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

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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.

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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

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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 (kW/m^2/μm/sr)
I_0^+	spectral intensity (kW/m^2/μm/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 (kW/m^2/μm)
q_0^+	spectral heat flux (kW/m^2/μm)
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

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 [11–14]. 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 radiative transfer equation for intensity $I(s,\mu)$ in the layer of non-scattering liquid is

$$\mu\frac{dI(s,\mu)}{ds} = -\kappa I(s,\mu) \tag{1}$$

where $\mu \equiv \cos(\theta)$ and θ is the angle between the beam direction and the surface normal. The inward flux at depth s in liquid can, in principle, be calculated as a plane-parallel integral of Eq. (1) using the incoming flux as a boundary condition [15]

$$q^+(s) = 2\int_0^\infty q_0^+(\lambda)E_3(\kappa(\lambda)s)d\lambda \tag{2}$$

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 the exponential decay of intensity I^+ in a direction perpendicular to the pool surface.

$$I^+(s) = \int_0^\infty I_0^+(\lambda)\exp(-\kappa(\lambda)s)d\lambda \tag{3}$$

The two flux method (or the Schuster–Schwarzschild approximation) is a very simple form of a discrete ordinates methods [15]. In this method, the intensity is assumed to be constant over the hemispheres covering forward ($I = I^+$) or backward ($I = I^-$) solid angles, and thus only a function of position s. Integrating Eq. (1) over the forward solid angle $\mu > 0$ leads to

$$\frac{dI^+(s)}{ds}\underbrace{\int_0^1 \mu d\mu}_{=1/2} = -\kappa I^+(s)\underbrace{\int_0^1 d\mu}_{=1} \tag{4}$$

Integrating Eq. (4) over s gives us the following equation for the heat flux at depth s and also Eq. (12) for transmittance

$$q^+(s) = \int_0^\infty q_0^+(\lambda)\exp(-2\kappa(\lambda)s)d\lambda \tag{5}$$

Effectively, the absorption coefficient of the two-flux method is multiplied by factor two in comparison to Lambert–Beer law.

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. (2)–(5) 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

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