A NON-EQUILIBRIUM MONO-COMPONENT EVAPORATION MODEL FOR HEATING AND EVAPORATION OF ALKYL ALCOHOLS

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Abstract - Droplet heating and evaporation is a phenomenon which has become an indispensable part of industry and technology such as evaporative cooling, fuel combustion, spray drying and it is also important to cloud physics, pre-mixing of air-fuel, pollution control, nanofabrication etc. Evaporation is an unsteady problem, associated with both mass and heat transportation. The present analytical work focuses on the modelling of heating evaporation of a single component droplet, for different types of fuel like ethanol, propanol, methanol. A non-equilibrium Langmuir-Knudsen model for a mono-component droplet at rest is developed to obtain several evaporation parameters. The intentness of droplet interior is considered as identical throughout its area. The evaporation model has been extensively studied and suitably implemented into a CFD code, in order to compute the evaporation process of a mono-component droplet. This comprehensive work, undertaken highlights the comparison of the evaporation characteristics among ethanol, propanol, methanol and we have observed some interesting phenomenon in our result.

Keywords - Langmuir-Knudsen Model, Single-Component Droplet, Evaporation, Knudsen Layer, Non-Equilibrium

I. INTRODUCTION

The theoretical analysis of spherical fuel droplet evaporation has been intensively studied since the past few decades [1]. The prediction of evaporation rate of liquid droplet is a scientific approach, especially in mechanical engineering application under high pressure and temperature [2]. It has a wide range of uses in industrial applications majorly in the field of thermal science, Fire suppression, automobile, spray combustion, turbines and space engineering [3]. Spray cooling technology involving water and certain additives is becoming very renowned in the steel industry which provides large scope for research in this particular field. There are lot of models available but the accurate prediction of vaporization characteristics such as geometryor position for a single or multicomponent fuel droplet is also significantly depends on selected model [4]. This current work is conducted assuming the droplet is stationery and unit Lewis number in the gas phase. The forced convectional effect near the droplet is taken into account with the help of Nusselt number and some other physical properties are neglected also. Adequate description of the heat transfer at the boundary of the liquid droplet is the most important part of the evaporation model. The molecular velocity in Knudsen layer, which is adjacent to droplet surface, can change the evaporation rate strongly and become different from local equilibrium value [5]. The Knudsen layer thickness is thin, under low temperature for the droplet of large diameter and it can be neglected. So, the traditional gas-dynamic approach is valid for this condition. But for a droplet with small diameter under high temperature, there will be some intensive vaporization and condensation as well [5]. So, the evaluation of Knudsen layer thickness should be done very carefully. The purpose of the present paper is to perform an evaluation of different parameters of a mono-component droplet using a non-equilibrium Langmuir-Knudsen model. We have plotted all necessary parameters such as temperature, droplet mass and diameter with respect to time for pure methanol, pure propanol and pure ethanol. The significance of non-equilibrium effects and reference conditions for property evaluations are highlighted.

II. MATHEMATICAL FORMULATION

We model an isolated perfectly spherical stationary droplet. As it remains at rest the Lagrangian Equations for the velocity and position may be neglected. The evaporation process is assumed to be quasi-steady, that is, at each small time-step, the droplet behaves as if the evaporation is steady. This permits us to avoid coupled partial differential equations. We also neglect internal temperatures for the model, which is equivalent to the use of a lumped-system for heat transfer calculations.
The governing Equations are [3]:

$$\frac{dT_d}{dt} = \frac{f_2 Nu}{3Pr_G}\left(\frac{\theta_1}{\tau_d}\right)(T_G - T_d) + \left(\frac{L_V}{C_L}\right)\left(\frac{\dot{m}_d}{m_d}\right) \quad (1)$$

$$\frac{dm_d}{dt} = -\frac{Sh}{3Sc_G}\left(\frac{m_d}{\tau_d}\right)\ln(1 + B_{M,neq}) \quad (2)$$

Where: T_d and m_d are the temperatures and masses of the droplet, T_G is the ambient gas temperature, C_L, L_V are the specific heat capacity and latent heat of vaporization of the liquid fuel respectively. The gas phase Prandtl Number (Pr_G) and Schmidt number (Sc_G) in terms of specific heat capacity ($C_{p,G}$), density (ρ_G) viscosity (μ_G), thermal conductivity (k_G)

of the gas and the Specific Diffusivity of fuel vapor with respect to air (Γ_G) are: $Pr_G=(\mu_G C_{p,G})/k_G$ and $Sc_G=\mu_G/(\rho_G \Gamma_G)$, and $\theta_1=C_{p,G}/C_L$. If the density of the fluid is ρ_d and the droplet diameter D, then $\tau_d=\rho_d D^2/(18\mu_G)$ is the time constant of stokes-flow.

The widely used Ranz-Marshall correlations are used to model the Sherwood Number(Sh) and Nusselt Number(Nu):

$$Nu = 2 + 0.522Re_d^{1/2}Pr_G^{1/3} \quad (3)$$

$$Sh = 2 + 0.522Re_d^{1/2}Sc_G^{1/3} \quad (4)$$

TwoReynolds Numbers, are defined:

$$Re_b = \frac{\rho_G u_b D}{\mu_G}, \dot{m}_d = -\pi\rho_G D^2 u_b \quad (5)$$

$$Re_d = \frac{\rho_G u_s D}{\mu_G}, u_s = |u - v| \quad (6)$$

In our problem, the slip velocity u_s is constant, and must be equal to the ambient air velocity, v, as the droplet velocity u=0.

The heat transfer correction is obtained from a quasi-steady solution of the gas field equations coupled to the drop surface boundary conditions, given by $f_2 = \frac{\beta}{e^{\beta}-1}$, β being obtained from the Langmuir-Knudsen Evaporation model.

EVAPORATION MODEL

According to the Langmuir-Knudsen evaporation model, which also takes into account the flow of vapors from the ambient air back to the droplet surface, the non-equilibrium mole fraction is evaluated from the equation [3]:

$\chi_{s,neq} = \chi_{s,eq} - \frac{L_K}{D/2}\beta$; L_K is the Knudsen Length: (7)

$$L_K = \frac{\mu_G\sqrt{2\pi T_d \bar{R}/W_V}}{\alpha_e Sc_G P_G} \quad (8)$$

$$\beta = -\left(\frac{3Pr_G\tau_d}{2}\right)\frac{\dot{m}_d}{m_d} = Pr_G Re_b/2 \quad (9)$$

Where $\bar{R}$ is the universal gas constant, W_V is the molecular wt. of the vapor, P_G is the ambient gas pressure, and α_e is the molecular accommodation coefficient, assumed to be equal to 1.

$\chi_{s,eq}$refers to the equilibrium vapor concentration on the droplet surface, which may be evaluated from the Clausius-Clapeyron Equation. The Spalding Transfer Number, given by

$$B_{M,neq} = \frac{\chi_{s,neq}}{\chi_{s,neq} + \frac{(1-\chi_{s,neq})W_G}{W_V}} \quad (10)$$

where $W_G$is the molecular weight of the carrier gas.

This completes the outline of all necessary equations and quantities used in the model. Equations (2) and (7) are coupled in a non-linear manner for $\dot{m}_d$,so at a given time-step, a single-point iteration scheme is applied for the solution of $\dot{m}_d$. Having obtained $\dot{m}_d$, we apply the necessary value to Eq(1), and a second order backward-difference scheme is applied for the solution of the updated temperature at that instant. The updated mass is calculated and divided by the density to find the updated volume, from which the updated diameter is calculated. The convergence criteria for the simulation is set in such a way that the simulation will stop when the droplet diameter is less than 1.2 nm. All the above models were derived under the assumption of constant spatial gas and vapor properties. Consequently, we must select suitable average constant property values that approximate account for the variation of thermal and spatial properties. Based on the suggestion of [3] all necessary property values were evaluated on the basis of the wet-bulb temperature. On the event the specific data or correlations were unavailable, they were evaluated at the boiling point, since it has been shown in [3] that reasonable results are obtained therein as well.

III. RESULTS AND DISCUSSION

Three different alcohols, propanol ethanol and methanol, are considered for our simulation. The Initial conditions for droplets are: initial diameter =1.2 mm, mass fraction= 1, droplet temperature = 293.15 K, ambient air pressure and temperature = 1 bar and 475 K, ambient gas velocity = 2 m/s. The gas is assumed to be perfectly dry so there is no effect of water vapor on the results. Experimental data for evolution of surface area as shown in Figure (1) is taken from [7,8]. The simulation result for pure ethanol droplet shows that the simulation results and the droplet lifetime are in much closer agreement with experimental results compared to [6]. Thus, the accuracy of the model is established.

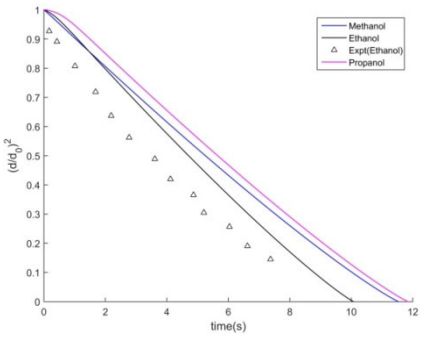

Figure (1): Droplet surface area withtimefor various pure alcohol droplets. Initial conditions: droplet diameter = 1.2 mm, droplet temperature = 293.15 K, ambient pressure and temperature = 1 bar, 475 K

In figure (1), the symbols show experimental results of [7,8] and the solid lines show simulation result. The black solid line represents ethanol, blue solid line represents methanol, and pink solid line represents propanol. The ethanol is highly volatile which is the reason behind rapid evaporation of pure ethanol droplet. It should be noted however, that the linear D^2-law for droplet evaporation is not observed in either the simulation results or the experimental results [7,8]. At the initial stage, this may be attributed to the initial transient rise of droplet

temperature, and linear D^2 variation is observed only when the temperature is steady. At the final stage, when the ratiod/$d_0$becomes very less, surface effects and variable transport parameters become predominant. A critical parameter for validating numerical results, the droplet gasification rate, however is not present currently.

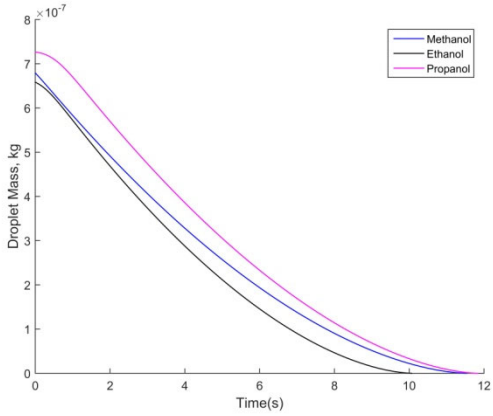

Figure (2): Droplet massversus timefor various pure alcohol droplets. Initial conditions: droplet diameter = 1.2 mm, droplet temperature = 293.15 K, ambient pressure and temperature = 1 bar, 475 K

In figure (2), the change of the mass of the droplet is plotted versus time. Ethanol has the smallest mass of all the three alcohols (for the same droplet size). This happens because the density of ethanol is lower compared to the other two elements. Also, as seen in the simulation, ethanol has the smallest droplet lifetime, followed by methanol and propanol.

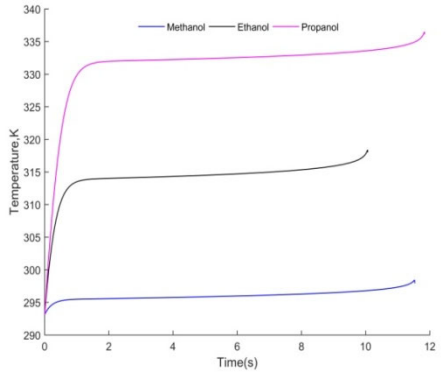

Figure (3): Droplet temperature withtimefor various pure alcohol droplets. Initial conditions: droplet diameter = 1.2 mm, droplet temperature = 293.15 K, ambient pressure and temperature = 1 bar, 475 K

Figure (3) shows surface temperature variation with time for methanol, ethanol and propanol droplets of same size. After the initial heating period, the droplets remain at constant surface temperature for most of their lifetime. The initial droplet heating results in an abrupt increase in a surface temperature of the droplet. During this period of initial heating, a non-linearity is observed in the $(\frac{d}{d_0})^2$ versus time curve (Figure (1)). Also, during the last few seconds of droplets' lifetime, there is a small increase in droplet surface temperature as well. However, it should be noted that, for small size droplets, the model is not guaranteed to give accurate results.

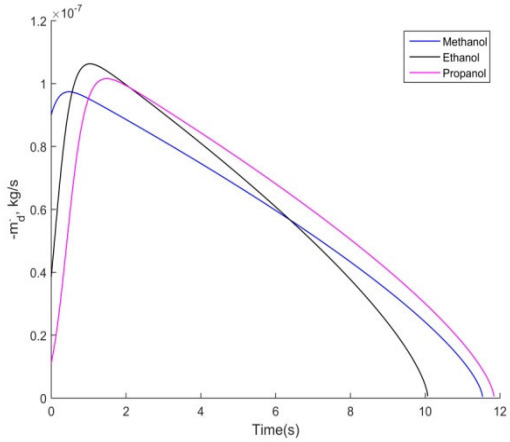

Figure (4): Droplet surface area withtimefor various pure alcohol droplets. Initial conditions: droplet diameter = 1.2 mm, droplet temperature = 293.15 K, ambient pressure and temperature = 1 bar, 475 K

From figure (4), it is observed that the initial evaporation rate of methanol is higher than that of ethanol and propanol. However, for a long time, up to 7 seconds, the evaporation rate of ethanol is significantly higher than that of methanol. This explains the smaller lifetime of ethanol compared to methanol. The slightly larger droplet lifetime of propanol can be attributed to its larger density and initial very low rate of initial rate of evaporation compared to the other two alcohols.

IV. CONCLUSION

An analytical approach to a spherical symmetric fuel droplet is extensively studied and presented in this paper to compare the vaporization characteristic among three different alkyl alcohols- ethanol, methanol and propanol. A non-equilibrium evaporation model has been developed to determine the different important parameters related to evaporation of single-component droplet. This computational code has been found to give an accurate description of the evaporation of the different droplets and also demonstrate the concomitant evolution of droplet diameter, mass, temperature and surface area as well.Different graphs of various parameters are plotted on the basis of this model and based on that the comparison is made successfully among three different fuels with the resultof ethanol validated with an available experimental result. From the above study, it is clear that the non-equilibrium effects are significant for small diameter droplet evaporation and should be accounted for.

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