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SENSITIVITY ANALYSIS FOR THE TEMPERATURE OF INCIDENT INTENSITY IN APPLYING FSCK METHOD FOR LIQUID FUELS

Farid Alinejad
Hadi Bordbar
Department of Civil Engineering, School of Engineering, Aalto University, Finland
farid.alinejadalmachovan@aalto.fi, hadi.bordbar@aalto.fi

Simo Hostikka
Department of Civil Engineering, School of Engineering, Aalto University, Finland
simo.hostikka@aalto.fi

Abstract. *In this paper, a sensitivity analysis is presented for the equivalent temperature of the incident intensity in applying the full spectrum correlated-k (FSCK) method for liquid fuels. Simulations have been done for radiation penetration within liquid heptane and toluene subjected to incident radiation with equivalent Planck temperature of 500-2000K. Presented relative difference between results of the simulations with and without considering liquid emission revealed the relative importance of the incident intensity and liquid emission for the considered equivalent temperatures. Liquid emission shows a considerable effect on the results for the equivalent Planck incident radiation up to 1300 K and 1400 K for heptane and toluene, respectively. With applying of the equivalent temperature of the incident intensity as the reference temperature in FSCK method, emission of the liquid is not correctly. However, this error does not have significant effect on the overall accuracy of FSCK calculation for the cases with high Planck temperatures of the incident intensity due to the lower relative importance of the liquid emission. However, for the cases subjected to low Planck incident intensity, the error of neglecting liquid emission is significant.*

Keywords: *Sensitivity analysis, liquid emission, FSCK method, reference temperature, radiation penetration within liquid fuels.*

1. INTRODUCTION

Due to the spectral behavior and directional dependency, thermal radiation is known as the most complex mode of the heat transfer. For estimation of the radiative heat source and heat flux within the participating media, radiative transfer equation (RTE) needs to be solved for whole spectrum and each direction. Radiative absorption and emission from the participating media depend on the absorption coefficient that drastically changes with wavelength. Hence, the RTE should be solved within a very small wavelength spectral intervals with constant absorption coefficient. However, solving RTE for a large number of intervals is computationally demanding. To solve this issue, different models such as weighted sum of gray gases (WSGG) model (Modest (1991);Bordbar *et al.* (2014)), spectral-line based sum of gray gases (SLW) (Sun and Zhang (2018);Solovjov *et al.* (2016)), and full spectrum k-distribution (FSK) method (Modest and Zhang (2000);Wang *et al.* (2019)) have been presented in the past years.

Most of these developments have been done for the gas phase as the main products of the combustion. However, in some applications like the pool fires and flame-droplet interaction within the fires and spray combustors, radiation penetration into the liquid phase should be considered. The main heat source for the evaporation in liquids that provides the needed fuel vapor for the combustion comes from the radiation (Hamins *et al.* (1994);Kim *et al.* (2019)). Therefore, modeling of the radiation heat transfer within the liquids may improve the overall simulation of heat and fluid flow of the systems. However, in modeling of evaporation, the liquid fuels have been conventionally considered as gray media and their radiation modeling has been done by solving RTE for an averaged value of the absorption coefficient that is called gray mean absorption coefficient (Sikanen and Hostikka (2016)). Due to some characteristics of the liquid fuels such as lower fluctuations of the absorption coefficient, lower temperatures, and strong absorption, it has been a common sense that spectral modeling of the thermal radiation transfer for them is not needed and using very simple methods such as gray method provides reasonable accuracy. However, some recent studies showed that by applying of gray methods, the radiative heat source and heat flux can not be estimated accurately. In one of the first attempts for the modeling of spectral thermal radiation transfer within the liquid fuels, Isojärvi *et al.* (2018) applied the k-distribution method for estimation of the transmissivity of the thermal radiation within the liquid heptane. In this study, the liquid emission was neglected

and the k-distribution using the incident intensity spectral profile for weighting the spectral absorption of the liquid. They showed that applying the gray method for liquid fuels results in a low accuracy in estimation of the transmissivity and applying the k-distribution method improves the results substantially even with lower numbers of quadrature points (QP).

Recently, the full spectrum correlated-k (FSCK) method has been developed for liquid fuels in our previous report (Alinejad *et al.* (2020)) and look-up tables were presented for five liquid fuels including decane, ethanol, ethylene glycol, heptane, and toluene. This paper improved the modeling of radiation penetration within the liquid fuels by including their emission into the RTE and providing the look-up tables that gives the needed coefficient at different local and reference temperatures. One of the most important results in that research was about the role of reference temperature. We showed that using the flame temperature or equivalent temperature of the incident intensity as the reference temperature in FSCK model gives the most accurate results for the simulation of the radiation heat transfer inside the liquids. In the present paper, the investigation of the role of reference temperature is further investigated. The radiation intensity at the boundary of the liquid layers in our previous work (Alinejad *et al.* (2020)) was selected as 1450K as experimentally measured as the flame temperature of heptane pool fire. However, in the present paper, we expand our investigations and will study how selecting the equivalent Planck temperature of the boundary incident as the reference temperature in FSCK will work for other flaming conditions from very low irradiation equivalent temperature to very large one, i.e. 300-2000K.

Applying large irradiation spectra in our previous study showed the negligible effect of the liquid emission within the simulations and one can conclude that neglecting liquid emission is a valid assumption for modeling the radiation transfer within the liquids. However, here we further assess this statement by considering various flame equivalent Planck temperatures for the incident radiation at the boundary of a liquid layer. This changes the relative size of the liquid emission compared to the radiation coming from the flame and therefore introduced the cases with various relative importance of the liquid emission. The sensitivity analysis of the present paper will provide an insight of importance of liquid emission and the conditions in which it can be safely ignored in FSCK calculations.

2. MODEL DESCRIPTION

Equations for the RTE and solution procedure in this paper are the same as Alinejad *et al.* (2020) and are briefly reviewed in following sections.

2.1 High-resolution method for solving spectral RTE

To calculate the radiative heat source within the liquid fuel, RTE should be solved for each fine enough spectral interval in different directions. To account for the direction of the intensity, two-flux method has been selected due to its simplicity of the calculations. Nonetheless, the results of the investigations are equally valid for more complex directional RTE solvers such as discrete ordinates (DO) and finite volume methods (FVM). RTE for the forward direction is written as:

$$\frac{1}{2}\frac{dI_\lambda^+}{dx} = \kappa_\lambda(I_{b\lambda} - I_\lambda^+) \tag{1}$$

In above equation, λ, I_λ^+, $I_{b\lambda}$ x, and κ_λ are wavelength, spectral forward intensity, blackbody intensity, path length, and spectral absorption coefficient, respectively. RTE for the backward direction is written in the similar way. To numerically solve the Eq. 1, the whole spectrum should be divided into very narrow intervals within which the absorption coefficient can be considered constant. We call this method as high-resolution method and its results have been applied as benchmark in this paper. After calculation of the intensity for each wavelength in forward and backward directions, the spectral heat flux for forward and backward directions is obtained by applying the $(\dot{q}_\lambda'')^+ = \pi I_\lambda^+$ and $(\dot{q}_\lambda'')^- = \pi I_\lambda^-$ respectively. Using the spectral heat flux, the spectral heat source is obtained from the following equation:

$$\dot{q}_\lambda''' = \frac{d(\dot{q}_\lambda'')^+}{dx} + \frac{d(\dot{q}_\lambda'')^-}{dx} \tag{2}$$

Then, the total heat flux is calculated from:

$$\dot{q}''' = \int_0^\infty \dot{q}_\lambda''' d\lambda \tag{3}$$

Similarly, the total heat flux for forward direction is obtained as:

$$(\dot{q}'')^+ = \int_0^\infty (\dot{q}_\lambda'')^+ d\lambda \tag{4}$$

Total heat flux for the backward direction is calculated in a similar way. Finally, transmissivity can be obtained from the following equation:

$$\tau = \frac{(\dot{q}'')^+}{\dot{q}_{in}''} \tag{5}$$

In above equation, $\dot{q}''_{in}$ is the incident heat flux from the upper wall which for instance represents the liquid pool surface in pool fire scenario.

2.2 Full spectrum correlated-k distribution (FSCK) method

One of the popular global methods for modeling the radiation transfer is the FSCK method. Due to high fluctuation of the absorption coefficient spectrum, in high-resolution method, solving of the RTE is done for a same value of absorption coefficient several times resulting high computational time. To avoid this repetition and decreasing the simulation time, FSCK method by using the weights, reorders the wavelengths and transforms it into a monotonically increasing function. For doing this reordering, a k-distribution is defined using the following equation (Modest and Zhang (2000)):

$$f(T,k) = \frac{1}{I_b}\int_0^\infty I_{b\lambda}\delta(k-\kappa_\lambda)d\lambda \tag{6}$$

where, I_b, k, and δ are total blackbody intensity, considered k-distribution, and delta function, respectively. Above equation uses the blackbody intensity for determining a weight for different wavelengths. By multiplying the both sides of the Eq. 1 with applied delta function in Eq. 6 and integrating for whole spectrum, following equation is achieved:

$$\frac{1}{2}\frac{dI_k^+}{dx} = kf(T,k)I_b - kI_k^+ \tag{7}$$

In above equation, I_k^+ is defined with:

$$I_k^+ = \int_0^\infty I_\lambda^+\delta(k-\kappa_\lambda)d\lambda \tag{8}$$

For the extremum points of the absorption coefficient, $f(T,k)$ goes to infinity. Therefore, working with this function is not easy in solving the RTE. Hence, a cumulative form of the k-distribution is applied that produces a monotonically increasing function with reordered wavelength. This function is defined with following equation:

$$g(T,k) = \int_0^k f(T,k)dk \tag{9}$$

In above equation, $g(T,k)$ is called cumulative k-distribution function and defines a new space for describing the radiative intensity through the following equation:

$$\frac{1}{2}\frac{dI_g^+}{dx} = k^*(T_{ref},g_{ref})(a(T,T_{ref},g_{ref})I_b - I_g^+) \tag{10}$$

where, subscript ref shows the reference state and I_g^+ and k^* are the forward intensity in the g space and the correlated-k distribution, respectively. Equation 10 was derived by dividing both sides of the Eq. 7 to a k-distribution function in a constant temperature. This constant temperature called reference temperature that can be different from the temperature of the medium. In Eq. 10, I_g^+ is defined by:

$$I_g^+ = \frac{I_k^+}{f(T,k)} \tag{11}$$

and $a(T,T_{ref},g_{ref})$ is defined by the following equation:

$$a(T,T_{ref},g_{ref}) = \frac{f(T,k)}{f(T_{ref},k)} = \frac{dg(T,k)}{dg_{ref}(T_{ref},k)} \tag{12}$$

In Eq. 10, $a(T,T_{ref},g_{ref})$ establishes a correlation between k-distributions of the local and reference temperatures. For the same local and reference temperature, this parameter equals unity and therefore is vanished from the RTE. According to the presented results by Alinejad *et al.* (2020) using the flame temperature or equivalent temperature of the incident intensity as the reference temperature gives the highest accuracy where FSCK is applied to a liquid layer. Therefore, in all the simulations using the FSCK method in this paper, the reference temperature is the temperature of the upper wall. After calculation of the intensity from the Eq. 10, total intensity for the forward direction is obtained from the following equation:

$$I^+ = \int_0^1 I_g^+ dg \tag{13}$$

For solving the above integral, Gauss-Chebyshev quadrature method is used with an appropriate number of QP. In this paper, the solutions are presented for the 7 QP as optimal number of QP and 32 QP as the size of the reported look-up tables in Alinejad *et al.* (2020).

2.3 Boundary conditions

For the high-resolution method, boundary condition for the upper wall is described using the following equation:

$$I_{\lambda}^{+} = \varepsilon_{wu}\varepsilon_{flame}I_{b\lambda}(T_{wu}) + \frac{1-\varepsilon_{wu}}{\pi}\int_{2\pi} I_{\lambda}^{-}|\hat{n}.\hat{s}|d\Omega \tag{14}$$

Boundary condition for the backward direction has the similar equation. In above equation, I_{λ}^{-}, ε_{wu}, ε_{flame}, T_{wu}, $\hat{n}$, $\hat{s}$, and Ω are the backward spectral intensity, emissivity of the upper wall, emissivity of the flame, temperature of the upper wall, unit normal vector of the surface, direction vector, and solid angle, respectively.

For the RTE of the FSCK method, the boundary condition for the upper wall is described as:

$$I_{g}^{+} = \varepsilon_{wu}\varepsilon_{flame}I_{b}(T_{wu}) + \frac{1-\varepsilon_{wu}}{\pi}\int_{2\pi} I_{g}^{-}|\hat{n}.\hat{s}|d\Omega \tag{15}$$

In above equation, I_{g}^{-} is the backward intensity in the g space. For the backward direction, the boundary condition is:

$$I_{g}^{-} = \varepsilon_{wb}a(T_{wb}, T_{ref}, g_{ref})I_{b}(T_{wb}) + \frac{1-\varepsilon_{wb}}{\pi}\int_{2\pi} I_{g}^{+}|\hat{n}.\hat{s}|d\Omega \tag{16}$$

where, ε_{wb} and T_{wb} are the emissivity and temperature of the bottom wall respectively. The difference between Eq. 15 and Eq. 16 is the appearance of the $a(T_{wb}, T_{ref}, g_{ref})$ in the boundary condition of the backward radiation. Due to applying the temperature of the upper wall as reference temperature, $a(T_{wb}, T_{ref}, g_{ref})$ is vanished from the boundary condition of the forward direction.

3. GEOMETRY AND CONSIDERED CASE STUDIES

Analysis of this paper have been done for the same geometry as one used by Alinejad *et al.* (2020) and is shown in Fig. 1. A one-dimensional 8 mm layer of liquid fuel has been considered between two walls with constant temperature and diffused emissivity. For different liquid fuels, Suo-Anttila *et al.* (2009) measured the arrived radiative heat flux to the surface of the liquid and showed that this heat flux can be approximated by the blackbody radiation at 1450 K with emissivity of 0.4. In the considered geometry in this paper, upper wall presents the flame condition for the pool fires and according to the reported results by Suo-Anttila *et al.* (2009), an emissivity of 0.4 has been assumed for the incoming thermal radiation from the flame. This emissivity is different from the defined emissivity of the upper wall in Eq. 14 and Eq. 15. Upper wall has been considered to be the black wall, therefore its emissivity is equal to 1.

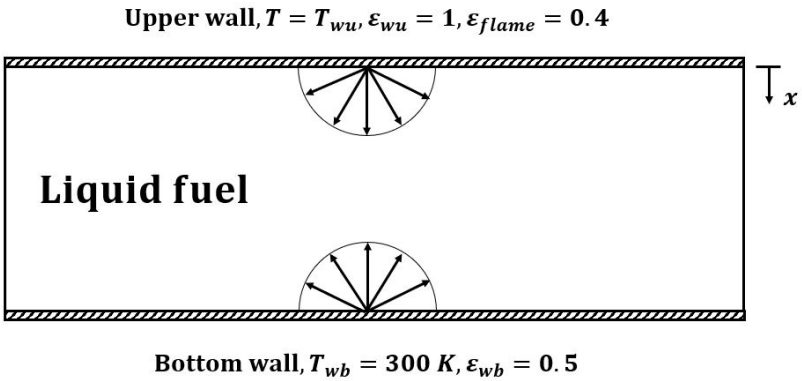

Figure 1. Considered geometry for the liquid fuels.

In this paper, using the reported experimental data (Inamura *et al.* (1992);Vali *et al.* (2015)), a nonlinear temperature profile for the liquid heptane and toluene have been assumed according to the shown diagrams in Fig. 2. Equations of the nonlinear temperature profiles in Fig. 2 has been given in the Tab. 1.

Table 1. Applied nonlinear temperature profiles for the liquid fuels.

$T(x) = a.exp(-\frac{b(x-x_0)}{s}) - c.exp(-\frac{d(x-x_0)}{s})$						
Fuel	a	b	c	d	x_0	s
Heptane	373.3	0.1519	6.496	2.5	0.002938	0.003526
Toluene	449.3	0.2466	69.75	1.055	0.002938	0.003526

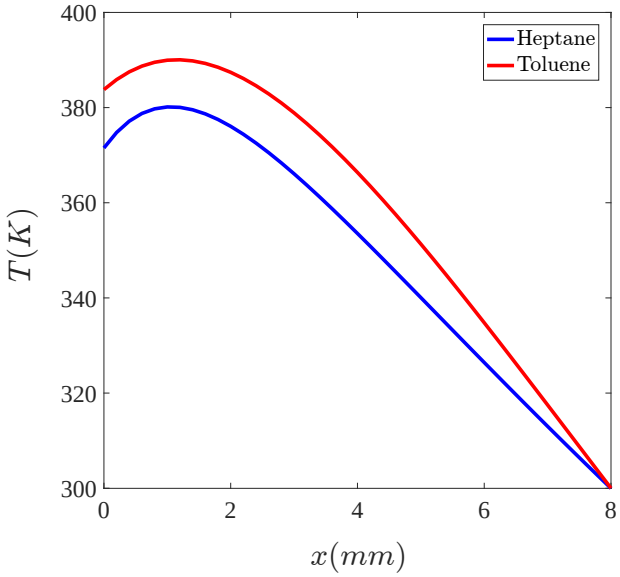

Figure 2. Assumed temperature profiles for the liquid fuels.

To solve the RTE with high-resolution method, the absorption coefficients of the considered liquid fuels and for simulation with FSCK method, the data of look-up table for the k^* and a should be known. These information have been given in Alinejad *et al.* (2020).

4. RESULTS AND DISCUSSIONS

Due to the strong absorption of the liquid fuels, most part of the incident intensity is absorbed within a thin layer (e.g. a few millimeters) of the liquid under the surface. For calculation of the radiative heat source within liquid, this part of the liquid has higher importance. Therefore, weighted arithmetic mean is applied for calculation of the relative error of the simulations to give higher weight to the very first layer of the liquid under the surface. According to the weighted arithmetic mean, averaged relative error for the heat source is calculated using the following equation:

$$\text{Relative error of } \dot{q}''' = \sum_{i=1}^{n} w_i \frac{|\dot{q}'''_{\text{HR},i} - \dot{q}'''_{\text{FSCK},i}|}{|\dot{q}'''_{\text{HR},i}|} \times 100 \tag{17}$$

In above equation, subscript HR stands for the high-resolution method and w_i is the weighting parameter and is calculated by:

$$w_i = \frac{|\dot{q}'''_{\text{HR},i}|}{\sum_{i=1}^{n} |\dot{q}'''_{\text{HR},i}|} \tag{18}$$

Similarly, the averaged relative error for the transmissivity is calculated using the following equation:

$$\text{Relative error of } \tau = \sum_{i=1}^{n} w_i \frac{|\tau_{\text{HR},i} - \tau_{\text{FSCK},i}|}{\tau_{\text{HR},i}} \times 100 \tag{19}$$

The weighting parameter in above equation is calculated by applying the forward heat fluxes in:

$$w_i = \frac{(\dot{q}''_{\text{HR},i})^+}{\sum_{i=1}^{n} (\dot{q}''_{\text{HR},i})^+} \tag{20}$$

To address the relative importance of the liquid emission, the value of the liquid emission in high-resolution calculations sets to zero. Then, its results are compared with the result of high-resolution method with considering of the liquid emission and the difference has been reported in the form of averaged relative difference. Similar to radiative heat source and transmissivity, averaged relative difference has been calculated using the weighted arithmetic mean. Results have been presented in Fig. 3.

As seen in Fig. 3, it is clear that liquid emission has sensible effect for boundary temperatures up to 1300 K and 1400 K for heptane and toluene, respectively. Therefore, the estimation of the liquid emission using the FSCK method affects the accuracy of the simulations. To investigate the sensitivity of the results to equivalent temperature of the incident intensity, simulations have been done for FSCK and high-resolution methods and the averaged relative errors for these

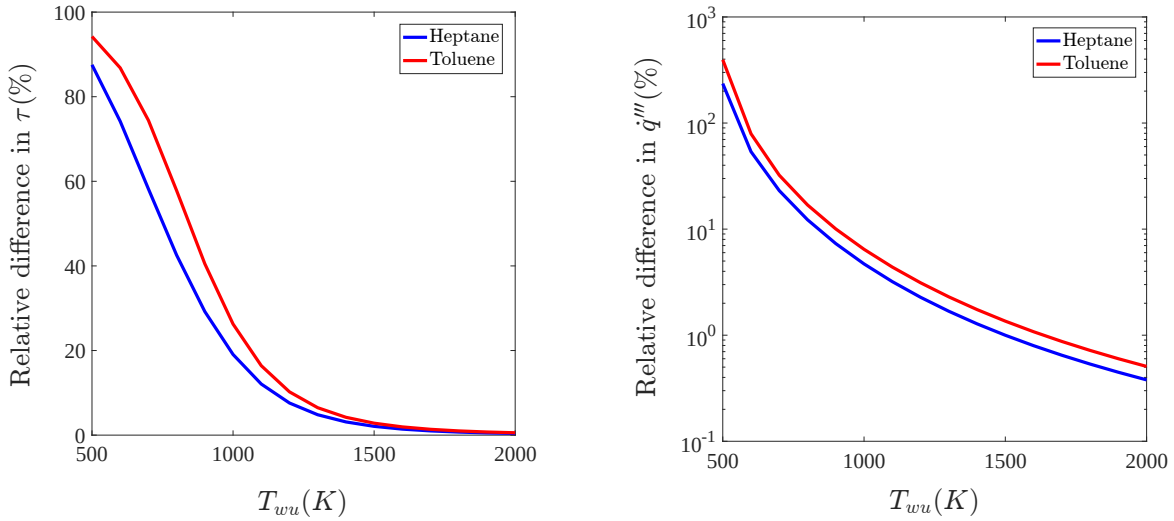

Figure 3. Averaged relative difference between the results of two simulations using HR method with and without considering liquid emission for transmissivity (left) and radiative heat source (right) for various temperature of boundary temperature.

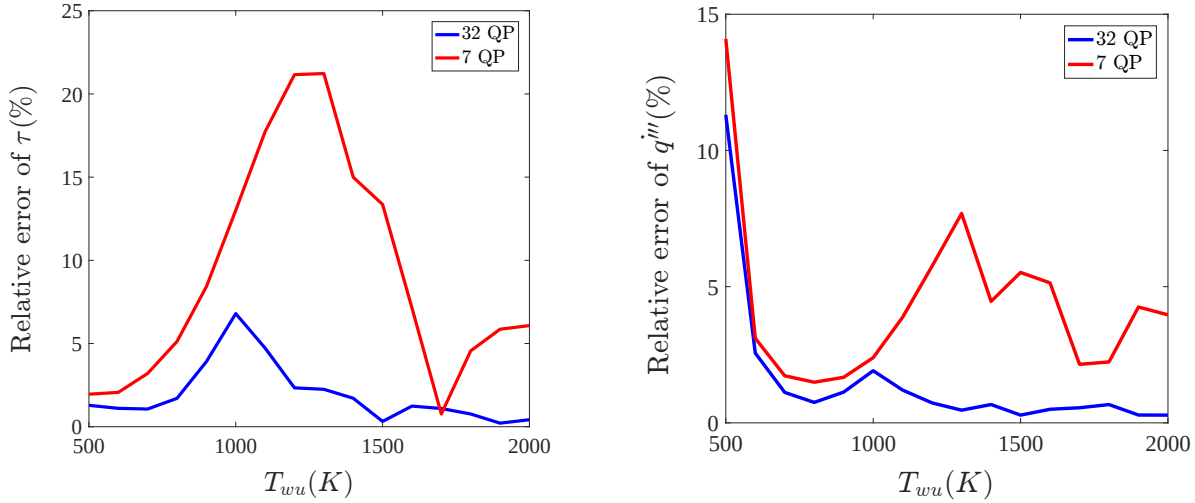

Figure 4. Averaged relative error in estimation of the transmisivity (left) and radiative heat source (right) of the liquid heptane using 7 and 32 QP in FSCK method.

calculations have been shown in Fig. 4. Simulations have been done for the equivalent temperature of incident radiation at the boundary in the range of 500 K to 2000 K with step of 100 K.

Results in Fig. 4 show that the error for lower boundary temperatures is higher. In addition, there are some peaks in the diagrams that are related to the strong absorption of the liquid in that temperatures. Strong absorption alters the shape of the intensity spectrum and causes an error in applying of FSCK method. Higher error for the lower temperatures shows that liquid emission was not estimated accurately by FSCK method when boundary temperature has been used as the reference temperature. For low temperatures of the incident intensity, the relative importance of the liquid emission is higher, therefore its estimation causes considerable effect on the accuracy of the simulations by FSCK method. Figure 5 shows normalized blackbody intensity at 500 K as the equivalent temperature for the incident intensity and 352 K as the volume-averaged temperature of the liquid heptane. The two intensity profiles have different correspondency with the absorption spectrum of the liquid. Therefore, their k-distributions are not same and using the equivalent temperature of the incident intensity as reference temperature can not accurately estimate the liquid emission.

The averaged relative error of the radiative heat source and transmissivity for toluene has been shown in Fig. 6. For toluene, the simulations have been done using the same conditions as liquid heptane. Results show a good accuracy in applying of the FSCK method for different temperature of the incident intensity.

Similar to heptane, the error is higher when low temperatures were used as equivalent temperature of the incident intensity. There are also some peaks in the diagrams that are due to the strong absorption of the liquid. To explain the inaccuracy seen in low equivalent temperatures of the incident intensity, the given explanations for heptane is valid for

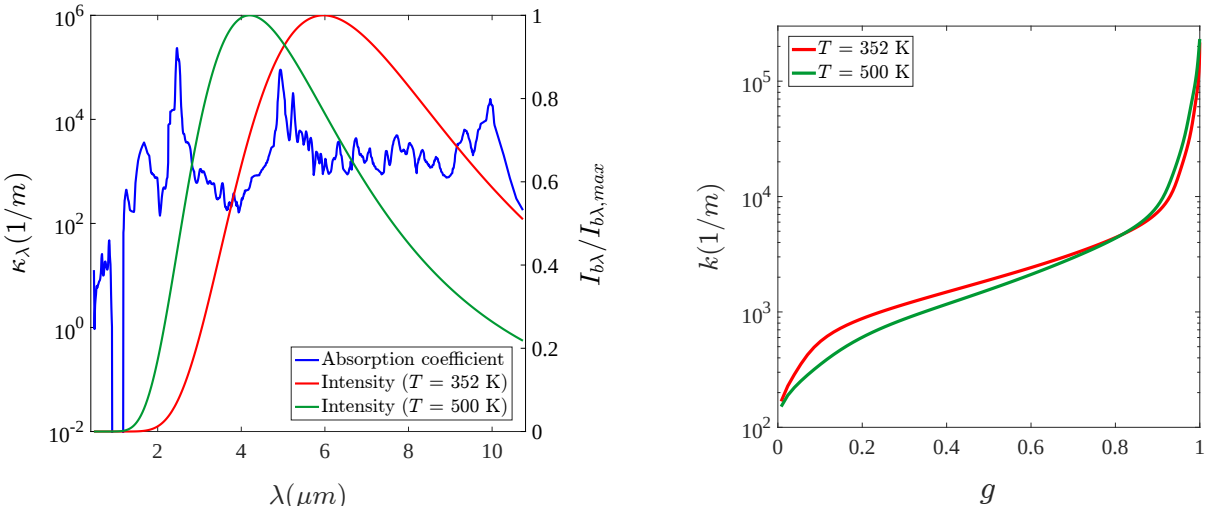

Figure 5. Spectrum of the intensity and absorption coefficient for the liquid heptane (left) and k-distributions in two different temperatures (right).

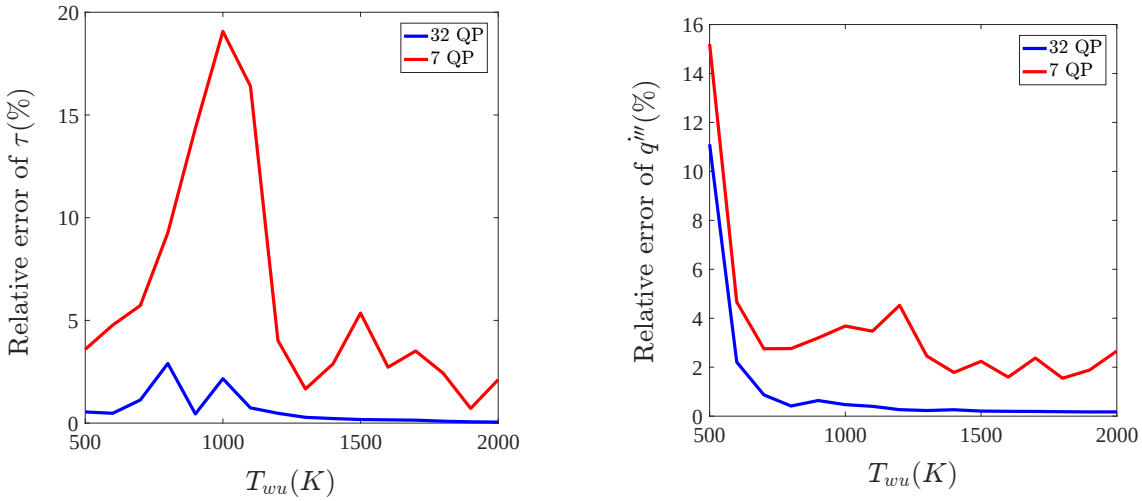

Figure 6. Averaged relative error in estimation of the transmisivity (left) and radiative heat source (right) of the liquid toluene.

toluene, as well. Figure 7 shows the Planck intensity profiles of the temperatures of 500 K as the temperature of incident intensity at the boundary and 362 K as volume-averaged temperature of the liquid. The differences in correspondences to the absorption coefficient spectra causes a small difference in the k-distributions of the two temperatures. This difference in k-distribution that is shown in the logarithmic scale in Fig. 7 causes the inaccuracy seen in the cases with error for low boundary temperatures.

The presented results in this paper are for the liquid heptane and toluene that have relatively low boiling temperature. For the other liquid fuels with higher boiling temperature like ethylene glycol and decane, the inaccuracy of FSCK when using the boundary temperature as the reference temperature is seen even in the cases with larger boundary temperature. In addition, the flame emissivity considered at the upper wall is given for the direct flame which means that it represents the upper bound for the flame emissivity as reported in Suo-Anttila *et al.* (2009). Using this value of emissivity overestimates the penetrated thermal radiation from the flame into the liquid fuel due to the neglecting of the fuel surface reflectivity. In addition, for other conditions, such as receiving radiation from other sources or radiation from inclined flames, a view factor should be considered together with the flame emissivity that reduces the amount of the penetrated incident intensity into the liquid fuels. Therefore, the relative importance of the incident intensity will be reduced that enhances the effect of the liquid emission in different temperatures.

5. CONCLUSION

In this paper, a sensitivity analysis has been performed for the different equivalent temperatures of the incident intensity in range of 500 K to 2000 K as the reference temperature in FSCK method for liquid fuels. Relative difference between the

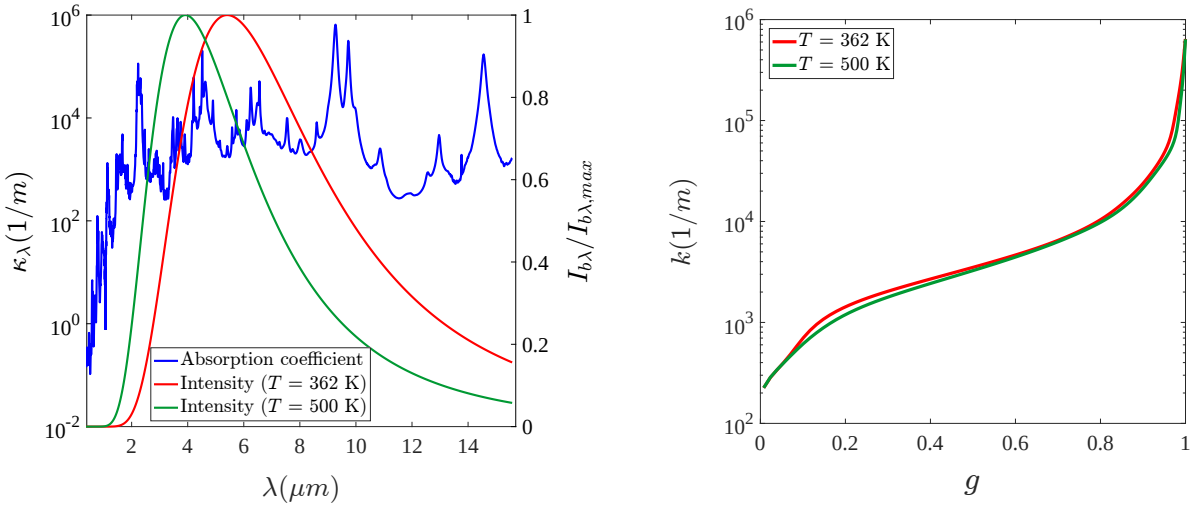

Figure 7. Spectrum of the intensity and absorption coefficient for the liquid toluene (left) and k-distributions in two different temperatures (right).

results of the simulations with and without considering liquid emission showed that liquid emission for the temperatures up to 1300 K and 1400 K has considerable effect. For the FSCK method, simulations have been done for liquid heptane and toluene with using of 32 QP and 7 QP. The results were shown in the form of averaged relative error for the radiative heat source and transmissivity. The results showed that FSCK method is accurate for different temperature of the incident intensity. Applying of the equivalent temperature of the incident intensity as reference temperature causes an error in estimation of the liquid emission. Due to the high relative importance of the liquid emission in low temperatures, this error has significant effect on the total accuracy of the simulation. The role of liquid emission is more highlighted when the incident radiation reaching the liquid surface is weak either due to a weak source or view factor.

6. ACKNOWLEDGEMENTS

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