
This is an electronic reprint of the original article.
This reprint may differ from the original in pagination and typographic detail.

Isojärvi, Teemu; Bordbar, Hadi; Hostikka, Simo

Spectrally resolved calculation of thermal radiation penetration into liquid n-heptane in pool fires

Published in:
International Journal of Heat and Mass Transfer

DOI:
[10.1016/j.ijheatmasstransfer.2018.08.108](https://doi.org/10.1016/j.ijheatmasstransfer.2018.08.108)

Published: 01/12/2018

Document Version
Peer-reviewed accepted author manuscript, also known as Final accepted manuscript or Post-print

Published under the following license:
CC BY-NC-ND

Please cite the original version:
Isojärvi, T., Bordbar, H., & Hostikka, S. (2018). Spectrally resolved calculation of thermal radiation penetration into liquid n-heptane in pool fires. *International Journal of Heat and Mass Transfer*, 127, 1101-1109. <https://doi.org/10.1016/j.ijheatmasstransfer.2018.08.108>

This material is protected by copyright and other intellectual property rights, and duplication or sale of all or part of any of the repository collections is not permitted, except that material may be duplicated by you for your research use or educational purposes in electronic or print form. You must obtain permission for any other use. Electronic or print copies may not be offered, whether for sale or otherwise to anyone who is not an authorised user.

Spectrally resolved calculation of thermal radiation penetration into liquid n-heptane in pool fires

Tecmu Isojärvi*, Hadi Bordbar* and Simo Hostikka**

* Department of Civil Engineering, Aalto university, Espoo, Finland
Address: Rakentajanaukio 4 A, Espoo PL 12100, 00076 AALTO

★ Corresponding author: simo.hostikka@aalto.fi

Abstract

The radiative heat transfer in a volatile hydrocarbon pool fire was investigated by obtaining the transmittance of infrared radiation through fuel (n-heptane) layers of different depths. The incident radiation spectrum was assumed to be either the same as a spectrum obtained experimentally for a 2 meter pool fire, or to be a Planck distribution corresponding to the approximate flame temperature. The transmittances were calculated by integrating either the single-ray Lambert-Beer formula, the two-flux method or the analytical plane-parallel monochromatic/gray solution of the radiative transfer equation over wavelength, using the liquid spectral absorption coefficients found in literature. The obtained results are validated against earlier 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 in the liquid with a fractional error of only about 5% being attainable even with a 3-point quadrature method. The use of the k-distribution, more known and used in gas phase thermal radiation calculations, significantly speeds up the calculations. It was found out that in the calculation of total transmitted fractions of radiation, the flame spectrum can be approximated with a Planck distribution of an appropriate temperature.

Keywords: Spectral radiation, k-distribution, liquid n-heptane, pool fire, numerical modeling

Nomenclature

Latin

E_3	The 3rd exponential integral function	
g	Cumulative k-distribution	
g_i	An array of abscissas of a Gaussian quadrature	
I	Spectral intensity	$\text{kW}/\text{m}^2/\mu\text{m}/\text{sr}$
I_0^+	Spectral intensity	$\text{kW}/\text{m}^2/\mu\text{m}/\text{sr}$
$I_{0,n}^+$	Dimensionless relative intensity	
k	Spectral absorption coefficient	m^{-1}
L	Characteristic length of a flame	m^{-1}
q	Spectral heat flux	$\text{kW}/\text{m}^2/\mu\text{m}$
q_0^+	Spectral heat flux	$\text{kW}/\text{m}^2/\mu\text{m}$
s	Path length	m
w_i	An array of weights for a Gaussian quadrature	

Greek

α	Decay rate constant in an exponential function $e^{-\alpha x}$	
β	A parameter related to thermal emissivity of a fuel in Eq. 12	m^{-1}
ϵ	Dimensionless flame emissivity factor	
κ_{mean}	Mean absorption coefficient	m^{-1}
λ	Wavelength	m
τ	Transmittance	

1 Introduction

Radiative heat transfer has an important role in energy transfer in many energy conversion systems, such as combustion systems [1,2], fires [3] and rocket engines [4]. The calculation of radiative heat transfer is significantly more difficult than that of other heat transfer mechanisms because the governing equation of radiative heat transfer is an integro-differential equation which requires solution methods different from ordinary differential or partial differential equations. Moreover, the radiative properties of participating media are wavelength dependent and especially in gases are very difficult to be accurately included in radiation heat transfer models [3]. During the last decade many researches have been dedicated to develop models to include the spectral features of radiative properties of participating media in solution of radiative transfer equation [3].

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 reaching the pool from the flames above is the most important heat transfer mechanism for large scale pool fires. It controls the mass loss and heat generation rate in combustion through the evaporation rate on the pool

surface. Any model attempting to predict the liquid pool evaporation rate must take into account the rate of radiation absorption. Simple energy balance-based models assume that all the absorbed radiation is available for evaporation [5]. This is equivalent to assuming that the radiation does not penetrate into the pool. Some other models assume that it is absorbed to the entire depth, leading to a uniform, steady-state temperature distribution over the liquid depth. In either case, the transient nature of the pool evaporation rate cannot be captured. Using numerical simulations Sikanen and Hostikka showed [6] that the rate of sub-surface absorption affects the transient burning rate of liquid pools. According to their results, it was not possible to define a single (gray) absorption coefficient that would yield accurate pool temperatures both close to the surface and in-depth. The same phenomenon has been investigated experimentally by Inamura et. al. [7], by measuring the time required for a water sublayer below a combusting water-insoluble fuel to start boiling, and Suo-Anttila et. al. [8] who for the first time attempted to include spectral details of radiation in their theoretical considerations.

In principle, the radiative transfer inside the pool could be calculated by solving the radiative transfer equation (RTE) with high resolution spectral locations. This would, however, be too costly for the practical fire calculations. The goal of the current research is to develop a numerically efficient method to take into account the spectral dependence of the radiation penetration. The method needs to be applicable for different fuels, and possible to implement within the state-of-the-art fire CFD models [9]. The method may also find applications in combustion of fuel sprays where the evaporation of the fuel droplets depends on the absorption of thermal radiation. Similar situation is found in the pyrolysis of solid polymers: a polymer that allows thermal radiation to pass to a significant depth will last longer in the fire before melting, decomposing and igniting [10].

An important part of this research has been dedicated to implement k-distribution method for solving the radiation penetration within a liquid fuel pool. Different versions of the k-distribution method including the full-spectrum correlated-k method (FSCK) have been widely used in modeling of spectral radiative heat transfer in gaseous media [11,12,13,14]. It is based on reordering the wavenumber in order to obtain a monotonically increasing function of k which is much easier to be numerically integrated. While this kind of global models can not provide the spectral radiation heat flux (or heat source), they can accurately predict the total integrated values of these parameters by using the spectrally integrated radiative properties of the media. The usefulness of this approach is that integrations over the wavelength λ in the rapidly varying spectrum $\kappa(\lambda)$ require a much more dense set of data points than integrating an increasing function. In the gas phase this is especially important because the spectrum consists of sharp absorption lines with width that is much smaller than the total wavelength interval which has to be considered.

2 Methods and materials

2.1 Numerical solution of 1D RTE

By ignoring the emission of the liquid at low temperatures, the inward radiation flux at depth s in liquid can, in principle, be approximately calculated by integrating the monochromatic plane-parallel RTE solution of a non-scattering and non-emitting medium [15] over the relevant wavelength interval, using the incoming flux as a boundary condition.

$$q^+(s) = 2 \int_0^\infty q_0^+(\lambda) E_3(\kappa(\lambda)s) d\lambda \quad (1)$$

The function E_3 here 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 intensity.

$$I^+(s) = \int_0^\infty I_0^+(\lambda) \exp(-\kappa(\lambda)s) d\lambda \quad (2)$$

A more accurate approximation is the two-flux model given by

$$q^+(s) = \int_0^\infty q_0^+(\lambda) \exp(-2\kappa(\lambda)s) d\lambda. \quad (3)$$

The two flux method is a way to partially take into account the fact that all of the thermal radiation penetrating the liquid is not advancing to a direction normal to the surface of the liquid pool, while ignoring the variation of the intensity inside each hemisphere of directionality.

The emission by liquids depends on temperatures, which are naturally below their boiling point in a pool fire, and hence are quite small compared to the absorption by the liquid which depends on the incoming radiation from the flame. In this work we aimed to obtain the transmissivity of the n-heptane pool, and we have assumed that emission by the liquid is negligible and can be ignored compared to the absorption term.

2.2 k-distribution method

Using the high resolution spectral data for the incident flame spectrum and absorption of the liquid, the integrations of Eqs. 1,2 and 3 over the entire spectrum can be computationally very demanding when performed within large scale CFD computations. The so called global models aim at providing a fast and accurate means to calculate the total values of radiation heat transfer with spectral absorption coefficients of media. One of the most well-known global models is k-distribution method which is based on converting the complex spectral absorption coefficient profile $\kappa(\lambda)$ to a much simpler function of k which is easier to integrate [11,12].

To find these functions, we first take the function $I_0^+(\lambda)$, and multiply it with a constant C that normalizes its integral to unity: $\int_0^\infty CI_0^+(\lambda) d\lambda = 1$. Denoting $I_{0,n}^+ = CI_0^+$, we can define

$$f(k) = \int_0^{\infty} I_{0,n}^+(\lambda) \delta(k - \kappa(\lambda)) d\lambda. \quad (4)$$

It represents the integral of normalized intensity over the spectrum for the wavelengths where the $\kappa(\lambda)$ equals a certain k value. A cumulative form of this function is defined as

$$g(k) = \int_0^k f(k') dk'. \quad (5)$$

The $g(k)$ has a quite easily visualized interpretation, it is the same as integral

$$g(k) = \int_{D(k)} I_{0,n}^+(\lambda) d\lambda \quad (6)$$

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

$$D(k) = \{\lambda \in \mathbb{R} \mid \kappa(\lambda) < k\}. \quad (7)$$

Next the the inverse function of $g(k)$, i.e. $k(g)$, needs to be obtained and finally the transmittance through a path length of s , assuming Lambert-Beer law, is found by integrating

$$\tau(s) = \int_0^1 \exp(-k(g)s) dg, \quad (8)$$

or equivalently with the exponential integral decay law

$$\tau(s) = 2 \int_0^1 E_3(k(g)s) dg, \quad (9)$$

or the two-flux model

$$\tau(s) = \int_0^1 \exp(-2k(g)s) dg. \quad (10)$$

An advantage of this kind of calculation is that, as the functions $g(k)$ and $k(g)$ are monotonically increasing and therefore do not contain any rapid oscillations, the integral can be very accurately approximated with a Gaussian quadrature, using a small number of quadrature points. For an integral of a function $f(g)$ over interval from 0 to 1, a quadrature formula of order n is like

$$\int_0^1 f(g) dg \approx \sum_{k=1}^n w_k f(g_k), \quad (11)$$

where the w_k :s are called weights and the g_k :s are called abscissas. The calculations become more complicated than presented here, if it is not assumed that the temperature, pressure and chemical composition conditions are the same across the whole liquid layer that the radiation is passing through. In those cases, the functions f and g depend on additional variables describing the local and reference states of the medium [11,12]. Assuming a homogeneous condition in this study is expected to be acceptable as most of the temperature and composition changes in a liquid fuel pool

occur in the very first layer of the pool facing the incident radiation, except maybe at the boilover stage of a pool fire with a high boiling point fuel.

2.3 Boundary conditions and n-heptane properties

2.3.1 Boundary conditions

To solve the radiative transfer equation, boundary conditions are needed as in the solution of any differential equation. In the case of flame radiation penetrating a liquid fuel, the relevant BC is the spectral radiation intensity on the surface of the liquid. 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

$$\epsilon = 1 - \exp(-\beta L), \quad (12)$$

where the constant β 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 ϵ in Eq. (12) is actually a function of the wavelength λ and affects the relative intensities at different wavelengths. In the calculations in this paper, we circumvent the problem of finding the parameter ϵ by calculating transmittances instead of absolute intensity values.

As a boundary condition, either an extended experimentally measured flame spectrum, or a Planck function corresponding to an approximate flame temperature, can be assumed as the spectral intensity on the surface of the liquid fuel. The experimental absorption and flame spectra of n-heptane have been collected from sources [8,17,18] (the absorption spectrum) and source [8] (the flame spectrum), and shown in Figs. 1 and 2, respectively. The spectral data was in the form of absorption coefficients in Ref. [17], but as transmittances measured through a known path length in [8,18]. The transmittances had to be converted to absorption coefficient values $\kappa = -\log(\tau)/\Delta x$. Δx is the path length. The spectral resolution was also different in each source. The flame spectrum in the article of Suo-Anttila et al. [8] was given in the form of spectral intensity from 1 to 5 micrometers wavelength. It was measured for a 2 meter diameter n-heptane pool. As Ref. [8] reports that the Planck distribution of 1450 K temperature and emissivity 0.4 is closest to the actual flame spectrum, we extend the experimental data to wavelengths longer than $5\mu\text{m}$ with that Planck function.

2.3.2 N-heptane liquid properties

N-heptane is a colorless, flammable liquid with chemical formula C_7H_{16} and boiling point 98 °C. It is often used in pool fire experiments because it is less dangerous than many lower-boiling fuels.

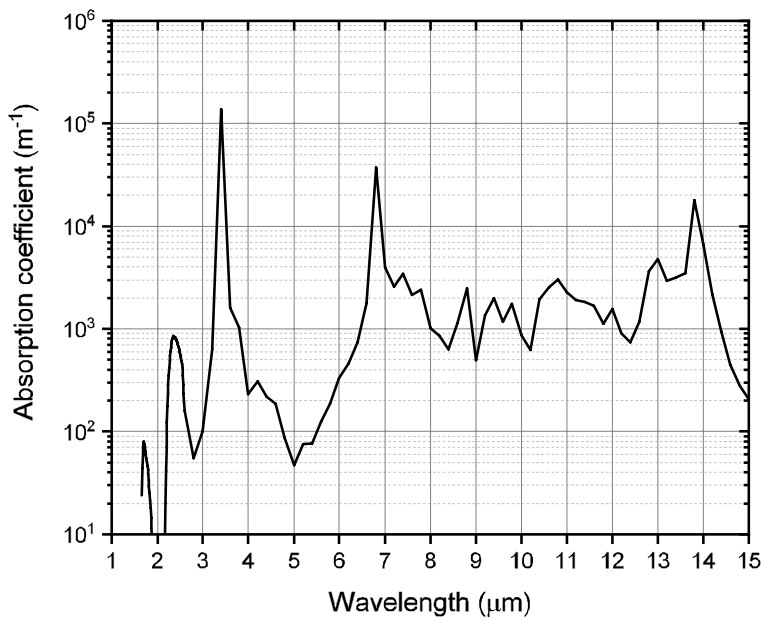


Figure 1: *The infrared absorption spectrum of liquid n-heptane.*

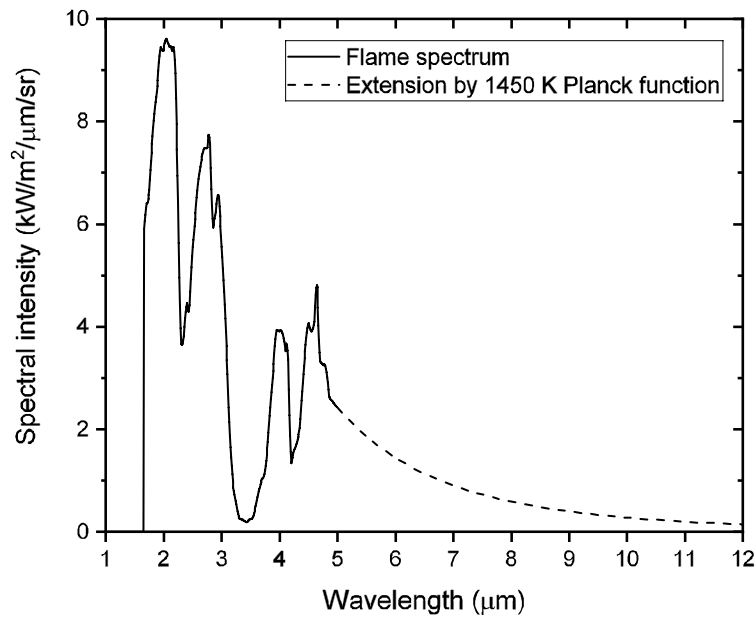


Figure 2: *The flame spectrum of a 2 meter diameter n-heptane pool fire reaching the liquid surface of the pool, measured by Suo-Anttila et al. [8] with an extension to longer wavelengths with 1450 K Planck radiation.*

3 Results and discussion

3.1 Spectral characteristics of the in-depth radiation

Using Eq. 2 with either the measured flame spectrum or the 1450 K Planck distribution as the surface boundary condition, it is possible to plot the spectrum of the radiation that is left at different depths in the liquid. This has been done in Fig. 3 that shows the spectral intensities at 1,2 and 8 mm below the liquid surface. In the case of an initially continuous spectrum (bottom figure), the absorption happens most effectively at wavelengths close to $3.5 \mu\text{m}$ and at $7 \mu\text{m}$. These wavelengths correspond to the two most important liquid heptane absorption peaks (Fig. 1). In the top figure of Fig. 3, there is no incoming radiation near the $3.5 \mu\text{m}$ peak, indicating that these wavelengths have been absorbed already by the fuel vapor above the liquid pool. The $7 \mu\text{m}$ region of the incoming spectrum was approximated by the Planck function, thus showing identical behavior in these two cases.

The initially different intensity profiles of the flame and Planck function BCs become quite similar once the radiation has passed through a path length of several millimeters. This result indicates that beyond the immediate region close to the surface, the penetrated heat flux is more sensitive to the liquid absorption spectrum than the assumed boundary condition. Within the first mm, the shape of the incoming spectrum may become important for the amount of absorbed energy.

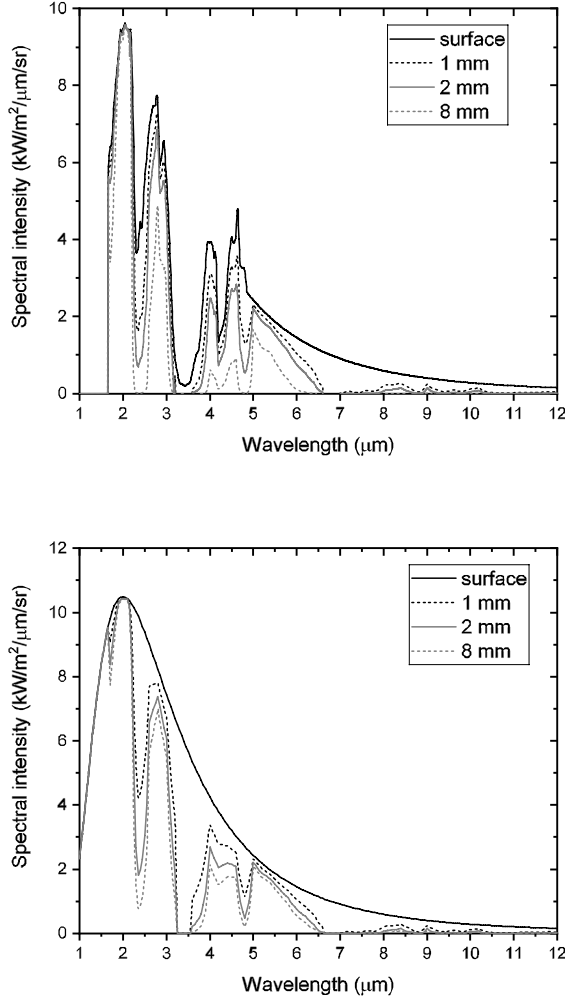


Figure 3: *The remaining radiation spectrum after having passed through different depths of n-heptane, assuming the radiation model of Eq. 2. Top: boundary condition is the extended experimentally measured intensity profile of [8]. Bottom: boundary condition is the Planck distribution of 1450 K.*

3.2 Total heat fluxes at different depths

3.2.1 Effect of the RTE solution method

Zhao et al. [19] measured total (spectrally integrated) radiative heat fluxes in heptane pool fires, ranging from 10 to 30 centimeters in length scale. Functions with a decaying exponential function plus a constant were fitted to the data and the fitting parameters reported. This is equivalent to assuming that the radiation consists of a rapidly absorbed part and a part that will not be absorbed at all. A similar function of form $y = y_0 + A \exp(-\alpha x)$, in which y_0 , A and α are fitting parameters, fits well to the Sandia laboratories transmittance data [8] when tested with the Origin Pro nonlinear curve fit.

In Fig. 4, the results of our single-ray (Eq. 2), two-flux method (Eq. 3) and exponential integral (Eq. 1) calculations are compared to the 20 cm curve fit given in [19]. The integrations were done with all the resolution of the available spectral data, so they were spectrally accurate. When the heat fluxes are converted to dimensionless transmittances beginning from 1 at $s = 0$ mm by multiplying with a normalization factor, the curve fits reported in [19] describing the heat flux in 10, 20 and 30 cm pool fires are almost identical but distinguishable. This makes the plot in Fig. 4 practically the same as the one that would be obtained for a 10 or 30 cm pool. This is an indication that the relative amounts of wavelengths in the flame spectrum do not change much in small changes of the size of the pool.

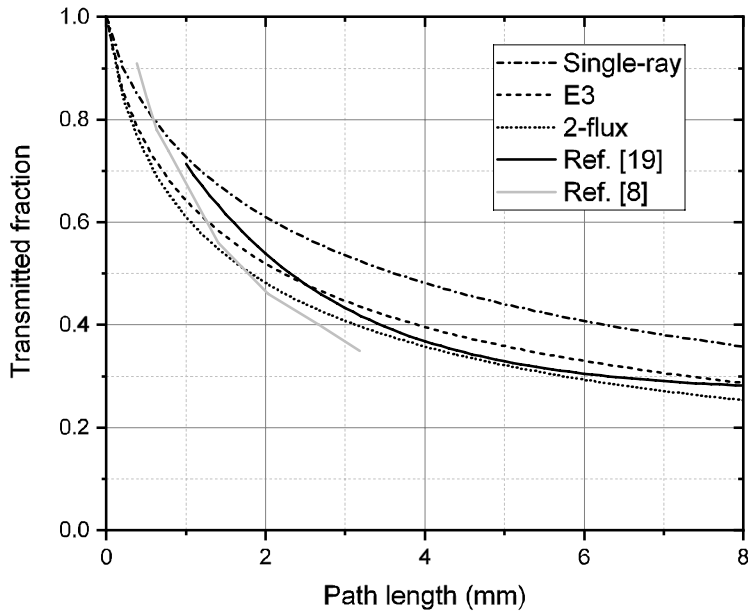


Figure 4: *Calculated transmittances, either with Lambert-Beer law, two-flux method or plane parallel gray medium exact solution as the RTE solution method, compared to a curve fit made in [19] into measured heat fluxes under the surface of an ignited 20 cm heptane pool.*

In Fig. 4, it is seen that the RTE solution with the E_3 function has best correspondence to the experimental data, and that the single-ray approximation is the least accurate.

To find out how accurately the real experimental flame spectrum of n-heptane can be approximated with a blackbody spectrum in these calculations, we obtained the LBL single-ray transmittances by using Planck functions with temperatures 1000, 1200 and 1400 K as the boundary condition on the fuel surface. The comparison of these to the LBL single-ray result of Fig. 4 is shown in Fig. 5. From the result it is apparent that an optimal blackbody spectrum in this approximation would have a temperature of about 1400 Kelvin, which is similar to an actual flame temperature expected in hydrocarbon fires.

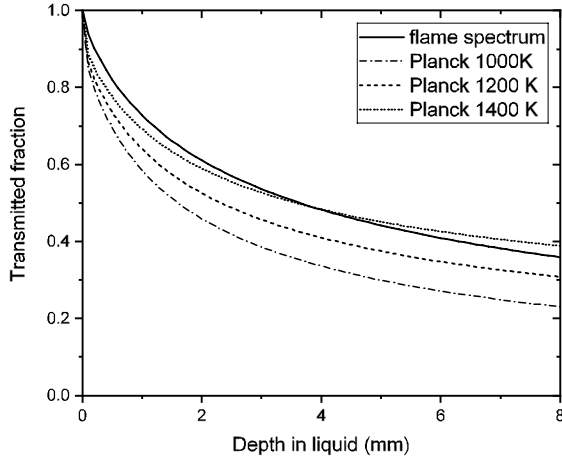


Figure 5: *The transmitted fraction of radiation as function of depth in n-heptane pool, calculated by the line-by-line method using either the experimental n-heptane flame spectrum or Planck functions corresponding to different flame temperatures.*

3.2.2 Solution by k-distribution method

To verify the implementation of the k-distribution method, we first performed a calculation where the number of integration points for the $k(g)$ function was identical to the number of spectral data points. Next, we investigated the capability of the k-distribution method in providing approximate solutions to the transmitted radiation with a small number of integration points. Figure 6 compares the k-distribution results with 3 points and with 15 points of Gauss-Chebyshev quadrature against the line-by-line result of Eq. 1. The results of both quadratures are found to be close to the line-by-line solution. This verifies the implementation and indicates the level of uncertainty that is the price of computational efficiency. Similar good agreement with the line-by-line results was found in the case of Planck distribution as the surface boundary condition, or when the calculation was done for the single-ray solution of Eq. 2.

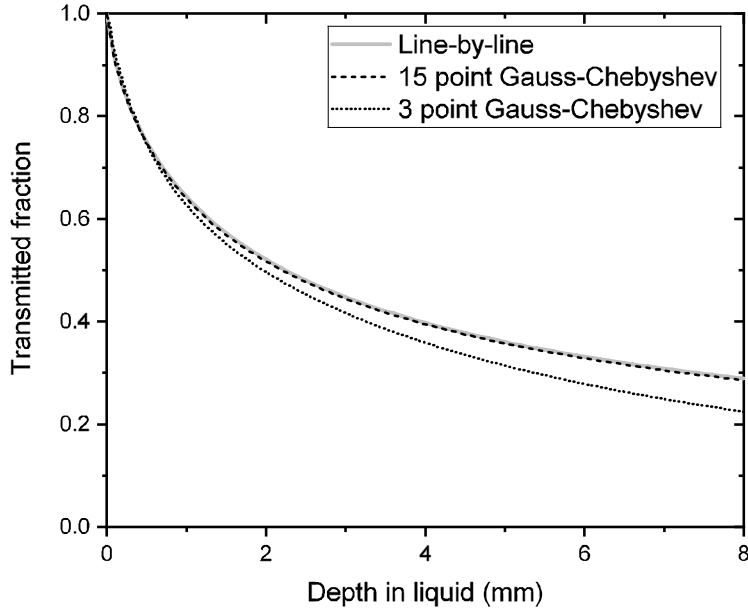


Figure 6: *Transmitted fraction of radiation in the pool using line-by-line solution and k-distribution method with 3 and 15-point Gauss-Chebyshev quadratures.*

The abscissae g_i and weights w_i for a 3-point Gauss-Chebyshev quadrature, as well as the values of the function $k(g)$ at the quadrature points, are shown in Table 1 as an example. The version of the quadrature that is used here is the same as described by Wang and Modest [20], and has the property of points g_i becoming more dense when approaching the endpoint $g = 1$.

Table 1: *The quadrature points g_i , the corresponding weights w_i of Eq. 11 and the function values $k(g_i)$, for the 3-point Gauss-Chebyshev quadrature as described in [20] and applied to the problem of experimentally measured flame radiation passing through liquid n-heptane.*

i	1	2	3
g_i	0.22252	0.62349	0.90097
w_i	0.44629	0.32679	0.22692
$k(g_i) / (\text{m}^{-1})$	57.2	287.7	1505.2

The rate of convergence of the Gauss-Chebyshev quadrature was tested by calculating the root mean square error of the transmittance on the depth interval $0 \text{ mm} \leq s \leq 8 \text{ mm}$, with the quadrature order varying from 2 to 15. The radiation model was the E_3 solution of Eqs. 1 and 9. The theoretical speedup compared to an LBL solution is expected to be n_l/n_q where n_l and n_q are number of lines in LBL calculations and number of quadratures in k-distribution method, however the observed speedup for standalone radiation solutions is somewhat less due to the

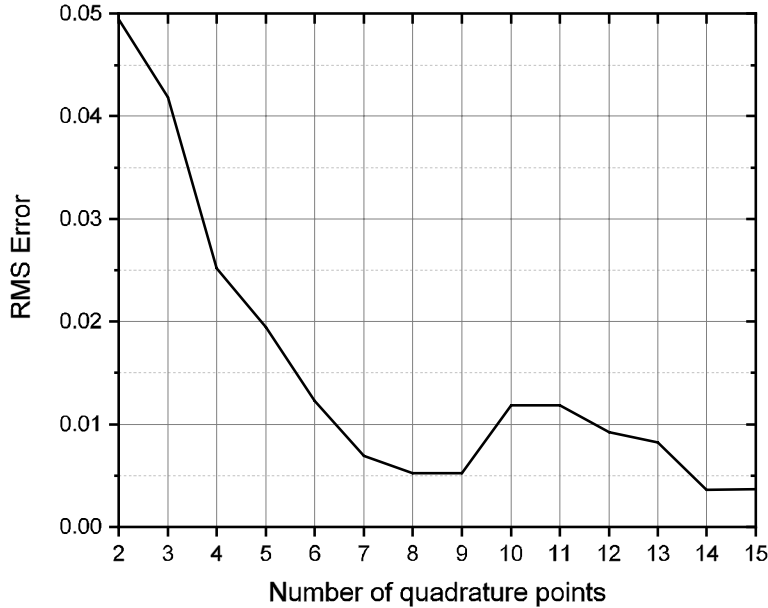


Figure 7: The convergence of Gauss-Chebyshev quadrature described in [20], when applied to the problem of calculating flame thermal radiation transmittance through path lengths of 0 to 8 mm liquid n-heptane.

compiler and operating system -related efficiency. Note that for the homogeneous media, the $k(g)$ data points can be obtained beforehand from the spectral data as for instance reported for three points G-C quadrature scheme in Table 1 and therefore the calculation time of obtaining $k(g)$ quadrature points is not considered in the above mentioned ratio of n_l/n_q . For the heterogeneous thermal condition as seen for instance in gaseous combustion, $k(g)$ should be obtained for each computational cell either from the LBL data or from the published correlations [13,14] or look-up tables [21]. This decreases the speeding factor. The G-C quadrature scheme has been widely used in k-d literature [20,21]. Due to dense quadrature points near to $g = 1$ in G-C scheme, it better includes the effect of spectral regions with larger absorption coefficients which are more important in total radiative transfer. It is why we selected G-C for reporting the parameters of k-d distribution in Table 1. The same 3-point quadrature calculation can also be done by Gauss-Legendre (GL3) and trapezoidal (TQ3) quadratures. In Fig. 8 it is seen that these results do not differ dramatically, and the Gauss-Legendre quadrature (GL3) has the least root mean square error. However, our results showed that G-C shows its privileges compared to G-L in $n_q = 5$ and larger which is due to its better capability of including large spectral absorption coefficients as explained.

3.2.3 Solution by mean absorption coefficient

Finally, the calculations were performed using two alternative mean absorption coefficients. The first coefficient is the flame spectrum weighted mean absorption coef-

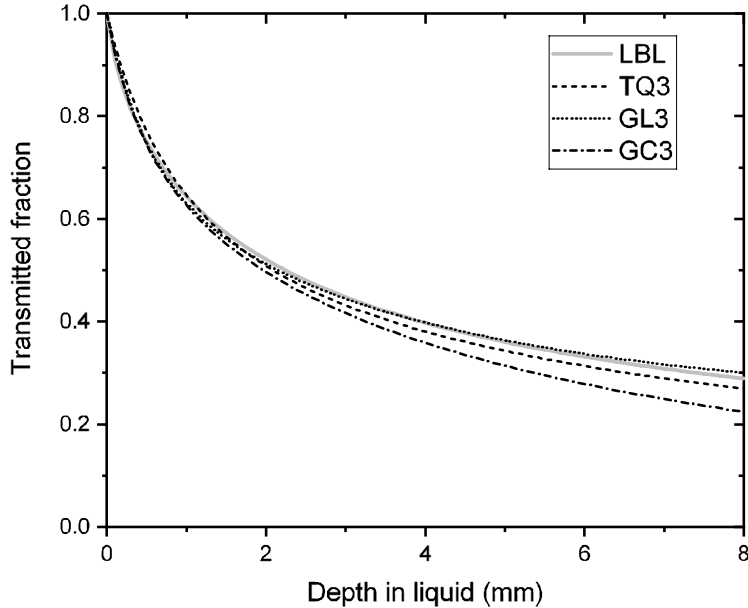


Figure 8: *The effect of using three different 3-point quadrature methods for the integration in Eq. 9.*

ficient defined in Eq. 13.

$$\kappa_{mean} = \frac{\int_0^\infty I_0^+(\lambda) \kappa(\lambda) d\lambda}{\int_0^\infty I_0^+(\lambda) d\lambda}. \quad (13)$$

Numerical integration gave a value of $\kappa_{mean} = 1210 \text{ m}^{-1}$. The mean absorption coefficient of this type does not change if the flame spectrum BC is multiplied by a constant, it only depends on the relative amounts of different wavelengths. This can be seen from the Eq. 13 where in both the numerator and denominator there is a linear dependence on any constant multiplier of I_0^+ .

Another way to define a mean absorption coefficient is to choose the k in the function $\exp(-ks)$ so that it produces correct experimentally measured transmittance at the bottom ($s = 8 \text{ mm}$) of the pool. This kind of calculation leads to value $\kappa_{mean} \approx 158 \text{ m}^{-1}$. In Figure 9 it is seen that with the former case most the radiation is absorbed at unrealistically short path length of $s < 1 \text{ mm}$, while with the latter the total heat flux decreases almost linearly as a function of depth. The obtained results are consistent with those obtained previously in [6]. Figure 9 shows that using of mean absorption coefficients cannot predict the observed experimental measurements, while the LBL calculation of Eq. 1 can do so with much better accuracy.

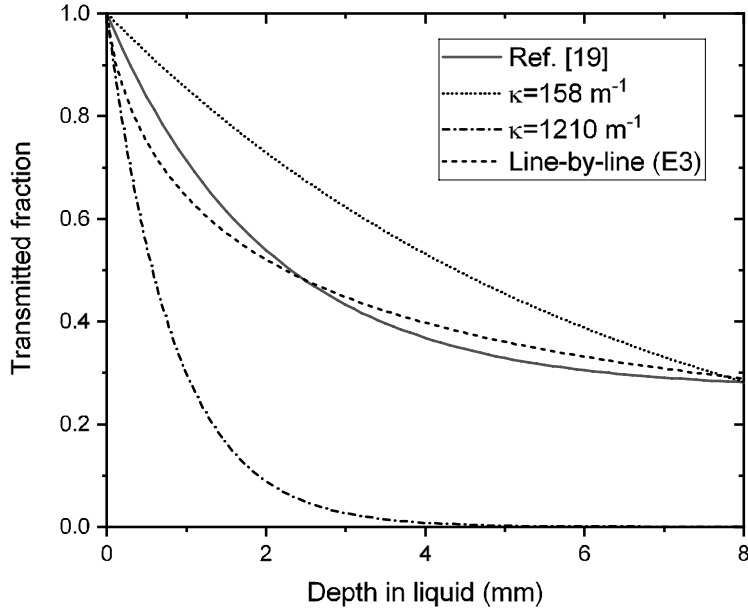


Figure 9: Calculation of the transmitted fraction of thermal radiation under the n-heptane pool surface, done with two different mean absorption coefficient models, and compared to the curve fitted in [19] to experimental data, and the line-by-line solution of Eq. 1.

4 Conclusions

Radiation transmission through n-heptane liquid pools has been modeled using three different solution methods implemented within the line by line spectral integration. The previously published spectrum of the incident flame radiation reaching the pool surface, and the spectral absorption coefficient of liquid n-heptane have been used in our simulations. The accuracy of the solution methods has been addressed by comparing them with the literature experimental results. The k-distribution method which has been widely used before for the radiation heat transfer in gaseous media, has been used, to our knowledge for the first time, to calculate transmittance within the liquid fuel. Using the results of the present spectral solutions, the problems of the previously used gray methods have been addressed.

Comparing the spectrally integrated predictions of the different solution methods with the available experimental data, we found out that the analytical E_3 solution for a 1D slab, Eq. 1, provides the best accuracy among the three studied methods. None of the gray solutions, with different ways of obtaining the mean absorption coefficients, showed good accuracy in the whole depth of the n-heptane pool while the present spectral LBL methods are constantly in a good agreement with the experimental data in the whole studied depth of 8 mm.

Implementing a k-distribution method to spectrally solve radiation transmission within the liquid layer significantly speeds up the computation with almost no loss

of accuracy, compared to the LBL solutions. The predictions of the k-distribution method were also in good agreement with the experimental data. Although the accuracy of the k-distribution method improves with increasing number of quadrature points, the predictions using as few as three points were found to be close to the LBL solution data. Hence, the coefficients of the three-point k-distribution method in Gauss-Chebyshev scheme have been tabulated for the use by other researchers. Three different quadrature schemes have been tested (G-L, G-C and T-Q) and all three showed quite the same level of accuracy. In addition, we found that for the k-distribution calculations, the spectral radiation incident from the flame can be approximated with a Planck distribution profile corresponding to typical temperatures. There is quite limited information found in literature for the flame spectrum reaching the surface of the pool and the absorption spectrum of the liquid fuel. It should be noted that the current results and the model parameters have been obtained with the current available spectral data of n-heptane. Obtaining and implementing higher resolution and more accurate experimental spectral data both for the flame intensity and the fuel absorption which is a part of our ongoing research can alter the reported model parameters and will improve the modeling capabilities.

The k-distribution model and the data presented in this paper can be used in overall CFD modeling of n-heptane pool fires. Through the improved radiation calculation, significant enhancement is expected in the accuracy of the evaporation modeling, thus paving the way towards fully predictive simulations of the liquid fuel fires. Testing this hypothesis and addressing the issues of the radiation passing through the gas-liquid interface form the objectives of our future work.

Acknowledgements

This work has been partially funded by the Academy of Finland under Grant No 314487 and the State Nuclear Waste Management Fund of Finland in the scope of the SAFIR-programs.

References

- [1] M. H. Bordbar, T. Hyppänen, "The Correlation Based Zonal Method and its Application to the Back Pass Channel of Oxy/Air-Fired CFB Boiler", *Applied Thermal Engineering*, 78 (2015) 351-365.
- [2] H. Bordbar, T. Hyppänen, "Line by line based band identification for non-gray gas modeling with a banded approach", Accepted to be published in IJHMT 2018, MS. No HMT16560.
- [3] M. H. Bordbar, G. Wećel, T. Hyppänen, "New Line by Line Based Weighted Sum of Gray Gases Model for Inhomogeneous CO₂-H₂O Mixture in Oxy-Fired Combustion", *Combustion and Flame* 161 (2014) 2435-2445.
- [4] D. Byun, S. W. Baek, "Numerical investigation of combustion with non-gray thermal radiation and soot formation effect in a liquid rocket engine", *International Journal of Heat and Mass Transfer* 50 (2007) 412-422.
- [5] D. Drysdale, "An Introduction to Fire Dynamics, 3rd ed.", 2011 John Wiley &

Sons, Ltd.

- [6] T. Sikanen, S. Hostikka, "Modeling and simulation of liquid pool fires with in-depth radiation absorption and heat transfer", *Fire Safety Journal* 80 (2016) 95-109.
- [7] T. Inamura, K. Saito and K. A. Tagavi, "A Study of Boilover in Liquid Pool Fires Supported on Water. Part II: Effects of In-depth Radiation Absorption", *Combustion Science and Technology*, 86 (1992) 105-119.
- [8] J. M. Suo-Anttila, T. K. Blanchat, A. J. Ricks, A. L. Brown, "Characterization of thermal radiation spectra in 2 m pool fires", *Proceedings of the Combustion Institute* 32 (2009) 2567-2574.
- [9] K. B. McGrattan, R. J. McDermott, C. G. Weinschenk, G. P. Forney, "Fire Dynamics Simulator, Technical Reference Guide, Sixth Edition", National Institute of Standards and Technology, 2013.
- [10] J. Gong, Y. Chen, J. Jiang, L. Yang and J. Li, "A numerical study of thermal degradation of polymers: Surface and in-depth absorption", *Applied Thermal Engineering* 106 (2016) 1366-1379.
- [11] M. Modest, H. Zhang, "The Full-Spectrum Correlated-k Distribution for Thermal Radiation From Molecular Gas-Particulate Mixtures", *Journal of Heat Transfer*, 124 (2002) 30-38.
- [12] A. Bansal, M. F. Modest and D. A. Levin, "Correlated-k Distribution Method for Atomic Radiation in Hypersonic Nonequilibrium flows", 47th AIAA Aerospace Sciences Meeting and Exhibit, 5-8 Jan 2009, Orlando, Florida.
- [13] M. F. Modest, R. S. Mehta, "Full spectrum k-distribution correlations for CO₂ from the CDSD-1000 spectroscopic databank", *International Journal of Heat and Mass Transfer* 47 (2004) 2487-2491.
- [14] H. Zhang, M. F. Modest, "Multi-group full spectrum k-distribution database for water vapor mixtures in radiative transfer calculations", *International Journal of Heat and Mass Transfer* 46 (2003) 3593-3603.
- [15] M. F. Modest, *Radiative Heat Transfer* 3rd ed., Elsevier Science, 2013, pp. 454-479 and 626-693.
- [16] J. Ma, B. Li, J. R. Howell, "Thermal radiation heat transfer in one- and two-dimensional enclosures using the spectral collocation method with full spectrum k-distribution model", *International Journal of Heat and Mass Transfer*, 71 (2014) 35-43.
- [17] A. Tuntomo, C. L. Tien, S. H. Park, "Optical constants of liquid hydrocarbon fuels", *Combustion Science and Technology*, 84 (1992) 133-140.
- [18] NIST Chemistry WebBook, SRD 69,
<https://webbook.nist.gov/cgi/cbook.cgi?JCAMP=C142825&Index=2&Type=IR> (6 Jul 2018).
- [19] J. Zhao, H. Huang, H. Wang, Z. Zhao, Q. Liu, Y. Li, "Experimental study on burning behaviors and thermal radiative penetration of thin-layer burning", *Journal of Thermal Analysis and Calorimetry* 130 (2017) 1153-1162.

- [20] A. Wang, M. F. Modest, "High-accuracy, compact database of narrow-band k-distributions for water vapor and carbon dioxide", *Journal of Quantitative Spectroscopy & Radiative Transfer* 93 (2005) 245–261.
- [21] C. Wang, W. Ge, M. F. Modest and B. He, "A full-spectrum k-distribution look-up table for radiative transfer in nonhomogeneous gaseous media", *Journal of Quantitative Spectroscopy and Radiative Transfer*, 168 (2016) 46-56.