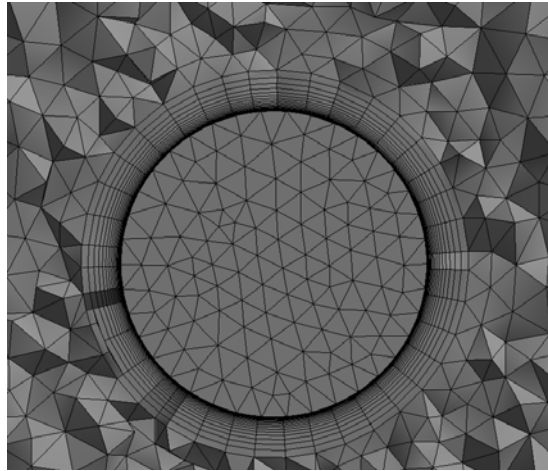


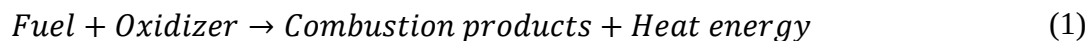
Figure 3 Inflation layer example

2.4 Transient time step

Transient analysis is the simulation of a flow field over a specified time period. In the case of the transportation accident fire simulation problem, fire duration is the specified time period. Transient simulations are solved by computing a solution for many discrete points in time. The time step size is the amount of time between each successive solve points in time. Transient time steps essentially discretize the analysis in the time dimension. The transient time step must be sized appropriately to capture changes in the flow field so that details of important parameters are preserved from one time step to the next. Time step sizing can be guided by the Courant Number metric, discussed in more detail in the ANSYS documentation [2]. The Courant Number basically approximates how many mesh elements the fluid passes through in one time step. The Courant Number is typically calculated in the area of interest, which is the fire zone in the case of the transportation accident fire simulation model. Typical recommendation for Courant Number value is between 1 and 10 [2].

2.5 Combustion modeling

Combustion is a highly complex phenomenon where fuel molecules interact with oxidizer molecules through many chemical reaction steps to produce combustion products and heat. Fortunately, the overall behaviour of typical combustion reactions can each be summarized in a respective global reaction equation. For example, equation (1) shows the general format of global reaction equations.



The most common oxidizer is air as it contains oxygen and is readily available. The amount of fuel compared to amount of air in a reaction can be expressed as the air-to-fuel ratio (A/F). The stoichiometric A/F is the ratio at which the exact amount of oxidizer is available to completely consume all fuel.

Combustion problems can be broadly categorized into two categories: premixed and non-premixed combustion, depending on how the fuel and oxidizer enter the reaction zone. Premixed combustion, as its name suggests, models the situation where fuel and oxidizer are already mixed before entering a reaction zone. Premixed combustion problems are characterized by a known and relatively constant A/F. In contrast, fuel and oxidizers in non-premixed combustion problems enter the reaction zone in separate streams. A kerosene pool fire is an example of non-premixed (also called diffusion)

combustion. In a pool fire, evaporated fuel vapors encounter and mix with oxidizers (oxygen) in the surrounding air. A large pool fire generates turbulent air flow, which makes the fuel/air mixing boundary highly dynamic. Modeling non-premixed combustion problems requires tracking the dynamic fuel-oxidizer mixture, as well as tracking combustion of that mixture.

Transportation accidents that lead to severe, large scale fires likely involve burning large quantities of spilled petroleum fuel. Such fuel spill fires are examples of non-premixed combustion. Therefore, this work focuses on modeling non-premixed combustion to simulate severe transportation accident fires.

A number of combustion models are available for modeling non-premixed combustion. The models are first divided into two categories: finite rate chemistry models and infinitely fast chemistry models. Finite rate chemistry models are appropriate for problems where flow characteristics change very quickly, within the same time scale as the combustion chemical reaction rate; or for problem where the analyst is interested in microscopic effects of turbulence on the combustion process. For example, modeling jet engine performance would require finite chemistry models as the flow is fast enough to potentially disrupt the combustion process. In contrast, fast chemistry models are appropriate for problem where turbulent flow characteristics change much more slowly compared with the chemical reaction rates. That is, the chemical reaction proceeds so quickly that the slow flow does not have time to disturb the chemical reaction on the molecular level. 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 likely change at a 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, fast chemistry models are most suitable for simulating fuel spill fires.

Fast chemistry models available in Fluent are: Species Transport models, Premixed Combustion models, Non-Premixed Combustion models, and Partially Premixed Combustion models. Premixed and Partially-Premixed models are not appropriate since a fuel spill fire is a non-premixed problem (as discussed earlier). Species Transport models and Non-Premixed models are the remaining model options.

Species Transport models model the mixing and transport of chemical species such as fuel, air (oxygen, nitrogen, etc.), and combustion products (carbon dioxide, carbon monoxide, water vapor, etc.). The combustion itself is simulated by enabling the 'Volumetric Reaction' feature, which activates Fluent's built-in reaction mechanism equations. Those reaction equations calculate production of combustion products (including heat) from interaction between fuel and oxidizer species. A number of sub-models are available within the Species Transport models category, from which, Eddy Dissipation model is the only fast chemistry model. In the simplest terms: Eddy Dissipation model assumes that combustion proceeds whenever turbulence is present. Mixing of fuel and oxidizer is directly related to the turbulence characteristics of the flow. Combustion is then modeled as a one-step reaction according to a global reaction equation. That is, as soon as reactants (fuel and oxidizer) come into contact through turbulent mixing, they are immediately converted into combustion products (carbon monoxide, carbon dioxide, water vapor, and heat) according to the global reaction equation for that particular fuel. Complete stoichiometric combustion is assumed at the mixing boundary. This idealized assumption leads to maximum heat output in this simplified model, producing conservative results with respect to simulating severe fire conditions. The ease of use and conservative results makes the Species Transport Eddy Dissipation model an ideal starting point for modeling combustion in transportation accidents.

The Non-Premixed Combustion model is also an appropriate choice for simulating fuel spill fires. Setup and tuning of the Non-Premixed Combustion model is more complex than the Eddy Dissipation model and is outside the scope of this work.

2.6 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. Liquid flow and even vaporization of liquid flow are relatively simple to simulate. However, the interactions between liquid fuel flow, vaporization, and combustion of that fuel vapor are very difficult to model. The domain must become much larger, detailed terrain geometry would add to mesh element count, and the addition of liquid flow models, vaporization models, and two-way coupling of those models with combustion models dramatically increase complexity. Computational cost would rise exponentially. A more practical approach would be to decouple the liquid fuel spread (and vaporization) modeling from the combustion modeling. That is, simulate liquid fuel spread in a separate analysis to estimate fuel pool shape, size, and volume. The combustion of those fuel pools can then be simulated with a combustion model. Modeling of liquid fuel spread and vaporization is not considered in the transportation accident fire simulation model and is therefore outside the scope of this paper.

The transportation accident fire simulation 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. The mass flow rate at that fuel pool boundary condition is set to $0.054 \text{ kg/m}^2\text{s}$, the kerosene burning rate estimated from pool fire experimental data [3]. Modeling the fuel inlet with a constant mass flow rate essentially assumes that fuel vaporization is uniform across the entire fuel pool surface. This is not absolutely accurate as in reality, fuel vaporization is variable across the fuel pool surface. Many factors contribute to variations in local fuel vaporization rate, chief among them is temperature distribution across the fuel pool surface. For example, the centre of a large circular pool fire can be starved of oxygen and burn relatively cool compared to the fire's outer edge. Fuel vaporization rate at the cooler centre would be lower than vaporization rate at the hotter outer edges. The current uniform fuel vaporization rate assumption is a good starting point for the transportation accident fire simulation model; future work will investigate non-uniform fuel vaporization profiles on the fuel inlet or even couple the flame temperature together with the fuel vaporization profile.

2.7 Material

The Eddy Dissipation combustion model requires the use of mixture type materials that model various components of oxidizer, fuel, and combustion products. The Fluent built-in kerosene-air mixture material is most appropriate for this transportation accident fire simulation. Kerosene is a hydrocarbon fuel similar to gasoline and diesel and therefore represents the types of fuels that could be encountered in a transportation accident.

Two solid materials are needed for this simulation work: steel and ground surface material. Thermal conductivity is the only parameter of interest in solid materials for this combustion analysis. The built-in Fluent steel material is sufficient to model the thermal characteristics of the transportation packages (test specimen) under study. Heat transfer into the ground is an unimportant parameter in this combustion analysis. For simplicity, the ground is assumed to have similar thermal conductivity

characteristics as concrete. Therefore, the built-in Fluent calcium-oxide material is used to model the ground surface.

2.8 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. The most accurate approach would discretize flow into tiny fluid parcels and calculate the properties of each fluid parcel as it interacts with its neighbouring fluid parcels. This approach, an extremely simplified explanation of Direct Numerical Simulation (DNS), would resolve all details of the flow down to near molecular level. This DNS approach carries extremely high computational cost and is considered impractical for most engineering applications. The more practical approach is to model turbulence and calculate only its general, time-averaged effects. The most widely used approach for industrial flows is the Reynolds Averaged Navier-Stokes Simulation (RANS) approach. Most practical applications are only concerned with the time-averaged effect of turbulence so the RANS approach is an excellent compromise unnecessary accuracy for much reduced computational cost. Numerous RANS models have been developed through years of experimentation and research.

The two approaches discussed thus far represents ends of the turbulence modeling approach spectrum. At one end, the DNS approach directly calculates turbulence characteristics at impractically high computational cost. At the other end, the RANS approach models turbulence and calculates only its generalized, averaged effects at very low computational cost. In between these two ends of the spectrum lie a range of approaches called Scale Resolving Models. The Scale Resolving models mix DNS and RANS approaches and treat turbulence with models in some areas and with direct calculation in other areas. The most widely used Scale Resolving model is the Large Eddy Simulation (LES) model.

RANS models are very useful for studying generalized behaviour of a flow problem. However, it is unsuitable for modeling dynamic fires as much of the transient details would be lost through time-averaging of turbulence characteristics.

The LES model is described in extensive detail in an ANSYS LES quick start guide [4]. Accurate application of LES requires very fine and square mesh near walls [2][4]. The inflation layer mesh shown in section 2.3 is dense only in the direction perpendicular to the boundary. LES models would require very fine mesh in directions both perpendicular and parallel to the boundary. This fine mesh requirement leads to exponential growth in element and grid point count. LES model also have strict time step size requirement. The recommended Courant Number for LES simulation is 0.5 [4]. This combination of fine mesh and small time step requirements grow the computational cost exponentially, rendering the LES models impractical for all but the simplest geometry problem over very short analysis duration. The transportation accident fire simulation involves large test specimen at the meters scale and analysis domain at the tens-of-meters scale. The fine mesh element required for LES simulation is likely to be at the millimeters scale. Meshing such a large domain with such tiny elements would require an impractical element count in the millions or billions. The fine mesh resolution requirement further compounds into finer time discretization requirements. In order to achieve the recommended Courant Number of 0.5, the time step size may need to be in the millisecond range. Discretizing transportation accident fires, which could have duration in the minutes to hours range, into tiny millisecond time steps would require a massive number of time steps. Fully simulating a transportation accident fire could mean repeatedly solving a billion grid points at very small time steps

for millions of time steps. Simulating the transportation accident fire problem using the LES model carries an impractical computational cost.

Scale-Adaptive Simulation (SAS), a hybrid between the RANS models and LES models, is a compromise between solution resolution and computational cost. In principle, SAS uses RANS models to simulate boundary flow and uses LES models to resolve eddies in the flow field away from boundaries. SAS have much more forgiving mesh density and time step size requirements compared to LES models. The inflation layer mesh like the example shown in section 2.3 can be used. The recommended Courant Number for SAS simulation is 1. Detailed description of the SAS model is outside the scope of this paper; more details can be found in the ANSYS documentation and in the ANSYS SAS turbulence modeling guide [2][5]. SAS is the preferred approach for the transportation accident fire simulation problem. SAS is capable of simulating the dynamic nature of a fire by simulating turbulent mixing of fuel and oxidizer with LES-like quality at reasonable computational cost.

2.9 Radiation modeling

The dominant mode of heat transfer in fires is typically radiation heat transfer. Fluent has many radiation models to choose from. 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]. Based on ANSYS examples, the following settings are deemed appropriate for the transportation accident fire simulation problem: theta divisions, phi divisions of 5, and theta pixels, phi pixels of 3.

Computational cost of the DO radiation model can also be tuned in the time dimension via the parameter – Energy Iterations per Radiation Iteration. With this parameter, the analyst can choose the number of regular flow calculation iterations to run between each radiation calculation iteration, essentially reducing the total number of radiation calculation iterations and reducing overall run time. In the case of the transportation accident fire simulation, radiation is the dominant mode of heat transfer and therefore should be calculated accurately. The Energy Iterations per Radiation Iteration parameter is set to 1 to ensure that radiation calculations are run at each flow iteration.

Activating radiation modeling in a combustion analysis has implications on material properties. In particular, the kerosene-air mixture material must have its Absorption Coefficient property set to “wsggm-domain-based.” The Weighted Sum of Gray Gas Model (WSGGM) is a built-in Fluent model to account for different absorptivities of CO₂ and H₂O species within the reacting mixture. This setting contributes to correct modeling of radiation absorption properties of flow within the simulated fire.

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 transportation accident fire simulation is the steel surface of the test specimen. Steel can have a wide range of emissivity values depending on surface finish. Soot deposition in a fire can drastically change the surface finish of a test specimen. For simplicity, the test specimen is assumed to be fully covered in soot throughout the analysis duration. This assumption is expressed as a constant surface emissivity

value of 0.8 for the test specimen. This conservative emissivity value is supported by the accident conditions of transport thermal test requirements in the IAEA regulations [1].

2.10 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.

2.11 Fluid-solid interface

Fluid-solid interface (FSI) is a feature in ANSYS workbench that couples CFD analysis with FEA analysis. The transportation accident fire simulation is well suited for FSI modeling. A CFD domain simulates the dynamic fluid environment of a severe fire, while an FEA domain models heat conduction and temperature distribution throughout the solid test specimen. The two separate analyses are coupled together through a fluid-solid interface at the test specimen surface. Heat flux values are passed from the CFD domain to the FEA domain and temperature values are passed from the FEA domain back to the CFD domain. This so called two-way coupled system solves both the CFD domain and FEA domain in each time step, simulating the interaction between the solid test specimen with its fluid surroundings.

FSI coupling of separate analysis domains focuses different solvers on their respective areas of specialization. That is, Fluent focuses on simulating fluid flow in the CFD domain while calculation of heat conduction in the test specimen is delegated to ANSYS Mechanical, a solver better suited for solid FEA. Mesh within each domain can be optimized for its respective solver without compromising mesh quality in the other domain.

The use of FSI coupling also minimize computational cost of simulating the post-fire cooldown phase. The cooldown phase simply subjects the post-fire test specimen to quiescent ambient conditions until temperatures at all points within the specimen are decreasing. Simulating that ambient condition does not require sophisticated CFD models. At the end of the fires phase, Fluent is no longer needed and ANSYS Mechanical takes over to model the cooldown phase using simple convection and radiation boundary conditions on the test specimen surface. FEA simulation of the simple cooldown phase is far more practical then CFD simulation of those same conditions.

3. Model validation

General purpose CFD analysis tools such as Fluent are extremely powerful and flexible. However, it is very easy for a well-meaning analyst to build a simulation model that does not 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 transportation accident fire simulation model[6]. The Kramer experiment subjected a large cylindrical steel calorimeter to a 30-minute hydrocarbon pool fire to simulate Type B package testing under regulatory fire conditions. The pool fire in this experiment was fueled by JP-8 jet fuel, a hydrocarbon fuel similar to kerosene. The fuel consumption rate in this experiment was estimated to be $0.050 \text{ kg/m}^2\text{s}$, corroborating the mass flow rate estimated in section 2.6. A number of thermocouples installed in the calorimeter captured its response to the pool fire. Flame temperatures and even wind data were also captured.

The simple geometry and conditions of the Kramer experiment were modeled in the transportation accident fire simulation 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 a little bit. The mesh is less fine than ideal and the inflation layer leads to average y^+ values around 4 rather than the desired value of 1 as discussed in section 2.3. A coarse time step is also used that results in Courant Number between 2 and 3 rather than the desired value of 1 as discussed in section 2.4. Despite these computational cost reduction efforts, the analysis still took nearly 3 days to complete on a very powerful, high-end business grade analysis workstation.

The simulation was initialized at a uniform 20°C , the same quiescent starting conditions as the real world fire test. The model then simulated a 30-minute fire around the test specimen. Figure 4 and Figure 5 compare the simulated flame temperature distribution to photos taken during the experimental pool fire test [6]. 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 transportation accident fire simulation model is capturing the dynamic turbulent nature of real fires.

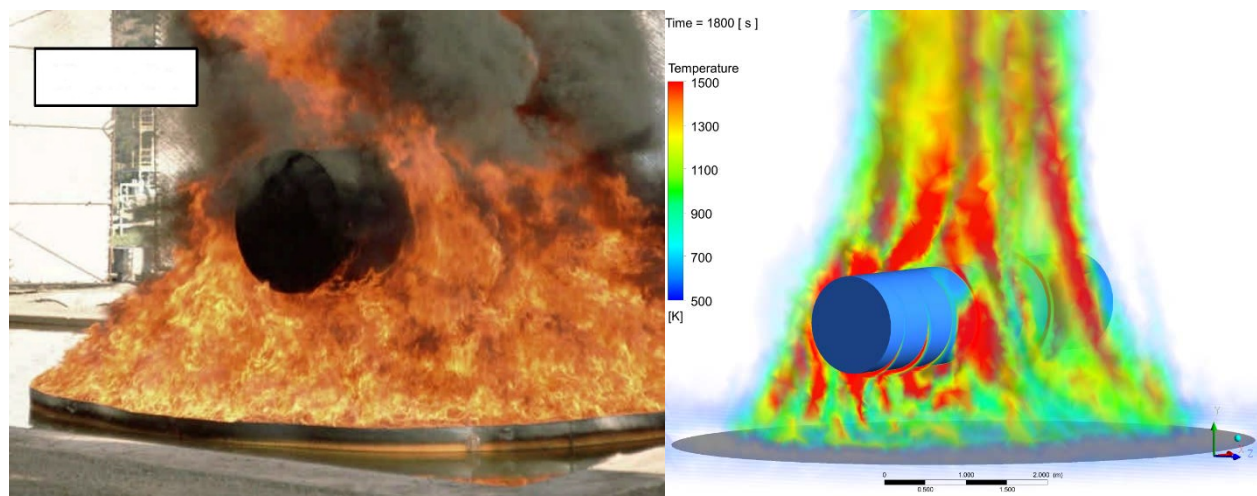


Figure 4 Comparison of experimental pool fire (left) with simulated pool fire (right)[6]

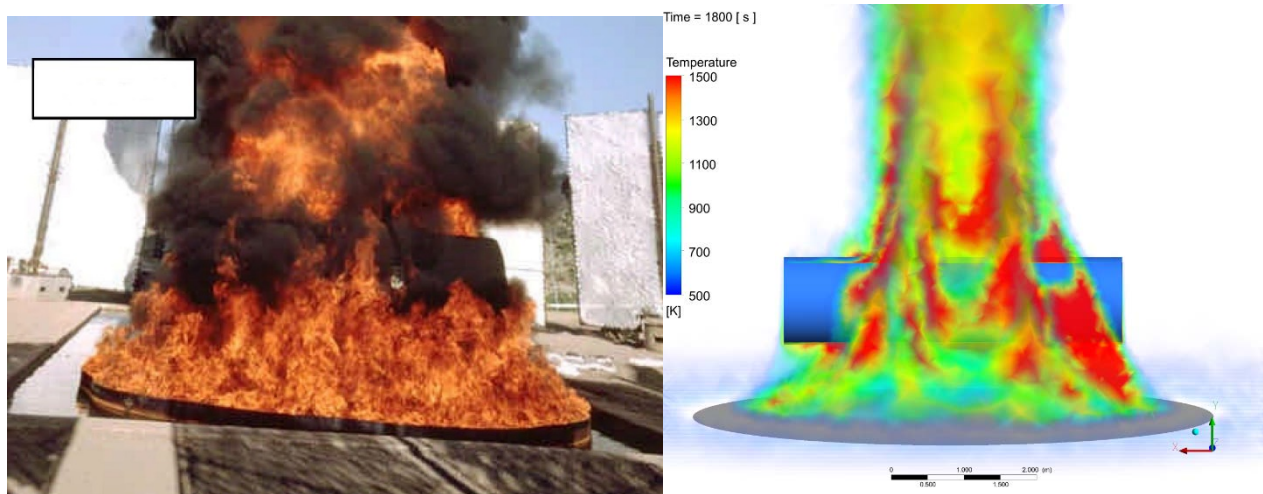


Figure 5 Comparison of experimental pool fire (left) with simulated pool fire (right), second angle[6]

Thermocouple readings throughout the calorimeter during the pool fire test are summarized in Figure 6. Corresponding probe readings from the transportation accident fire simulation model are shown in Figure 7.

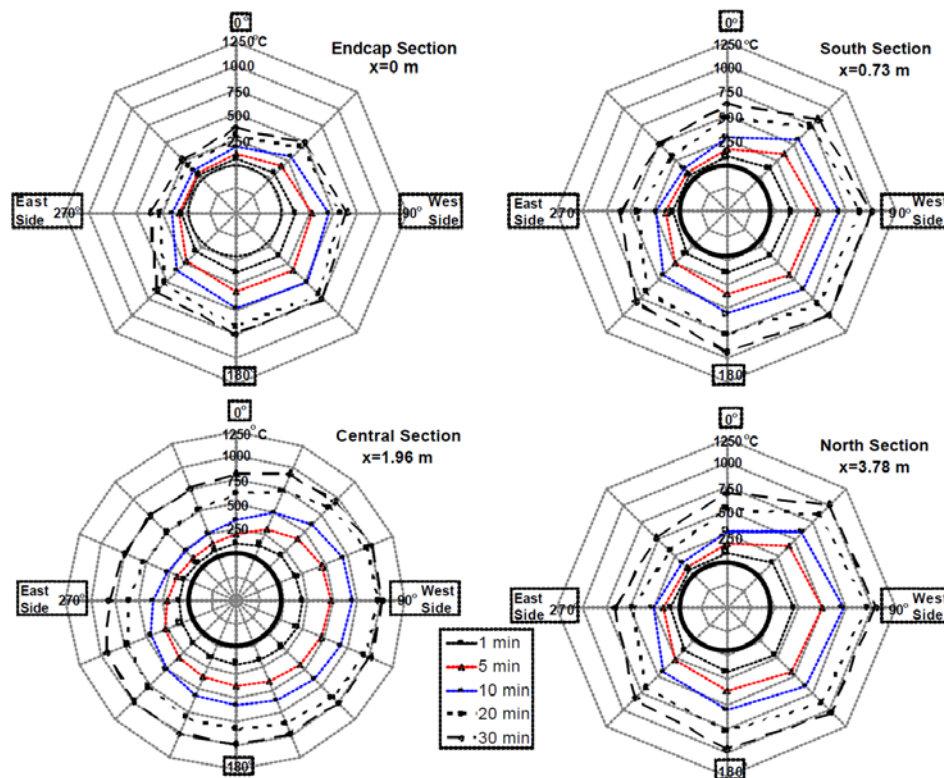


Figure 6 Thermocouple readings at various locations in the pool fire calorimeter [6]

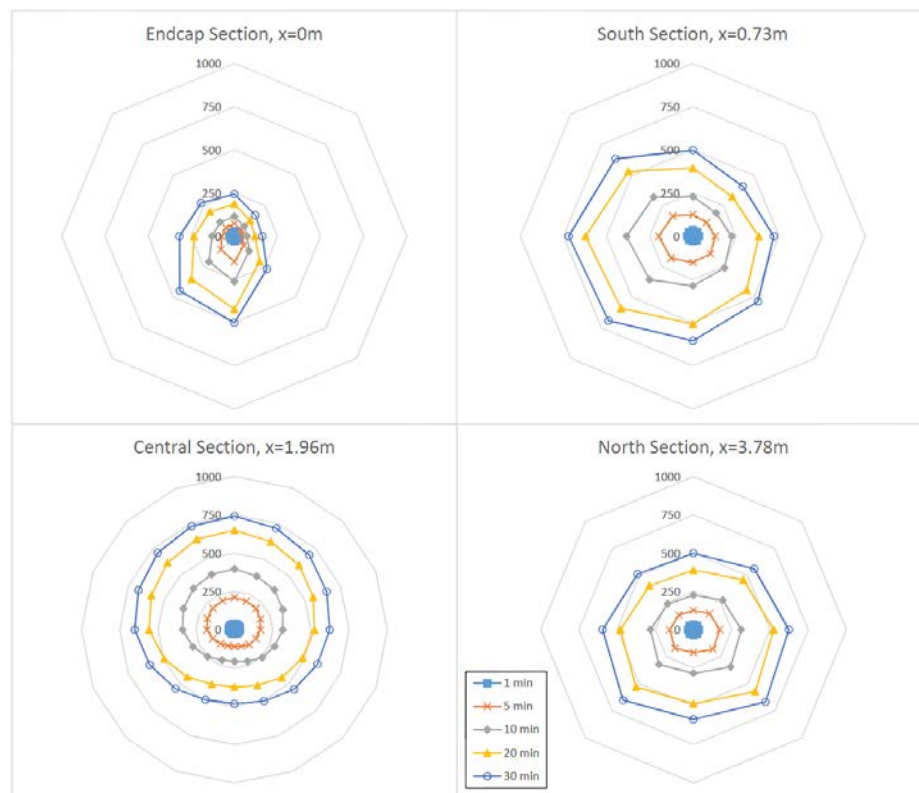


Figure 7 Corresponding temperature readings in simulated fire test specimen

A comparison between Figure 6 and Figure 7 show that the simulated temperature distribution is non-uniform around the calorimeter as expected from the readings in the real-world fire test. This suggests that the simulation is capturing dynamic heat transfer characteristic of a fire. However, the simulated temperature distribution is lower than that recorded in the real world pool fire test. This suggests that the transportation accident fire simulation model is not yet fully validated. Some components of heat transfer are not captured correctly by the simulation.

One factor that could have contributed to the simulation model deficiency is the simplistic fuel inlet assumption. As discussed in section 2.6, 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 in those hotter areas. The simulated fire could be smaller than it should have been, reducing overall heat input into the test specimen. Future work will explore non-uniform or dynamic fuel flow profiles to better simulate fuel vaporization.

A second factor that could have contributed to the simulation model deficiency is the relative coarseness of the mesh. 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. As discussed in section 2.5, 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 turned out to be still a little bit too thick. Y^+ values at the specimen surface averaged around 3, which is still quite good but y^+ values closer to 1 should lead to more accurate heat transfer calculations. The next step to rectify this issue is to refine the mesh in the fire zone and inflation layer with smaller elements.

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. As discussed in section 2.8, 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.

Finally, 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.

4. Conclusion

NWMO has performed some preliminary work in building a computer model for simulating transportation accidents involving severe, long duration fires. A coupled CFD-FEA model was developed to simulate the response of large steel test specimen to large, dynamic pool fires. Compared against real-world pool fire validation test, the so-called transportation accident fire simulation model does capture the dynamic behaviour of fires but underestimates total heat input into the test specimen. Some possible reasons for this discrepancy were discussed and future work planned.

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

5. References

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