Applied Thermal Engineering 104 (2016) 497–503

Contents lists available at ScienceDirect

Applied Thermal Engineering

journal homepage: www.elsevier.com/locate/apthermeng

Research Paper

Transient heating and evaporation of moving mono-component liquid fuel droplets

Chungen Yin

Department of Energy Technology, Aalborg University, 9220 Aalborg East, Denmark

HIGHLIGHTS

- A droplet evaporation model addressing internal heat/mass transfer is developed.
- The model is developed in a generic 3D framework and presented in a repeatable way.
- The code is validated by evaporation data of n-Heptane and n-Decane droplets.
- The model can be readily and reliably extended for more generic applications.

ARTICLE INFO

Article history:
Received 11 December 2015
Revised 12 April 2016
Accepted 17 May 2016
Available online 17 May 2016

Keywords:
Heating
Evaporation
n-Heptane
n-Decane
Generic model

ABSTRACT

This paper presents a complete description of a model for transient heating and evaporation of moving mono-component liquid fuel droplets. The model mainly consists of gas phase heat and mass transfer analysis, liquid phase analysis, and droplet dynamics analysis, which address the interaction between the moving droplets and free-stream flow, the flow and heat and mass transfer within the droplets, and the droplet dynamics and size, respectively. For the liquid phase analysis, the droplets are discretized into a number of control volumes along the radial, polar and azimuthal directions, on each of which the flow and energy transport equations are numerically solved using the finite volume method. The computer code for the model is developed in a generic 3D framework and verified in different ways (e.g., by comparison against analytical solutions for simplified cases, and against experimental or modelling results of heating and evaporation of n-Heptane and n-Decane droplets in literature), so that the model can be readily and reliably extended to more generic applications (e.g., heating and evaporation of multi-component liquid fuel droplets, thermochemical conversion of commercially available biomass pellets).

1. Introduction

The transient heating and evaporation of spray droplets in turbulent two-phase flows is important for many engineering applications, e.g., internal combustion engines, spray drying, fire suppression, and reliable testing and modelling of droplet heating and evaporation is essential to these applications. Great efforts have been successfully made in this regard [1–12]. Many results have been published including a number of widely known monographs and review papers, as comprehensively reviewed in [1].

Models of droplet heating and evaporation can be classified into six groups in the order of increasing complexity: (1) models based on assumption that the droplet surface temperature is uniform and does not change with time, (2) models based on assumption that there is no temperature gradient inside droplet (infinite thermal conductivity of liquid), (3) models taking into account finite liquid thermal conductivity, but not the flow recirculation inside droplet (conduction limit), (4) models taking into account both finite liquid thermal conductivity and the recirculation inside droplets via introduction of a correction factor to the liquid thermal conductivity (effective conductivity models), (5) models describing the recirculation inside droplets in terms of vortex dynamics (vortex models), and (6) models based on the full solution of the Navier–Stokes equation.

The importance of accounting for the impacts of finite thermal conductivity and internal recirculation in the droplets has been generally accepted by the engineering community. Models of group 4, i.e., effective conductivity models, show great advantages over other groups of models, in terms of both the accuracy and computational efficiency required by computational fluid dynamics (CFD) modelling. The effective conductivity models employ an effective, liquid Peclet number-dependent thermal conductivity,

E-mail address: chy@et.aau.dk

http://dx.doi.org/10.1016/j.applthermaleng.2016.05.098
1359-4311/

instead of the actual liquid thermal conductivity, and can correctly predict the average droplet surface temperature which is the most important parameter in many practical applications [1].

This study is a part of a European Union's Seventh Framework Programme (FP7)-funded project which aims at producing the 2nd generation bio-oil from biomass and wastes based on a microwave-assisted catalytic pyrolysis technology and upgrading the bio-oil for utilization in transportation and for the production of lubricants [13]. Among the various tasks of different partners (e.g., production and characterization of the raw bio-oil, dewatering of the raw bio-oil, refining of the dewatered bio-oil), testing and modelling of atomization, evaporation and combustion of the refined bio-oil will be performed. Thermochemical conversion of the biomass pellets in the microwave-assisted pyrolysis reactor is also one of the key issues. This paper presents the effort towards a generic model for heating and evaporation of single droplets of the refined bio-oil. A kind of vortex model (group 5) for the transient heating and evaporation of moving mono-component liquid droplets is developed first, which mainly consists of gas phase heat and mass transfer analysis, liquid phase analysis, and droplet dynamics analysis. The model is developed in a generic 3D framework and validated in various ways, so that it can be readily and reliably extended to predict the heating and evaporation of the multi-component pyrolysis bio-oil droplets as the next step.

2. Modelling approach

The droplet heating and evaporation model is based on the two commonly used assumptions. One is that the droplet retains its spherical form even in the process of its movement. The other is that the temperature over the entire droplet surface is the same (although it varies with time), which is expected to be a good approximation in the case of a stationary or very fast moving droplet [2]. In the intermediate conditions, the uniform droplet surface temperature assumption is also acceptable, without producing any remarkable errors [1]. Among the references on modelling of droplet heating and evaporation [1,2,4–6,8–10], the modelling works in [2,5,6,8] make the backbone to formulate the model description here. It has to be mentioned that a lot of inconsistencies exist in the literature, due to the fact that there are many different models to evaluate the external heat and mass transfer and to address the internal recirculation and heat and mass transfer. The model description below integrates not only the key findings in the literature bus also theoretical derivation and comparison, in order to secure a clear, reliable and repeatable model formulation and structure.

Given all the parameters of the free-stream flow and droplet at time t, the droplet parameters at the next time ($t + \Delta t$) can be evaluated by the three sub-models (i.e., gas phase heat and mass transfer analysis, liquid phase analysis, and droplet dynamics analysis) in the following steps.

1. Based on the droplet surface temperature T_s from the initial condition or from the previous solution, the molar and mass fraction of the fuel vapor at the droplet surface χ_{Fs} and Y_{Fs} can be evaluated.

$$\chi_{Fs} = P_{\mathrm{sat}}(T_s)/P_\infty \tag{1}$$

$$Y_{Fs} = \frac{\chi_{Fs}\mathrm{MW}_F}{\chi_{Fs}\mathrm{MW}_F + (1-\chi_{Fs})\mathrm{MW}_{\mathrm{air}}} \tag{2}$$

where $P_{\mathrm{sat}}(T_s)$, P_∞, MW_F and $\mathrm{MW}_{\mathrm{air}}$ represent the saturated fuel vapor pressure evaluated at droplet surface temperature, free-stream flow pressure, molecular weight of fuel vapor and air, respectively.

2. Calculate the average physical properties of the fuel vapor/air mixture in the gas film around the droplet, i.e., density ρ_g [kg/m^3], thermal conductivity λ_g [W/(m K)], specific heat $C_{p,g}$ [J/(kg K)], binary diffusion coefficient D_g [m^2/s], dynamic viscosity μ_g [kg/(m s)], Prandtl number $Pr = C_{p,g}\mu_g/\lambda_g$, Schmidt number $Sc = \mu_g/(\rho_g D_g)$, and Lewis number $Le = Sc/Pr$, based on the '1/3 rule' reference conditions (T_{ref}, $Y_{j,\mathrm{ref}}$).

$$T_{\mathrm{ref}} = T_s + \frac{1}{3}(T_\infty - T_s) \tag{3}$$

$$Y_{j,\mathrm{ref}} = Y_{j,s} + \frac{1}{3}(Y_{j,\infty} - Y_{j,s}) \tag{4}$$

in which T_∞, $Y_{j,\infty}$ and $Y_{j,s}$ denote the free-stream flow temperature, mass fraction of gas/vapor species j in the free stream and at the droplet surface, respectively. Fuel-vapor specific heat $C_{p,F}$ [J/(kg K)] is calculated also based on the reference temperature, since $C_{p,F}(T_\infty - T_s)$ represents the thermal energy required to heat up the fuel vapor leaving the droplet surface to the ambient temperature.

3. Calculate the Reynolds number (Re) based on the viscosity of the fuel vapor/air in the gas film (μ_g) and the free-stream density (ρ_∞) since it is interpreted as a ratio of inertia to viscous forces, and then the drag coefficient (C_D) and the Nusselt and Sherwood numbers for a non-vaporizing droplet ($Nu_0$and Sh_0),

$$Re = \rho_\infty \cdot U_{\mathrm{rel}} \cdot 2R_d/\mu_g \tag{5}$$

$$C_D = \max\left(\frac{24}{Re}\left(1 + \frac{Re^{2/3}}{6}\right), 0.424\right) \tag{6}$$

$$Nu_0 = 1 + (1 + RePr)^{1/3}\max(1, Re^{0.077}) \tag{7}$$

$$Sh_0 = 1 + (1 + ReSc)^{1/3}\max(1, Re^{0.077}) \tag{8}$$

where R_d is the droplet diameter and U_{rel} is the relative velocity calculated from the free-stream gas velocity ($\mathbf{u}_g$) and droplet velocity ($\mathbf{v}_d$) as $U_{\mathrm{rel}} = |\mathbf{u}_g - \mathbf{v}_d|$.

4. Calculate the Spalding mass transfer number B_M, diffusion film thickness correction factor F_M (due to Stefan flow effect), the 'modified' Sherwood number Sh^* by accounting for the Stefan flow effect, the actual Sherwood number of the refined model Sh, and the mass vaporization rate from the droplet surface $\dot{m}$ [kg/s].

$$B_M = (Y_{Fs} - Y_{F\infty})/(1 - Y_{Fs}) \tag{9}$$

$$F_M = (1 + B_M)^{0.7}/B_M \cdot \ln(1 + B_M) \tag{10}$$

$$Sh^* = 2 + (Sh_0 - 2)/F_M \tag{11}$$

$$Sh = Sh^*/B_M \cdot \ln(1 + B_M) \tag{12}$$

$$\dot{m} = 2\pi\rho_g R_d D_g \cdot Sh^* \cdot \ln(1 + B_M) = 2\pi\rho_g R_d D_g \cdot Sh \cdot B_M \tag{13}$$

where $Y_{F\infty}$ is mass fraction of fuel vapor in the free stream and D_g is binary diffusion coefficient evaluated at T_{ref} and $P_{ref} = P_\infty$.

5. Calculate the correction factor for the thermal film thickness, $F_T = F(B_T)$, using the value of the Spalding heat transfer number from the previous iteration ($B_T = B_T^{old}$). As an initial estimate at beginning of each time-step, the final value of B_T from the previous time-step can be used.

$$F_T = (1 + B_T)^{0.7}/B_T \cdot \ln(1 + B_T) \tag{14}$$

6. Calculate the 'modified' Nusselt number Nu^*, parameter φ, and the corrected value of the Spalding heat transfer number B_T,

$$Nu^* = 2 + (Nu_0 - 2)/F_T \tag{15}$$

$$\varphi = (C_{p,F}/C_{p,g})(Sh^*/Nu^*)/Le \tag{16}$$

$$B_T = (1 + B_M)^\varphi - 1 \tag{17}$$

Return to Step (5) if $|B_T - B_T^{old}| > \varepsilon_B$, where ε_B is the desired accuracy of the calculation of B_T. In the present study, a few iterations were usually sufficient to achieve the required accuracy of $\varepsilon_B = 10^{-4}$.