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Model Evaluation Protocol for Fire Models Involving Fuels at Liquefied Natural Gas Facilities (Version 2)

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ABSTRACT

This document provides a description of the model evaluation protocol (MEP) for pool fires, jet fires, and fireballs involving liquefied natural gas (LNG) and processing fuels at LNG facilities. The purpose of the MEP is to provide procedures regarding the assessment of a model's suitability to predict heat flux from fires. Three components, namely, a scientific assessment, model verification, and model validation comprise the MEP. The evaluation of a model satisfying these three components is to be documented in the form of a model evaluation report (MER). Discussion of models for the prediction of fire, detailed information on each of the three MEP components, the MEP procedure regarding new versions of previously approved models, and the format of the model evaluation report (MER) are provided.

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ACRONYMS AND DEFINITIONS

Abbreviation	Definition
CFD	Computational Fluid Dynamics
EDC	Eddy Dissipation Concept
LES	Large Eddy Simulation
LNG	Liquefied Natural Gas
MEP	Model Evaluation Protocol
MER	Model Evaluation Report
PHMSA	Pipeline and Hazardous Materials Safety Administration
RANS	Reynolds-Averaged Navier-Stokes
SEP	Surface emissive power

1. INTRODUCTION

The approval process in siting liquefied natural gas (LNG) facilities by the Pipeline and Hazardous Materials Safety Administration (PHMSA) involves meeting federal safety standards which require that an operator or governmental authority control the activities around an LNG facility to protect the public from hazards associated with fires and flammable vapor-gas dispersion. In meeting federal safety standards an operator must evaluate the exclusion zones from these hazardous events which require the use of an analytical or numerical model. The objective is to predict thermal exclusion zones which demark regions of thermal injury and damage from radiant heat exposure from a fire. The extent of thermal damage will depend on the radiant heat exposure, expressed in terms of a flux, that is heat per unit time per unit area, and the duration of exposure. To have confidence in a model's predictive capability it must be evaluated with regards to its suitability.

To carry out model evaluation PHMSA required the development of a model evaluation protocol (MEP) for fires involving LNG and processing fuels. Thus, PHMSA contracted with Sandia National Laboratories to develop a MEP. Similar in spirit to the MEPs developed for LNG dispersion by the Health and Safety Laboratory [1] [2] and BLUE Engineering and Consulting [3], this MEP includes three components, namely, a scientific assessment, model verification, and model validation. The scientific assessment, model verification, and model validation results are to be documented in the form of a model evaluation report (MER) and provided to PHMSA.

The purpose of the scientific assessment is to provide a description of the various features of a model, namely, its mathematical equations, assumptions, limitations, numerical aspects, and general user information. Verification involves the petitioner reporting on verification activities performed by the model developers that demonstrate the software met specifications and ensured that the implementation of the model is correct. Validation is carried out by comparing model results to experimental data that includes pool fires, jet fires, and fireballs.

In addition to the present document, there are two accompanying documents to the MEP, one describing the experimental database for validation and another that is in the form of a spreadsheet which includes the experimental data [4] [5]. To facilitate the ease in carrying out the validation process, entries are provided for a user to enter model results in the spreadsheet. The spreadsheet then automatically calculates statistical performance measures and generates graphical comparisons of model predictions to experimental data.

The data included in the MEP are from experiments using liquefied natural gas (LNG) and fuels involved in the processing of LNG at facilities. The processing fuels include:

- Refrigerants: Ethane/Ethylene, Propane, Butane, and Iso-pentane as single or mixture release.
- Stabilized condensate or C5+: mixture of butane, pentane, and hexane.
- Diesel fuel

Note that anhydrous ammonia and hydrogen sulfide are also fuels involved in processing but are not included in the MEP since experimental data is not available. The lack of data for anhydrous ammonia is due to difficulties in sustaining a flame, and for hydrogen sulfide data is lacking due to safety considerations.

The MEP database also includes data on the thermal response of concrete walls that could serve as thermal barriers. The motivation to include the data is due to the potential for current LNG facilities requiring the installation of radiant thermal barriers to satisfy the factor of uncertainty criteria within

the MEP. These facilities were built before the MEP for fires was developed, hence the potential need for thermal barriers.

The following provides discussion of models for the prediction of fire, detailed information on each of the three components that comprise the MEP, the MEP procedure regarding new versions of previously approved models, the format of the MER, and a checklist for petitioners and reviewers.

1.1. Version Changes

The main changes in this document from Version 1 to Version 2 are the rearrangement of the introduction by moving the description of the fuels further down in the section to improve contextual flow. Also, Table 5-1 and Table 5-4 have been modified to include the additional test series described in item 1 of the list below. The itemized list below pertains to the main changes from Version 1 to Version 2 of the MEP database [4] [5]. Note that future versions may be released if corrections are necessary and/or improvements are recommended by users.

1. The addition of 10 non-LNG fire experiments and 2 concrete wall thermal experiments. The experiments include:
 - a. 3 jet fires (ethane, ethylene, and isopentane)
 - b. 4 pool fires (ethane, ethylene, propane, and isopentane)
 - c. 3 fireballs (ethane, ethylene, and isopentane)
 - d. 2 concrete walls (formed and masonry)
2. The recently added Sandia pool fire test series provides data for a propane (99+%) pool fire and has replaced the 'USN' test series. Since it's uncertain whether the 'USN' test series used LPG with propane as the main constituent, it has been removed from the MEP. LPG is commonly comprised of either mostly butane or propane and will contain other components such as propene, methane, and ethane.
3. In the comparison plot in the 'Montoir_T1' worksheet, the line for 'model' was corrected since it was not showing on the graph of 'predicted vs. measured' for the period of 130-170 sec. Also, the radiant fraction has been removed from the worksheets for the Montoir test series since it was derived by the MEP Database author and not provided in the experimental reports.
4. Worksheet 'CERTEC summary' indicated an error internal to Excel where the data was not linked. The worksheet now functions correctly after a new worksheet with the same data and formulas was created and replaced the non-functioning worksheet.
5. The data for comparison in the worksheets for the 'HSL-BG' experiments has been simplified and is now commensurate with the data provided for other fireball test series.
6. The radiative fraction for the experiment 'Phoenix T2' has been corrected from 0.3 to 0.24.

7. In the MEP Database spreadsheet, the listing of cells where data is entered in the Master List sheet has been removed due to the high number of worksheets now in the database spreadsheet, however a list of the worksheets remains.
8. Section 2.2 has been revised to improve clarity in describing the equations used to determine performance in the Database spreadsheet.
9. In section 2.3, the probability criteria used to determine the uncertainty factor has been changed from 0.01 to 0.025 to reflect a 95% confidence interval.

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2. FIRE MODELS

The following sections provide a general description and discussion of models used to predict the behavior of fire, with a focus on pool fires, jet fires, and fireballs. First, the general features of fire models are presented, followed by more detailed discussion of the different fire types included in the MEP.

2.1. General Features

The approach to modeling fires ranges from the very simple, such as a point source representation, to the very complex, such as using computational fluid dynamics (CFD) for turbulent reacting flow. A common class of simplified models includes integral or solid flame models. Parameters required as input for these models to determine heat flux external to the fire include the average surface emissive power, burn rate, flame length, transmissivity, and burn rate which are based on empirical correlations. For simple flame geometries, and where parameters are well known for the scale under consideration, these models provide good agreement with experimental data in the far-field, for example at distances greater than approximately two characteristic widths of the fire away from the source. In the case of circular pool fires the diameter is taken to be the characteristic width of the fire. Solid flame models are only appropriate for fires not impinging on or engulfing surrounding infrastructure. By federal requirements, spills are designed to have a spill containment which directs the fire to a remote impoundment within a boundary demarked by a heat flux of 5 kW/m² (1600 BTU/ft² hr). This heat flux level is commonly used as a criterion to specify exclusion zones for emergency personnel [6]. For reference, this heat flux level causes 2nd degree burns to bare skin after about 30 seconds of exposure [7]. Effects on people from exposure to different levels of radiant heat flux is provided in Table 2-1. Damage to structures and some materials after 30 minutes exposure to different heat flux levels is provided in Table 2-2. Since federal regulations required that impoundments are remote, that is, not impacting infrastructure, integral models are often used to determine thermal radiation from a fire.

Table 2-1: Effect on people from exposure to different levels of radiant heat flux [7].

Radiant heat flux (kW/m ²)	Pain or Injury
1.0	No harm – solar constant on a summer day.
2.1	Pain after 1 minute.
5	Pain after 10 s. 1 st degree burn after 20 s. 2 nd degree burn after 30 s exposure to bare skin.
10	2 nd degree burns after 20 s.
30	3 rd degree burns to bare skin and 50% lethality after 30 seconds exposure.

Table 2-2: Damage to structures and materials from radiant heat flux [8].

Radiant heat flux (kW/m ²)	Damage after 30 minutes
12.5 -15	Piloted ignition of wood
18 - 20	Cable insulation degrades
25 - 32	Unpiloted ignition of wood. Steel deformation.
35 - 37.5	Process equipment and structural damage
100	Steel structure collapse

CFD models can address environments both with and without influences from surrounding infrastructure since they can include models for engulfed objects, irregular geometries, fire and smoke

propagation, and combustion of solids. Key sub-models required to predict fire behavior include fluid mechanics, chemical reaction, radiation, and soot. A CFD model will include all of these in addition to a turbulence model. Figure 2-1 shows the various branches of the required sub-models. If modeling solid phase combustion is applicable, then additional sub-models to address solid decomposition and conductive heat transfer are required along with the associated material properties. Note that equations of state, transport properties of the gas phase and radiative properties of the combustion products are included in the suite of required sub-models.

A CFD model may include a suite of sub-models that address a particular physical phenomenon. The MEP does not specify the choice of sub-model, but rather provides validation data with which a proper selection can be made. There is no prescriptive approach with regards to the choice of sub-models having appropriate physics, rather the selection is performance based and must be determined by investigation for a particular application and model. The investigative process includes performing exploratory simulations, reviewing the literature on relevant studies, reviewing the user manual, and user forums. The following sections provides more detailed discussion of the fire types covered in the MEP and related sub-models. Note that integral models use empirical relations to predict pertinent parameters required to predict heat radiating to an object external to the flame. If there are several different correlations available within a model, then they could be evaluated against the MEP.

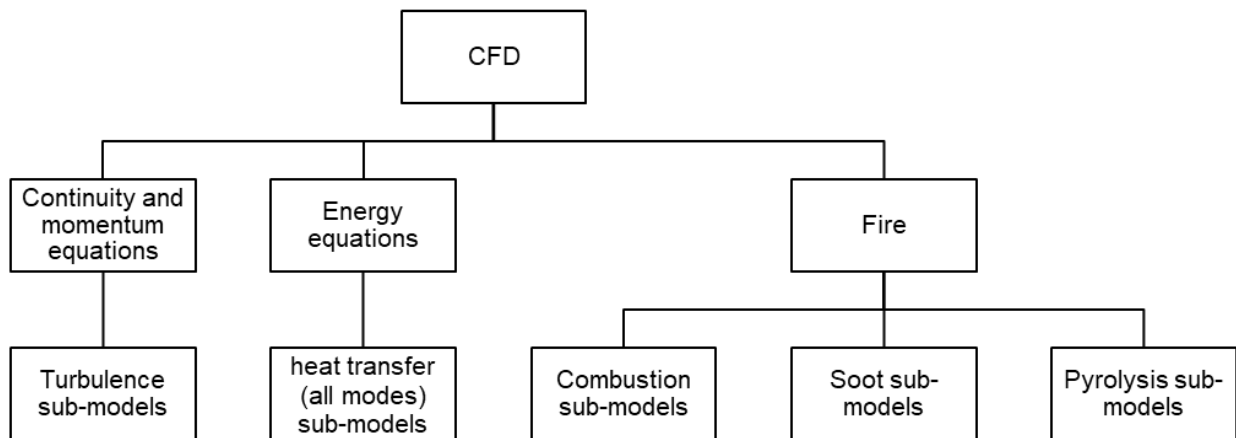


Figure 2-1. Models required to simulate the behavior of fire for CFD models.

2.1.1. Pool fires

A pool fire is defined as a horizontally oriented fuel burning upwardly in free convection. They can occur, for example, whenever a liquid fuel is spilled, and an ignition source is present. Due to the low momentum nature of pool fires they are affected by atmospheric conditions such as wind speed, wind direction, temperature, and humidity and consequently thermal exclusion zones are affected. Jet fires and fireballs are less affected due to their high momentum and/or short duration. Wind-driven pool fires will tilt in the downwind direction, and the base dimension of the flame will extend in the downwind direction, also termed flame drag, while the upwind and crosswind dimensions remain relatively unchanged. For pool fires contained in a pan, the extent of drag depends on the lip height above the fuel surface where increasing lip height results in reduced drag. The effect of flame tilt and

drag is to either increase or decrease the thermal hazard distances in the downwind direction depending upon the degree of tilt and the distance from the fire. Also, the angle of the wind is important with regards to impacting downwind infrastructure if it results in flame impingement. For wind-driven fires it has been found experimentally that an object engulfed in the fire will experience extremely high heat flux levels on their leeward side, up to 400 kW/m² [9]. Furthermore, increasing wind speeds can cause an increase in the burn rate. Other atmospheric factors which can affect thermal exclusion distances and pertains to all types of fires considered in the MEP include atmospheric temperature and humidity by means of the transmissivity, which is a measure of the attenuation of radiation by absorption and scattering through the atmosphere. The transmissivity will decrease with increasing levels of relative humidity and atmospheric temperature. Thus, a model must account for the above features to predict radiant thermal hazard zones from a pool fire.

2.1.1.1. Solid flame models for pool fires

In predicting the radiant thermal exclusion zones for LNG facilities, as noted previously integral or solid flame models are often used. An integral model represents the surface of a circular pool fire with a simple, usually cylindrical or conical, geometry as shown in Figure 2-2. The radiative heat flux as a function of distance is determined from the equation, $q'' = EF\epsilon\tau$. The thermal radiation, E, is uniformly emitted from the model surface and is the average surface emissive power (SEP). For an assumed geometry, the geometric view factor, F, which is the fraction of radiant energy from the fire that is received by a target object's field of view, can be determined exactly for the assumed geometry. The flame emissivity, ϵ , ranges from values of 0 to 1 but is typically assumed to be 1 for large-scale fires. The transmissivity, τ , ranging from values of 0 to 1 is the degree of atmospheric attenuation due principally to H₂O and CO₂. To capture the tilting of the flame due to wind, a tilted cylindrical flame shape is used. Flame length, tilt and drag necessary to determine flame shape and view factors are based upon empirical correlations. Parameter inputs that solid flame models require include the view factor for a given pool size and shape, burn rate, surface emissive power, flame emissivity, atmospheric quantities such as wind speed and direction, temperature, and humidity. For each of these parameters, numerous correlations have been developed by several researchers all providing different results due to different approaches, experimental data, and assumptions used to determine the parameters.

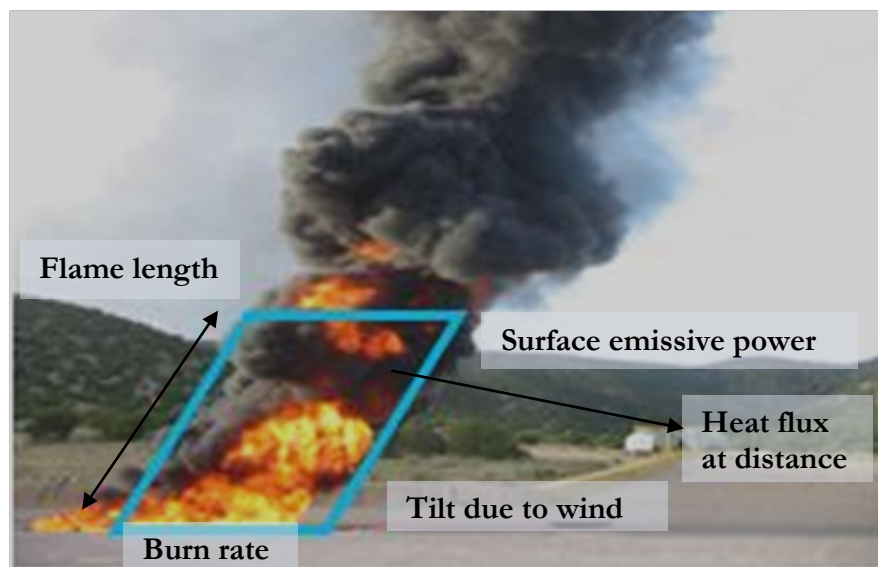


Figure 2-2: Tilted cylinder representation using solid flame model.

Flame length correlations are an example of this. The majority of flame length correlations are based on a combination of flame length measurements and dimensional arguments such as the model by Thomas [10] and Moorhouse [11], or experimental measurement combined with theoretical mathematical models such as the model by Steward [12]. The correlation by Moorhouse is based on 29 LNG experiments involving square pools with aspect ratios from 1 to 2.5. Assuming a circular pool, the equivalent pool diameters ranged from 6.9 m to 15.4 m. Thomas based his correlation on square wood crib fire experiments up to 2 meters. These correlations illustrate the very different experimental configurations used to develop correlations, that is, different fuels and scales which explains why different flame lengths for a given hydrocarbon at a specified pool diameter are predicted among the correlations. As shown in Figure 2-3, predicted flame height or length to pool diameter ratios (L/D) for LNG can vary by a factor of 2 to 3 for a given pool diameter.

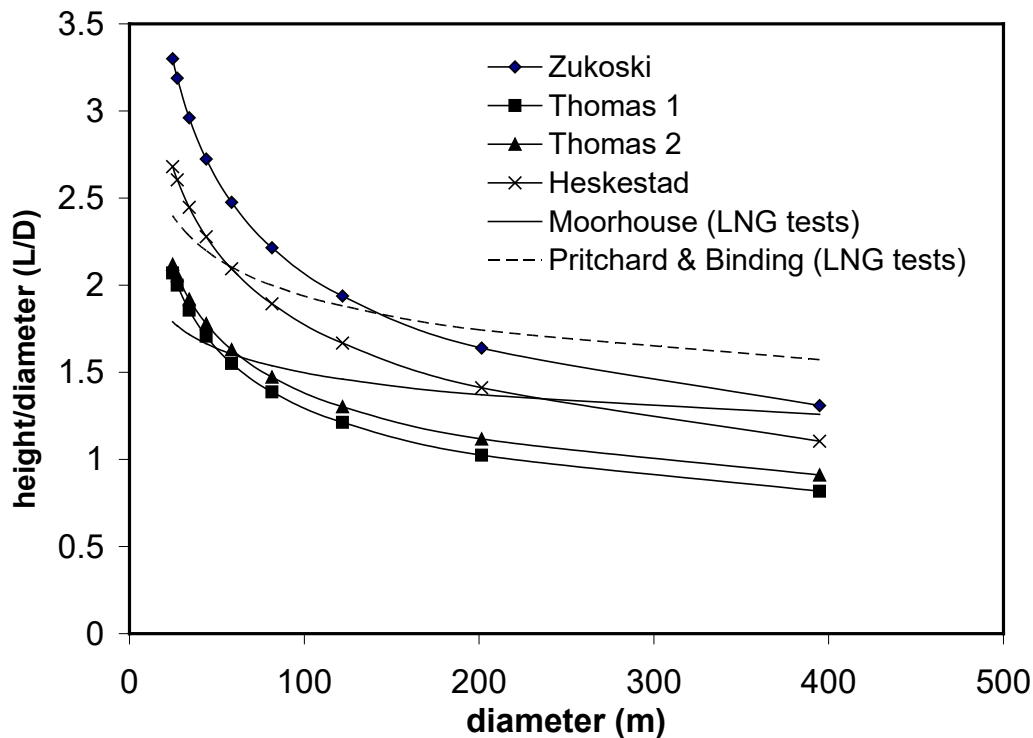


Figure 2-3: Flame height correlations as a function of pool diameter for LNG.

There are at least twenty correlations, but only a few are plotted in Figure 2-3 to indicate the range of disagreement. The variation among the correlations may be due to differences in the pool geometry tested and environmental conditions, as well as differences in the measurement technique and definition of flame height. It should also be noted that these correlations assume that the flame is characterized by a single temperature and gas composition regardless of the flame size or soot concentration in the flame. They also do not consider fuel radiation properties, or turbulent mixing either from the mechanisms due to the fire or induced by the atmosphere. Thus, this justifies their classification of ‘correlation’ as well as their associated uncertainty. To determine the flame length, the burn rate is a required as an input into these correlations. Similar to the flame length, burn rate correlations will vary due to differences in the data used for their development, that is, fuel type, pool size, pool shape, atmospheric conditions, and whether the fuel is on land or water.

Additionally, the surface emissive power used in the solid flame model will vary depending on the assumed flame shape and length. It's typically derived from experiments by using heat flux measurements from radiometers and an assumed flame shape and length. The derived average surface emissive power will greatly depend on the assumed flame shape and length. More accurate methods of determining the surface emissive power is achieved by using video analysis to perform detailed mapping of the flame over time synchronized with radiometers measurements. As an example of how assumed flame shape and height can affect SEP, the analysis performed for the Montoir pool fire experiments using these two different approaches resulted in an SEP about 100 kW/m² lower using a solid flame model compared to determining the flame shape through video analysis [13].

The intent of the above discussion regarding solid flame models is to point out that correlations applicable to all hydrocarbons and pool diameters does not exist. Since solid flame models are based on empirical correlations, they are valid for the experimental configuration and conditions for which the correlations are derived. Extrapolating too far outside the applicable range may provide very inaccurate results. Thus, in using a solid flame model it is recommended that correlations are used which apply as close as possible to the scale and fuel type of interest to minimize error if extrapolation is necessary.

2.1.1.2. CFD models for pool fires

The other class of models used to evaluate radiant thermal exclusion zones for pool fires are CFD models. In using CFD models there are several notable features to highlight that pertain to their sub-models which include flow regime, combustion, radiative transport, and soot production. Since pool fires are buoyancy-controlled, low-momentum diffusion flames, they can be modeled using the low-Mach number approximation, applicable to flow speeds below a Mach number of about 0.3. The advantage of such an approximation is that the characteristic time scale comes either from chemical reaction, diffusion, or convection times, rather than acoustic times linked to the pressure field. Resolving acoustic waves in a model can be computationally expensive. This approximation allows the elimination of these acoustic waves, but the resulting equations still allow for large density variations due to the temperature field that occurs in reacting flows. Thus, this approximation would be appropriate for the pool fires considered in the MEP.

The flame structure of pool fires is strongly dependent on the pool diameter. Pool fire flames are considered laminar for pool diameters below approximately 5 cm, in transition between 5 cm and 1 m, and fully turbulent above 1 m. The pool fires included in this MEP are considered to fall within the fully turbulent regime and thus, a turbulence model is required. Typically, Reynolds-Averaged Navier-Stokes (RANS) or Large Eddy Simulation (LES) turbulence models and their variants are used for fire applications, though several other model types have been used. LES offers the advantage that it can capture the unsteady flow of large-scale flow structures, whereas with RANS unsteady turbulent motion is unresolved over the range of time and length scales of the application, necessitating turbulence closure models to account for the unresolved physics.

As found experimentally, for most of the duration of an LNG fire nearly pure methane will burn and will provide the highest radiative heat flux compared to the later stages of the fire where burning of heavier components such as ethane and propane occurs. The chemical reactions involved in burning methane are numerous as evident from the GRI-Mech 3.0 mechanism involving 53 species and 325 elementary chemical reactions [14]. For the LNG pool fires included in the MEP, the chemical reaction mechanism can be simplified to a single-step reaction involving fuel, oxidant, and products

since they allow for the total heat release from the flame to be reasonably captured. Additionally, it is considered acceptable to not resolve the chemical reaction time scale and to assume chemical equilibrium. Since pool fires are diffusion flames, the times scale of mixing dominates that of the chemical reaction time scale allowing for this assumption. Thus, combustion models based on the mixing-controlled assumption, such as the eddy-dissipation-concept (EDC) or a laminar-flamelet model, are often used in pool fire simulations and are considered acceptable for use for the pool fires considered in the MEP, though the use of other models is not precluded.

Pool fires will be optically thin up to a certain diameter and then transition to becoming optically thick where the flame is no longer transparent, and the local soot production becomes saturated to the point that local radiation emission is absorbed within the flame envelope. In the optically thin regime gas band radiation from water vapor and carbon dioxide is significant, whereas in the optically thick regime soot radiation dominates, resulting in a much higher radiative heat flux. The radiation emitted on the outer surface of the flame envelope originates at a layer near the surface. At the soot saturation point the surface emissive power (SEP), which is the energy emitted per unit time per unit area, is then a function of the surface area of the flame and not the volume, which would be the case for optically thin fires. The pool fires included in the MEP are considered optically thick with the possible exception of the Sandia indoor gas burner tests which indicate that the soot saturation point has not been reached based on comparative heat flux measurements to larger diameters. Radiative heat transfer is a key feature of reacting flow and thus a method for the solution of the radiative transport equation is required. The discrete transfer radiative method, discrete ordinates method, and finite-volume method can span the entire range of optical thicknesses, thus represent appropriate model choices to use when simulating the pool fire tests included in the MEP. These models have the disadvantage of displaying ray effects which is due to angular discretization of the radiative intensity. The result is a pattern of discrete rays emanating from the fire to the surroundings. If an object external to fire, e.g. a radiometer, lies along the trajectory of one of the rays a much higher heat flux will result than if the object lies between two rays. To reduce the ray effect a high-order angular discretization can be used. Thus, when comparing to radiometer measurements it is recommended that a high-order angular discretization is used.

Some CFD models require specifying the fraction of the heat generated by the fire that radiates to the surroundings, termed the radiative fraction, rather than predicting it. Experimentally the radiative fraction is typically determined by using wide angle radiometer data along with a simplified geometrical representation of the flame such as a point source or cylindrically shaped source. For experiments that report the radiative fraction, the values are provided in the MEP database [5]. For experiments not reporting the radiative fraction it is recommended that various values be investigated since it can have a significant effect on the results for heat flux. A reasonable range is 0.2 to 0.4. Additionally, some CFD models require specifying a path length for radiative transport which may be based on either the flame volume or the entire domain volume if the atmosphere is considered a participating media. Thus, it is important to identify the appropriate path length to use based on sub-model assumptions.

The local absorption and emission of combustion products also require models which differ in their ability to handle spectral radiation. The simplest approach is to use a gray gas assumption by prescribing a constant absorption/emission coefficient across the full spectrum. However, for most fire applications the absorption and emission characteristics will vary with temperature and mixture composition thus other methods, such as the weighted sum of gray gases or wide-band and narrow-band models, are typically used. All such approaches are considered acceptable for use to simulate the pool fires included in the MEP. However, it should be noted that using the gray gas assumption may

not produce predictions for the Sandia gas burner tests which are as accurate as predictions made using the other models.

With regards to radiative heat flux, predicting local soot concentrations allows for the evaluation of the absorption coefficients of gas-soot mixtures which is used in the radiative transport equation. The effect of soot can be included by using various sub-models that include, in order of increasing complexity: a user-specified soot yield, single-step equation for soot mass fraction with a source term, semi-empirical two-equation models for soot particulate number density and soot volume fraction, and the population balance model. Within increasing complexity, the computational run time increases, thus in practical engineering applications the first two types of models are often used, though the others are not precluded.

An additional model that addresses the prediction of the burn rate requires that the model can capture multi-phase behavior. Accurately predicting the burn is a complex problem in that it requires resolving the dynamics of the liquid phase of the fuel while coupled to the gas-phase which encompasses all model types provided in Figure 2-1. Although outside the scope of datasets included in the MEP, a spreading pool adds additional complexity since the substrate will contribute to the heat transfer to the pool and affect the spread rate. The height of the spreading pool will require a very fine grid relative to the rest of the domain, greatly increasing the number of computational elements involved. Thus, it is computationally infeasible to include the burning pool in this fashion for large scale pool fires. To provide an approximation of the burn rate, there are models that use simplified, semi-empirical, sub-grid models. If a model has such a sub-model, it can be applied to the pool fires included in the MEP conducted outdoors, though it is acceptable to prescribe the burn rate as a boundary condition using the values provided in the database. The mass flux of the Sandia indoor gas burner tests was controlled so does not require a burn rate model.

Note that regarding grid resolution traversing the pool, at least 20 cells are typically required. This is because a key feature of pool fires is the periodic formation of a toroidal vortex or ‘donut’ that begins at the base of the fire and propagates upward due to buoyancy forces. This periodic process is responsible for the ‘puffing’ frequency of pool fires. Thus, in looking at a cross-section of this toroidal vortex where counter-rotating vortices can be seen, at least 10 cells for each vortice allow the rotational motion to be resolved. These structures affect the average flame shape which in turn have a significant effect on the prediction of near field radiant heat flux and less so on the far field prediction. Additional guidance involving grid resolution can be found in reference [15].

2.1.2. Jet fires

Jet fires are classified as turbulent, high-momentum, diffusion flames. They can result from high pressure releases as created by pumps, compressors, or at the base of an LNG storage tank. Although they typically will result in smaller exclusion zones compared to a pool fire, they can cause severe thermal damage to nearby infrastructure from flame impingement which could lead to cascading events. The convective heat flux is similar in magnitude to the radiative heat flux to engulfed objects due to the jet’s high velocity. This contrasts with pool fires wherein engulfed objects are subject predominantly to radiative heating. The high velocity release also provides a higher rate of air entrainment into the jet resulting in more efficient combustion than pool fires. Consequently, engulfed objects are subject to a higher heat flux from a jet flame compared to a pool fire flame.

The jet release can be in the form of a pure liquid or a gas-liquid mixture that arises from rapid depressurization. Two-phase releases have been found to result in higher radiative heat flux levels than single-phase releases. For two-phase releases, the rapid release to atmospheric pressure will most likely

cause the liquid to break up into droplets which are quickly vaporized when the jet is ignited. The release configurations for jet fires are more numerous than pool fires since the flame can be released in either vertical, inclined, or horizontal orientations. If the release velocity is high enough, the flame can lift off from the release point. Additionally, horizontal jets can have the tip of the flame lift due to buoyancy which is observed more often with gaseous jets versus liquid jets. Wind effects the behavior of jets by causing an increase in entrainment rates along the flame, thereby increasing the rate at which the fuel reaches the lower flammability limit which in turn causing a reduction in flame length.

2.1.2.1. Multipoint source and solid flame models for jet fires

Various modeling approaches have been developed to predict the thermal radiant heat emitted by jet fires include multi-point source, solid flame, and CFD models. Multi-point models use weighted point emitters placed equally along a line emitting in all directions along the flame length. A single-point source model can be considered a special case of the multi-point source model. This approach requires correlations for the flame length and radiant fraction. Solid flame models are often used to predict the thermal radiant exclusion zones for jet fires since they can include correlations that account for flame trajectory, effects of wind, and provide a better representation of flame shape. They often represent the geometry of the flame as either a cylinder or a truncated frustum of a cone. These models use empirical correlations for the jet momentum flux, surface emissive power or radiative fraction, flame length, flame lift off, buoyancy forces, and the effect of wind [16]. Surface emissive power is often determined by the product of an empirical correlations for radiant fraction with the heat release of the fire divided by the area of the idealized shape. Solid flame correlations typically require the orifice diameter, mass flow rate, and wind speed as input.

Flame length correlations applicable to different flow regimes have been developed for subsonic, transitional, choked, and supersonic flows based on dimensionless parameters such as Q^* and U^* [17]. Q^* is defined as $Q^* = \dot{Q} / (c_p T_u \rho_u g^{1/2} D^{5/2})^{-1}$ where c_p is the mean specific heat of the fuel at constant pressure and T_u is the temperature of the unburned gas. U^* includes the maximum laminar burning velocity and Reynolds number to account for specific combustion parameters and turbulence. The dimensionless U^* is defined as $U^* = (u / S_L) Re_L^{-0.4} (P_i / P_a)$ where u is the fuel flow mean velocity at the exit plane, S_L is the maximum laminar burning velocity, $Re_L = DS_L / \nu$, P_i the initial stagnation pressure, and P_a the atmospheric pressure. Flame length correlations based on Q^* and U^* were developed in reference [17] using 880 experiments where flame lengths ranged from 0.08 to 110 m. They identified the subsonic regime by $Q^{*2/5} < 100$ and the choked and supersonic regime by $Q^{*2/5} > 100$. Using U^* scaling, they identified the buoyancy and turbulent subsonic regime by $U^* < 10$, the transition regime by $10 < U^* < 230$, and the choked and turbulent supersonic regime by $U^* > 80$. Note that the flame length correlations for subsonic flow encompass the buoyancy regime which applies to pool fires. Thus, different flame length correlations apply depending on the flow regime. For the jet fires considered in the MEP the correlations for the choked and supersonic regime would be appropriate.

2.1.2.2. CFD models for jet fires

For CFD models the same sub-models applicable to pool fires apply to jet fires though there are some notable differences. The 'LU' and 'A-S' jet fire experiments included in the MEP are supercritical, under-expanded gaseous jets. Thus, the flow field in the immediate vicinity of the jet is very complex with the occurrence of shock waves and multi-phase flow which require a model that can model multi-phase, compressible flow of real gases. To resolve this region would require extensive computational time given the disparate time and length scales between this region and the flame and domain. For the

MEP, it not expected that this region is resolved given the computational expense. Thus, it is acceptable to use semi-empirical models to identify a subsonic region downstream of the release point to provide a boundary condition for the simulation of the jet fire. Alternatively, a de-coupled approach could be used in which the near-field region is resolved, and its results are used to identify the boundary conditions in a subsonic region that would then be utilized for the simulation of the jet fire.

The jet fire experiments included in the MEP also displayed lift-off which is a region just beyond the release point that does not ignite due to the thermodynamic state and high speed of the flow field. Beyond the lift-off region, a non-luminous premixed blue flame forms which is followed by the luminous flame forming the main body of the jet fire. To predict the lift-off region, a model that captures turbulence-induced high strain rates resulting in flame quenching is required. In regions of high strain rate, the chemical time scales are comparable to mixing time scales, thus a model must take chemical kinetics into account, that is, incorporate finite-rate chemistry. If a model does not have this feature, then a simulation can still be performed but the model assumptions and limitations should be reported.

An additional element of these tests is the presence of an engulfed pipe in which embedded calorimeters measured total incident heat flux and radiometers measured radiative heat flux to the pipe. Thus, both radiative and convective heat transfer must be modeled to accurately predict the total incident heat flux to the calorimeters. This requires capturing the thermal boundary layer near the surface of the pipe which is coupled to the turbulent boundary layer. Typically, two approaches are used. The first involves resolving the flow in the near-wall region with a fine grid, which is computationally difficult or infeasible for large scale applications. The second approach is to use semi-empirical wall functions which are algebraic sub-grid models that bridge the region where viscous forces dominate, that is, the viscous sublayer and the region above this layer where turbulence dominates. These models obviate the need to resolve the viscous and transition layers thereby saving on computational expense. Note that the standard law of the wall will not provide accurate results for the pipe engulfed in the jet fire. The standard law of the wall model assumes negligible pressure gradients, local equilibrium of turbulence, and a constant stress layer near the wall. These assumptions do not apply to flow around a cylinder from an impinging jet such as in the stagnation region where high pressure gradients occur. Thus, non-equilibrium wall functions are required to obtain accurate results. Another consideration involving the heat transfer to the pipe is identifying the convective heat transfer coefficient. Often an overall Nusselt number correlation is used where the overall Nusselt number is based on averaging the circumferential values. Rather than using a global circumferential value for the Nusselt number, local average values can be used. The circumferential variation in the Nusselt number could be approximated using the equations fitted to experimental data for average Nusselt number over a range of angles as function of Reynolds number as provided in reference [18]. Note that in creating the solid model for the pipe, separate boundaries for each segment would have to be delineated to apply the functions to each segment. A CFD model that does not have the above capabilities could still provide reasonable results. The intent of pointing out these features is to provide an indication of possible causes for a model providing poor agreement to data.

2.1.3. Fireballs

Fireballs can arise when a tank containing fuel is heated sufficiently to a thermodynamic state that will result in rapid phase change and cause the tank to rupture through thermal (or mechanical) damage. Fragments may also be thrown, thus presenting an additional hazard. Most of the models discussed for pool fires also pertain to fireballs. The main difference between the two types of fires is that fireballs are partially pre-mixed diffusion flames which rapidly combust due to enhanced turbulent

mixing and atomization. Thus, their distinguishing feature is the rapid consumption of fuel on the order of seconds to tens of seconds rather than minutes to hours. The other difference is the early time dynamics that occur with fireballs. Typically, the release is from a failed tank that occurs at very high speeds (~ 100 m/s). Note that the speed of the expanding fireball does not support a shock wave, though a shock wave can be generated from the rapid expansion of the highly pressurized release and from the rapid phase change when releasing superheated fuels.

2.1.3.1. Solid Flame models for fireballs

Solid flame and CFD models are used to predict the thermal radiant heat emitted by fireball. Solid flame models typically represent the fireball as a sphere and use correlations for fireball diameter, rise height, duration, and surface emissive power. These quantities vary in time and as such the transient functions can be incorporated into correlations. However, due to the lack of available time-varying data, the traditional approach is to use empirical correlations that identify maximum or averaged parameter values.

Empirical correlations have been developed by several researchers for these parameters [19]. Most are based on data from small-scale experiments, typically using fuel masses below 50 kg. The empirical correlations are of the form of a power law in which the fuel mass is raised to some exponent, b , and then the result multiplied by some factor, a . The factors ‘ a ’ and ‘ b ’ are determined by fitting a power-law curve to data. The values of these factors have not been consistent among various researchers because of differences in test configuration, scales, fuel-types, instrumentation, and parameter definitions. Reflective of fire experiments in general, significant variation occurs in results even for repeat tests. For example, fireball experiments using propane, butane, diesel, and kerosene fuel indicated variation of about $\pm 20\%$ for measurements of maximum diameter, radiated energy, and surface emissive power [20] [21].

There is consensus, however, that the exponent on fuel mass used to determine maximum diameter is approximately $1/3$, thus this parameter has the least variation among researchers [19]. This agreement can be anticipated given that most hydrocarbon fuels require a similar volume of air for complete combustion. The growth of the fireball has also been shown to have a $1/3$ power dependence where the growth is proportional to $t^{1/3}$, where ‘ t ’ is time (s) [19].

The greatest variation among the equations exists for fireball duration, basically due to the use of different criteria for what defines duration and release configurations. The duration can also be affected by release configuration, for example if a test vessel ruptures in a way that allows fuel to be released close to the ground, the fireball will expand initially along the ground and then begin liftoff, whereas if a test configuration allows for only an upward vertical release, then the expansion phase along the ground is circumvented. Large variation also exists for rise height due to differences in definition which include: the height at which the fireball breaks up, height at which maximum diameter occurs, and height at which the fireball area is steady state.

Correlations have not been developed for the surface emissive power mainly due to the lack of measurement of this parameter. It has been measured for a limited number of experiments and most have used indirect approaches by employing radiometer measurements in conjunction with video coverage. More direct measurements are infrared cameras which offer the additional advantage of tracking the fireball over time to provide more detailed information. The surface emissive power is not amenable to a power law form.

2.1.3.2. CFD Models for fireballs

For CFD models, most of the sub-models discussed for pool fires pertain to fireballs. The initial conditions defining the release however is uncertain. The initial shape of the fireball will depend on the mode of release which in turn will affect the timing of the fireball such as the height at maximum diameter, height at burn out, and duration. The effect on the timing ultimately affects the radiant heat flux from the fireball to an external object. Since experiments typically don't measure the initial momentum of the fuel, a viable approach to address this issue is to perform several different release configurations that vary the initial trajectory of the fuel, that is, explore different partitions between the horizontal and vertical directions of release. Also, note that for the fireball tests included in the MEP the fireball dimensions differed when viewed along the east-west direction compared to the north-south direction which can be due to the test vessel configuration, failure pattern, and/or wind conditions.

To avoid having to resolve high speed flow that occurs right after failure, the release duration can be increased thereby reducing the mass release rate. It is recommended that exploratory simulations of different release durations be performed since it is also another uncertainty. Additionally, if a model has a sub-model for partial pre-mixed combustion, then the initial mixed state of the fuel can be explored, though the fireball is sufficiently fuel-rich, a diffusion flame model can be applied. If simulations are performed exploring different trajectories and release durations, the results are to be reported in the MER.

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3. SCIENTIFIC ASSESSMENT

As previously mentioned in the Section 1, the purpose of the scientific assessment is to provide a description of the various features of a model, namely, its mathematical equations, assumptions, limitations, numerical aspects, and general user information. The following provides more detail on what information should be included in these areas. Different sub-sections comprise the scientific assessment, including:

- General description
- Development, availability, and version
- Documentation
- Governing equations and assumptions
- User input
- Output quantities
- Limitations

Each sub-section is to be reported in the MER using Table 3-1 through Table 3-7 where descriptions are to be entered in the second column. The text in parenthesis in the second column is provided for clarification and can be removed from the table that is provided in the final MER.

3.1. General description of the model

Table 3-1 provides features that are to be described pertaining to general modeling capability, model types, and boundary conditions. Features that are applicable to only CFD models are noted.

Table 3-1. General description of model features

Feature	Description
Model type	(e.g. integral type, CFD)
Flow regimes (CFD models only)	(e.g. laminar, incompressible, compressible)
List of sub-model types	(CFD models: pertaining to turbulence, combustion, radiation, gas radiation properties, soot, burn rate, and wall functions) (Integral models: list correlations used)
Instrumentation sub-grid models (CFD models only)	(e.g. thermocouples, radiometers, directional flame thermometers)
Mesh features (CFD models only)	(e.g. Cartesian, body-fitted, axisymmetric, adaptive grid, etc)
Cell types (CFD models only)	(hexahedral, tetrahedral, polyhedral, etc.)
User-defined capabilities (CFD models only)	(e.g. pertaining to boundary conditions, initial conditions, and subroutines)
Boundary condition types available (CFD models only)	(e.g. velocity inlet, open, symmetry, etc. and capability of time and spatial variation of boundary conditions)
Spatial and temporal schemes	(CFD models: list available schemes and provide spatial and temporal accuracy of schemes)

Feature	Description
	(Integral models: provide description of geometrical shapes modeled and view-factor model)
Other	(provide general description of any other notable feature)

3.2. Model development, availability, and version

Table 3-2 provides the features that are to be described pertaining to model development, availability and the current version used to carry out the MEP.

Table 3-2. Description of model development, availability, and version

Feature	Description
Developers of the model	(past and current)
Availability	(open source or commercial)
OS platforms and parallel capability	(e.g. Linux, Windows and parallel capability describing any limitations)
How to obtain model	(provide website and/or contact information)
Version of the model used for MEP	(version and OS platform)

3.3. Model documentation

Table 3-3 lists the types of model documentation to specify and where to obtain them.

Table 3-3. Description of model documentation

Feature	Description
Theory manual	(provide citation and where to obtain)
User manual	(provide citation and where to obtain)
Verification	(provide citation and where to obtain)
Validation	(provide citation and where to obtain)
User training, support, and forums	(provide information on user training and support, i.e., if classes are offered online or in person) (provide user forums for support and website if applicable)
Other	(other information pertaining to model documentation or user support)

3.4. Governing equations and assumptions of sub-models

Table 3-4 provides the information regarding a model's governing equations and assumption that are to be provided in the MER. Some models encompass a vast number of sub-models which may not be applicable to the MEP database. Thus, only sub-models applicable to the MEP database are to be described. Features applicable to either CFD models or solid flame models are noted.

Table 3-4. General description of governing equation and assumptions of models

Feature	Description
Fluid dynamics (CFD models only)	(provide description of governing equations and assumptions of available turbulence models applicable to MEP database; include burn rate model if applicable)
Combustion (CFD models only)	(provide description of governing equations and assumptions of available combustion models applicable to MEP database)
Radiation (CFD models only)	(provide description of governing equations and assumptions of available radiation models applicable to MEP database)
Soot (CFD models only)	(provide description of governing equations and assumptions of available soot models applicable to MEP database)
Gas radiation properties (CFD models only)	(provide description of governing equations and assumptions of available gas radiation property models applicable to MEP database)
Thermodynamic and material properties (CFD models only)	(provide general description of thermodynamic and material database. Also available equation of state models)
Empirical correlations (Solid flame models only)	(provide description of equations used for correlations, view factor, atmospheric attenuation, as well as assumptions and parameter values)

3.5. Required user input

Table 3-5 provides the input required by a user to perform simulations. Features that are applicable to only CFD models are noted.

Table 3-5. Required user input for a model

Feature	Description
Solid model (CFD models only)	(capability to create solid model, i.e. domain, within model or requires separate software package)
Mesh (CFD models only)	(capability to mesh solid model within model or requires separate software package. Provide accepted file extensions for mesh such as *step, *iges, etc.)
Mesh decomposition (CFD models only)	(mesh automatically decomposed for parallel processing within model or external software required)
Thermodynamic properties	(Available within model or requires user input)
Material properties (CFD models only)	(Available within model or requires user input)
Fuel properties for combustion	(combustion properties to input including those pertaining to reaction mechanisms and kinetics)
Initial conditions (CFD models only)	(input to provide)
Boundary conditions (CFD models only)	(input to provide for boundary conditions pertinent to MEP database)

Feature	Description
Model input	(required model input parameter for models pertinent to MEP database)
Model output	(input required by user for output of quantities)
Numerical parameter input (CFD models only)	(Provide all solver selections that are required and specify those that are automatic, e.g., is time-step automatically selected by model or requires user input?)
Other	(other user inputs pertinent to model used)

3.6. Output quantities

Table 3-6 provides the output features that should be described and provided in the MER.

Table 3-6. Output quantities and model output features.

Feature	Description
Variables	(What quantities are available pertinent to MEP database?)
User defined variables	(Are user-defined variables possible?)
Output format	(What is the format of the output? e.g. *.csv, *.e, etc. Also, whether quantities can be output at points, along a line, a plane, and the entire domain volume)
Other	(other pertinent output quantities)

3.7. Limitations

Table 3-7 lists features to address regarding a model's limitations. Features applicable to either CFD models or solid flame models are noted.

Table 3-7. Description of model limitations

Feature	Description
Fluid dynamics (CFD models only)	(provide limitations related to fluid dynamics models and turbulence models)
Combustion (CFD models only)	(provide limitations of combustion models)
Radiation (CFD models only)	(provide limitations of radiation models)
Soot (CFD models only)	(provide limitations of soot models)
Gas radiation properties (CFD models only)	(provide limitations of gas radiation property models)
Thermodynamic properties (CFD models only)	(provide limitations of thermodynamic and material property capability)
Mesh (CFD models only)	(provide limitations of available mesh types)

Feature	Description
Correlations (Solid flame models only)	(provide limitations of correlations, e.g. what fuel type and scale for which they were developed)
Other	(other limitations?)

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4. VERIFICATION

The objective of model verification is to determine if the discretized form of the relevant governing equations is correct and are being solved correctly and to reveal coding mistakes that affect the order of accuracy. Verification of integral based models can be carried out by a thorough systematic review of the equations to determine if either algebraic and/or solution errors exist. A CFD model can be verified by various methods, traditionally by comparison with exact solutions, benchmark solutions, other model solutions, as well as checking for symmetry behavior. The most rigorous verification method having high versatility is the method of manufactured solutions [22]. This method can help in determining where coding errors exist and to ascertain the order of accuracy. Note that even in high-quality scientific journals, peer verification of the mathematical implementation is often not systematically performed, and thus should not be relied upon as a method of verification. A formal quality assurance process by developers involving a suite of verification cases in which to check results after model modifications is the most reliable approach. For the MER, verification methods and any formal process used to carry out verification should be described by the petitioner. There should also be verification cases presented demonstrating the model's ability to conserve energy.

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5. VALIDATION

Validation is to be carried out by comparing model results to the MEP database that include datasets for pool fires, jets fires, and fireballs provided in Table 5-1. Comparison to the wall experiments is also to be provided if applicable. A spreadsheet and accompanying document [4] [5] provide information on the datasets, measurement comparisons, format of the spreadsheet, statistical measures, and evaluation of thermal exclusion zones based on model performance. Thus, the information is not repeated here but other information regarding sensitivity analysis and the MEP process for updated versions of a previously approved model is provided.

Note that the trench fire test series, BGC, is classified as a pool fire, but the pool is rectangular rather than circular. Although trench fires pose lower risk to the public comparing to pool fire and jet fire scenarios, the radiant heat from trench fire may compromise adjacent equipment and result in cascading damage. Additionally, the test series is included due to the size of the fires, the quality and reporting of data, and their applicability in exercising the same physical models applicable to circular pool fires for CFD models. However, integral models require different models to represent the shape of the flame to determine the view factor.

Table 5-1. Validation datasets for MEP database

Test Series	Fuel	Fire Type	Number of tests	Pool diameter or length (m)	Flame length or height (m)	Land/water	Engulfed object?
Sandia gas burner [23]	LNG	pool (circular)	28	3	1.1-6.9	land	no
Phoenix [23]	LNG	pool (circular)	2	27, 56	70, 146	water	no
Montoir [13]	LNG	pool (circular)	3	35	70-85	land	no
BGC trench [24] [25]	LNG	pool (rectangular)	13	4.4-52	1.5-7.7	land	no
LU [26]	LNG	jet	3	na	20- 50	land	yes
Shell [27]	LNG	fireball	3	na	42-56*	land	no
USN [28]	propane	pool	4	14.9-16.9	51.9-54.9	water	no
SNL-indoor [29]	crude oil	pool	1	2	4.4	land	no
SNL-outdoor [30]	crude oil	pool	1	5	4.5	land	yes
CERTEC [31] [32]	diesel	pool	5	1.5-6	~3-12	land	no
Sandia pool fire [33]	ethane, ethylene, propane, isopentane	pool	4	5	~10-25	land	no

Test Series	Fuel	Fire Type	Number of tests	Pool diameter or length (m)	Flame length or height (m)	Land/ water	Engulfed object?
TAMU [34] [35] [36]	propane	jet fire	4	na	2-4	na	no
A-S [37]	crude oil	jet fire	2	na	22-23	na	yes
Sandia jet fire [33]	ethane, ethylene, isopentane	jet fire	3	na	~12-17	na	no
HSL-BG [38]	propane	fireball	4	na	54-72*	na	no
BG propane [21] [39]	propane	fireball	1	na	65*	na	no
BG butane [21] [39]	butane	fireball	4	na	60-76*	na	no
SNL-fireball [30]	crude oil	fireball	3	na	60-69*	na	no
Sandia fireball [33]	ethane, ethylene, isopentane	fireball	3	na	72-84*	na	no
SNL concrete wall [33]	Insulated formed concrete	na	1	na	na	na	na
SNL masonry wall [33]	Masonry brick wall	na	1	na	na	na	na

5.1. Sensitivity Analysis

The MEP includes assessing the sensitivity of a model to input parameters, including the grid, numerical parameters, initial conditions, boundary conditions, and the choice of simulation domain. A simple way to carry out the sensitivity analysis is to vary the parameters one by one from a 'base case' that uses nominal, best-estimate parameter values. The results from the parameter variation cases can then be compared to the base case to assess the effects. The intent of sensitivity analysis is to provide direction on appropriate parameters, sub-models, conditions, and grids to use to carry out the validation. Sensitivity analysis provides a greater understanding of model behavior by identifying which parameters significantly contribute to uncertainty in the response quantities. This allows identification of appropriate models and areas where improvements to the model can be made to reduce uncertainty. There are several ways to determine the most impactful factors based on the results from a sensitivity analysis. Linear regression analysis is one simple approach to provide a ranking of the parameters for uncertainty importance. The resulting linear correlation coefficients from this analysis indicate the strength and positive/negative relationships of any linear or near linear correlations. Scatter plots of the input/output variables can be used to reveal if a strong nonlinear relationship exists for cases with a weak linear correlation coefficient. Also, a Pareto chart which combines a bar chart of frequency overlaid with a line chart of cumulative frequency can be used to reveal the most impactful factors [40].

Since the model type and the selection of associated parameters are not universal for a specific application, a good strategy is to first perform the sensitivity analysis before moving on to performing simulations for a test series. The parameter variation exercise will help identify which models and parameters provide more favorable comparison. The parameters that are varied should not require developer knowledge and access but rather should be accessible to a general user. Note that once pertinent models and parameters within a model have been identified for each fire type and are evaluated using the MEP, they are to be applied when assessing thermal exclusion zones for siting purposes. Note that the parameters in this case pertain to those associated with a sub-model for CFD and correlations for integral models. They do not include experimental input parameters such as the burn rate. The input parameters chosen when performing hazard analysis should be able to be justified from experimental data and should be as close to the scale being simulated as possible. If it is desired to have the flexibility to use different sub-model options within a model for siting purposes, e.g. turbulence models or flame length, drag, and tilt correlations, then that model is to be assessed using the MEP. The information gained by performing a sensitivity analysis on one or more tests can then be applied to the rest of the test series. The following provides discussion on each of the areas involving sensitivity analysis to be included in the MER.

5.1.1. Correlation Parameters (Solid flame models)

Sensitivity analysis of solid flame models can be carried out by assessing the effect of varying the parameters applicable to the model. However, common parameter variations for pool fires include surface emissive power, flame shape, flame length, tilt, drag, and transmissivity. Common parameter variations for jet fires include jet momentum flux, surface emissive power or radiative fraction, flame length, flame lift off, buoyancy forces, and wind effects. Common parameter variations for fireballs include fireball diameter, rise height, duration, and surface emissive power. For many of these parameters their values will cover a range of values based on experimental data. Using a combination of parameters based on their low- and high-end values can result in very significant differences [41]. Thus, the sensitivity evaluation should involve assessing different combination of parameters to understand the potential range of values that can result. The rationale for the nominal parameter values used in a model should also be provided. In instances where software packages do not allow for correlation parameters to be changed by a user it is recommended that users contact the developers for assistance.

5.1.2. Grid resolution (CFD models)

For simulations, it is desirable to demonstrate grid independence where quantities of interest don't change in value significantly with further grid refinement. The term 'grid sensitivity' is used for this section, rather than 'grid independence' since often for large scale problems involving fire it is difficult to reach true grid independence due to the computational requirements in using a sufficiently refined grid. Additionally, prevention of grid independence can be due to physical models and numerical methods as discussed in [42]. Not achieving grid independence does not mean that a model cannot provide useful predictions for practical engineering applications. Thus, demonstrating grid independence is not required, rather reporting on trends in the results using different grid resolutions is to be provided.

Grid sensitivity is to be carried out by performing simulations on at least three different grid resolutions where each successive cell size is reduced preferably by one half. The results for experimental quantities at their respective measurement locations are to be provided in the form of a bar graph from which predominant trends from the different grid resolutions can be revealed. The

word “predominant” is used since trends most likely will not be consistent in behavior at each measurement location. The predominant trends can help identify grid resolutions that indicate more asymptotic behavior than others and can potentially reveal the grid resolution that optimizes validation performance and computational expense, that is, further grid refinement doesn’t significantly change the results but allows much less computation time. The absolute value of the percent difference in results between successive grid resolutions for each measurement location and for each quantity is to be reported in the MER. The net effect of grid refinement is to be evaluated by the average of these values which is also to be reported. If the average is greater than 10% then this is considered a significant change. If the average is less than or equal to 10% then the coarser grid of the comparison should be used. The results are to be entered in the sensitivity worksheet for each test series and the graphical comparison is to be provided in the MER.

5.1.3. Sub-models (CFD models)

Many models will have a suite of models to choose among, thus the intent of a model sensitivity study is to evaluate the use of different models and their associated sub-models as well as pertinent parameters for each experimental series. For instance, different turbulence models could be explored as well as treatments of turbulent viscosity. Other model types involving combustion, radiation, and soot can also be investigated. However, the number of simulations to perform can easily become overwhelming given the number of models, and their associated parameters, potentially available within a model. CFD models that have extensive validation and a large user base will often be a good source to narrow the scope of the analysis by providing information on applicable models to explore, as well as their sub-models and parameters. The results for experimental quantities at their respective measurement locations are to be provided in the form of a bar graph to indicate the effect. The results are to be entered in the sensitivity worksheet for the test identified in the MEP database report and a graphical comparison is to be provided in the MER. If a linear regression analysis is performed this should also be reported.

5.1.4. Initial conditions, boundary conditions, and simulation domain (CFD models)

All outdoor fires included in the MEP were subject to wind which significantly affects the flame dynamics. Thus, it is important to capture the velocity profile and direction of the wind before starting the fire. Many CFD models require several time iterations before achieving a steady state for the wind conditions, however some models allow for the wind profile and direction to be set as an initial condition, in which case the initial iterations are not necessary. The real-time required to achieve a steady profile well as any other useful related information should be provided in the MER.

With regards to boundary conditions, it is important to identify those that allow for the wind and fire source to be appropriately captured. The tests included in the MEP did not measure the magnitude and direction of the wind impacting the full extent of the flame, thus the entire vertical wind profile is uncertain. The wind profile depends upon the stability of the atmosphere which was not characterized. It would be ideal to fully map wind conditions at boundaries reflective of those used in a simulation, but this is rarely ever provided due to the expense. Thus, it is recommended a sensitivity analysis using different profiles be performed along with different levels of turbulence intensity if applicable to the model. This sensitivity analysis is recommended only for pool fires due to the wind’s significant impact. Additionally, the simulation should be checked for non-physical behavior arising from boundary conditions, such as perturbations or back-flow. And, if using wall function models, y+

values should be evaluated to ensure that that grid placement does not violate the assumptions of the model.

The boundary condition at the surface of a burning of a pool fire involves specifying a velocity or mass flux and if applicable to the model, the turbulence intensity. Different turbulent intensities could be assessed as part of the sensitivity analysis. Regarding the jet fire simulations, the selected approach to modeling the region near to the fuel release will require evaluation of parameters associated with the boundary condition representing the release. This is also true of the representation and boundary treatment regarding the engulfed pipe as discussed in Section 2.1.2 of the MEP database document [4]. Similarly, the fireball simulations will require a sensitivity analysis of the boundary conditions representing the release, as mentioned in Section 2.1.3 of the MEP database document [4].

Domain boundaries placed too close to a fire can affect results due to the violation of assumptions regarding the boundary condition at open boundaries, such as zero fluxes and constant pressure. Thus, a sensitivity study should be performed to make sure that the domain extent is large enough to not affect results. Sensitivity analyses performed on boundary conditions or the domain should be reported in the MER.

5.2. Process for updated versions of a model

The MEP process for an updated version of a previously evaluated model is based on the extent of revision, categorized as minor, major, and significant. Their definitions and the process required for each are provided in Table 5-2 and Table 5-3, respectively. For minor changes, only a subset of the MEP database cases need be performed, whereas for significant changes all cases in the MEP database are to be performed. The subset cases are provided in Table 5-4.

Major and significant changes both require providing a change-log report which describes changes made between the updated version and previously approved version of the model. The change-log report is to follow the format of the MER but with the additional feature of describing and discussing changes pertinent to each section. In the scientific assessment section, a third column labeled ‘modification’ is to be added to Table 3-1 through Table 3-7 where descriptions of changes are to be entered. All changes to the model are to be provided even if not applicable to MEP datasets, including those pertaining to changes in physical model and/or numerical methods.

Table 5-2. Definition of change categories for model revisions

Category	Definition
Minor	<ul style="list-style-type: none"> • Correction of software bugs or flaws within the software that make it perform less than optimally • Graphic User Interface (GUI) • Addition of new compatible hardware support • Models not relevant to pool fires, jet fires, and fireballs pertaining to LNG and processing fuels of LNG • There is no difference in results between the updated and previously approved version of the model for MEP database subset
Major	<ul style="list-style-type: none"> • May encompass minor changes but includes new and/or improved modification to models relevant to pool fires, jet fires, and fireballs pertaining to LNG and processing fuels of LNG

Category	Definition
	<ul style="list-style-type: none"> The average value of the absolute change in results for all measurements in a test series between the updated and previously approved version of the model for MEP database subset is $\leq 1\%$
Significant	<ul style="list-style-type: none"> May encompass minor changes but includes new and/or improved modification to models relevant to pool fires, jet fires, and fireballs pertaining to LNG and processing fuels of LNG The average value of the absolute change in results for all measurements in a test series between the updated and previously approved version of the model for MEP database subset is $> 1\%$

Table 5-3. Review process based on modification category

Category	Process
Minor	<ul style="list-style-type: none"> Perform a subset of cases included in the MEP database (Table 5-4) Provide a short report describing the changes made to the model since its previous version Provide input files for the subset cases MEP database spreadsheet which has results for subset cases Provide access to the new version of the model
Major	<ul style="list-style-type: none"> Provide a change-log report Provide input files for all cases in MEP database MEP database spreadsheet which has results for all cases with sensitivity analysis Provide access to the new version of the model
Significant	<ul style="list-style-type: none"> Provide a change-log report Provide input files for all cases in MEP database MEP database spreadsheet which has results for all cases with sensitivity analysis Provide access to the new version of the model

Table 5-4. MEP case subset

Type	Test series	Test
Pool fire	Sandia gas burner	T1
	Montoir	T2
	Phoenix	T1
	BGC	T6
	USN	T1
	SNL-indoor	Bakken 2.1
	SNL-outdoor	Tight 1 (Bakken)
	CERTEC	T14_D4
	Sandia pool fire	Ethylene
Jet fire	LU	T2

Type	Test series	Test
	TAMU	T19f
	A-S	T2a
	Sandia jet fire	Isopentane
Fireball	Shell	T4
	HSL-BG	T4
	BG	T1
	SNL-fireball	Tight 2
	Sandia fireball	Isopentane

In the verification section, any changes to the quality assurance or verification process are to be described. In the validation section a quantitative comparison of results obtained between the new and previous version of the model are to be provided where both versions are configured identically. If there are changes to the configuration, then a description and explanation of the changes should be provided. Cases that produce a significant difference in results should be highlighted by explaining the cause of the difference. Any potential impact that changes have on the application of the model for LNG siting studies is to be discussed as well as how the updated version of the model potentially affects current suitability, limitations, and uncertainty factors as specified in PHMSA's Final Decision Letter for the previously approved version of the model.

6. MODEL EVALUATION REPORT FORMAT

The MER should include the following sections.

1. Scientific Assessment

Provide Table 3-1 through Table 3-7 with information provided in second column.

2. Verification

Describe verification process.

3. Validation

3.1 Pool fires

3.1.1 Test series (specify name of test series, e.g., Sandia gas burner tests, etc.)

3.1.1.1 *Computational specifications.* Table 6-1 provides the information to include for each test series. Those that pertain to CFD models only are specified.

Table 6-1. Computational specifications for Sandia gas burner tests

Specification	Description
Domain extent (CFD models only)	(x, y, z)
Mesh elements (CFD models only)	(N _x , N _y , N _z)
Element cell size (CFD models only)	If stretched provide details in mesh section below. If non-stretched provide cell size for each direction
Cell type (CFD models only)	e.g. hexahedral, tetrahedral, polyhedral, cartesian, mix of cell types.
Real time (minutes or seconds) (CFD models only)	
Computational time (days or hours) (CFD models only)	
Number of processors (CFD models only)	
Hardware platform	
Operating system	
Models	List all types of models used for test series
Assumptions	List any assumptions regarding the models

3.1.1.1.1 *Domain*

Provide picture of domain and label the transverse and vertical directions. If different domains are used for tests within a test series, then describe each one.

3.1.1.1.2 *Mesh*

Provide pictures of mesh and provide information on stretched grids, i.e., how it was stretched and smallest and largest cell sizes. If different meshes are used for tests within a test series, then describe each one.

3.1.1.1.3 *Initial conditions*

Provide initial conditions and time required to develop wind profile if applicable. If different initial conditions and/or different wind development times are used for tests within a test series, then describe each one.

3.1.1.1.4 *Boundary conditions*

Indicate boundary conditions on domain figure by a number. Provide a description of the boundary conditions in a table (Table 6-2) for each numbered location. If different boundary conditions are used for tests within a test series, then describe each one.

Table 6-2. Boundary conditions for ‘test series name’

Boundary location	description
1 (corresponds to boundary number pointed out on domain figure)	Provide type of boundary condition used
2	
Etc.	

3.1.1.2 *Results*

- Provide results from sensitivity analysis using different model parameters and/or models. Provide a bar graph indicating results at each measurement location as a function of variation. Note some test series may require several graphs to span all measurement locations. If ranking of parameters for impact is performed, then provide results.
- Provide the summary table and graphical results for the test series automatically generated in the MEP database spreadsheet. These are the worksheets labeled as ‘Test series name summary’ in the MEP database spreadsheet. If a summary worksheet isn’t provided for a test series due to insufficient data for the statistical parameters report results in tabular form.

3.1.1.3. *Discussion*

- Discuss results from sensitivity analysis including which factors had the greatest effect on the results.
- Provide discussion of the MEP database results for that test series. Include discussion of any anomalous or outlier behavior and possible causes of behavior.

3.1.2 through 3.1.8: Repeat sections 3.1.1 through 3.1.1.3 for each of the remaining pool fire datasets

3.1.9 Overall pool fire results

- Provide the summary table and graphical results from worksheets labeled ‘LNG pool fire summary’ and ‘non-LNG pool fire summary’ automatically generated in the MEP database spreadsheet.
- Provide discussion of results highlighting any outlier behavior and possible causes.

3.2 Jet fires

3.2.1 through 3.2.3: Repeat sections 3.1.1 through 3.1.1.3 for each jet fire test series.

3.2.4 Overall jet fire results

- Provide the summary table and graphical results from worksheets labeled ‘LNG jet fire summary’ and ‘non-LNG jet fire summary’ automatically generated in the MEP database spreadsheet.
- Provide discussion of results highlighting any outlier behavior and possible causes.

3.3 Fireballs

3.3.1 through 3.3.5: Repeat sections 3.1.1 through 3.1.1.3 for each jet fire test series.

3.3.6 Overall fireball results

- Provide the summary table and graphical results from worksheets labeled ‘LNG fireball summary’ and ‘non-LNG fireball summary’ automatically generated in the MEP database spreadsheet.
- Provide discussion of results highlighting any outlier behavior and possible causes.

4. Discussion

- Provide discussion of overall performance of model against MEP database.
- Provide any lessons learned or recommendations from models used.

7. CHECKLIST FOR MEP PETITIONERS AND REVIEWERS

Table 7-1 provides potential sources of error by an analyst performing the simulations for the MEP and Table 7-2 provides a checklist pertaining to these sources of error, useful for the both the MEP petitioner and reviewer. These are provided as beneficial aids to reduce the occurrence of errors. Thus, the checklist does not have to be provided in the MER.

Table 7-1. Potential sources of error in steps to perform simulations

Step	Sources of Analyst Error
1. Understanding problem	Not including appropriate physics for problem
2. Model selection	Inadequate model for problem
3. Model parameters	Inappropriate specification of parameters (model dependent)
4. Geometry creation	Incorrect dimensions specified Boundaries placement – i.e. boundary placement is affecting flow field
5. Mesh creation	Cell quality Inadequate resolution
6. Boundary conditions	Inappropriate boundary specified – e.g. wall instead of inlet Specified conditions – e.g. incorrect inlet velocity
7. Initial conditions	Incorrect conditions specified Not allowing the external flow field to develop before ignition – e.g. wind profile development
8. Material properties	Incorrect specification
9. Output comparison	Incorrect locations for point comparisons Reported output not corresponding to correct output results Incorrect comparison of quantities – e.g. comparing simulated gas temperatures to thermocouple measurements
11. Documentation	Not reporting the correct simulation description – e.g. assumptions, parameters, etc.

Table 7-2. Checklist for analysts and reviewers

Step	Checklist	
1. Understanding problem	Are the appropriate physics being addressed?	Yes <input type="checkbox"/> No <input type="checkbox"/>
2. Model selection	Are appropriate models being used to address the physics?	Yes <input type="checkbox"/> No <input type="checkbox"/>
3. Model parameters	Are the specified parameters correct for the specific models?	Yes <input type="checkbox"/> No <input type="checkbox"/>
4. Geometry	Are the dimensions correct for each geometric object? Are the boundaries interfering with the flow field?	Yes <input type="checkbox"/> No <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/>
5. Mesh	Are the cells overly skewed or have too large of an aspect ratio? Is the mesh resolution adequate? Has a mesh scaling study been performed?	Yes <input type="checkbox"/> No <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/>
6. Boundary conditions	Are the specified boundary types appropriate? Are the boundary conditions correctly specified?	Yes <input type="checkbox"/> No <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/>
7. Initial conditions	Are the correct initial conditions specified? If applicable, is the external flow field developed before ignition?	Yes <input type="checkbox"/> No <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/>
8. Material properties	Are the material properties appropriate and correctly specified?	Yes <input type="checkbox"/> No <input type="checkbox"/>
9. Output comparison	Are the results reasonable? Are the correct measurement locations being compared to? Do the reported results come from the correct simulation case? Are similar variables being compared?	Yes <input type="checkbox"/> No <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/>
11. Documentation	Is everything accurately documented?	Yes <input type="checkbox"/> No <input type="checkbox"/>

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