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Numerical investigation of evaporation of a single ethanol/iso-octane droplet

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HIGHLIGHTS

- Non-uniform vortices inside liquid droplet due to shearing interaction with the gas phase.
- Droplet temperature has the most significant effect on evaporation rate.
- Droplet composition and predominant evaporating species affects overall droplet temperature.
- Droplet composition affects rate of change in droplet diameter.

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ABSTRACT

Numerical study has been performed to analyse evaporation of a single droplet composed of a binary mixture of ethanol and iso-octane. The Navier–Stokes equations are solved in conjunction with VOF multiphase model to track the liquid/gas interface over time. Ethanol and iso-octane form a highly non-ideal mixture and therefore the UNIFAC group contribution method was used to determine the vapour–liquid equilibrium (VLE). Source terms due to interfacial mass transfer were implemented in the continuity, momentum, energy and species equations. Commercial computational fluid dynamics solver, Ansys Fluent 13.0 was used in this study. VLE, mixture transport properties and source terms due to interfacial mass transfer were implemented using user defined functions. Parametric study to analyse the effect of free stream temperature and composition, droplet temperature and composition was performed.

1. Introduction

Multicomponent droplet evaporation is important in many industrial and engineering applications and once such application is evaporation of fuel droplets during fuel injection and atomization [1]. Due to environmental concerns, alcohol blended gasoline is being increasingly considered as an alternative fuel for SI engines [2]. Several experimental and numerical studies have been performed to understand the fuel injection process and has been previously reviewed by Drake and Haworth [3] and Jiang et al. [4]. Godsave [5] and Spalding [6] were the first to propose an evaporation model based on the d^2-law for a single fuel droplet, where the droplet temperature remained constant at the wet bulb temperature. Law [7] proposed an evaporation model based on the Infinite Conduction Model, where the temperature changed with time but was spatially constant inside the droplet. Later this restriction on constant spatial temperature distribution inside the droplet was relaxed using the Finite Conduction Model [8]. Sirignano and Law [9] included effect of internal circulation on droplet evaporation. Haywood et al. [10,11] have performed detailed flow field analysis for axisymmetric flow by solving the Navier–Stokes equation for stationary and deforming droplets. Miller et al. [12] compared equilibrium and non-equilibrium evaporation models for many-droplet gas–liquid flow. More recently, Abarham and Wichman [13] studied evaporation/condensation of a single droplet in presence of background fuel vapour.

The above studies were performed for single component droplets. However, fuels used in many engineering applications are complex multicomponent fluids. Researchers have used various models to represent heat and mass transfer for multicomponent fluids. Bhattacharya et al. [14] have performed a theoretical investigation on a bi-component hydrocarbon droplet composed of n-hexane and n-hexadecane. Their study included the effect of finite diffusion and rapid mixing on droplet evaporation. Sezen [15] derived analytical expression for a single multicomponent droplet based on Infinite Conduction Model. Nadykto et al. [16] derived expressions for mass flux from multicomponent droplet evaporation and condensation under non-isothermal condition. Zeng and Lee [17] used a third order polynomial to model temperature and concentration profiles for multicomponent fuel film vaporization. Yao [18] used film theory to model multicomponent droplet evaporation for high and low pressure environments. Sazhin and his group have reported a number of studies on multi-component

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Nomenclature

C_p	specific heat (J/kg-K)
D, D_{ij}	binary diffusivity (m/s^2)
E	specific energy (J/kg)
$\boldsymbol{F}$	body force (N/m^3)
$\mathbf{g}$	acceleration due to gravity (m/s^2)
h	enthalpy (J/kg)
$\boldsymbol{J}$	species flux (kg/m^2-s)
k	thermal conductivity (W/m-k)
m_i'''	mass transfer/volume (kg/m^3)
p	pressure (Pa)
S_e	energy source term (W/m^3)
S_m	momentum source term (N/m^3)
$S_{\alpha q}$	source term VOF eq. (kg/m^3)
T	temperature (K)
t	time (s)
u, $\mathbf{u}$	velocity (m/s)
U_∞	free stream velocity (m/s)
V	volume (m^3)
X	liquid mole fraction
x	gas phase mole fraction
Y	liquid phase mass fraction
y	gas phase mass fraction

Greek symbols

α	volume fraction
γ	activity coefficient
μ	viscosity (Pa s)
ρ	density (kg/m^3)
σ	surface tension (N-m)

Subscripts

b	bulk
d	droplet
dp	dew point
g	gas phase
i	initial value
l	liquid phase
q	qth phase
s	saturated value
vap	vapour
∞	free stream

Superscript

i,j	i or jth species

Abbreviations

VOF	Volume of Fluid
UNIFAC	Universal Functional Activity Coefficient
SIMPLEC	Semi-Implicit Method for Pressure Linked Equations-Consistent

droplet evaporation. They have reported evaporation models based on analytical solutions of heat conduction and species diffusion for two-component droplet [19] and arbitrary number of species [20]. They have also reported the effect of replacing complex multicomponent fuel with relatively few quasi-components having average properties similar to the representative group of actual components [21].They included effects of temperature gradient and quasi-component diffusion inside the droplet. However, according to Aggarwal and Mongia [22], evaporation characteristics of a bi-component fuel can be effectively represented by a single surrogate component fuel (50% boiling point) at high pressures because evaporation is more sensitive to droplet heating models than to droplet composition.

In all the above mentioned multicomponent evaporation models, the number of components that have been used is relative few in number. However, petroleum fuels are complex multicomponent fluids which are composed of several hundred different components and therefore tracking all the components becomes computationally very expensive. Researchers have used alternative methods to represent such complex multicomponent fluids. Burger et al. [23] have used Distillation Curve Model (DC model) to represent aviation fuels like JP-4, Jet-A1, etc. The DC model describes fractional boiling during droplet evaporation process as a function of the mean molar molecular weight of the fuel. As the model is based on algebraic equations, it is computationally less expensive. In a similar approach, multicomponent fuel composition can be represented using Continuous Thermodynamics [24,25]. Here the fuel composition is represented using a probability distribution function based on one or more macro-properties. Researchers [26–28] have used this approach to solve transport equations to determine evaporation rate and composition time history of multicomponent droplets. In all the above mentioned studies, the effect of droplet deformation was not taken into account.

Alcohols like ethanol have a relatively high polarity compared to hydrocarbons. Therefore, a mixture of alcohol and hydrocarbons is highly non-ideal. It has been shown previously [29] that a binary mixture of ethanol and iso-octane has a higher vapour pressure compared to its individual components. Therefore, interfacial mass flux of such mixtures is also correspondingly higher. Droplet shape, thermal and mass diffusion is expected to have a strong bearing on the evaporation rate of alcohol and hydrocarbon mixtures. Interface of two immiscible fluids has been tracked using different interface tracking methods like VOF [30], Level-Set [31], Front-tracking or immersed boundary method [32] and their variants [33]. The VOF method has been previously used to simulate heat and mass transfer in droplets [34,35], bubbles [36] and film boiling [37,38]. More recently, Tanguy et al. [39] reported evaporation of a 2D moving droplet using Level-Set/Ghost Fluid Method; Schlottke and Weigand [40] used VOF method to perform DNS studies on evaporating 3D droplet with high density ratio; and Strotos et al. [41] again used VOF method to study evaporation of a bi-component 3D droplet suspended from a spherical suspender. In their analysis they used a binary mixture of n-heptane and n-decane in various proportions. As various aspects of droplet evaporation have been studied for several decades, the literature review presented above can no way be considered exhaustive and therefore has been restricted to the context to the study reported here. The author would suggest excellent review articles reported elsewhere [42–44] for more detailed discussion on various droplet evaporation models.

The present study is aimed at understanding the effects of droplet internal and near vicinity flow physics for non-ideal multicomponent droplet evaporation time history. In keeping with the aforementioned objective, a 2D droplet composed of a binary mixture of ethanol and iso-octane has been investigated in this paper. This work is an extension of a previous study reported elsewhere [45]. An evaporation model suitable for such mixtures has been