# SIMULTANEOUS OPTICAL MEASUREMENT OF SOOT VOLUME FRACTION, TEMPERATURE, AND $\mathrm{CO}_{2}$ IN HEPTANE POOL FIRE 

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#### Abstract

Detailed measurements of the temperature, soot volume fraction, and $\mathrm{CO}_{2}$ have been performed for a 10 cm diameter heptane fire. In addition, the concentrations of $\mathrm{H}_{2} \mathrm{O}$ and CO were inferred from generalized state relationships. The heat feedback to the surface was calculated by using a reverse Monte-Carlo method in conjunction with RADCAL. The calculated heat fluxes to the surface with and without gas emission indicate that the contributions from the gaseous combustion products to total radiation are significant for heptane due to its mildly sooting nature.

Simultaneous optical measurements using two probes were performed to investigate the importance of temporal correlations on the heat transfer calculations. Measurements made throughout the fire indicate that nonsimultaneous data sets can be used to accurately predict the heat transfer to the fuel surface.


## Introduction

For liquid pool fires, the dominant mode of heat feedback to the fuel surface is related to the size of the pool [ 1,2 ]. For small fires (less than 10 cm ) that produce quasi-laminar llames, conduction and convection are the dominant modes of heat transfer. However, for intermediate to large fires, it has been found that radiation plays a significant role in the heat transfer process. Therefore, detailed examination of the radiative heat transfer mechanism is crucial to the understanding of the burning rate and the flame spread rate. These processes are key factors in assessing potential fire hazards.
Thermal radiation from the fire to the fuel surface is controlled by the emission from the soot and product gases. Radiation analysis using average temperature, average species concentrations and constant cylindrical flame shapes can diminish the turbulent enhancement of the heat flux [3]. Thus, accurate modeling of turbulent radiative heat transfer requires the instantaneous distribution of the local temperature and emissivity within the region between the fuel surface and the flame.
In a previous study that analyzed radiative heat feedback to the surface, the relative importance of gas emission was considered negligible for a llame with high levels of soot concentration [4,5]. Whereas

[^0]this assumption yields reasonable results for fuels like toluene, for mildly sooting fuels such as heptane, neglecting gas emission may significantly underestimate the overall heat transfer to the surface [6]. Thus, accurate assessment of the surface heat transfer requires radiation contributions from gaseous combustion products.
The goal of this study is to perform a parametric study investigating the importance of the radiative component of the heat transfer to the fuel surface for different fuels and pool dimensions. In this paper, results for a $10-\mathrm{cm}$-diameter (intermediate sized) heptane pool fire are presented.

The local instantaneous temperature, soot volume fraction, and $\mathrm{CO}_{2}$ concentrations were measured throughout the flame. The measured $\mathrm{CO}_{2}$ concentrations were used to estimate the concentrations of $\mathrm{H}_{2} \mathrm{O}$ and CO using the generalized state relationship developed by Sivathanu and Faeth [7]. The distributions of $T$, $f_{v e}, \mathrm{CO}_{2}, \mathrm{H}_{2} \mathrm{O}$, and CO were used to calculate the radiative heat feedback to the surface using a reverse Monte-Carlo heat transfer model that incorporated the RADCAL radiation model developed by Grosshandler [8]. RADCAL is a model that solves the equation of transfer for a nonhomogeneous emitting/absorbing medium composed of soot and gaseous combustion products.
Accurate modeling of the nonsteady heat feedback to the surface requires the instantaneous temperature and emissivity distributions above the pool surface. However, acquiring such information is not practical, considering the turbulent three-dimensional nature of these large fires. In order to understand the importance of simultaneous measurements


Fic. 1. Diagram of the experimental apparatus.
on the radiative heat transfer calculations, experiments were performed using a dual probe assembly to obtain simultaneous emission information at various locations throughout the fire.

## Experimental Technique

The schematic diagram of the experimental apparatus is shown in Fig. 1 [9]. Probes A1 and A2, which were used for temperature and soot volume fraction measurements, consisted of 6.4 mm diameter stainless steel light guides (length 15 cm ), and were surrounded by water-cooled jackets. The emission intensity from the luminous path ( $L$ in Fig. 1) was carried through two bifurcated fiber optic bundles. The emission intensity was monitored at central wavelengths of 900 and 1000 nm (both with 60 nm half-bandwidths) using two separate biased silicon photodiodes. The use of the fiber optic bundle facilitated the movement of the probes through the fire, circumventing the cumbersome task of moving the burner with respect to the probes. Probe B1 was used to monitor emission from $\mathrm{CO}_{2}$ and consisted of a 6.4 mm diameter light guide attached to an aluminum box housing a PbSe infrared detector, 4350 nm central wavelength filter (with 180 nm half-bandwidth),
a mechanical chopper, and an infrared lens. Nitrogen was purged slowly through ports labeled I (in Fig. 1) at a rate of $2.5 \mathrm{~cm}^{3} / \mathrm{min}$ to prevent thermophoretic deposition of soot. The detection systems were calibrated using a high-temperature bblackbody source and calibration factors were checked frequently and were found to be constant before and after the experiments. The burner was 10 cm in diameter and was water cooled. The fuel was gravity fed and maintained 0.5 cm below the rim of the bumer.

## Temperature and $f_{c \varepsilon}$ Measurements

The temperature and soot volume fraction measurement technique is similar to that used by Klassen and coworkers $[4,5]$. The emission intensities measured at two wavelengths were simultaneously solved to determine the local soot volume fraction, $f_{v e}$, and temperature, $T$.

$$
\begin{align*}
I_{900} & =\frac{\int I_{b \lambda} F_{900 \lambda}\left(1-e^{-K i f f_{v 0 L} L \lambda}\right) d \lambda}{\int F_{900 \lambda} d \lambda}  \tag{I}\\
I_{1000} & =\frac{\int I_{b \lambda} F_{1000 \lambda}\left(1-e^{-K i f_{v} L / \lambda}\right) d \lambda}{\int F_{1000 i} d \lambda} \tag{2}
\end{align*}
$$



Fig. 2. Average temperature and $f_{\text {ve }}$ measurements as a function of radial position at an axial position of 10 cm above the pool surface.
where $F_{i}$ is the wavelength-dependent sensitivity of the detection svstem, $K_{i}$ is the dimensionless soot absorption constant. $L=15 \mathrm{~mm}$ was the distance maintained between probes Al and Bl , and $I_{b}$, is Planck's function:

$$
\begin{equation*}
I_{b, k}=\frac{2 / c^{2}}{i^{3}\left(e^{j_{1+c} / k, h}-1\right)} \tag{3}
\end{equation*}
$$

where $h$ is Planck's constant. $c$ is the speed of light. $k_{b}$ is Boitzmann's constant, and $T$ is the temperature of the radiating particles. Equations (1) and (2) were solved iteratively for the two unknowns, temperature, $T$, and soot volume fraction, $f_{c y}$.
To be consistent with the practice employed by researchers in the fire community $[4,8,12]$, the dimensionless soot absorption constant used in this work was determined from the indices of refraction of soot reported by Dalzell and Sarofin [10]. The uncertainty in the temperature measurements is approximately $50^{\circ} \mathrm{C}$. and the uncertainty in $f_{u c}$ is approximately $10 \%$ [9,11].
Figure 2 displays the measurements of the average temperature and soot volume fraction as a function of radial location at an axial position 10 cm above the pool surface. The data was acquired at 200 Hz for a period of 50 s . The average root-inean-square ( rms ) values of the temperature and soot volume fraction were 350 K and 0.40 ppm , respectively. The symmetry exhibited by the data in Figure 2 indicates that measurements performed over half the radial domain (from $r=0-5 \mathrm{~cm}$ ) were sufficient. It was also found that, for fires of this size, positions beyond 30 cm above the pool surface produce only sporadic periods during which the emission from soot or gaseous products can be measured [6]. Thus, most of the thermal radiation emanates from positions below 30 cm .

## $\mathrm{CO}_{2}$ Measurements

For typical temperatures encountered in fires, the $\mathrm{CO}_{2}$ emission spectra extends from 4100 to +700 nm [8]. The contributions of the various components to the total emission detected by the PbSe detection system were analyzed using RADCAL for a typical condition: $T=1500 \mathrm{~K}, f_{\mathrm{cc}}=1 \mathrm{ppm}$, and mole fractions of $\mathrm{CO}_{2}, \mathrm{H}_{2} \mathrm{O}, \mathrm{CO}$, and $\mathrm{N}_{2}$ equal to $0.1,0.1,0.1$. and 0.7 , respectively. The interference filter (4350nm central wavelength) was chosen to provide transmission of only the radiation emitted by $\mathrm{CO}_{2}$ and reject emission from the other species. The contribution from $\mathrm{CO}_{2}$ emission to the total intensity measured by the present PbSe detection system was approximately $94 \%$, whereas the contributions from CO and $\mathrm{H}_{2} \mathrm{O}$ emission were negligible and the contribution from soot emission was only $5 \%$.

The PbSe detection system was calibrated with a blackbody source at vanious temperatures ( $150^{\circ} \mathrm{C}$ $1000^{\circ} \mathrm{C}$ ). Using the temperatures deternined from emission at 900 and 1000 nm [Eqs. (1) and (2)], the $\mathrm{CO}_{2}$ concentrations were calculated iteratively until the emission intensity (between +100 and 400 nm transmitted through the filter function) predicted by RADCAL was equal to the intensity measured by the PbSe detection system.

Because of the nonsteady nature of fires of this size, the emission data exhibited sporadic periods during which the emission signals at 900 and/or 1000 nm were too low to determine the temperature and soot volume fraction. Typically. "low" emission periods occurred from 5 to $15 \%$ of the observation time. depending on location. For these periods, the temperature was set at 1000 K . which is the approximate lower-limit temperature for the detection of soot particle emission [19], and this temperature was used in the RADCAL calculations for determining the $\mathrm{CO}_{2}$ concentrations. The $\mathrm{CO}_{2}$ gas temperatures are expected to be somewhat higher than the soot temperatures [20]. Although the choice of temperature affects the calculated $\mathrm{CO}_{2}$ concentration. calculations show that the impact on the $\mathrm{CO}_{2}$ radiation intensity is small, typically less than $10 \%$.

## Simultaneous Emission Measurements

As mentioned in the Introduction. the calculation of the radiative heat flux to the fuel surface requires the spatial and temporal measurement of the fluctuating temperature and soot volume fraction. The flame for the 10 cm heptane pool exhibits buovancyinduced fluctuations with an average frequency of approximately 11 Hz [13]. To determine the importance of using nonsimultaneous data for heat transfer calculations, simultaneous information at various locations must be obtained. The sensitivity of the cal-
culated heat transfer to this effect can be determined by uncorrelating the simultaneous data sets.

For this purpose, simultaneous emission measurements were performed using two pairs of identical probes (see Fig. 1). The vertical separation distance between the probes is defined as $H$. The horizontal distance between the probes was maintained at $L=$ 15 mm . The simultaneous temperature and soot volume fraction information at two discrete locations was determined [from Eqs. (1) and (2)] and was used to calculate the radiative heat transfer (using RADCAL) from the top probe position through the lower probe position to the plane just below the bottom probe.

The effect of temporal correlation of the simultaneous data sets from two locations on the radiative heat transfer was tested by shifting one time series with respect to the other. In effect, the simultaneous (therefore correlated) data sets were effectively uncorrelated. The average of the shifted heat transfer normalized by $Q_{0}$ is defined as $a$ :

$$
\begin{equation*}
a=\frac{1}{21} \sum_{n=-10,10} \frac{Q_{n}}{Q_{0}} \tag{4}
\end{equation*}
$$

which is an indication of the effect of the time shift on the heat transfer calculations. The term $Q_{0}$ corresponds to the time-averaged heat transfer calculated with the simultaneous data sets; $Q_{1}$ corresponds to the time-averaged heat transfer calculated with a 1 s shift in the time series; and $Q_{2}$ corresponds to the time-averaged heat transfer calculated with a 2 s shift in the time series, and so on. The heat transfer was calculated for time shifts between -10 and +10 s in 1 s increments. A value of $a$ close to unity suggests only a small change in the heat transfer as a function of the time shift.

Simultaneous emission measurements were performed for the following conditions: $L=15 \mathrm{~mm}$ and $H=15,20,25$, and 30 mm . The center of the probe assembly was placed at $x=10 \mathrm{~cm}$ and $r=0 \mathrm{~cm}$. Using the shifted time series modifies the instantaneous heat fux calculations, however, the average value of the heat flux was relatively insensitive to time shifts. For all of the probe separation distances, the calculated $a$ was near unity with a standard deviation less than $\pm 5 \%$. Thus, for positions above the pool surface and the various separation distances, uncorrelating the simultaneous data sets had negligible effects on the calculated heat transfer.

Measurements of $a$ were also performed at various locations above the pool surface along the center line using $L=15 \mathrm{~mm}$ and $H=30 \mathrm{~mm}$. The center of the assembly was placed at axial positions, $x$, between 3 and 30 cm (with $r=0 \mathrm{~cm}$ ) in increments of 3 cm . The calculated $a$ for all positions was near unity with a standard deviation less than $\pm 5 \%$. This suggests that there is no effect of correlation between the simultaneous data sets on the calculated heat transfer.

For pool fires, periodic fluctuations (caused by buoyancy) of the outer flame surface occur along both the vertical and horizontal axes. Along the centerline (only vertical fluctuations are present because of the symmetry exhibited by the fire), temporal shifting of the simultaneous data sets does not affect the heat transfer calculations. This was verified by shifting the time series in increments of 0.005 s for a period of 0.5 s (which corresponds to approximately five flame pulsation periods) and calculating the $a$. Even for the time shifts producing maximum cross correlation between the data sets ( $H$ divided by the fluid velocity), the a values varied by only $1 \%$. However, it is unclear how the correlations will affect the radiative heat transfer when both modes of fluctuation are present. Experiments performed for various radial positions ( $r$ from 0 to 5 cm ) at $x$ locations of 5 , 10 , and 15 cm also indicated only small changes in heat transfer as a function of time shifting of the data sets.
These findings suggest that, throughout the fire, the heat transfer calculation is relatively insensitive to the temporal correlation between data sets. This is important because it suggests that nonsimultaneous data acquired at different locations can be used to calculate the heat transfer to the pool surface. This practice will be employed for the heat transfer calculations discussed in the next section.

## Reverse Monte-Cario Technique

Because of the complexity of the problem, early attempts at modeling the nonsteady radiative heat feedback mechanism involved several limiting assumptions, including the use of average flame emissivity and constant or mean flame temperatures and absorption/emission coefficients as a function of height and effective flame shapes. However, it has been demonstrated that the use of mean radiative properties to calculate heat feedback can lead to significant differences between the predicted and measured fuel burning rates in these turbulent fires [3,4,5].

In this study, a reverse Monte-Carlo integration technique was used to calculate the incident flux at the fuel surface. The technique is equivalent to the technique described by Carter et al. [14] and Walters and Buckius [15].

The approach has several important advantages. First, it avoids aliasing errors that can be important if the "hot" volumes (localized regions of high temperature or high soot volume fraction) are small. Furthermore, the number of directional ravs can automatically be determined by setting acceptable sample standard deviations. The sample standard deviation is an indication of the magnitude of the error in the results.

The incident radiative flux $q_{i}$ received at area el-
ement $d A$ on the fuel surface is given by the following equation:

$$
\begin{equation*}
q_{i}=\int_{2 x} i_{i}\left(\theta_{i}, \phi_{i}\right) \cos \theta_{i} d \omega_{i} \tag{5}
\end{equation*}
$$

where the integral.is over the hemisphere of incident directions above $d A$ and $i_{i}\left(\theta_{i}, \phi_{i}\right)$ is the incident total intensity. The total incident intensity is given by

$$
\begin{align*}
i_{i}= & \int_{0}^{\infty} \int_{0}^{s} K_{\lambda}\left(s^{\bullet}\right) i_{b_{i} \lambda}\left(s^{\bullet}\right) \\
& \cdot \exp \left(-\left[K_{\lambda}(s)-k_{\lambda}\left(s^{*}\right]\right\} d s^{\bullet} d \lambda\right.  \tag{6}\\
& k_{\lambda}(s)=\int_{0}^{s} K_{\lambda}\left(s^{\bullet}\right) d s^{*} \tag{7}
\end{align*}
$$

and the coordinate $s$ is measured along a path in direction $\left(\theta_{i}, \phi_{i}\right)$.

Equation (6) can be rewritten as

$$
\begin{align*}
q_{i}= & \int_{0}^{2 x} \int_{0}^{\sqrt{2} 2} \pi i_{i}\left(\theta_{i}, \phi_{i}\right) \\
& \cdot\left[2 \cos \theta_{i} \sin \theta_{i} d \theta_{i}\right]\left[d \phi_{i} /(2 \pi)\right] . \tag{8}
\end{align*}
$$

That is, the flux is equal to $\pi i_{i}\left(\theta_{i}, \phi_{i}\right)$ integrated over $\theta_{i}$ and $\phi_{i}$ with weighting functions of $2 \cos \theta_{i} \sin \phi_{i}$ and $1 / 2 \pi$, respectively. The flux can be estimated then by taking the average of many trial values of $\pi i_{i}\left(\theta_{i}, \phi_{i}\right)$ evaluated at random values of $\theta_{i}$ and $\phi_{i}$ chosen using the weighting functions as probability density functions (pdfs).

The evaluation of the flux requires the selection of a random direction ( $\theta_{i}^{\prime}, \phi_{i}^{\prime}$ ) and then the evaluation of the incident intensity along that path. Using the appropriate pdfs, the random direction is chosen using

$$
\begin{equation*}
\phi_{i}^{\prime}=2 \pi R_{\infty} \quad \theta_{i}^{\prime}=\arcsin \left(R_{\theta}\right) \tag{9}
\end{equation*}
$$

where $R_{\phi}$ and $R_{\theta}$ are random numbers. After $N$ trials using $N$ directions, the estimated $q_{i}^{\prime}$ is

$$
\begin{equation*}
q_{i}^{\prime}=\pi \sum_{j=1}^{N} \frac{i\left(\theta_{j}, \phi_{j}\right)}{N} . \tag{10}
\end{equation*}
$$

The magnitude of the error in this estimate is indicated by the sample standard deviation:

$$
\begin{equation*}
\Delta q_{i}^{\prime}=\pi \sqrt{\frac{1}{(N-1)} \sum_{j=1}^{N}\left(i_{j}^{\prime}\right)^{2}-\frac{\left(q_{i}^{\prime}\right)^{2}}{\pi^{2} N}} . \tag{11}
\end{equation*}
$$

The line integral in Eq. (7) needs to be evaluated for each trial. For each line integral, a ray is followed through the cylindrical geometry in which $T$, soot volume fraction, and mole fractions of the gaseous


Fic. 3. Calculated heat flux to the pool surface as a function of radial position using $10,100,1,000,10,000$, and 100,000 random rays.
products are known at a set of discrete values of $r$ and $x$. The integration is performed by considering the cylindrical geometry as a stack of cylindrical rings. For each cylindrical ring, the ray pierces the distance through the ring, and the data for that ring are stored in an array. The array of data is then passed to RADCAL, which performs the integral given in Eq. 6.

Figure 3 displays the irradiance along the pool surface as a function of the number of rays used in the calculations. The use of 10 rays produced very large errors and standard deviations in the heat flux due to aliasing errors. Both the errors and standard deviations decreased as the number of rays increased until the calculation converged for 10,000 rays. For the cases in which 10,000 and 100,000 rays were used, the irradiance decreased smoothly as a function of radial position with the highest value occurring at the pool center. These results indicate that arbitrarily choosing the number of ravs can produce large uncertainties in the heat flux calculations.

## Generalized State Relationships

In this study, the emission and absorption characteristics of hydrocarbons and pyrolysis gases were not considered. However, in the 10 cm heptane fire, the impact on the total radiative heat transfer calculations is estimated to be modest. The concentrations of hydrocarbons decreased rapidly both as a function of radial and axial positions above the pool surface [18]. Orloff [21] also estimated that the radiation blockage due to pyrolysis gases was not important for fires of this size.

To incorporate the effects of radiation from gaseous combustion products, $\mathrm{CO}_{2}$ emission at 4350 nm was monitored. $\mathrm{CO}_{2}$ produces a well-defined emis-
sion band that can be distinguished from the emission of other components [16]. For example, the emission line for $\mathrm{H}_{2} \mathrm{O}$ at 2700 nm is difficult to separate from the $\mathrm{CO}_{2}$ emission at 2700 mm . CO radiation at 4600 nm cannot be extracted from the dominant emission from $\mathrm{CO}_{2}$.

To estimate the concentrations of $\mathrm{H}_{2} \mathrm{O}$ and CO , the generalized state relationships for gas-phase components of diffusion flames [7] were used in conjunction with the measured concentrations of $\mathrm{CO}_{2}$. However, there are two solutions for the concentrations of $\mathrm{H}_{2} \mathrm{O}$ and CO from the $\mathrm{CO}_{2}$ measurements, depending on whether the local equivalence ratio is lean or rich. In this work, the concentrations were calculated for both the rich and lean conditions.

Figure 4 displays the time-averaged measurements of $T, f_{c c}$, and $\mathrm{CO}_{2}$, and inferred values of $\mathrm{H}_{2} \mathrm{O}$ and CO distributions calculated assuming rich conditions. Both the average temperature and soot concentration are highest along the centerline above $x$ $\sim i \mathrm{~cm}$. The reduction of the average $T$ and $f_{c e}$ as a function of radial position occur due to the realizations of low emission data. The distributions of the average gaseous species concentrations look similar because the $\mathrm{H}_{2} \mathrm{O}$ and CO concentrations were derived from the $\mathrm{CO}_{2}$ measurements.

Figure 5 compares the instantaneous heat flux integrated over the pool surface using time series of the temperature, soot volume fractions, and species concentrations from all locations above the pool surface for both the rich and lean cases. For the rich case, the average heat flux was approximately $10 \%$ greater than the average heat flux calculated for the lean case. This is expected since higher concentrations of gaseous products are formed under rich conditions and therefore can contribute to the total radiation. The difference in the total heat flux was modest, partly because the dominant radiation emanates from soot particles. Thus, in consideration of this small variation in the calculated heat flux between the lean and rich cases, the remainder of the paper will discuss results obtained using the rich conditions.

## Contributions from Gas Emission

Figure 6 displays the heat flux integrated over the entire pool surface using the nonsimultaneous $T, f_{\text {te }}$, $\mathrm{CO}_{2}, \mathrm{H}_{2} \mathrm{O}$ and CO data as a function of time step. Figure 6 also displays the running time average. For this case, both gas and soot emissions were considered. There were significant time-varving fluctuations in the instantaneous heat flux to the surface (due to fluctuations in the temperature and/or species concentrations). However, within 400 time steps (corresponding to 2 s ), the heat flux reached a steadystate value of $17.7 \pm 1 \mathrm{~W}$. The heat fux required to vaporize the fuel (including the heat of vaporization
and the energy required for fuel heat-up using the measured fuel consumption rate of $0.08 \mathrm{~g} / \mathrm{s}$ ) is 43.2 $W$. Thus. the radiative flux to the surface of the 10 cm diameter heptane fire represents $40 \%$ of the total heat required for fuel vaporization, which is a significant fraction. The remainder of the heat feedback was attributed to convection, which is important for pool fires of this size [17].

Figure 6 also displays the radiative heat flux calculations for the same condition when gas emissions were suppressed. The average value also asvimptoted to a steady-state value within 2 s for this calculation. The steadv-state value of $11.6 \pm 1 \mathrm{~W}$ represents nearly a $40 \%$ decrease in the heat flux to the surface compared to the case in which gas emission was included. The radiation from soot represents approximately $60 \%$ of the total radiative heat Hux to the surface. Thus. for heptane pool fires of this dimension. gas emission represents a significant fraction of the total flame emission and therefore must be included in the heat transfer calculations. This is in contrast to a very sootv fuel like toluene where calculations performed using centerline measurements indicate that the contributions from the gaseous combustion products represent approximately $10 \%$ of the total radiation to the surface $[4,5]$.

## Average vs Instantaneous Values

Fischer et al. [18] reported a significant difference in the calculated radiant intensities when time-averaged values of the temperature were used instead of the instantaneous values. Using the time-averaged values of $T, \mathrm{CO}_{2}, \mathrm{H}_{2} \mathrm{O} . \mathrm{CO}$. and $f_{t r}$ can diminish the effects of turbulent fluctuations of temperature and species concentrations on the radiative heat transfer as a result of the nonlinear dependence of radiation on these parameters. Furthermore the occurrence of low emission periods will reduce the magnitude of the average values and increase the magnitude of the rms values [19]. Thus, the use of time-averaged values does not provide a true representation of the time-averaged heat transfer.
The radiative heat transfer calculations were also performed for the case using time-averaged values. For this case, the calculated heat flux was approximately $14.0 \pm 1 \mathrm{~W}$. As stated earlier, the average heat flux calculated using the instantaneous values was $17.7 \pm 1 \mathrm{~W}$. This suggests the importance of using local instantaneous measurements from various locations above the pool surface for calculating the heat transfer to the fuel surface. This finding is in qualitative agreement with the results reported by Fischer et al. [18].

Temperature


CO
$\mathrm{CO}_{2}$
$\mathrm{H}_{2} \mathrm{O}$





Soot
Fic. 4. Time average distributions of temperature, $\mathrm{CO}_{2}, \mathrm{H}_{2} \mathrm{O}, \mathrm{CO}$, and $f_{\mathrm{w}}$ above the pool surface.


Fic. 5. Comparison of the (calculated) integrated heat flux to the pool surface as a function of time for rich and lean cases.


Fic. 6. Calculation of the instantaneous integrated heat flux to the pool surface as a function of time for the case considering gas (rich) and soot emission. The running averages of the cases with and without gas emission are also plotted.

## Conclusions

Detailed measurements of the temperature, soot volume fraction, and $\mathrm{CO}_{2}$ distributions have been made for a 10 cm diameter heptane fire. The emissions from the gaseous combustion products, both measured (in the case of $\mathrm{CO}_{2}$ ) and estimated from the generalized state relationship (for $\mathrm{H}_{2} \mathrm{O}$ and CO ), were calculated using RADCAL in conjunction with the reverse Monte-Carlo method.

Simultaneous emission measurements made for various locations above the pool fire surface indicate relative insensitivity of the heat transfer to the temporal correlation between the data sets. This finding suggests that the use of nonsimultaneous data is adequate to predict the heat transfer to the surface for large fires where simultaneous measurement over the entire flame volume is impractical.

The results indicate that, for the case of a 10 cm diameter pool fire burning heptane (which is a mildly sooting fuel), radiation contributions from the gas phase represent a significant fraction of the total radiative heat transfer to the surface of the pool. However, this fraction is a function of the amount of soot produced by the flame and therefore a function of the fuel structure and pool dimension. The effect of using average values of $T, f_{v e}, \mathrm{CO}_{2}, \mathrm{H}_{2} \mathrm{O}$, and CO indicates that the heat Hux was underpredicted when compared to the case in which instantaneous values were used.

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## REFERENCES

1. Blinov, V. I., and Khudiakov, G. N., Dok. Akad. Nauk. USSR 113:241 (1957).
2. Burgess, D., and Hertzberg, M., Heat Transfer in Flames (N. H. Afgan and J. M. Beer, Eds.), Hemisphere Press, New York, p. 413, 1974.
3. Hamins, A., Yang, J. C., and Kashiwagi, T., "A Simple Model for Predicting the Burning Rate of Liquid Pool Fires," Fire Safety J.; submitted.
4. Klassen, M., Ph.D. Thesis, University Of Maryland, College Park, MD, 1992.
5. Klassen, M., Sivathanu, Y. R., and Gore, J. P., Combust. Flame 90:34 (1992).
6. Choi, M. Y., Hamins, A., Rushmeier, H., Hubbard, A., and Kashiwagi, T., "Simultaneous Optical Measurements of Soot Volume Fraction and Temperature in Heptane Pool Fires," Eastern States Section of the Combustion Institute, Princeton, NJ, October 25-28, 1993.
7. Sivathanu, Y. R., and Faeth, G. M., Combust. Flame 82:211 (1990).
8. Grosshandler, W. L., "RADCAL: A Narrow-Band Model for Radiation Calculations in a Combustion Environment," NIST Technical Note 1402, 1992.
9. Choi, M. Y., Hamins, A., Mulholland, G. W., and Kashiwagi, T., "Simultaneous Optical Measurements of Soot Volume Fraction and Temperature in Premixed Flames," Combust. Flame, in press.
10. Dalzell, W. H., and Sarofim, A. L., J. Heat Transfer 91:100 (1969).
11. Choi, M. Y., Mulholland, G. W., Hamins, A., and Kashiwagi, T., "Comparisons of Soot Volume Fraction Measurements Using Optical and Isokinetic Sampling Techniques," Eastern States Section of the Combustion Institute, Princeton, NJ, October 25-28, I993.
12. Sivathanu, Y. R., and Faeth, G. M., Combust. Flame 81:150 (1990).
13. Hamins, A., Yang, J. C., and Kashiwagi, T., TwentyFourth Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, 1992, p. 1695.
14. Carter, L. L., Horak, H. G., and Sanford III, M. T., J. Comput. Phys. 26:119 (1978).
15. Walters, D. V., and Buckius, R. O., Int. J. Heat Mass Transfer 35(12):3323 (1992).
16. Sivathanu, Y. R., and Gore, J. P., Combust. Sci. Technol. 80:1 (1991).
17. Hottel, H. C., Fire Res. Abstr. Rev. 1:41 (1959).
18. Fischer, S. J., Hardouin-Duparc, B., and Grosshandler, W. L., Combust. Flame 70:291 (1987).
19. Klassen, M., and Gore, J. P., Combust. Flame 93:270 (1993).
20. Best, P. E., Chien, P. L., Carangelo, R. M., Solomon. P. R., Danchak, M., and Ilovici, I., Comb. Flame 85:309 (1991).
21. Orloff, L., Eighteenth Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, 1981, p. 549.

## COMMENTS

Patrick J. Pagni, University of Califomia, Berkeley, USA. Have you compared your soot volume fractions with the pool-fire soot volume fraction measurements in the literature [1,2]?

## REFERENCES

1. Bard, S., et al., "Spatial Variation of Soot Volume Fractions in Pool Fire Diffusion Flames," in Fire Safety Sci-ence-Proceedings of the First International Sympo-
sium (C. Grant et al., Eds.), Hemisphere, New York, 1986, pp. 361-369.
2. Markstein, G. H., "Measurements on Gaseous-fuel Pool Fires with a Fiber-Optic Absorption Probe," Combust. Sci. Technol. 39:215 (1984).

Author's Reply. Comparisons with the pool fire results in the literature [1-4] reveal that the time-averaged soot volume fractions measured in the present experiments are of the same order of magnitude. In a previous study performed in a steady-state and homogeneous environment of premixed flames [5], the soot volume fraction measurements were found to be very sensitive to the refractive index used to calculate the soot optical properties. In the present study, the refractive indices of Dalzell and Sarofim [6] were used to be consistent with previous investigations of radiative characteristics of liquid pool fires [3,7].

## REFERENCES

1. Bard, S., et al., "Spatial Variation of Soot Volume Fractions in Pool Fire Diffusion Flames," in Fire Safety Sci-ence-Proceedings of the First International Symposium (C. Grant et àl., Eds.), Hemisphere, New York, 1986, pp. 361-369.
2. Bard, S., and Pagni, P. J., J. Heat Transfer 103:357 (1981).
3. Klassen, M., Sivathanu, Y. R., and Core, J. P., Combust. Flame 90:34 (1992).
4. Sivathanu, Y. R., and Faeth. G. M., Combust. Flame 81:150 (1990).
5. Choi, M. Y., Hamins, A., Mulholland, G. W., and Kashiwagi, T., "Simultaneous Optical Measurement of Soot Volume Fraction and Temperature," Combust. Flame, in press, 1994.
6. Daizell, W. H., and Sarofim, A. L., J. Heat Transfer 91:100 (1969).
7. Klassen, M., Ph.D. Thesis, Department of Mechanical Engineering, University of Maryland, 1992.
Y. R. Sivathanu and J. P. Core, Purdue University. You had indicated that the temporal correlation between adjacent points or the spatial correlation does not affect your heat flux calculations. What was the minimum distance between the adjacent points for your measurements? Could you comment on the minimum distance for which your observation is valid? Do your findings essentially agree with those of Kounalakis et al. [1] in that the spatial correlation coefficients have negligible influence on the radiation properties?

Author's Reply. In turbulent fire studies, researchers have to reconstruct the temperature and emissivity distribution using mean values from sets of nonsimultaneous data collected at various locations within the fire [1,2]. The purpose of the present study was to directly measure the effects of using nonsimultaneous data on the radiative heat transfer process without relying on the use of mean temperatures and soot volume fractions and the statistical variation of these parameters. In this work, the radiation characteristics were measured simultaneously in pairs of two spatial locations with separations of $H$ equal to $15,20,25$, and 30 mm (with the lower limit being determined by the dimensions of the optical probes). These separation distances are of the order of the integral scale lengths reported in the work by Kounalakis et al. [3]. Since the emission data were acquired simultaneousiy for the top and bottom probes, this study provided a unique opportunity to determine the spatial correlation coefficients as a function of time shift between the data sets. The spatial correlation coefficients were calculated for the $\mathrm{H}=30 \mathrm{~mm}$ case for heights ranging from 3 to 30 cm above the burner surface. The average coefficient was approximately 0.2 for zero time shift and 0.5 for cases when the time shift was equal to $H / u$ (where $u$ is the local velocity of the flame). Based on measurements at the smaller separation distances, the magnitude of these coefficients is expected to decrease as $H$ is increased beyond the integral scale lengths. The reconstruction of the temperature and emissivity distribution using the data (collected at more than 100 locations above the fire) is equivalent to a random temporal ordering. Although the instantaneous heat transfer between the two locations changes as a function of time shift, the integrated heat transfer varied negligibly with random time shifting.

## REFERENCES

1. Klassen, M., Sivathanu, Y. R., and Gore, J. P., Combust. Flame 90:34 (1992).
2. Klassen. M., and Gore, J. P., Combust. Flame 93:270 (1993).
3. Kounalakis, M. E., Gore, J. P., and Faeth, G. M., J. Heat Transfer 111:1021 (1989).
J. Gore and Michael Klassen, Purdue University, USA. In previous multiray radiation calculations [1,2], fewer rays were necessary to obtain heat flux values. For example, Klassen et al. (1993) [2] utilized between 22 and 450 rays and 5000 realizations to calculate converged heat feedback in $30-\mathrm{cm}$ toluene pool fires. Please comment on the necessity of using a large number of rays ( $\geq 10,000$ ) to obtain converged heat fluxes in your information.

## REFERENCE

1. Kounalakis, M. E., Gore, J. P., and Faeth, C. M., J. Heat Transfer 111:1021-1030 (1989).

## REFERENCES

1. Gore, J. P., Ip, U.-S., and Sivathanu, Y. R., "Coupled Structure and Radiation Analysis of Acetylene/Air

Flames," J. Heat Transfer Trans. ASME 114:487-493 (1992).
2. Klassen, M., Gore. J. P., Sivathanu, Y. R., Hamins, A., and Kashiwagi, T., "Radiative Heat Feedback in a Toluene Pool Fire," Twenty-Fousth Symposium (International) on Combustion, The Combustion Instifute, Pittsburgh, pp. 1713-1719.

Author's Reply. In the present study, the fadiative heat transfer characteristics for the $10-\mathrm{cm}$ heptane pool fire were modelled as an aggregate of small emitters and receivers. The turbulent fluctuations of the location of the "hot" emitting volumes above the pool surface required dense sampling using a large number of rays generated in random directions to prevent aliasing errors. The number of rays chosen for these calculations was determined for some initial "pilot" calculations rather than determining the
number of rays interactively [1]. To achieve a systematic determinant for convergence, the sample standard deviation was maintained at $1-2 \%$. At a particular time step, the geometry of the radiation field may require less than 10,000 rays to produce a standard deviation less than the determined threshold. However. it has been found that 10,000 rays always provided this level of accuracy for each time step [2].

## REFERENCES

1. Kirk, D., and Arvo, J., Comput. Graphics 25(4):153 (1991).
2. Kushmeier, H., Hamins, A., and Choi. M. Y., "Volume Rendering of Pool Fire Data." IEEE/ACM Volume Visualization Symposium. Washington, DC. Oct. 1994.

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