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Assessment of Simulation Predictions of Hydrocarbon Pool Fire Tests

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Assessment of Simulation Predictions of Hydrocarbon Pool Fire Tests

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Abstract

An uncertainty quantification (UQ) analysis is performed on the fuel regression rate model within SIERRA/Fuego by comparing to a series of hydrocarbon tests performed in the Thermal Test Complex. The fuels used for comparison for the fuel regression rate model include methanol, ethanol, JP8, and heptane. The recently implemented flamelet combustion model is also assessed with a limited comparison to data involving measurements of temperature and relative mole fractions within a 2-m diameter methanol pool fire. The comparison of the current fuel regression rate model to data without UQ indicates that the model over predicts the fuel regression rate by 65% for methanol, 63% for ethanol, 95% for JP8, and 15% for heptane. If a UQ analysis is performed incorporating a range of values for transmittance, reflectance, and heat flux at the surface the current model predicts fuel regression rates within 50% of measured values. An alternative model which uses specific heats at inlet and boiling temperatures respectively and does not approximate the sensible heat is also compared to data. The alternative model with UQ significantly improves the comparison to within 25% for all fuels except heptane. Even though the proposed alternative model provides better agreement to data, particularly for JP8 and ethanol (within 15%), there are still outstanding issues regarding significant uncertainties which include heat flux gauge measurement and placement, boiling at the fuel surface, large scale convective motion within the liquid, and semi-transparent behavior.

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NOMENCLATURE

ASC	Advanced Simulation and Computing Program, formerly Accelerated Strategic Computing Initiative
BVG	Bouyant Vorticity Generation
DOM	Discrete Ordinates Method – a radiation solution technique
DSMAG	Dynamic Smagorinsky LES turbulence model
DTM	Discrete Transfer Method – a radiation solution technique
EDC	Eddy Dissipation Concept
FUEGO	ASCI developed fire loads simulation tool
KSGS	Subgrid-scale Kinetic Energy One-equation LES turbulence model
LES	Large Eddy Simulation
LDRD	Lab Directed Research and Development
RANS	Reynolds Averaged Navier Stokes
SIERRA	ASC developed computation infrastructure for multiphysics integration
SNL	Sandia National Laboratories
SYRINX	ASC developed participating media radiation simulation tool
TTC	Thermal Test Complex
TFNS	Temporally Filtered Navier Stokes
UQ	Uncertainty Quantification
V&V	Verification and Validation ASC program

1 Executive Summary

The objective of this work is to perform a validation and uncertainty quantification (UQ) analysis of the fuel regression rate model within SIERRA/Fuego/Syrinx, the fire code developed at SNL through the Advanced Simulation and Computing (ASC) Program. The recently implemented flamelet combustion model is also assessed with a limited comparison to data. Two different experimental data sets are used for comparison. One of the data sets provides measurements of fuel regression and heat flux at the pool surface of 2-m diameter hydrocarbon pool fires. The fuels used for comparison for the fuel regression rate model include methanol, ethanol, JP8, and heptane. The other data set used for comparison provides measurements of temperature and relative mole fractions within a 2-m diameter methanol pool fire. Due to the commonality of the use of methanol for these two independent data sets, this fuel is used for comparison for the gas phase predictions using SIERRA/Fuego/Syrinx.

The comparison of the current fuel regression rate model to data without UQ indicates that the model over predicts the fuel regression rate by 65% for methanol, 63% for ethanol, 95% for JP8, and 15% for heptane. If a UQ analysis is performed incorporating a range of values for transmittance, reflectance, and heat flux at the surface the current model predicts fuel regression rates within 50% of measured values. An alternative model which uses specific heats at inlet and boiling temperatures respectively and does not approximate the sensible heat is also compared to data. The alternative model with UQ significantly improves the comparison to within 25% for all fuels except heptane. Even though the proposed alternative model provides better agreement to data, particularly for JP8 and ethanol (within 15%), there are still outstanding issues regarding significant uncertainties which include heat flux gauge measurement and placement, boiling at the fuel surface, large scale convective motion within the liquid, and semi-transparent behavior. It is recommended that these areas are the focus of future research.

For the gas phase comparison several turbulence models were compared to data for heat flux at the fuel surface, as well as temperature and relative mole fractions of H₂/N₂ and O₂/N₂ 1-m above the center of the pool. The models that provide the best agreement to data for the spatially and temporally averaged heat flux at the pool surface are the Temporally-Filtered Navier Stokes Reynolds average model (TFNS) and the Subgrid-scale Kinetic Energy One-equation LES model (KSGS). These two models provided a mean over-prediction of about 25%, while the Dynamic Smagorinsky LES model (DSMAG) provided an mean over-prediction of about 43%. The Buoyant Vorticity Generation Reynolds Average model (BVG) proved not to have sufficient dynamic behavior and predicted a very low flame. All models, except for the BVG model, predict a temporally mean temperature 1-m above the center of the pool of about 1200K, within the range of measured values. Simulation results were also compared to data showing plots of temperature versus relative mole fractions 1-m above the center of the pool. The TFNS model provides the best agreement to these plots with a peak temperature of 1800K compared to 2000K from data. The KSGS and DSMAG models predicted a peak temperature of 1600K, while the BVG model predicted a temperature of 580K. These findings are not an indication of general model performance due to the limited comparison to data. Thus no conclusions should be drawn with regards to model performance outside the range of this specific comparison.

2 Introduction

The objective of this work is to perform a validation and uncertainty quantification (UQ) analysis of simulations of hydrocarbon pool fire experiments performed in the Thermal Test Complex at Sandia National Laboratories (SNL). Two different experimental data sets are used for comparison. One of the data sets, funded by the Nuclear Weapons Engineering Campaign 6 (FY2008) program, measured fuel regression and heat flux at the pool surface of 2-m diameter hydrocarbon pool fires for the purpose of development and validation of the fuel regression rate model within SIERRA/Fuego/Syrinx, the fire code developed at SNL through the Advanced Simulation and Computing (ASC) Program. Methanol was tested as well as various other fuels. The other data set which was funded by Lab Directed Research and Development (LDRD) measured temperature and relative mole fractions within a 2-m methanol diameter pool fire. Thus, due to the commonality of the use of methanol for these two independent data sets, this fuel is used for comparison for the gas phase predictions using SIERRA/Fuego/Syrinx. The results for the various other fuels tested in the Campaign 6 experiments will also be discussed pertaining to the fuel regression rate model. While the main objective is to evaluate the fuel regression rate model, a further objective is to provide an initial evaluation of the flamelet based combustion model recently implemented within SIERRA/Fuego/Syrinx since the heat flux from the flame is the driving source for the fuel regression. The following first provides a discussion of the physical dynamics of a burning liquid surface, a description of the fuel regression rate and flamelet combustion models used within SIERRA/Fuego/Syrinx, a brief description of the experiments and simulations, as well as the UQ matrix, and finally the results and discussion are provided.

2.1 Mass and Heat Transfer at Pool Surface

A distinguishing feature of pool fires is the interdependence of the heat and mass transfer at the pool surface, that is, the supply of fuel is a function of the heat transferred from the fire back to the fuel surface and the heat generated from the fire is a function of the fuel supply rate, thereby generating a feedback mechanism. The supply of fuel will significantly affect the total heat release rate from the fire and ultimately the potential heat radiated to objects external to the fire, thus it is important to be able to predict the fuel regression rate. In general the fuel regression rate will be different than the burning rate since not all of the fuel vaporizing from the liquid will contribute towards combustion.

For pools of sufficient diameter, the heat from the flame will be principally transferred to the surface via radiation and convection modes, with radiation dominating in contribution with increasing diameter. Not all of the heat arriving from the flame to the pool surface will contribute to vaporization of the fuel. A portion of the incident radiation will be reflected at the pool surface, while some will be both absorbed and transmitted through the fuel. If the fuel layer is sufficiently thin and/or enough energy is transmitted there will be losses through the bottom of the pan. Part of the heat will also be lost through conduction at the pan rim, but becomes

fractionally negligible with increasing pool diameters. The fuel surface at nearly its boiling temperature will also be emitting radiation. Thus, the net incident heat transfer at the pool surface can be expressed as the following.

$$\dot{Q}_{net}'' = \alpha q_{radiation} + q_{convection} - q_{conduction} - q_{emittance} \quad (1)$$

The fraction of energy absorbed, α , will be balanced by the amount reflected and transmitted through the liquid fuel, that is,

$$\alpha = 1 - \rho - \tau \quad (2)$$

These quantities are spectral and depend on the wavelength of incident radiation. In the gas phase there is also spectral absorption in the fuel rich core which alters the radiant heat flux arriving to the pool surface.

Water condensation is another effect that can alter the amount of energy available to vaporize the fuel. Water from the combustion products can condense on the surface of the pool and become absorbed into the fuel and thereby increase the effective density of the liquid as well as other thermal properties. For methanol and for the length of time these tests were conducted approximately a 2% increase in density is expected (Corlett and Fu, 1966). This is a relatively small effect and thus is neglected in this analysis. The term $q_{conduction}$ in eq. (1) for conduction losses to the pan rim is also assumed to be negligible since the pan sidewall thickness is relatively thin, 6.4 mm, and the pan diameter relatively large, 3 m.

There is also convective motion occurring within the liquid. This is principally due to variation in heat flux from the flame to the pool surface which results in variation of mass flux. The variation in mass flux in the vertical direction must result in lateral fluid motion in order to conserve mass. This convective motion can be considered an energy loss with respect to the energy that can contribute towards vaporization of the fluid. The extent that this convective motion affects the mass flux is unknown. One of the objectives of the C6 experiments was to determine if this convective motion within the liquid is significant, but as will be discussed in a subsequent section it is uncertain if the approach taken was sufficient to answer this question due to possible competing effects.

Within the liquid the following equation for energy applies, along with the conservation of momentum and mass which are not explicitly stated here.

$$\rho c_p \frac{DT}{Dt} = k \nabla^2 T - \nabla \cdot q_r \quad (s(t) \leq x < L) \quad (3)$$

with the following boundary conditions at the surface, $x = s(t)$, where $s(t)$ moves with a velocity of the fuel vapors.

$$\dot{m}'' H_v = \dot{Q}_{net}'' + k \left. \frac{\partial T}{\partial x_i} \right|_{x=s(t)} \quad (4)$$

$$T = T_{boil} \quad x = 0 \quad (5)$$

Various boundary conditions could exist at the bottom of the pool at $x = L$ depending upon the scenario under consideration so none is explicitly stated here. Equation (3) assumes that the fluid has convective motion and is three dimensional. The current fuel regression rate model neglects these effects. Part of the objective of the C6 experiments and this current effort is to determine whether the current simplified model is adequate to reasonably predict fuel regression.

2.2 Current Fuel Regression Rate Model

Ideally, the governing equations within the liquid fuel would be solved for any given pool fire simulation, but due to the disparity of the length scale of the liquid versus the gas phase region it is computationally cost prohibitive. Thus, the current fuel regression rate model within SIERRA/Fuego/Syrinx uses a model which solves for the mass flux using an algebraic expression and does not computationally resolve liquid phase dynamics.

The current implemented model within SIERRA/Fuego/Syrinx to determine the mass flux of fuel vapor from the pool surface is one dimensional and assumes that radiative heat transport and convective motion does not occur within the liquid. A thermodynamic balance is used on the entire liquid region which is the control volume, that is,

$$\dot{Q}_{CV}'' = \dot{m}'' [(h_s - h_i) + g(z_s - z_i) + \frac{v_s^2 - v_i^2}{2}] \quad (6)$$

The net heat transfer at the surface of the pool can be expressed as

$$\dot{Q}_{CV}'' = \dot{Q}_{net}'' - \dot{m}'' H_v \quad (7)$$

For the C6 experiments the fuel is supplied at the same rate at which it is being consumed, thus the ‘inlet’ and ‘exit’ velocities, v_s , and v_i , are equal and the potential energy from gravity is negligible (~ 1) for these tests. Then using eq. (6) and (7) the following equation can be obtained where T_{boil} and T_{pool} are the boiling and pool temperatures, respectively.

$$\dot{Q}_{net}'' = \underbrace{\dot{m}'' H_v}_{Q_{evap}} + \underbrace{\dot{m}'' c_{p_l} (T_{boil} - T_{pool})}_{Q_{heat}} \quad (8)$$

An approximation is used to determine what fraction of the net energy arriving at the pool is going towards Q_{heat} which is the amount of sensible heat required to heat the fuel.

$$\frac{\dot{Q}_{heat}''}{\dot{Q}_{net}''} = f_{sensible} = \max(\min(\frac{T_{boil} - T_{pool}}{T_{boil} - T_{flash}}, 0.7), 0) \quad (9)$$

where $T_{flash} = T_{boil} - 125(K)$. This approximation (eq. 9) is based on curve fitting data for several fuels. The fraction of sensible heat is zero when the temperature of the fuel has reached the boiling point. Note that the temperature of the fuel is assumed constant with depth and the fuel temperature is not allowed to exceed the boiling temperature. Once the temperature of the fuel has reached the boiling temperature the mass flux is calculated by assuming that all of the heat arriving to the pool is contributing towards vaporization, that is,

$$\dot{Q}_{net}'' = \dot{m}'' H_v \quad (10)$$

The model assumes that conductive heat transfer is negligible which then reduces equation (1) to

$$\dot{Q}_{net}'' = \alpha q_{rad} + q_{conv} - \varepsilon \sigma T_{pool}^4 \quad (11)$$

The emittance is assumed to be equal to the absorptance, that is, $\varepsilon = \alpha$. The change in temperature and height with time as well as the mass loss rate are calculated by

$$\frac{dT_{pool}}{dt} = \frac{\dot{Q}_{net}'' f_{sensible}}{\rho c_p z_{pool}} \quad (12)$$

$$\frac{dh}{dt} = \frac{\dot{Q}_{net}'' (1 - f_{sensible})}{\rho H_v} \quad (13)$$

$$\frac{dm}{dt} = \frac{\dot{Q}_{net}'' A (1 - f_{sensible})}{H_v} \quad (14)$$

where z_{pool} is the height of the pool and A is the pool area. The equations are discretized and applied at every element at the fuel surface in a simulation and thus results in a variable mass flux across the surface due to variation in calculated surface heat flux values.

Alternatively, if eq. (9) is not used where no approximation of the sensible heat is made then the thermodynamic balance for a control volume of the entire fuel region using eq. (8) and (11) is

$$\dot{m}'' = (\alpha q_{rad} + q_{conv} - \varepsilon \sigma T^4) / [H_v + c_{p_l} (T_{boil} - T_{inlet})] \quad (15)$$

The temperature, T_{inlet} , is the temperature of the incoming fuel and does not change with time. The current model within Fuego treats the entire liquid volume as one temperature which changes with time and hence is more applicable to thin layers of fuel and is not representative of a layer of fuel which has a significant temperature differential between the incoming fuel and the

fuel at the surface. Section 8.1 of this report compares this equation as well as the current fuel regression rate model, eqs. (9 -14), to experimental data in order to determine the effect of the approximation for the sensible heat (eq. 9) on predicted mass flux values. Note, that the current model does not include specific heat as a function of temperature, but rather is based on an average specific heat between initial fuel temperature and the boiling temperature of the fuel.

To include variable specific heat with temperature, eq. (12) can be altered as

$$\frac{d(c_p T_{pool})}{dt} = \frac{\dot{Q}_{net}'' f_{sensible}}{\rho z_{pool}} \quad (16)$$

The computational expense would increase by this alteration since the equation now becomes an implicit polynomial equation in temperature which would have to be solved at every time step and location. Equation 15 uses an average specific heat evaluated between the inlet and surface temperatures. A more accurate representation would be to evaluate the specific heat at the inlet and surface temperatures respectively, that is,

$$\dot{m}'' = (\alpha q_{rad} + q_{conv}) / [H_v + c_{pT_s} T_s - c_{pT_i} T_i] \quad (17)$$

A comparison of using an average specific heat versus a specific heat evaluated at respective inlet and surface temperatures (eq. 15 and 17) is also provided in the section 8.1. Note that the fuel regression rate model within Fuego with or without the approximation of eq. (9) does not account for any kind of volumetric heat absorption. It will be shown in a following section that radiative heat transport occurs within certain fuels such that heat is partially absorbed and transmitted through the fuel layer and thus can be considered semi-transparent for the depths of fuels tested. The amount of energy absorbed can also be affected by the presence of bubbles on the fuel surface which can increase the reflectivity in equation (2) which is discussed in a later section.

2.3 Flamelet Combustion Model

As noted previously, an additional objective of this work is to compare predicted heat flux values at the fuel surface using the flamelet based combustion model within SIERRA/Fuego/Syrinx to experimental data. The following provides a brief description of the model. A more detailed description can be found in Hewson (2007) and Glaze (2007).

The steady laminar flamelet model for non-premixed combustion represents turbulent flames as an ensemble of laminar diffusion flames (Peters, 1984). This model is based on the idea that chemical time scales are much shorter than characteristic turbulent time scales and that the fuel and oxidant react in locally thin one-dimensional structures normal to the stoichiometric contour. The structures resemble the flame sheets responsible for combustion in a laminar flame and thus

have been termed laminar flamelets. The effect of strain and stretching from turbulence on these flamelets are accounted for in the model.

A laminar flamelet database, which provides variable relationships such as for temperature, species mass fractions, and density as a function of the mixture fraction and strain rate, is generated by the solution of equations for a one-dimensional, laminar, counter-flow, diffusion flame which are transformed into mixture fraction space.

The library covers the expected range of strain rates for reacting flows and is characterized in terms of a reference scalar dissipation rate at a reference mixture fraction which is typically the stoichiometric mixture fraction value or the maximum mixture fraction value. The flamelet library is a pre-calculated database of interpolated variables which are a function of mixture fraction and the reference scalar dissipation rate. The effect of turbulence on the ensemble of flamelets is accounted for by a statistical model which provides filtered state variables required for averaged conservation equations such as that used in LES and RANS formulations. The mixture fraction and the scalar dissipation rate are assumed to be statistically independent. A beta probability density function (PDF) is used for mixture fraction and the PDF of the scalar dissipation rate is modeled as the delta function.

One of the main advantages of the flamelet combustion model is that it can incorporate much more detailed chemistry than the other combustion model within Fuego, namely the Eddy Dissipation Concept (EDC) model by Ertesvag and Magnussen (2000). Detailed chemistry can easily be incorporated in the flamelet model since the flamelet library contains information about major and minor species.

2.4 Description of Experiments for Comparison

A brief description of the experiments used for comparison for this study is provided here. More detailed descriptions can be found in Ricks and Blanchat (2007) and Frederickson, et al. (2008). For the C6 funded experiments (Ricks and Blanchat, 2007), many different fuels were tested measuring fuel regression, spectral absorption coefficients in the vapor dome above the fuel surface (Suo-Anttila, et al., 2008), total heat flux at the fuel surface, and the effect of large scale convective transport within the fuel on fuel regression. In a non-fire environment and using a black body source the reflectivity at the fuel-air interface and the transmittance through the fuel were also measured (Suo-Anttila, et al., 2008). The tests were performed in the Thermal Test Complex at Sandia using a pan diameter of 2-m. The fuels tested include methanol, ethanol, JP8, heptane, and toluene, along with fuel blends of various proportions of methanol/toluene and ethanol/toluene. A constant liquid level depth was maintained with a liquid level control system. The fuel depths ranged roughly from 45 to 55 mm among the tests. In order to assess the effect of convective motion within the liquid fuel on the fuel regression rate, experiments were performed with small crushed glass pebbles within the fuel with the intent of suppressing large scale motion. The fuel regression rate and heat flux measurement at the fuel surface were used

for comparison for this study. Further details regarding this experiment will be discussed in the section presenting the results.

The LDRD funded experiments (Frederickson, et al., 2008) were also performed in the TTC for a 2-m diameter methanol pool fire. The optical technique of coherent anti-Stokes Raman Spectroscopy (CARS) was used to measure temperature and relative mole fractions of O_2/N_2 and H_2/N_2 at a location of 1 m above the center of the fuel surface. The measurement control volume was an ellipsoid with dimensions of 0.01 cm by 1 cm. These measurements were also used for comparison to simulation results for this study.

2.5 Simulation Specifications

2.5.1 Computational Suite

A suite of coupled codes, Sierra/Fuego/Syrinx (Moen, et al., 2002), was used to perform these calculations. Sierra provides a general framework for multi-physics coupling that allows Fuego and Syrinx to interact via volume and surface transfers for either one-way or two-way coupling. Fuego computes the fluids region and Syrinx computes the participating media radiation field. Fuego can simulate three-dimensional low Mach number turbulent reacting flows on heterogeneous topological meshes, e.g., a mixture of hexahedral, tetrahedral, pyramid, and wedge. An approximate projection algorithm is used with Control Volume Finite Element Method (CVFEM) discretization. SIERRA/Syrinx uses a discrete ordinates method assuming a grey non-scattering medium in which radiative sources include soot as well as gases.

Four different turbulence models were tested for this study: a variant of the standard $k-\epsilon$ turbulence subgrid closure model (Jones and Launder, 1972) for the Reynolds Averaged Navier Stokes (RANS) equations, a Temporally Filtered Navier Stokes (TFNS) closure model, the Dynamic Smagorinsky LES model, and the Subgrid-scale Kinetic Energy One-equation LES model.

The first model involves a modification to the production of turbulent kinetic energy for highly buoyant flows. The standard $k-\epsilon$ turbulence model can perform very poorly in fires since this model does not produce enough turbulent shear production in the first half diameter of elevation. Strong turbulent mixing occurs in this region due to density gradients. Thus, a term has been added to the production of turbulent kinetic energy to capture the buoyant vorticity generation (BVG) (Nicolette, et al., 2005). The term has the form

$$G_B = \frac{0.35\mu_t}{\rho^2} \|\vec{\nabla}\rho \times \vec{\nabla}p\|. \quad (18)$$

The term attempts to model the time-averaged effect of the roll-up of the large vortices that are characteristic of puffing fires as an additional turbulent kinetic energy production source term. The effects of both buoyant and shear production are contained in the eddy viscosity. Herein, this model is referred to as the BVG model.

The second treatment is the temporally-filtered Navier-Stokes (TFNS) model which temporally filters the k - ϵ turbulence subgrid closure model by applying a filter width, τ , (Tieszen, et al., 2005) and has the following form

$$\mu_t = c_\mu \rho k \tau \quad (19)$$

This definition for the eddy viscosity is also used in the turbulent kinetic energy and dissipation equations and results in source terms that are proportional to the filter width, τ , as opposed to the integral turbulence timescale, k/ϵ . Since the large scales are resolved, as opposed to modeled, Eq. 18 is not used with TFNS.

The Dynamic Smagorinsky LES model, herein denoted as the DSMAG model, is similar to the standard Smagorinsky LES closure model in that the subgrid eddy viscosity is modeled by the mixing length approximation. The expression for the subgrid eddy viscosity has a coefficient which must be determined which in the case of the DSMAG model is dynamically calculated instead of set to a constant value as in the standard model. The coefficient is dynamically calculated based on scale similarity in the inertial range of the turbulence spectrum near the minimum resolved scales. Thus, the coefficient does not have to be tuned beforehand for a particular problem application.

The Subgrid-scale Kinetic Energy One-equation LES model, herein denoted as the KSGS model, includes a transport equation for the subgrid turbulent kinetic energy which is used to compute the subgrid turbulent eddy viscosity and dissipation of turbulent kinetic energy.

These four models were tested using the flamelet combustion model within SIERRA/Fuego/Syrinx to compare predicted heat flux values at the fuel surface to the data obtained from C6 funded experiments performed in the TTC as well as the temperature and relative mole fractions obtained from the LDRD funded experiments.

2.5.2 Simulation Parameters

The fluid region was initialized with the values in **Table 1**. The fuel used for all simulations is methanol which has the following properties as shown in **Table 2**.

Table 1: Initial values for fluid region.

u-velocity (downstream velocity)	0 m/s
v-velocity (cross stream velocity)	0 m/s
z-velocity (vertical velocity)	0 m/s
Pressure above atmospheric	0 N/m ²
Temperature	300 K
turbulent kinetic energy*	1.5e-7 m ² /s ²
turbulent dissipation*	2.7e-5 m ² /s ³

*TFNS and BVG models

Table 2: Properties of methanol.

Molecular formula	CH ₃ OH
Molecular weight	32.04 kg/kmol
Liquid fuel density	791 kg/m ³
Vapor mid-boiling point	337 K

A time step of about 0.005 s was used for all simulations using the TFNS model, with a time filter of 0.04 s and CFL<1. Simulations using the BVG model had variable time steps also restricted by a CFL number of 1. Two non-linear iterations were taken for the energy equation, while for all other equations one non-linear iteration was taken. The quadrature order (QO) used for all simulations was 4 using the TN algorithm. The projection scheme used was "fourth order smoothing with timestep scaling." The linear equation residual norm tolerance was set to 1.E-04 for the continuity equation and 1.E-03 for the scalar and momentum equations. A MUSCL upwind scheme with Van Leer limiting was used. The first order upwind factor was set to 0.2 for all fluid equations except k and epsilon.

2.5.3 Geometry and Mesh

The TTC is cylindrical with a diameter of 18.3 meters and has sloped ceiling of approximately 18 degree where the height transitions from 12.2 m to 14.6 m (Fig. 1). The outlet is at the center of the ceiling and is 4.9 m in diameter and exits to a rectangular 3.0 by 3.7 m duct. The walls of the facility are water cooled to prevent radiation interactions. The burner at the center of the facility is surrounded by a 12.7 m diameter steel plate and air is provided from a ring at the floor of the facility. Also shown in Fig. 1 is the geometric model used for all simulations where nodes were clustered towards the fuel burner. The number of hexahedral elements used for each mesh is provided in Table 3. The medium size mesh was used to perform the uncertainty quantification analysis simulations.

Figure 1: a) Flame Test Cell at the Thermal Testing Complex b) Simulation geometry model.

Table 3: Number of hexahedral elements for each mesh and cell size.

	coarse	medium
Number of elements	330 K	2.5 M
Average smallest cell size (m)	0.1	0.05

2.5.4 Boundary Conditions

All simulations used the boundary conditions as listed in Table 4.

Table 4: Boundary conditions used for UQ simulations.

Surface	Boundary Type	Specifications TFNS and BVG	Specifications DSMAG and KSGS
Pool surface	Inflow	X_velocity = 0.0 m/s Y_velocity = 0.0218 m/s Z_velocity = 0 m/s Mixture Fraction = 1.0 Scalar Variance = 0.0 Turbulent kinetic energy = $1.8e-4 \text{ m}^2/\text{s}^2$ Turbulent dissipation = $1e-6 \text{ m}^3/\text{s}^3$ Temperature = 337 K	X_velocity = 0.0 m/s Y_velocity = 0.0218 m/s Z_velocity = 0 m/s Mixture Fraction = 1.0 Temperature = 337 K
Air ring	Inflow	X_velocity = 0.0 m/s Y_velocity = 0.854 m/s Z_velocity = 0 m/s Mixture Fraction = 0.0 Scalar Variance = 0.0 Turbulent kinetic energy = $2.74e-3 \text{ m}^2/\text{s}^2$ Turbulent dissipation = $4.7e-5 \text{ m}^3/\text{s}^3$ Temperature = 300 K	X_velocity = 0.0 m/s Y_velocity = 0.854 m/s Z_velocity = 0 m/s Mixture Fraction = 0.0 Temperature = 300 K
TTC walls	Wall	X_velocity = 0.0 m/s Y_velocity = 0.0 m/s Z_velocity = 0.0 m/s	X_velocity = 0.0 m/s Y_velocity = 0.0 m/s Z_velocity = 0.0 m/s
TTC outflow	Open	Pressure = 0.0 Characteristic Length = 2.5 m Mixture Fraction = 0.0 Temperature = 300 K	Pressure = 0.0 Characteristic Length = 2.5 m Mixture Fraction = 0.0 Temperature = 300 K
TTC floor	Wall	X_velocity = 0.0 m/s Y_velocity = 0.0 m/s Z_velocity = 0.0 m/s	X_velocity = 0.0 m/s Y_velocity = 0.0 m/s Z_velocity = 0.0 m/s

3 Uncertainty Quantification Matrix

The model used to predict fuel regression rate within Fuego has three parameters that can significantly impact predicted values due to the large range of uncertainty. These parameters include the fuel absorptance, α , the radiative heat flux from the flame to fuel surface, and the convective heat flux from the flame to the fuel surface. Since the convective heat transfer is under 10% of the total heat flux the radiative component has a much more significant effect (Modak and Croce, 1977, Iqbal and Quintiere 1994). Thermal properties have a much lower range of uncertainty and thus their expected variation has a minor effect on predicted regression rates.

The exact range of uncertainty for the significant parameters is difficult to determine based upon several indications. First, the amount of heat absorbed into the fuel is a function of the amount reflected off of the surface where the reflectance is a function of wavelength and angle. One of the factors that can affect the reflectance is the bubbling of the fuel surface which was observed in the C6 experiments for several fuels. Reflectance measurements for the C6 experiments were taken, however not in a fire environment, but rather at a laboratory scale for a quiescent sample without bubbling as shown in Figures 4 and 5 in section 4.1. The values ranged from about 0.01 to almost 0.1 depending on the fuel, angle, and wavelength. The reflectance measurements for the angle of 60 degrees display negative values which may indicate that the measurements are not accurate. Thus, the 20 degree measurements are taken as more valid for this analysis. Attempts were made to take measurements for a disturbed surface, but the measuring apparatus proved not to be appropriate for such an application.

In the literature, there has been laboratory scale work performed which indicates that the presence of bubbles can significantly alter the reflectance. Yavas, et al. (1993) used a pulsed-laser to induce boiling for a $1 \times 1 \text{ cm}^2$ sample of various liquids which included ethanol and methanol. They found that the reflectance displayed transient behavior as a function of bubble growth, incident angle, and the angle of a polarized beam. They also found that the formation of a bubble layer can increase the reflectance by about 25% for an angle of 26° for methanol. Although this was at a laboratory scale and not in a fire environment, the results from this study indicate that bubbling could potentially have a significant effect. Thus, in the absence of measurements indicative of bubble formation in a fire environment, the range of uncertainty for the reflectance assessed for the UQ analysis is 0.02 – 0.1.

The absorptance is also a function of the amount of radiation transmitted through the fuel. Transmittance measurements were obtained for the fuels presented here and are reported in Suo-Anttila, et al. (2008). The range of uncertainty was not reported. Consequently, the range of values used for the UQ analysis includes an uncertainty up to $\pm 20\%$ based upon discussion with the experimentalist and the extent of extrapolation required for particular fuels.

There is also uncertainty associated with the Schmidt-Boelter water-cooled thermopile gauges. These are total heat flux gauges which measure both radiative and convective heat transfer. The manufacture provides an uncertainty of $\pm 3\%$, but work by Nakos (2005) has shown that the

uncertainty in fire environments can vary from $\pm 20\%$ to $\pm 40\%$. The low end of this range, $\pm 20\%$ pertains to situations in which convective heat transfer contributes roughly 10% to the total heat transfer to an object. For 2-m diameter pool fires it is expected that the convective contribution of heat transferred to the surface from the flame should be under 10%. Thus, the lower end of this uncertainty range is more applicable to this study.

There are several factors that can affect the total heat flux measurement such as soot collection on the gauge surface, condensation of fuel or water on the gauge surface if the gauge is not cooled above respective boiling points, and the convective heat transfer uncertainty. Additionally, small variations in the heat flux gauge placement above the pool surface could also introduce some error. For the C6 tests, the 12 heat flux gauges were placed approximately 1.27 cm above the surface. Subsequent smaller scale experiments, 1 ft in diameter have indicated that a 1.27 cm placement can result in a 20% higher reading than if placed at the surface. This percent difference may not apply to the 2-m fires since the aspect ratio of placement distance to pool diameter is different. Only further experiments at the 2-m scale could determine what the difference would be if the gauges were flush with the surface. For this study, an uncertainty range of $\pm 30\%$ will be used for the total heat flux gauge measurements to account for all of these various factors. Note that further research is required to more accurately determine the range of uncertainty associated with heat flux gauges particular to this experimental configuration, not only intrinsic to the nature of the gauges, but also to how they are being utilized. Thus, the range of uncertainty explored for this study is still an open question.

As previously mentioned, the experimental results for heat flux to the fuel surface is also being used as a metric for comparison in addition to single point temperature and relative mole fractions. This comparison tests the capabilities of the newly implemented flamelet based combustion model. For this initial validation effort of the new model, the UQ analysis will assess the affect of different turbulence models as described previously in section 2.5.1, namely, the TFNS, DSMAG, KGSG, and BVG turbulence models. Methanol is the only fuel that is assessed since it is currently the only fuel available for this new model. The addition of other fuels is currently in progress, but they will not be implemented before the completion of this study.

A segregated approach is used in which the flamelet combustion model and the fuel regression rate model are decoupled by the specification rather than calculation of the pool mass flux using the fuel regression rate model. Similarly, the fuel regression rate model is evaluated by the specification of the heat flux back to the fuel rather than using calculated values. This approach allows for an isolated evaluation of predicted fuel regression rate and surface heat flux values. In reality, the heat flux will vary across the fuel surface and hence the mass flux will vary. The predicted heat flux may be altered by specifying a constant mass flux compared to allowing the mass flux to change according to the heat flux received at the surface. Since the main objective of this work is to fully evaluate the fuel regression model and to provide a relatively cursory evaluation, rather than a comprehensive UQ analysis, for the flamelet combustion model, the uncertainty introduced in the simulation results by this segregated approach is not addressed in this work.

4 Results and Discussion

4.1 Comparison of Fuel Regression Rate Model with Data

The fuel regression rate model is compared to experimental data by using the measured total heat flux values at the pool surface and eqs. (9) – (14) to calculate mass flux. These values are then compared to measured mass flux values assuming $\alpha = 1$. Note that this comparison is provided in order to facilitate discussion of features of the current model and to propose a new model. A UQ assessment is presented following this initial discussion.

The total measured heat flux is comprised of

$$q_{\text{total}} = q_{\text{rad}} + q_{\text{conv}} \quad (20)$$

Equation 11, however, has the radiative term reduced by the absorptance factor based on the fuel radiative properties. Thus, when q_{total} is substituted into eq. 11 it is multiplied by the absorptance, that is,

$$\alpha q_{\text{total}} = \alpha (q_{\text{rad}} + q_{\text{conv}}) \quad (21)$$

which is not equivalent to the segregation of the convective component in eq. 11, that is,

$$\alpha (q_{\text{rad}} + q_{\text{conv}}) \neq \alpha q_{\text{rad}} + q_{\text{conv}} \quad (22)$$

or

$$\alpha q_{\text{conv}} \neq q_{\text{conv}} \quad (23)$$

Since convection comprises 10% or less of the heat transferred to the fuel surface, though methanol may be an exception with possibly 20%, this error introduced from this substitution should be relatively minor with an upper limit of about 3% and a most probable value closer to 1% depending upon the amount of convective contribution and the absorption for particular fuels.

Table 6 shows the results of this comparison for four different fuels tested. The fuel properties used are provided in Table 5. Note that the ethanol used was not pure and composition values are listed in the Appendix in Table A1. It is very difficult to calculate heat of vaporization of mixtures (Ito, 1996), thus for this comparison pure property values are used. The calculated values over-predict the mass flux by almost a factor of two for all fuels except heptane. This is with the assumption that all of the energy is absorbed into the liquid. The initial height and temperature of the liquid are 0.05 m and 303 K, respectively. An average specific heat between the initial and boiling temperature is used and the calculated mass flux values are an average over the time it takes to deplete the fuel. Note that the results are independent of the initial height specified.

Table 5: Fuel properties.

Fuel	Molecular weight	Boiling Point (K)(C)	Heat of Vaporization (kJ/kg)	Heat of Combustion (kJ/kg)	Density (kg/m ³)	Thermal Conductivity (W/mK)
Methanol	32.1	337 (65)	1101.0	19,718	791	0.20
JP8	160.8	488 (215)	280.0	45,854	808	0.15
Ethanol	46.1	352 (79)	837.0	25,603	789	0.17
Heptane	100.2	372 (98)	316.0	45,365	684	0.13

Table 6: Comparison of fuel regression rate model with data assuming $\alpha=1$.

Fuel	Measured heat flux* (spatial average) (kW/m ²)	Measured Mass Flux* (kg/m ² s)	Calculated Mass Flux (kg/m ² s)	Percent difference (%)
Methanol	40.5	0.020	0.034	+65
JP8	43.1	0.038	0.074	+95
Ethanol	43.3	0.027	0.044	+63
Heptane	30.0	0.061	0.070	+15

*average value among several tests

Now equations (15) and (17) are compared to experimental data, which are considered alternative models to the current fuel regression rate model within Fuego. Note that the enthalpy term in the denominator of eq. (15) uses a single value for specific heat which is approximated as the average of the specific heat values at the incoming fuel temperature and the fuel boiling temperature, that is,

$$c_{p\text{ average}} = \frac{c_p(T_b) + c_p(T_i)}{2} \quad (24)$$

Thus, the change in enthalpy between the incoming fuel and outgoing vaporizing fuel is calculated as

$$h_b - h_i = c_{p\text{ average}} (T_b - T_i) \quad (25)$$

This approximation of the specific heat can result in a significant difference in predicted mass flux values. Table 7 shows the difference between predicted mass flux values using an average specific heat versus using specific heats at respective temperatures as used in eq. (17), that is,

$$h_b - h_i = c_{p_b} T_b - c_{p_i} T_i \quad (26)$$

It can be shown that the difference between using eq. 25 versus eq. 26 is the quantity

$$\frac{(c_{pi} - c_{pb})(T_b + T_i)}{2} \quad (27)$$

Since the specific heat at T_i is always less than at T_b the result of eq. 27 will be negative. The change in enthalpy term is in the denominator of eq. 15 and thus by using eq. 25 a lower value is computed which results in a higher computed mass flux. The greater the difference in the specific heats and temperatures in eq. 27, the greater the disparity between the use of the approximation of eq. 25 versus that of using eq. 26. Hence, it is expected that JP8 would show the greatest disparity due to its much higher boiling temperature than the other fuels as indicated in Table 7. Mass flux values using the model within Fuego are also provided in Table 7 for comparison among the three models. The specific heats as a function of temperature used for all fuels are provided in the Appendix and the inlet temperature of 303 K was used for all fuels.

Table 7: Effect of using an approximate specific heat versus not approximate.

Fuel	Measured Mass Flux (kg/m ² s)	Calculated Mass Flux using model within Fuego (kg/m ² s)	Calculated Mass Flux using Eq. 15 (kg/m ² s)	Percent difference (%) Eq. 15 vs. measured	Calculated Mass Flux using Eq. 17 (kg/m ² s)	Percent Difference (%) Eq. 17 vs. measured
Methanol	0.020	0.034	0.033	+65	0.031	+55
JP8	0.038	0.074	0.055	+46	0.039	+2
Ethanol	0.027	0.044	0.044	+63	0.037	+37
Heptane	0.061	0.070	0.058	-4.2	0.050	-18

It can be seen that using eq. (17) improves the comparison results for all fuels except heptane. The improvement is very significant for JP8 due to its high boiling temperature and its respective specific heat at that temperature.

An under-prediction for heptane could be the result of fuel and or water condensation on the heat flux gauges that evaporated and cooled the gauge to result in a lower reading than without condensation and evaporation. This effect is expected to have been present with the other fuels as well with respect to water condensation, except for JP8 since its boiling temperature is above that of water. Thus, the total heat flux should have been higher than what was measured. Note that the measured average heat flux was 13 kW/m² lower compared to JP8 and ethanol. In order for the model predictions to match the fuel regression rate for heptane the average heat flux at the pool surface would have to be about 36 kW/m² or 20% higher over that measured which is within the expected range of uncertainty for the gauge measurements.

The difference between the results using the various models can partially be explained by assessing the approximation for the fraction of sensible heat in the current model within Fuego. Table 8 shows a comparison of the fraction of sensible heat determined by using eq. (28) below which utilizes experimental values for mass and heat flux versus that of using eq. (9). The net heat flux is calculated using eq. (11).

$$f_{sensible} = \frac{\dot{m}''(c_{p_b}T_b - c_{p_l}T_i)}{\dot{Q}_{net}''} \quad (28)$$

This sensible heat fraction using eq. (9) varies with time as shown in Figure 2 and thus an average was determined for comparison in Table 8. Note that eq. (28) is also an approximation because all losses including absorptance have not been accounted for, but it does give a good indication of what this fraction should be. If adjusted for losses, the value for this fraction would be higher since the net heat flux would effectively be reduced. It is appropriate here to compare without losses and a reduction in absorptance since these were not accounted for using the model within Fuego. Also provided in the last column is a comparison of the mass flux change if a constant value for the sensible heat is used as specified in the second column using the model within Fuego.

The comparison indicates that the model does not partition enough of the arriving heat flux towards sensible energy so that more is contributing towards vaporization, thereby resulting in over prediction. If the more appropriate sensible heat fraction is used then better agreement results, particularly for JP8 and heptane, but the predicted mass flux values are still much higher than using eq. (17). This is principally due to the use of a constant specific heat and to a minor extent on the assumption of a uniform temperature for the volume of the fuel. The model within Fuego assumes that the entire volume of fuel is at a single temperature which changes in time to approach the boiling temperature. Note that if the fraction of sensible heat based on eq. (15) with a constant specific heat is used within the Fuego model and the fuel surface temperature is not allowed to change in time then equivalent mass flux values to eq. (15) are obtained. Thus, the equations solved within Fuego are equivalent to eq. (15) if no approximation is made for the fraction of sensible heat and the surface temperature of the pool is not allowed to change in time.

Table 8: Comparison of sensible heats from experiment versus model approximation.

Fuel	Percentage of sensible heat based on steady state experimental values and eq. (28)	Percentage of <i>average</i> sensible heat from Fuego model	Calculated mass flux using Fuego model if eq. (28) is used and sensible heat is a constant as specified in 2nd column. Parenthesis is unmodified Fuego model (kg/m² s)
Methanol	8.8	6.2	0.033 (0.034)
JP8	71.6	49.7	0.040 (0.074)
Ethanol	18.9	10.6	0.041 (0.044)
Heptane	55.3	24.6	0.041 (0.070)

Figure 2: Fraction of sensible heat over time using model approximation.

Figure 3: Mass flux over time using current model within Fuego.

If a comparison is performed which takes into account variations of transmittance and reflectance, then agreement between predicted and experimental values improves. As previously mentioned the reflectance and transmittance was measured as shown in Figures 4-6. Figure 6 shows absorptance versus fuel thickness which is derived by calculating one minus the transmittance. These measurements do not correct for reflectance. Thus, the transmittance values should be higher or conversely the absorptance values should be lower. The correction required is relatively minor for small transmittance values such as for ethanol and methanol with a 0.00526 increase, assuming a reflectance of 0.05. For JP8 and heptane, the correction should be an increase of 0.0158 and 0.0211 respectively, calculated from values at the 3 mm depth. The

range of uncertainty due to extrapolation to greater depths is larger than this difference. Thus, the uncertainty analysis should cover these corrections.

Additionally, the experimental results indicate that there was heat transfer occurring at the bottom of the pan that held the liquid fuel. The bottom surface exposed to air was not insulated but had an attached thermocouple which typically increased in temperature during the tests by about 3 C. For convective heat transfer at the pan bottom, the surrounding air temperature and convection coefficient are uncertain. Thus, it's difficult to determine the heat transfer, but an estimate can be made for convective heat transfer. If the convective coefficient is assumed to be around $10 \text{ W/m}^2 \text{ K}$ with a temperature difference of 20 C, then the heat transfer would be roughly 0.2 kW/m^2 . This is a negligible loss, but there possibly could be other heat transfer mechanisms present, such as conduction into surrounding steel in contact with the pan. It is difficult to quantify the amount of heat transferred, but a loss of $1 - 2 \text{ kW/m}^2$ could be likely based upon results from small scale tests which will be discussed shortly. Thus, for the comparisons in Table 10 a heat loss of 2 kW/m^2 is assumed.

Another effective loss is the radiant heat emitted from the fuel surface which could be significant for certain fuels. The non-blended fuels that were tested in the C6 experiments are listed in Table 9 which indicates that all of the fuels emit a relatively small amount of radiation ($< 1 \text{ kW/m}^2$) except for JP8 which can emit roughly 7% of typical incident average heat flux values due to its high boiling temperature. Emittance values in the range of 0.8 to 0.9 are realistic based upon absorptance measurements, but to provide an upper bound estimate a value of $\epsilon = 1$ is used for all fuels to obtain values in Table 9. Note that the fuel surface can also emit in the direction of the liquid based on the aforementioned factors regarding semitransparent behavior.

Table 9: Heat flux emitted at fuel surface for several hydrocarbons.

Fuel	Methanol	JP8	Ethanol	Heptane
T_s, Boiling temperature (K)	337	488	351	371
Heat flux emitted (kW/m²) ($\epsilon \sigma T_s^4$)	0.73	3.2	0.86	1.1

Figure 4: Spectral reflectance measurements at a 20 degree angle for various fuels.

Figure 5: Spectral reflectance measurements at a 60 degree angle for various fuels.

Figure 6: In depth absorption for different fuels using a blackbody source.

Table 10 shows the comparison if absorptance values are used that are based on measured values of reflectance and transmittance for the respective fuels. A range of reflectance values are explored as previously mentioned in section 3. Also, a range of transmittance values are explored due to uncertainties of measurement and uncertainties for depths greater than 3 mm. Note that there are also clear indications that for JP8 there was fuel condensing on the surface of the heat flux gauges which resulted in roughly a 10% lower reading. This was due to the difficulty in maintaining the gauge at a temperature above the boiling temperature of JP8. This adjustment has been included for JP8 in Table 10. Fuel surface emittance and losses have also been accounted for.

DAKOTA [Adam, et al., 2010] is open-source software developed at Sandia for optimization, uncertainty quantification, parameter estimation, design of experiments, and sensitivity analysis. DAKOTA was used to provide 15 sets of combinations based upon ranges of heat flux, transmittance, and reflectance as indicated in Table 10. The Latin Hypercube method was used to provide the combination sets. The results were easily generated due to the algebraic formulation of the fuel regression rate model, as well as the specification of the heat flux. This would not be the case for a CFD simulation since the heat flux and hence mass flux would be dynamically calculated. Thus, it is important to realize it is typically not feasible to perform several CFD simulations that span the range. At this point, the most practical alternative is to use midpoint values for heat flux, transmittance, and reflectance provided in Table 10.

Table 10: Comparison of mass flux values using Dakota for ranges of values.

Fuel	Total heat flux (kW/m²)	Transmittance	Reflectance	Measured Mass Flux (kg/m²s)	Calculated Mass Flux using Fuego model (kg/m²s) (mean ± s.d.)	Calculated Mass Flux using equation (17) (kg/m²s) (mean ± s.d.)	Difference from mean for each model (%)
Methanol	40.5 ± 30%	0.05 – 0.15	0.02 – 0.1	0.020	0.026 ± 0.0051	0.025 ± 0.0047	+30 / +25
JP8	43.1 ± 30%	0.10 – 0.20	0.02 – 0.1	0.038	0.054 ± 0.012	0.032 ± 0.0064	+42 / -15
Ethanol	43.3 ± 30%	0.05 – 0.15	0.02 - 0.1	0.027	0.035 ± 0.0068	0.030 ± 0.0056	+30 / +10
Heptane	30.0 ± 30%	0.10 – 0.30	0.02 - 0.1	0.061	0.046 ± 0.0099	0.035 ± 0.0071	-25 / -43

The results indicate that predicted mean values for mass flux are within 50% of mean measured values using the current model within Fuego, while using eq. (17) the values are within 25% of measured values except for heptane. An increase of 13 kW/m² in the measured surface heat flux for heptane does bring the predicted fuel regression rate value within 16% of the measured value. This increase would be commensurate with the measured heat flux values for JP8 and ethanol. The variation in the transmittance, reflectance, and possible losses could allow for predictions to match data for heptane. Further testing is required to determine if the heat flux gauge measurements are low due to condensation, evaporation, and/or placement.

Even though the predictions are within 25% of the data using eq. (17), caution should be taken in assuming that the model is adequately capturing all significant physical mechanisms. There is enough uncertainty regarding the various parameters that a strong conclusion cannot be drawn. As mentioned previously, the crushed glass used in some of the experiments was used with the intent of suppressing large scale convective motion within the fuel to ascertain whether convective motion was significant enough to affect the mass flux. The results indicate that there was not a significant difference between the tests that did or did not used crushed glass. Thus, presumably the conclusion can be reached that large scale convective motion does not affect the mass flux. There are indications that this may not be the case. Smaller scale tests have clearly demonstrated that the presence of crushed glass induces vigorous boiling which as previously discussed can have the potential to increase the reflectivity. Thus, the glass may have been suppressing one ‘loss’, that is, convective motion, but inducing another, namely an increase in reflectivity, thereby provided a false conclusion that convective motion has no effect. This issue still is need of resolution and requires further research.

There is also indication that these fuels are semitransparent for fuel depths greater than just a few millimeters. The experiments had a thermocouple rake close to the edge of the pool and spaced as listed in Table 11 and graphically represented in Figure 8. A side view showing the general configuration of the pan is shown in Figure 7. Note that there was a significant lip for these experiments which most likely affected the convective heat transfer near the pan edges by

slightly reducing it from a no-lip configuration. Figures 9 - 12 show steady-state temperature profiles from the thermocouple rake for the four fuels. JP8 has the highest temperature gradient and boiling temperature. Figures 13 - 16 show the temperature rise of the thermocouple nearest the pan bottom at 7 mm. The temperature rise for methanol and ethanol is roughly 7 C with and without the glass pebbles, whereas for JP8 and heptane the temperature increase is about 20 C without the pebbles and about 10 C with the pebbles. It can be seen that the glass pebbles have a stabilizing influence on the temperature, particularly with JP8 and heptane.

The significant temperature increase for JP8 and heptane with and without the crushed glass indicate that heat transfer was occurring through the liquid layer. There is the assumption that the presence of the glass prevents significant liquid motion and hence this mechanism is not responsible for the immediate temperature rise. To fully determine if the pebbles prevented motion, visualization or velocity measurements within the liquid are required. Furthermore, the temperature increase over time at that depth was not due to thermal penetration from conductive heat transfer since the increase occurred faster than the expected time for the arrival of a conductive thermal wave. This is also the case for the crushed glass. Note that in Figures 13 - 16 the fuels were ignited approximately at 4 to 5 minutes at which time the temperature of the bottom-most thermocouple immediately starts to rise. Additionally, a series of smaller scale tests demonstrated that heat is transferred immediately at depths of about 50 mm. In these tests, a Schmidt-Boelter Medtherm gauge was placed about 50 mm below the fuel surface in a 0.11 m diameter tube to measure heat flux penetration in depth. For all fuels the gauge immediately responded with a reading of about 1 kW/m² at 50 mm. Thus, all of these factors indicate that radiative heat transfer must have been responsible for the temperature increase and that JP8 and heptane, particularly, can be regarded as semitransparent mediums in which conduction and radiation are simultaneously occurring. For certain scenarios which have a thin layer of fuel such as when fuel is allowed to freely spread, this semitransparent behavior is significant since it will affect the temperature gradient below the fuel which in turn affects the vaporization. This finding is very significant and should be incorporated into future research and development.

Table 11: Thermocouple placement.

TC#	height (mm)
1	7.0
2	14.0
3	21.0
4	27.9
5	34.9
6	41.3
7	42.3
8	43.3
9	44.3
10	45.3
11	46.3
12	47.3
13	48.3

14	49.3
15	50.3
16	51.3
17	52.3
18	53.3
19	54.3
20	55.3
21	56.3
22	57.3
23	58.3
24	59.3
25	60.3
26	66.7
27	77.5
28	88.3
29	99.1
30	109.9
pan lip

Figure 7: Side view of 2-m pan.

Figure 8: Thermocouple in depth locations within the fuel.

Figure 9: Fuel in-depth temperature profile for methanol, all tests.

Figure 10: Fuel in-depth temperature profile for JP8, all tests.

Figure 11: Fuel in-depth temperature profile for ethanol, all tests.

Figure 12: Fuel in-depth temperature profile for heptane, all tests.

Figure 13: Methanol temperature rise in liquid for tests with and without crushed glass. Lowest thermocouple (7 mm from pan bottom).

Figure 14: JP8 temperature rise in liquid for tests with and without crushed glass. Lowest thermocouple (7 mm from pan bottom).

Figure 15: Ethanol temperature rise in liquid for tests with and without crushed glass. Lowest thermocouple (7 mm from pan bottom).

Figure 16: Heptane temperature rise in liquid for tests with and without crushed glass. Lowest thermocouple (7 mm from pan bottom).

It is of interest to determine if a correlation exists to predict the mass flux. If the ratio of the measured average heat flux at the fuel surface to the heat release versus the measured mass flux is plotted then the data falls along the line indicated in Figure 17. The measured heat of combustion values are provided in Table 5. The function is

$$\dot{m}'' = 0.0065 \left(\frac{Q_{surface}}{\dot{m}'' H_c} \right)^{-0.5} \quad (29)$$

This function can be approximated by

$$\dot{m}'' = (.0065)^2 \frac{H_c}{Q_{surface}} \quad (30)$$

Where H_c is in units of kJ/kg and $Q_{surface}$ is in units of kW/m².

Figure 17: Correlation of mass flux versus the ratio of surface heat flux to the heat release.

Note the relatively small amount of heat arriving to the surface compared to the total amount of energy theoretically available. One of the interesting aspects of Figure 17 is that heptane which has the highest mass flux requires only about 1% of the total theoretical heat release to vaporize the fuel. JP8 partitions about 3% towards vaporization which is higher than heptane but has a lower mass flux despite its lower heat of vaporization. Note that both fuels have similar heats of combustion. However, as previously discussed, the sensible heat is much higher for JP8 due to its higher boiling point compared to heptane. To have some measure of this comparison a plot of experimental mass flux versus the ratio of heat of vaporization plus sensible heat to the heat of combustion is shown in Figure 18. Even though a function can be fit to these points the curve should not be used universally to predict an average mass flux for every fuel since the mass flux may not asymptote for a particular fuel at this diameter and the data pertains to a particular fuel thickness. The function which fits the points in Figure 18 is the following.

$$\dot{m}'' = 0.0033 \left(\frac{H_v + c_{p,boil} T_{boil} - c_{p,inlet} T_{inlet}}{H_c} \right)^{-0.66} \quad (31)$$

Figure 18: Correlation of mass flux versus the ratio of surface heat flux to the heat release.

4.2 Comparison of Fuego Simulation Results with Data

As mentioned previously, a further objective of this work is to compare the newly implemented flamelet combustion model to data for different turbulence models using Fuego for a 2 m methanol pool fire. Specifically, results for heat flux at the pool surface are compared to data obtained from the C6 experiments, and results for temperature and relative mole fractions 1 m above the pool are compared to the data obtained from the LDRD experiments. The following sections provide these comparisons.

4.2.1 Comparison to Heat Flux Measurements at Pool Surface

For comparison to the measured heat flux at the pool surface, similar locations are sampled over time for the simulations. Twelve gauges were placed in the experiments such that if the pool was divided into 6 concentric rings, each ring would be of equal area and have 2 gauges in each ring, a primary and secondary. Each gauge was not completely flush with the pool surface, but was placed approximately 1.27 cm above the pool surface since it was necessary to prevent any fuel leaking down into the ‘basement’ of the facility. Table 12 provides the radii for the rings and Table 13 provides their X and Y placement. Figures 21 and 22 provide experimental time-

averaged heat flux values for primary and secondary gauges in each ring, as well as an average between the primary and secondary gauges. Figure 21 shows results for a test without crushed glass, while Figure 22 shows results for a test with crushed glass. It can be seen that there are minor differences in the measured total heat flux to the surface between the two tests. Thus, from these results it appears that the glass does not affect the total heat flux arriving to the surface.

Figures 23-25 provide simulation results using the TFNS, DSMAG, and KSGS turbulence models respectively using the flamelet combustion model. Each simulation was conducted for 40 to 50 seconds of real time with a computational run time of 4 days on 512 processors for the medium mesh (2.5 M nodes). For all simulations steady state behavior was reached within 10 seconds of real time. The TFNS and KSGS models have better agreement than the DSMAG model for the average among all the gauges to experimental data. The TFNS and KSGS models predict an average flux of 51.1 kW/m^2 and 50.8 kW/m^2 , respectively, which is approximately 28% higher than the measured value of about 40 kW/m^2 . The TFNS model performs better than both the DSMAG and KSGS models for prediction among the various rings. Note that the current model within Fuego for calculating radiation transport does not take into account all of the absorption that occurs in the fuel vapor dome. As part of the C6 experiments, spectral measurements were taken within the fuel vapor dome and the results indicate that there is significant spectral absorption by cold soot, CO_2 , H_2O , and fuel vapor which can cause the amount of incident radiation to the pool surface to be reduced (Suo-Anttila, et al., 2008). If absorption from all sources was incorporated into the radiation transport model then it is expected that better agreement would result. It is anticipated that this feature will be implemented into Fuego in the future to explore the possible impact to the heat flux arriving to the pool surface

It is also expected that a finer mesh would provide better agreement. The average heat flux using a coarse mesh shown in Figure 26 is 63.4 kW/m^2 compared to 51.1 kW/m^2 for the medium mesh. Thus, if a finer mesh is used the average heat flux should decrease according to this trend.

The BVG model proved to be extremely steady with no dynamic behavior and thus a full data extraction was not carried out. Results showing this behavior are shown in Figures 19 and 20. Figure 19 shows a plot of the temperature at an elevation 1-m above the pool which remained at a constant value of about 580 K which is about a factor of 2 lower than what experiment and the other models indicated. Figure 20 shows the heat flux to the pool surface and due to the very low flame is about a factor of 2 higher than the measured average heat flux.

For comparison a simulation was performed using the Eddy Dissipation Concept (EDC) model which was the only combustion model in Fuego before the recent implementation of the flamelet model. The simulation was conducted using the TFNS turbulence model. Figure 27 shows that the average heat flux to the pool surface is 42.9 kW/m^2 , which provides the best agreement to the experimental value. This better agreement compared to the flamelet model may be due to the higher predicted flame height of about 2 to 2.5 diameters using the EDC model versus about 1 to 1.5 diameters using the flamelet model. As mentioned with the BVG model, the predicted flame height was under 0.5 diameters which resulted in extremely high heat flux values to the pool.

surface. Thus, the prediction of where reaction occurs can significantly affect predicted pool surface heat flux values.

Figure 19: Temperature contours using the BVG model.

Figure 20: Heat flux to the pool surface using the BVG model.

Table 12: Radii of rings for 2-m pan.

ring #	inner radius (m)	outer radius (m)	Area (m ²)
1	0.000	0.408	0.524
2	0.408	0.577	0.524
3	0.577	0.707	0.524
4	0.707	0.816	0.524
5	0.816	0.913	0.524
6	0.913	1.000	0.524

Table 13: Position of heat flux gauges at the pool surface.

ring #	theta	radius (m)	x (m)	y (m)
1	-90	0.289	0.000	-0.289
1	135	0.289	-0.204	0.204
2	-150	0.500	-0.433	-0.250
2	75	0.500	0.129	0.483
3	150	0.645	-0.559	0.323
3	15	0.645	0.624	0.167
4	90	0.764	0.000	0.764
4	-45	0.764	0.540	-0.540
5	30	0.866	0.750	0.433
5	-105	0.866	-0.224	-0.837
6	-30	0.957	0.829	-0.479
6	-165	0.957	-0.925	-0.248

Figure 21: Experimental measurements of heat flux at the pool surface for methanol test without crushed glass.

Figure 22: Experimental measurements of heat flux at the pool surface for methanol test with crushed glass.

Figure 23: Simulation results for average pool surface heat flux values at various rings using the TFNS turbulence model.

Figure 24: Simulation results for average pool surface heat flux values at various rings using the DSMAG turbulence model.

Figure 25: Simulation results for average pool surface heat flux values at various rings using the KSGS turbulence model.

Figure 26: Simulation results for average pool surface heat flux values at various rings using the TFNS turbulence model, coarse mesh.

Figure 27: EDC model results. Simulation results for average pool surface heat flux values at various rings using the TFNS turbulence model, coarse mesh.

4.2.2 Comparison to Temperature Measurements

Temperature measurements were obtained at 1 m above the center of 2 m methanol pool fires in the LDRD funded experiments described previously. Figure 28 provides temperature histograms of two repeat experiments from those tests. Figures 29-31 show temperature histograms obtained from simulation using the TFNS, DSMAG, and KSGS models, respectively. The mean temperatures from all models compare favorably with the two experimental tests. The coarse mesh using the TFNS model shown in Figure 32 resulted in a higher average temperature of 1330 K versus 1209 K for the medium mesh. It is thus expected that a lower average temperature would result for a finer mesh according to this trend. Figure 33 shows results for temperature using the EDC combustion model and TFNS turbulence model and indicates an average temperature of $1080 \text{ K} \pm 206 \text{ K}$. Thus, the average temperature at this single point measurement is under-predicted using the EDC combustion model.

Figure 28: Experimental temperature histograms from repeat tests of a 2 m methanol fire taken at 1 m above center of pool.

Figure 29: Simulation temperature histogram of a 2 m methanol fire at 1 m above center of pool for TFNS model.

Figure 30: Simulation temperature histogram of a 2 m methanol fire at 1 m above center of pool for DSMAG model.

Figure 31: Simulation temperature histogram of a 2 m methanol fire at 1 m above center of pool for KSGS model.

Figure 32: Simulation temperature histogram of a 2 m methanol fire at 1 m above center of pool for TFNS model, coarse mesh.

Figure 33: EDC model results. Simulation temperature histogram of a 2 m methanol fire at 1 m above center of pool for TFNS model, medium mesh.

4.2.3 Comparison to Relative Mole Fraction Measurements

Simulation results are compared to relative mole fractions for O₂/N₂ and H₂/N₂ obtained at 1 m above the center of 2 m methanol pool fires in the LDRD funded experiments described previously. It should be realized that comparing the models to one location within the flame is a very limited indicator of model performance. A greater mapping of the flame experimentally would allow a more complete comparison to ascertain model performance. It is anticipated that additional data will be obtained in the future for such assessment.

Figure 34 provides temperature versus relative mole fractions from those tests. Figures 35-37 show relative mole fractions obtained from simulation using the TFNS, DSMAG, and KSGS

models, respectively. The overall shapes of the curves from simulation favorably compare qualitatively with experiment. The experimental results for the relative mole fractions of O₂/N₂ indicate a fairly even scatter distribution between 0.25 with a slightly higher density between 0.1 and 0.3. Data points are also clustered very near zero with a temperature range between 1000 K and 2000 K. The relative mole fractions of H₂/N₂ have a very high density of points occurring near zero ranging in temperature between atmospheric and 2000 K. The distribution is fairly uniformly scattered between H₂/N₂ values of 0.05 and 0.3 and then becomes very sparse. Note that there does seem to be an angled gap at around 0.2 which may be due to experimental origins. The greater scatter in the experimental result compared to simulation can be explained by the finer resolution with dimensions of 0.01 cm by 1 cm for an ellipsoid compared to the simulation cell size of approximately 5 cm. Thus, less averaging is occurring with the experimental measurements and more fluctuations are being captured compared to the simulations. Higher resolution simulations matching that of the experiment were not performed due to the extensive computational requirements of performing simulations using 10s millions of elements. The simulation results for all turbulence models do not capture the density differences that occur over the relative mole fraction ranges, particularly for H₂/N₂ values beyond 0.3 where the models over predict the amount of H₂ and/or under predict the amount of N₂ at this location in the flame.

The TFNS model performs better than the DSMAG and KSGS models with respect to peak temperature, 1800 K versus 1600 K, as compared to experiment with a value of approximately 2000 K. The DSMAG model is an LES based model and thus relies more on grid resolution than the TFNS model which is temporally averaged rather than spatially averaged. Thus, for equivalent mesh resolution it is expected that the TFNS model would provide more favorable agreement than the DSMAG model, provided the temporal resolution is sufficient for the TFNS model and that the solution has not reached essential grid independence for the DSMAG model. Note, however, that this statement cannot be applied generally given the wide array of different flow fields and the different treatment of modeling subgrid scale turbulence of these models.

Figure 38 provides results using the TFNS model using the coarse mesh and due to the larger cell size less scatter results. The coarse mesh also has a peak temperature of approximately 1600 K versus the medium mesh of 1800 K for the TFNS model. Thus, it is expected that a finer mesh would provide more scatter and a higher peak temperature providing more favorable comparison to experiment. Figure 39 provides results using the EDC combustion model and TFNS turbulence model. The general shape and distribution is not captured adequately using the EDC model at this measurement location. However, it should be kept in mind that this is a comparison to data obtained at a single location and thus may not be an indication of overall model performance. Due to the limited comparison, an accurate statement cannot be made regarding the general performance of these models at this time. In order to make a full assessment of model performance other characteristics should be measured such as flame geometry and heat flux at a distance, as well as obtaining data at several locations within the flame similar of this experimental study.

Figure 34: Temperature versus relative mole fractions of O₂/N₂ and H₂/N₂ from experiment.

Figure 35: Temperature versus relative mole fractions of O₂/N₂ and H₂/N₂ from simulation using the TFNS model.

Figure 36: Temperature versus relative mole fractions of O₂/N₂ and H₂/N₂ from simulation using the DSMAG model.

Figure 37: Temperature versus relative mole fractions of O₂/N₂ and H₂/N₂ from simulation using the KSGS model.

Figure 38: Temperature versus relative mole fractions of O₂/N₂ and H₂/N₂ from simulation using the TFNS model, coarse mesh.

Figure 39: EDC model results. Temperature versus relative mole fractions of O₂/N₂ and H₂/N₂ from simulation using the TFNS model.

5 Summary

The comparison of the current fuel regression rate model to data without UQ indicates that the model over predicts the fuel regression rate by 65% for methanol, 63% for ethanol, 95% for JP8, and 15% for heptane. This comparison was performed to facilitate discussion of the model, features of a proposed alternative model, and provide an indication of results using default values. If a UQ analysis is performed incorporating a range of values for transmittance, reflectance, and heat flux at the surface the current model predicts fuel regression rates within 50% of measured values. The proposed alternative model uses specific heats at inlet and boiling temperatures respectively and does not approximate the sensible heat. The alternative model with UQ significantly improves the comparison to within 25% for all fuels except heptane. It is recommended based upon these finding that no approximation is used for sensible heat as is assumed with the current model and that specific heats are evaluated at the temperature of the incoming fuel and the fuel surface. The recommended model is

$$\dot{m}'' = (\alpha q_{rad} + q_{conv}) / [H_v + c_{pT_s} T_s - c_{pT_i} T_i] \quad (32)$$

Further, it is recommended that absorptance values provided in Table 14 are used based upon mid-point values of transmittance and reflectance. Using mid-point values is recommended because when performing turbulent reacting flow simulations it is often too computationally expensive to perform a full UQ analysis covering a sufficient sampling space for the fuel regression model. If time permits it is recommended that a full UQ analysis is performed that spans the range of parameters. It should be kept in mind, however, that the fuel regression model is only one component of the many factors that must be incorporated to perform a UQ analysis of a turbulent reacting flow. It can quickly become unwieldy with regards to computational run time.

Table 14: Recommended absorptance values.

Fuel	Absorptance
Methanol	0.84
JP8	0.79
Ethanol	0.84
Heptane	0.74

Even though the proposed alternative model provides better agreement to data, particularly for JP8 and ethanol (within 15%), there are still outstanding issues regarding significant uncertainties which include heat flux gauge measurement and placement, boiling at the fuel surface, large scale convective motion within the liquid, and semi-transparent behavior. It is recommended that these areas are the focus of future research.

For the gas phase comparison several turbulence models were compared to data for heat flux at the fuel surface, as well as temperature and relative mole fractions of H₂/N₂ and O₂/N₂ 1 m above the center of the pool. The models that provide the best agreement to data for the spatially

and temporally averaged heat flux at the pool surface are the Temporally-Filtered Navier Stokes Reynolds average model (TFNS) and the Subgrid-scale Kinetic Energy One-equation LES model (KSGS). These two models provided an over prediction of about 25%, while the Dynamic Smagorinsky LES model (DSMAG) provided an over prediction of about 43%. The Bouyant Vorticity Generation Reynolds Average model (BVG) proved not to have sufficient dynamic behavior and predicted a very low flame. Consequently, the heat flux from the flame to the pool surface was over predicted by almost a factor of 2. All models, except for the BVG model, predict a temporally mean temperature 1 m above the center of the pool of about 1200 K, within the range of measured values. Simulation results were also compared to data showing plots of temperature versus relative mole fractions 1 m above the center of the pool. The TFNS model provides the best agreement to these plots with a peak temperature of 1800 K compared to 2000 K from data. The KSGS and DSMAG models predicted a peak temperature of 1600 K, while the BVG model predicted a temperature of 580 K. These findings are not an indication of general model performance due to the limited comparison to data. Thus no conclusions should be drawn with regards to model performance outside the range of this specific comparison.

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Appendix

The composition of Ethanol used in the C6 hydrocarbon tests was a mixture of various components as listed in Table A1.

Table A1: Composition of ethanol used in tests

SYNASOL	
PM-41	
190 proof	
Percent by Weight	
Ingredients	
Ethanol	83.47%
Methanol	3.52%
MIBK*	0.89%
Hydrocarbon	0.81%
(Hexanes)	
Ethyl Acetate	4.47%
Water	6.84%
total	100.00%

*MIBK (Methyl isobutyl ketone)

The specific heat as a function of temperature was determined from polynomial equations provided by the TPRC Data Series on Specific Heat for Nonmetallic Liquids and Gases (see references). For JP8 the specific heat was taken from the handbook of Aviation Fuel Properties. The functions used are the following.

Liquid Methanol:

Units for specific heat are in J/kg K and temperature is in K. ($181\text{ K} < T < 383\text{ K}$)

$$C_p = 1000 * 4.184 * (0.582485 - 3.75646 \times 10^{-4} T - 1.67844 \times 10^{-7} T^2 + 1.06214 \times 10^{-8} T^3)$$

Liquid Ethanol:

Units for specific heat are in J/kg K and temperature is in K. ($158\text{ K} < T < 383\text{ K}$)

$$C_p = 1000 * 4.184 * (0.504351 - 4.81584 \times 10^{-4} T - 9.21631 \times 10^{-7} T^2 + 1.14379 \times 10^{-8} T^3)$$

Liquid Heptane

Units for specific heat are in J/kg K and temperature is in K. ($230\text{ K} < T < 480\text{ K}$)

$$C_p = 1000 * 4.184 * (0.454958 - 3.45073 \times 10^{-4} T + 2.14820 \times 10^{-6} T^2 - 2.48653 \times 10^{-10} T^3)$$

Liquid JP8

Units for specific heat are in J/kg K and temperature is in K. (graph of linear function provided for 305 K < T < 457 K)

$$C_p = 4.309T + 685.69$$

Distribution:

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