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Numerical Simulations of a Methanol Pool Fire

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Abstract

Simulations of a turbulent methanol pool fire are conducted using both Reynolds-Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES) modeling methodologies. Two simple conserved scalar flamelet-based combustion models with assumed PDF are developed and implemented. The first model assumes statistical independence between mixture fraction and its variance and results in poor predictions of time-averaged temperature and velocity. The second combustion model makes use of the PDF transport equation for mixture fraction and does not employ the statistical independence assumption. Results using this model show good agreement with experimental data for both the 2D and 3D LES, indicating that the use of statistical independence between mixture fraction and its dissipation is not valid for pool fire simulations. Lastly, “finger-like” flow structures near the base of the plume, generated from stream-wise vorticity, are shown to be important mixing mechanisms for accurate prediction of time-averaged temperature and velocity.

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_m$</td>
<td>molecular diffusivity, $m^2/s$</td>
</tr>
<tr>
<td>$D_T$</td>
<td>turbulent diffusivity, $m^2/s$</td>
</tr>
<tr>
<td>$k$</td>
<td>turbulent kinetic energy, $m^2/s^2$</td>
</tr>
<tr>
<td>$I$</td>
<td>incomplete beta function</td>
</tr>
<tr>
<td>$P_Z$</td>
<td>probability density function (PDF) of $Z$</td>
</tr>
<tr>
<td>$P_{Z\chi}$</td>
<td>joint PDF of $Z$ and $\chi$</td>
</tr>
<tr>
<td>$\rho$</td>
<td>pressure, $N/m^2$</td>
</tr>
<tr>
<td>$r$</td>
<td>radial coordinate, $m$</td>
</tr>
<tr>
<td>$T$</td>
<td>temperature, $K$</td>
</tr>
<tr>
<td>$t$</td>
<td>time, $s$</td>
</tr>
<tr>
<td>$u$</td>
<td>axial velocity component, $m/s$</td>
</tr>
<tr>
<td>$u_i$</td>
<td>velocity component in $i^{th}$ direction, $m/s$</td>
</tr>
<tr>
<td>$W_s$</td>
<td>molecular weight of species $s$, $kg/kmol$</td>
</tr>
<tr>
<td>$x$</td>
<td>axial or stream-wise coordinate, $m$</td>
</tr>
<tr>
<td>$x_i$</td>
<td>coordinate in $i^{th}$ direction, $m$</td>
</tr>
<tr>
<td>$y, z$</td>
<td>transverse coordinates, $m$</td>
</tr>
<tr>
<td>$Y_s$</td>
<td>mass fraction of species $s$</td>
</tr>
<tr>
<td>$Z$</td>
<td>mixture fraction</td>
</tr>
<tr>
<td>$\beta_{1,2}$</td>
<td>parameters for the incomplete beta function</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>gamma function</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>dissipation rate of $k$, $m^2/s^3$</td>
</tr>
<tr>
<td>$\nu_s$</td>
<td>stoichiometric coefficient of species $s$</td>
</tr>
<tr>
<td>$\rho_s$</td>
<td>density, $kg/m^3$</td>
</tr>
<tr>
<td>$\sigma_Z$</td>
<td>mixture fraction variance (= $\overline{Z^2}$)</td>
</tr>
<tr>
<td>$\chi$</td>
<td>scalar dissipation rate, $1/s$</td>
</tr>
<tr>
<td>$\chi_f$</td>
<td>scalar dissipation rate fluctuation, $1/s$</td>
</tr>
<tr>
<td>$\omega_s$</td>
<td>chemical production rate of species $s$, $kg/s$</td>
</tr>
</tbody>
</table>

Subscripts

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F$</td>
<td>fuel property</td>
</tr>
<tr>
<td>$i, j$</td>
<td>indices for tensor notation</td>
</tr>
<tr>
<td>$O$</td>
<td>oxidizer property</td>
</tr>
<tr>
<td>$s$</td>
<td>species $s$</td>
</tr>
<tr>
<td>$st$</td>
<td>stoichiometric surface value</td>
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</table>

Superscripts

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\overline{\cdot}$</td>
<td>(overbar) Reynolds time-averaged or LES filtered quantity</td>
</tr>
<tr>
<td>$\sim$</td>
<td>(overtilde) Density weighted time or filtered quantity</td>
</tr>
</tbody>
</table>

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**Introduction**

An effort is currently underway to develop a computational tool to model the heat transfer from large-scale pool fires. This work is motivated by the need to insure the safety of nuclear weapons systems immersed in hostile thermal environments. Such a pool fire scenario could result from either an aviation fuel spill or an aircraft accident, therefore liquid hydrocarbon fuels are of primary interest.

A variety of different physical processes occur within the highly turbulent flame. The wide range of length and time scales of these processes combined with the fluid turbulence make direct numerical simulation, where all relevant physical processes are resolved on the grid, prohibitively expensive. The computational tool must therefore rely on a number of physical sub-grid models which introduce additional uncertainties into the calculation.

The heating rate from a pool fire has contributions from both convective and radiative heat transfer, with the latter generally being the major contributor.\(^1\) The radiative heat transfer arises primarily due to the presence of soot, which is strongly dependent on the location of the peak flame temperatures. The flame temperature, in turn, depends on both the chemistry and the transport properties within the flame.

![Fig. 1: Image of a 6x6 meter square pool fire from the Sandia National Laboratories Burn Site.](image)

Large pool fires are characterized as buoyancy driven turbulent diffusion flames. Initially, above the liquid pool of combustible fuel is a vapor dome of evaporated fuel. This is an oxygen starved region where no combustion can occur. At the interface between the vapor dome and the surrounding air, molecular diffusion of air and vapor fuel occur creating a stoichiometric surface where the flame resides. The depletion of reactants by chemical reactions typically occurs at a much more rapid rate than the mixing process and thus the rate of combustion is limited by the mixing process. The mismatch in the density and pressure gradients results in the generation of vorticity due to baroclinic torque. This vorticity manifests itself as large toroidal vorticities that are ejected at almost a constant frequency resulting in commonly observed flame puffing.\(^2\) (please see Ref. 3 for a more detailed discussion of the dynamics of large-scale pool fires).

The current fire modeling effort seeks an improvement over standard RANS methodologies through the use of LES technique. In LES, the large-scale turbulent flow structures are resolved in the calculation, while the smaller, more universally dissipative scales are modeled. The goals of this paper are to conduct preliminary validation of the combustion model and to assess the usefulness of LES approaches for pool fire simulation.

The initial effort will focus on the small-scale methanol pool fire studied experimentally by Weckman and Strong\(^4\) where the effects of soot and radiation are minimal. Following this introduction is a description of the methanol pool fire of interest followed by a brief summary of the different numerical approaches. The conserved scalar flamelet based combustion models are then detailed followed by a discussion of the results. Lastly, summary and conclusions are drawn.

**Problem Description**

The data set used for preliminary model validation is the 24.6 kW methanol pool fire of Weckman and Strong.\(^4\) The pool has a diameter of 31 cm and is fed by a liquid pumping system which provides a volumetric flow rate at the pool surface of 1.35 cm\(^3\)/s. This data set includes point laser doppler velocimetry and thermocouple measurements of both time-averaged and fluctuating velocity and temperature. The methanol pool is located at least 1 m from the floor and is enclosed by a wire mesh to minimize disturbances. Examples of the flame structure taken from the experiment are shown in Fig. 2. The local mixing of the flow field is controlled by the large scale stretched toroidal vorticities that are emitted at a puffing frequency of 2.8 Hz. In addition, smaller scale “finger-like” structures that lie near the base of the plume are clearly visible.
The following sections summarize the three numerical models investigated herein using an axisymmetric RANS and axisymmetric and 3D LES formulations.

2-D (Axisymmetric) RANS Model
The RANS model solves the Navier-Stokes equations in finite volume form using the standard high-Reynolds number k-e model to provide turbulence closure. The convective terms are discretized with the second order LDFSS upwind flux-difference splitting scheme of Edwards,\(^5\) while the diffusion terms are discretized with central differences. First order time accuracy is used to advance the solutions to a steady-state. This model uses a fully compressible formulation with local time-derivative preconditioning\(^6\) to alleviate the stiffness due to disparity between acoustic and convective time scales. Characteristic-based boundary conditions are used at the inflow and outflow boundaries. Solutions are obtained on three mesh levels (24x24, 48x48, and 96x96 cells) in order to assess grid convergence. In order to achieve a steady-state solution, the spatial accuracy of the RANS simulations was reduced from second order to first order. Richardson Extrapolation\(^7\) was used for the fine and medium grid levels in order to provide nominally second order accurate temperature and stream-wise velocity profiles. Unsteady RANS solutions were not attempted in this paper. The coarse grid is shown in Fig. 3. The code was run in serial on a Sun workstation.

2-D (Axisymmetric) LES Model
The axisymmetric LES model uses a Galerkin Least Squares finite element method to solve the filtered Navier-Stokes equations on an unstructured grid shown in Fig. 4.\(^8\) This model has an equal order pressure and velocity interpolation and provides SUPG-type stabilization. A second order Adams-Bashforth/trapezoidal rule time integration is used. The axisymmetric equations are solved in a fully coupled manner using an inexact Newton’s method. The grid consists of 5774 quadrilateral elements and uses linear basis functions. The simulations were run on a parallel computer using either 8 or 32 processors.

3-D LES Model
The 3-D LES model solves the filtered Navier-Stokes equations on a structured finite volume grid. A fifth order upwind biased stencil is used for momentum,\(^9\) while a fifth order Essentially Non-Oscillatory (ENO)
scheme is used for the energy and species equations. The equations are integrated in time with a fourth order Runge-Kutta scheme. Pressure gradient scaling is used to provide temporal stability for these low mach number flows. Sub-Grid Scale (SGS) modeling of momentum is achieved with the dynamic Smagorinsky model, while the SGS diffusion of mass and energy uses a dynamic gradient diffusion model. The size is 80x65x65 grid cells for approximately 340,000 grid nodes. The simulations were run on 16 processors using MPI and domain decomposition. The grid and domain decomposition is shown in Fig. 5.

Boundary Conditions

The liquid fuel flow rate in the experiment was measured to be $1.35 \times 10^{-6} \text{m/s}$ ($1.35 \text{ cm/s}$), which corresponds to an effective average gas-phase velocity of 0.0164 m/s ($0.1 \text{ cm/s}$) to provide a small co-flow stream for numerical stability. The time-averaged temperature specified from the experimental data in the fuel and air streams is 723.15 K and 300 K, respectively, and atmospheric pressure was imposed on all boundaries.

Combustion Models

The combustion models used in the current work are based on simple strained laminar flamelet models (SLFM) using assumed probability distribution functions (PDF). The chemistry is based on using infinitely fast single-step methanol reaction of the form:

$$\nu_{CH_3OH} + \nu_{O_2} \rightarrow \nu_{CO_2} + \nu_{H_2O}$$

The motivation for using infinitely fast chemistry is to obtain simple analytical expressions (i.e. computationally efficient) for combustion that will predict the overall heat release and products of major gas species. These approximations are considered reasonable for pool fire simulations where strong extinction and reignition events are rare. Under these assumptions the species may be written as functions of the mixture fraction only, i.e. $Y_s = Y_s(z)$. This expression can then be substituted in for the transport equation for $Y_s$ leading to the following expression for reaction rate:

$$\dot{\omega}_s = -\frac{1}{2} \frac{d^2 Y_s}{dz^2}.$$  

where $\chi$ is defined as the scalar dissipation rate. For a turbulent flow field the subgrid scale (SGS) combustion environment is envisioned as an ensemble of smaller laminar flames or flamelets. The average chemical production rate may then be found by integrating Eq. (2) over the joint PDF of mixture fraction and scalar dissipation rate, $P_{Z\chi}$:

$$\bar{\omega}_s = \frac{1}{2} \int_0^{\chi_{max}} \int_0^1 P_{Z\chi} \rho(Z) \frac{d^2 Y_s(Z)}{dz^2} dZ dz.$$  

The interpretation of $P_{Z\chi}$ is different for RANS as it is for LES. For RANS, $P_{Z\chi}$ represents the probability of finding a value of $Z$ and $\chi$ at a particular point in space over all time. For LES, the joint PDF represents the probability of finding $Z$ and $\chi$ in a subgrid volume weighted by a filtering function at a particular point in space and time (please see Ref. for further details). For the rest of the model development we will ignore these subtleties and assume that $P_{Z\chi}$ may either stand for the joint probability in a RANS or LES sense depending on the particular code implementation. In addition, the term “mean” used through the text may refer to either a time-averaged RANS quantity or a filtered LES quantity.

Two different assumed PDF approaches to evaluating Eq. (3) are explored in this study. In the first approach, denoted as SLFM #1 statistical independence is as-
sumed between the mixture fraction and the scalar dissipation rate, i.e.

\[ P_{Zf} = P_{Z}^2 \]

so that \( \langle \chi | \zeta \rangle = \bar{\chi} \) which valid under highly turbulent flow conditions.\(^2\) The time averaged (for RANS) or filtered (for LES) chemical production rate thus becomes:

\[
\bar{\omega}_{s} = \frac{1}{2} \bar{\chi} \left[ P_{Z}(\zeta) \rho(\zeta) \frac{d^2 Y_s(\zeta)}{d\zeta^2} \right].
\]

For infinitely fast chemistry, the second derivative of \( Y_s \) with respects to \( \zeta \) approaches a delta function at the stoichiometric surface allowing for an analytical solution to the convolution integral of Eq. (5).

\[
\bar{\omega}_{s} = -\frac{1}{2} C_s \bar{\rho}(z_{st}) \bar{\chi} P(z_{st})
\]

The constant \( C_s \) is a function of the stoichiometric coefficients and \( \bar{\chi} \) is the time averaged or filtered dissipation rate that requires additional modeling. For the LES, this term is closed using a scale-similarity based model.\(^2\)

\[
\bar{\chi} = 2 \left[ D_{m}(\bar{\chi}) \frac{\partial \zeta}{\partial x_j} \frac{\partial Y_s}{\partial x_j} + D_{m}(\bar{\chi}) \left( \frac{\partial \zeta}{\partial x_j} \frac{\partial \zeta}{\partial x_j} - \frac{\partial^2 \zeta}{\partial x_j^2} \right) \right]
\]

In the RANS formulation the following often used approximation is employed that is valid for highly turbulent flows:\(^1\)

\[
\bar{\chi} = 2 D_{m} \frac{\partial \zeta}{\partial x_j} \frac{\partial Y_s}{\partial x_j} = 2 D_{m} \frac{\partial^2 \zeta}{\partial x_j^2} = \bar{\chi}_f.
\]

where \( \bar{\chi}_f \) represents the fluctuating component of the time averaged dissipation rate. This quantity can then be modeled by assuming proportionally to the mixture fraction variance, \( \sigma^2 \), using the relation:\(^1\)

\[
\bar{\chi}_f = C_{\chi} \bar{\chi} \sigma^2
\]

where \( C_{\chi} \) is a constant of proportionality and is set equal to 2.\(^2\)

As will be highlighted in the Results and Discussion section, the predictions using the SLFM #1 tend to underpredict the extent of heat release and subsequently the temperatures and stream-wise velocities are too low. This problem is a consequence of the statistical independence assumption (please see results for further discussion) and so a second model is developed. In this approach (denoted as SLFM #2) statistical independence is not assumed. The model is derived by starting with the PDF transport equation for mixture fraction assuming constant density flows with equal and constant diffusivities.\(^2\)

\[
\frac{\partial \bar{P}_{Z}}{\partial t} = \frac{\partial}{\partial x_j} \left( \frac{1}{\rho} \bar{u}_{j} \right) + \frac{\partial}{\partial x_j} \left[ \frac{1}{\rho} \bar{u}_{j} \frac{\partial \bar{P}_{Z}}{\partial x_j} \right] = \frac{\partial^2 \bar{P}_{Z}}{\partial x_j^2}
\]

Modeling the subgrid mixing term using a gradient-diffusion model, i.e. \(-\partial \bar{P}_{Z}(u_j \zeta) / \partial x_j = D_{pZ} \partial^2 \bar{P}_{Z} / \partial x_j^2\), and solving for \( \langle \chi | \zeta \rangle \) results in the following expression:

\[
\langle \chi | \zeta \rangle = -\frac{1}{P_{Z}(\zeta)} \left[ \frac{D_{pZ}}{\rho} \int F(\xi) d\xi \right] + C_1(x_j, t) \zeta + C_2(x_j, t)
\]

where \( F \) is the cumulative distribution function defined as the integral of \( P_{Z} \), i.e. \( F(\xi) = \int P_{Z}(\zeta)d\zeta \) and \( C_1 \)

and \( C_2 \) are “constants” of integration and are in general functions of both time and space. In theory, these constants could possibly be obtained in terms of lower order moments of \( Z \) (i.e. \( \bar{Z} \) and \( \sigma^2 \)) by substituting Eq. (11) into moment equations derived from Eq. (10). For homogeneous flows these constants are identically zero.\(^2\) As a first step, it is assumed that these constant terms, as well as the diffusion subgrid mixing term, are small relative to the material derivative term leading to the following result.

\[
\langle \chi | \zeta \rangle = \frac{1}{P_{Z}} \frac{D_{pZ}}{\rho} \int F(\xi) d\xi
\]

The impact of this assumption on the predictions will
not be explored in this study but will be the focus of future efforts. Substituting Eq. (12) into Eq. (3) and using the infinitely-fast state relationships then the following analytical expressions can be derived for the mean reaction rate.

\[
\bar{\omega}_s = \frac{1}{2} C_s \bar{p}(z_{st}) \frac{DF(Z_{st})}{Dt}
\]  

(13)

where \(DF(Z_{st})/(Dt)\) is a Lagrangian derivative that is requires explicit calculation locally in space for the RANS and both time and space for the LES.

In addition, the filtered mass fraction is required for computation and found by simply integrating the state relationship over the PDF of mixture fraction:

\[
\bar{Y}_s = \int P_Z(\xi) Y_s(\xi) d\xi
\]  

(14)

In this study, a beta PDF is chosen and the filtered mass fraction may then be written as:

\[
\bar{Y}_s = a_2 + (a_1 - a_2) I_{z_{st}}(\beta_1, \beta_2)
\]

\[
+ (b_1 - b_2) \frac{\beta_1}{\beta_1 + \beta_2} \left[ I_{z_{st}}(\beta_1, \beta_2) + \frac{b_2}{b_1 - b_2} \right]
\]

\[
- \frac{\Gamma(\beta_1 + \beta_2)}{\Gamma(\beta_1) \Gamma(\beta_2)} \bar{Z}_{st} \frac{\beta_1}{\beta_1 + \beta_2} (1 - \bar{Z}_{st})^{\beta_2}.
\]

(15)

The constants \(a_1\) an \(b_1\) are functions of the stoichiometric coefficients and are obtained from the infinitely fast state relationship, i.e. \(Y_s(z) = a + bZ\), where the subscript 1 denotes the rich side of stoichiometric and 2 the lean side. An an example, Fig. 6 shows the filtered mass fraction of the \(CO_2\) product species for a range of variance values plotted as a function of mean mixture fraction. As the variance of the mixture fraction increases, the mean mass fraction of the product species is driven below the laminar value due to subgrid mixing.

\[
\bar{\omega}_s = -\frac{\rho_{\chi}}{2} \frac{\Gamma(\beta_1 + \beta_2)}{\Gamma(\beta_1) \Gamma(\beta_2)} \left( b_2 - b_1 \right) (b_1 - b_2) \bar{Z}_{st} \frac{1}{\beta_2 - 1} (1 - \bar{Z}_{st})^{\beta_2 - 1}.
\]

(16)

\[
\bar{\omega}_s = \frac{1}{2} (b_2 - b_1) \bar{p}(z_{st}) \frac{DF(Z_{st})}{Dt} \int I_{\beta_1, \beta_2} d\xi
\]

(17)

Figure 7 shows the chemical production rate for \(CO_2\) using Eq (16) and plotted as a function of mean mixture fraction. Note, in the laminar limit the when the variance approaches zero the reaction rate approaches a delta function at \(Z_{st}\) consistent with the infinitely fast state relationships.

\[
|\omega_s| \propto \bar{p}(Z)
\]

(18)

Fig. 6: Mean \(CO_2\) mass fraction for the infinitely fast flamelet model.

Fig. 7: Mean \(CO_2\) chemical production rate for the infinitely fast flamelet model.

The assumed beta PDF requires the specification the mean mixture fraction and the subgrid variance. For the LES approach, a scale similarity model is used.\textsuperscript{25}
\[ \varepsilon^2 = \sigma_z^2 = (\bar{z} - \bar{z})^2 \]  
(18)

For the RANS calculations, a transport equation is solved for the mixture fraction variance

\[ \frac{\partial \sigma_z^2}{\partial t} = \frac{\partial}{\partial \chi_j} \left( \tilde{\rho} \tilde{u}_j \sigma_z^2 \right) = P - D - \bar{\rho} \bar{X}_f \]  
(19)

where P is a production term and D represents diffusion due to turbulent fluctuations.

**Results and Discussion**

The mean reaction rate models based on Eqs. (16) and (17) are run for both the axisymmetric and 3D LES while just the former is used in the RANS calculations. Predictions of time-averaged temperature and streamwise velocity are compared to experimental data at heights of 0.02, 0.14 and 0.30 m above the pool surface to assess code (i.e. 2D versus 3D and RANS versus LES) and combustion model (i.e. SLFM #1 versus SLFM #2) performance. For the LES cases, time-averaged quantities are obtained by first allowing for initial time dependent transients to wash out of the computational domain and then statistics are collected over several (5-10) puff cycles for which the flow is considered statistical stationary.

**Time-averaged Temperature using SLFM #1**

Figures 8 through 10 present comparisons of time-averaged temperature for the three specified heights using SLFM #1. At 0.02 m above the surface (Fig. 8) the time-averaged temperature is under-predicted in all cases. At 0.14 m both LES approaches essentially give a mixing solution with very little heat release. The RANS approach shows good agreement with the data at the \( x = 0.14 \) m location, but under-predicts the mixing and hence the combustion at the centerline.

Fig. 10 shows time-averaged temperature at 0.30 m above the pool surface. The RANS approach greatly over-predicts the temperature while the LES cases greatly underpredict by almost a half.
Time-averaged Velocity using SLFM #1

Time-averaged profiles of axial velocity are extracted from the simulations and compared with experimental data at all three heights and presented in Figs. 11 through 13. At 0.02 m, the axial velocities are very near to the inflow values. At 0.14 m above the pool surface, the RANS model shows better agreement with the data, while LES approaches under-predict the stream-wise velocity, consistent with the temperature profile at the same location. The velocity trends in Fig. 13 (0.30 m) are consistent with the temperature profiles from Fig. 10. The RANS model over-predicts the axial velocity, while the 2D and 3D LES cases greatly underpredict by as great as a factor of 10.

In general, the behavior of the velocity field is closely linked to that of the temperature field. Temperature profiles from the LES model using the standard form of the flamelet model fall significantly below the experimental values, which then leads to an under-prediction of the stream-wise velocity. The heat release from the RANS model is larger than that seen in the experiment, leading to an over-prediction of the axial flow velocity. These discrepancies indicate that the assumptions used to de-
velop SLFM #1 are not well founded for this class of flows and an alternative model needs to be developed.

One of the main weaknesses in SLFM #1 is the assumption of statistical independence between $Z$ and $\chi$. This assumption is generally valid for highly turbulent flows but is breaks down in transitionally turbulent flows such as the very near field of a turbulent jet and so is also questionable for the transitionally turbulent pool fire flows in this study. In order to explore this assumption, a second combustion model is developed based on using the PDF transport equation of mixture fraction and makes no assumption regarding the statistical independence of $Z$ and $\chi$ outlined previously in the Combustion Models section. Results using this new model are presented next for the 2D and 3D LES.

**Time-averaged Temperature using SLFM #2**

Figures 14 through 16 present results of time-averaged temperature profiles at all three downstream location from the 2D and 3D LES. The results show significant improvement using the new combustion model (SLFM #2). The axisymmetric LES tends to underpredict the temperature near the centerline at all downstream locations and overpredict for $r > 0.04$ m at the $x = 0.3$ m location. The 3D LES overpredicts near the toe of the pool fire flame (i.e. $r = 0.15$ m) at $x = 0.02$ m but agrees reasonably well with the experiment at the other further downstream locations.

The most notable difference between the 2D-axisymmetric LES and the 3D LES is the strong bimodal shape of the 2D LES at the $0.02$ and $0.30$ downstream locations that do not appear in either the 3D LES nor the experimental data. The reason for this can be attributed to the axisymmetric assumption that doesn’t allow for any stream-wise vorticity to be generated. This is evident by comparing Figs. 17 and 18 showing representative snapshots of temperature contours from 2D and 3D LES flowfields, respectively. In the axisymmetric LES, two distinct flow regions are observed near the base of the
plume. The first region, near the plume centerline, consists of relatively high velocity that is being drawn upwards due to a previous puffing event. The second region is located away from the centerline and consists of slower moving fluid and a large toroidal vortical structure that was formed due to the presence of baroclinic torque. These two predominant flow features give rise to the bimodal shape observed in the time-averaged temperature profiles. In contrast, these structures are not as distinct in 3D LES of Fig. 18 due to the generation of stream-wise vorticity that rapidly mixes the flow. The generation of stream-wise vorticity gives rise to “finger-like” instabilities often observed in pool fires and shown in the experimental images of Fig. 2. These structures are also observed in the 3D LES as illustrated in Fig. 19 showing an isocontour plot of vorticity magnitude.

Time-averaged Velocity using SLFM #2

Figures 20 through 22 present time-averaged stream-wise velocity comparisons using SLFM #2. Good agreement is shown with comparison to experiment for both the 2D and 3D LES. Consistent with the temperature profiles, the 2D LES exhibits a strong bi-modal behavior at the 0.14 m and 0.30 m downstream locations due to the lack of secondary mixing previously noted.
Lastly, the puffing frequencies were determined from the unsteady LES calculations using both combustion models and presented in Table 1. Frequencies reported from the experiment and from simple Richard number based correlations of Ref. 2 are also tabulated. In all of the LES cases, better agreement to the experimental data and correlation using SLFM #2, consistent with the improved time-averaged velocity and temperature predictions.

**Table 1 Puffing Frequency**

<table>
<thead>
<tr>
<th>Source</th>
<th>Frequency (Hz)</th>
</tr>
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<tbody>
<tr>
<td>Experiment</td>
<td>2.8</td>
</tr>
<tr>
<td>Correlation (Ref. 2)</td>
<td>2.7</td>
</tr>
<tr>
<td>2D LES (SLFM #1)</td>
<td>3.1</td>
</tr>
<tr>
<td>2D LES (SLFM #2)</td>
<td>2.9</td>
</tr>
<tr>
<td>3D LES (SLFM #1)</td>
<td>1.8</td>
</tr>
<tr>
<td>3D LES (SLFM #2)</td>
<td>2.5</td>
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</table>

**Summary and Conclusions**

For pool fires, the velocity and temperature fields are tightly coupled. If the net amount of heat release is under-predicted, then the buoyant forces which drive the flow will be reduced leading to a subsequent reduction in the stream-wise velocity. This strong coupling between the temperature and velocity fields requires accurate predictions of the subgrid combustion processes. In this study, two different SLFM-based combustion models with assumed PDF were explored using 2D RANS, 2D LES and 3D LES codes. The use of SLFM #1 resulted in poor predictions of time-averaged temperature and stream-wise velocity for all cases. This behavior is attributed to the assumption of statistical independence between mixture fraction and its dissipation rate. This realization resulted in the development of a second combustion model combustion model (SLFM #2) that does not make use of the statistical independence assumption. The use of this model resulted in substantially better predictions of time-averaged temperature and velocity as well as puffing frequency for both the 2D and 3D LES. Lastly, a bimodal distribution is observed in the 2D LES and is attributed to the absence of stream-wise vorticity generation in the axisymmetric formulation that enhances secondary mixing.

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References


