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Calculation of radiation transmittance through n-heptane in a pool fire

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ABSTRACT

The radiative transfer mechanisms in a volatile hydrocarbon pool fire were investigated by solving the transmittance of infrared radiation through fuel (n-heptane) layers of different depths. The incoming radiation was assumed to have the same relative amounts of different wavelengths as a spectrum obtained experimentally for a 2 meter pool fire, and the transmittances were calculated by integrating either the single-ray Lambert-Beer formula, the two-flux (Schuster-Schwarzschild) method solution or the analytical plane-parallel monochromatic/gray solution of the radiative transfer equation over wavelength, using the liquid absorption coefficients from several sources. The obtained transmittances were compared to earlier heat flux measurements, and the possibility of calculating them with significantly less computation time by using a k-distribution method was investigated. The results managed to replicate the measured heat flux values at depths over 1 mm in the liquid with reasonable accuracy, and the use of the k-distribution, more known and used in gas phase thermal radiation calculations, significantly speeds up the calculations.

KEYWORDS:

pool fire; thermal radiation; hydrocarbon; transmittance; infrared spectra
INTRODUCTION

A pool fire, where an evaporating liquid undergoes combustion, is an important scenario in fire safety science due to large amounts of liquid fuels being stored in industrial facilities and carried between locations both by land and sea routes. A large pool fire can generate dangerous radiative heat fluxes at distances of tens of meters or more from the burning site, making it a large risk to surroundings. In addition to experiments on liquid pools, information about the relevant physics can be obtained by numerical simulations, which represent a complicated multiphysics problem with chemical reaction, hydrodynamics and radiation. The radiative heat transfer back to the pool from the flames above is the most important heat transfer mechanism for large scale pool fires, and it controls the mass loss and heat generation rate in combustion through the evaporation rate on the pool surface. In principle, the physics of this radiative transfer can be calculated by solving the radiative transfer equation (RTE), coupled to the hydrodynamic and reaction rate equations, by using FVM or some other numerical method.

It is, however, much simpler to measure empirical infrared flame spectra for pool fires of different surface areas and use this as the input data in an RTE calculation of radiative transfer downwards from the pool surface (using measured infrared absorption spectra of the liquid-phase fuels, from, e.g. Refs. [1,2,3]). The motivation for doing this is the attempt to find a radiative transfer model, usable in pool fire simulations, which would require less processing power through use of acceptable simplifications and empirical data instead of a full solution of the RTE. Earlier publications about radiation in pool fires, made by other authors, include Refs. [3,4,5], and some other sources discuss the more general problem of evaporation, heat transfer and flows in volatile liquid pools, which may contain mixtures of liquids instead of a single substance [7].

METHODS

Flame emissivity

As experimental flame spectra from different sources have been measured from pool fires of different sizes, there is a need to approximate the spectrum of a small pool fire by scaling the measured spectrum of a larger one. The simplest way to do this is to assume that the relative amounts of different wavelengths in the spectrum depends only on the fuel, and that the effect of pool size can be taken into account with a simple constant multiplicative factor, as in the commonly used equation of flame emissivity

$$\varepsilon = 1 - \exp(-KL), \quad (1)$$

where the constant $K$ depends on the fuel and $L$ is a characteristic length of the flame. This, of course, is not necessarily a justified assumption, and it is possible that the $\varepsilon$ in Eq. 1 is actually a function of the wavelength $\lambda$ and affects the relative intensities at different wavelengths. In this work it is assumed that it is not a function of $\lambda$ and the validity of this assumption is tested.

Absorption in a uniform medium with a simple geometry

The inward radiation flux at depth $x$ in liquid can, in principle, be approximately calculated by integrating the monochromatic (or gray-gas) plane-parallel RTE solution for non-scattering and non-emitting medium [8] over the relevant wavelength interval, using the incoming flux as a weight function.

$$q^+(x) = 2 \int_0^\infty q_0(\lambda) E_3(\kappa(\lambda)x)d\lambda$$

(2)

The function $E_3$ is the third exponential integral function. An approximate version of this is the single-ray approximation implementing the Lambert-Beer law that predicts exponential decay of flux/intensity.

$$q^+(x) = \int_0^\infty q_0^+(\lambda)\exp(-\kappa(\lambda)x)d\lambda$$

(3)

A more accurate approximation is the two-flux model [8], which predicts an inward radiative flux corresponding to 2 times larger absorption coefficient than in the Lambert-Beer result:

$$q^+(x) = \int_0^\infty q_0^2(\lambda)\exp(-2\kappa(\lambda)x)d\lambda.$$
The wavelength dependent quantity $q_\lambda^0(\lambda)$ is obtained from experimental data by multiplying with a flame size parameter equivalent to the $\varepsilon$ in Eq. 1. To obtain an intensity value, the corresponding radiative flux is divided by $\pi$ steradians.

**Significance of medium emission**

Adding a term corresponding to radiative emission by liquid material to Eqs. 2 and 4 would not be difficult, if temperature distribution as a function of depth were known. However, in this work it is assumed that the significance of this can be ignored. At the boiling point of n-heptane (about 371 K), the blackbody emissive power $\sigma T^4$ is about 1.1 kW/m$^2$, and at 50 °C it is about 0.62 kW/m$^2$, so it can be expected that medium emission is not among the most significant considerations. In the more accurate Eq. 2, the inclusion of emission in the liquid phase would mean having a term with an integration over the 2nd exponential integral function $E_2$ and in Eq. 4 there would be growing exponential term in the integrand in addition to the decreasing one. In pool fires with less volatile fuels, such as mineral spirits, with boiling temperature of 160-190 °C the thermal radiation from the liquid probably has to be considered.

**The k-distribution method**

The integrations in Eqs. 2, 3 and 4 can consume a lot of time if the flame spectrum and absorption spectrum have to be known in high resolution. A faster k-distribution method for calculating the fractional transmittances is based on converting the absorption coefficient function $\kappa(\lambda)$ into a monotone increasing function $g(k)$, which tells how large fraction of incoming radiation is on the wavelengths where the spectral absorption coefficient $\kappa(\lambda)$ is smaller than the variable $k$. To find this function, we first take the function $q_\lambda(\lambda)$, and multiply it with a constant that normalizes its integral to unity. If this normalized function is called $B_{n,n}(\lambda)$, we can calculate the function $g(k)$ as an integral

$$g(k) = \int_{D(k)} B_{n,n}(\lambda) d\lambda,$$

where $D(k)$ is defined as the set of wavelengths where the absorption coefficient is smaller than $k$:

$$D(k) = \{ \lambda \in \mathbb{R} | \kappa(\lambda) < k \}.$$

Next the function $g(k)$ is converted to the inverse function $k(g)$ and finally the transmittance through a path length of $s$ (assuming Lambert-Beer law) is found by integrating

$$\tau(s) = \int_0^s \exp(-k(g)s) dg,$$

or equivalently with the exponential integral decay law

$$\tau(s) = 2 \int_0^s E_2(k(g)s) dg.$$

An advantage of this kind of calculation is that, as the functions $g(k)$ and $k(g)$ are monotone increasing and therefore do not contain any rapid oscillations, the integral can be very accurately approximated with a Gauss-Legendre quadrature, using only a few quadrature points.

**Data measured by other researchers**

Data of the flame spectrum of a hydrocarbon (n-heptane) fire and the absorption spectrum of the liquid were found and combined from references [1,2,3]. The experimental data of the radiation penetration under the n-heptane liquid surface were obtained from [4].

The n-heptane IR absorption spectrum, combined from [1] and [3] is shown in Fig. 1.
The data in Suo-Anttila's work [3] was in the form of transmittances through a fixed path length (3.175 mm) of liquid, and the absorption coefficients in the Figure 1 are calculated by assuming Lambert-Beer law (exponential decay of intensity with increasing path length). The IR absorbance data in the NIST Chemistry Webbook for the range 2.65-20 µm has higher resolution than the data in Tuntomo's article [1], but as the former is from 1960 and the latter from 1992, the Tuntomo's results are used in these calculations. The measured IR emission spectrum of an n-heptane flame in the 2-meter pool fire of Suo-Anttila is in Fig 2., digitized from the original reported curve [3]. The article claims that the nearest blackbody equivalent of this spectrum has an absolute temperature of 1450 Kelvin and an emissivity of 0.4, and we assume that the spectrum outside this measured range of about 1.3-5.0 micron can be approximated with the corresponding Planck distribution of longer wavelengths (Fig. 2).

**RESULTS**

Zhao et al. [4] fitted simple curves to their measured heat fluxes as a function of depth, valid for the 10 cm, 20 cm and 30 cm diameter pools. Similarly, a function of form \( y = y_0 + A\exp(-kx) \), in which \( y_0 \), \( A \) and \( k \) are fitting parameters, fits well to the Sandia laboratories transmittance data (the graph on the right in Fig. 2) and the parameter \( k \) (describing the decay rate of intensity and not to be confused with the \( k \) in function \( g(k) \)) appears to have a value of about 0.83 mm\(^{-1}\), which is comparable to the values in the order of 0.5 mm\(^{-1}\) obtained in [4] when the very first datapoints with the lowest depth were ignored in the fitting by the authors of that article.

In Fig. 3, the results of single-ray, two-flux and exponential integral calculations are compared to the 20 cm and 30 cm curve fits given in [4]. When normalized to transmittances beginning from 1 at 0 mm, the curve fits describing the heat flux in 10, 20 and 30 cm pool fires are almost identical but distinguishable, which makes the two plots in Fig. 3 practically the same and is an indication that the relative amounts of wavelengths in the flame spectrum remain almost the same when the pool radius is multiplied by a small integer.
Fig 3: the calculated thermal radiation transmittances at different depths under the surface of a burning n-heptane pool, compared to curve fits (solid line) made in [4] to experimental heat flux data and to the results of calculation in [3].

When the k-distribution method of Eq. 7 is used for the calculation with single-ray Lambert-Beer model, the result is very similar to the result of Eq. 3 as seen in Fig. 4, and is expected to become identical when the k-distribution function g(k) is calculated with high enough resolution in the numerical integration. Also shown in Fig. 4 is the result of the integration when done with a Gauss-Legendre quadrature using only 3 quadrature points instead of adding quadrature points until convergence.

Fig 4: Left: the results of calculating the single-ray transmittance of flame radiation through n-heptane, done both with k-distribution and Eq. 3 (“Line by line”). The result of a Gauss-Legendre quadrature with only 3 nodes is also included. Right: Experimental results in [4] compared to two different mean absorption coefficient calculations.

Finally, the calculations were performed using two alternative mean absorption coefficients, revealing the problems of grey-medium calculations. The first coefficient is the flame spectrum weighted mean absorption coefficient of n-heptane, and the result of Eq. 3 was compared to a simple exponential decay using that absorption coefficient. Numerical integration gave a value of $k_{\text{mean}} = 1230 \text{ m}^{-1}$, and the corresponding graph is shown with dashed line in the right side of Fig. 4. From the image it is apparent that the absorption by the liquid cannot be described by a single absorption coefficient, and the result of such an approximation differs from the accurate result by a factor of 10 or more. Another way to define a mean absorption coefficient is to choose the $k$ in the function $\exp(-ks)$ so that it produces correct transmittance at the bottom ($s = 8 \text{ mm}$) of the pool. This kind of calculation gives the coefficient a value of about $158 \text{ m}^{-1}$, and the transmitted fraction decreases almost linearly when nearing the bottom as seen drawn with a dashed dot line on the right side of Fig. 4, which is clearly unrealistic.
CONCLUSIONS

In the results presented in this article, it is observed that the transmitted fraction of heat flux at different depths in the liquid phase of a pool fire can be calculated with reasonable accuracy from empirical flame spectrum and absorption coefficient data, and the effect of the size of the fire seems to be quite accurately taken in account by a simple multiplicative constant in the incoming intensity/flux. The calculations done with the two-flux method or with the exact plane parallel RTE solution are expectedly more similar to the experimental results than the single-ray calculation.

The most useful finding presented in this paper is that the results can also be obtained with similar accuracy by a k-distribution method in a similar manner to what is used for gas phase radiation calculations, and that the integrations in a k-distribution calculation can be done accurately with numerical quadrature involving a very small number of arithmetic operations, leading to fast computations. This kind of model can be implemented in fire simulation models attempting to predict liquid pool temperature distributions and evaporation.

REFERENCES


