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Numerical modeling of multi-component fuel spray evaporation process

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ABSTRACT

The overarching goal of this study is to implement computationally effective models that can predict the evaporation of multi-component fuel droplets/spray using a multidimensional Computational Fluid Dynamics (CFD) code. The new approach for modeling heat and mass transfer inside a droplet accounts for finite thermal conductivity, finite mass diffusivity, and turbulence effects within the atomizing liquid droplet/spray for multi-component fuel droplet evaporation. This model was developed and validated against experimental measurements for single droplet vaporization and one-way evaporating sprays previously, and is implemented into CFD code for two-way coupled numerical modeling study in this research. A new coalescence model for droplets with different mixture composition was also implemented into CFD code in this research. Thereby, the evaporation of multi-component diesel fuel surrogate spray in hot gas environment was predicted and compared with available experimental measurements. The model shows good predictive capability and was demonstrated to improve the accuracy of multi-phase flow simulations.

1. Introduction

In liquid fueled combustion systems such as gas turbine combustors, gasoline direct injection, and diesel engines, combustion performance depends strongly on the fuel type, liquid atomization, spray vaporization, and mixing process. Droplet size history during evaporation in a combustion chamber influences the dynamic behavior of droplets, while the variation of the gas-phase composition determines the distribution of the fuel compounds within the combustion chamber. Thus, a fundamental understanding of these processes is essential for modeling evaporating fuel sprays.

High pressure injectors, e.g., fuel line pressure of 400–1800 bars for diesel engines and 30–200 bars for Gasoline Direct Injection (GDI) engines, are utilized extensively to accomplish better and rapid air-fuel mixing. The fuel atomization process is influenced by a number of parameters, such as fuel property, injector geometry, combustion chamber gas density, fuel injection pressure, etc. Optimization of these parameters could lead to cleaner and more stable combustion.

Real fuels are typically composed of hundreds of complex compounds with different physical properties. In order to comprehensively model multi-component fuel evaporation process, it is critical to include the effects of several important thermo-physical processes. These include diffusion of components both inside the droplet and on the gas side, heat transfer inside of the droplets, effects of components on each other, and non-ideality of the mixture. Thus, the evaporation of multi-component droplets is a complex process.

In next section, the current state of knowledge associated with droplets/spray evaporation, droplet breakup, and droplets collision as relevant to the present paper is reviewed.

2. Literature review

There are several books, papers, and reports dealing with droplet evaporation, e.g., [3]. Most models for fuel sprays deal with single component fuels. Fuels are usually characterized by a single surrogate component in most evaporation models implemented in commercial and research computational fluid dynamic codes. However, single-component fuel models are insufficient to predict the complex behavior of complex fuels such as gasoline and diesel [4]. For predicting real fuel evaporation behavior, a method in which surrogate fuels are introduced can be used instead [5]. Surrogate mixtures are designed specifically to enable a reasonably accurate numerical simulation of complex mixtures using a small number of components.

A multi-component fuel modeling approach can increase the accuracy of prediction of evaporation rate, engine emissions, and overall engine performance, in contrast to single-component fuel modeling. Multi-component fuel models are classified into two types: Discrete Multi-Component models (DMC) and Continuous Multi-Component models (CMC). Studies have been performed on discrete multi-component fuel vaporization, e.g., Ra and Reitz

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Nomenclature

A	droplet surface area
B_0	constant (=0.61)
B_1	constant (=25.0)
C_a	constant (=0.0163)
c_p	specific heat at constant pressure
D	binary diffusion coefficient
h	heat transfer coefficient
J	mass transfer coefficient
k	thermal conductivity; turbulent kinetic energy
K_c	loss coefficient due to nozzle inlet geometry
L	latent heat of evaporation
L_t	characteristic length scale associated with droplet liquid turbulence length scale
L_w	characteristic length scale associated with surface wave motion
$\dot{m}$	mass transfer rate
M	molecular weight
P	pressure
Pr	Prandtl number
Q	heat transfer rate
r	instantaneous drop radius
r_p	product drop radius used in the secondary break up formulation
r_t	radial length scale associated with droplet liquid turbulence length scale
r_w	radial length scale associated with the wave motion
R	universal gas constant
Re	Reynolds number
Sc	Schmidt number
t	time
T	temperature
v	velocity
We	Weber number
X	mole fraction
Y	mass fraction

Greek letters

Λ	wavelength of fastest growing wave
ρ	density
σ	surface tension
ε	dissipation rate of kinetic energy in $k-\varepsilon$ model
τ	time associated with surface wave motion
τ_w	characteristic time scale associated with surface wave motion
τ_t	characteristic time scale associated with liquid turbulence time scale
δ	thermal layer or mass transfer layer thickness
μ	viscosity
ς	coalescence efficiency
Ω	maximum wave growth rate

Superscripts

d	associated with droplet
g	gas phase
l	liquid phase
o	initial condition
p	at the constant pressure
s	at the droplet surface
t	parameter associated with turbulence
∞	free stream condition

[4], Torres et al. [35], and Samimi Abianeh and Chen [1,6]. Tamim and Hallett [7], and Lippert and Reitz [8] are examples of CMC models. The DMC approach models a fuel with a limited number of components to match the actual fuel distillation curve. Other fuel surrogate properties such as thermal conductivity, density and heat capacity are not necessarily close to that for the real fuel [4]. Smith and Bruno [9] and Mueller et al. [10] have performed extensive experimental studies to generate distillation curves of real fuels with limited components and also generated several surrogates with limited number of components. In this research, the diesel surrogate of Ra and Reitz [4] with six components is used for predicting diesel fuel spray evaporation. The resulting distillation curve is in good agreement with the measurement of Butts [11].

Ra and Reitz [4] modeled the heat transfer within a droplet to predict the evaporation of gasoline and diesel fuel droplets at different temperatures and pressures. They modeled the heat transfer inside the droplet but assumed infinite mass diffusion (i.e., no gradient of mass fraction within the droplet). Sazhin et al. [12] used a binary-component mixture for modeling fuel droplet composition. They extended the Abramzon and Sirignano [13] model to include a mass diffusivity boundary layer thickness within an evaporating droplet. Their predicted time evolution of the average temperature is reasonably close to measured data, especially in the case of pure acetone and acetone-rich mixture droplets. The DMC approach has high computational overhead since additional transport equations have to be solved for each species in order to track the fuel composition and the vaporization behavior [4]. By contrast, in CMC models, the fuel composition is assumed to be a continuous distribution function of molecular weight or other appropriate parameters. However, when the CMC model is applied to combustion simulations, a description of the multi-component features of the fuel is inevitably limited, making it difficult to appropriately model the consumption of individual components [4]. The differences between continuous thermodynamics studies in the literature are mostly in the preference of the distribution function, e.g., gamma or Gaussian distributions, and the selection of the distribution variable, e.g., component molecular weight, boiling temperature and carbon number.

For modeling heat and mass transfer within fuel droplets, studies can be classified into two general categories: the infinite conductivity/diffusivity model and the finite conductivity/diffusivity model. The Infinite Conductivity Model or Rapid Mixing Model was introduced and implemented by Law and Sirignano [14]. This model assumes a well-mixed droplet without any temperature gradient within the droplet. The model produces reasonable results for slow and fast evaporation processes, when droplet internal heat conduction and diffusion does not have a major effect on the internal temperature and concentration profiles [3,15]. Also, this model could yield good agreement with experimental results when the boiling and initial temperature of the droplet is close to the surrounding gas temperature. On the other hand, if this condition is not met, it can lead to underestimation of the vaporization rate, droplet temperature, and droplet lifetime. Sommerfeld et al. [16] showed that the basic assumption of this model, viz., zero diffusion resistance, is inaccurate. The finite heat and/or mass transfer model refers to models in which the mass and heat transfer processes within a droplet are modeled. The