



Droplet evaporation characteristics due to wet compression under RCM conditions

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ABSTRACT

The vaporization characteristics of a single fuel droplet subjected to rapid gas-phase compression (i.e., wet compression) are computationally investigated using two spherically-symmetric models: quasi-steady (QS) and fully transient (TS). Features of the wet compression process under rapid compression machine (RCM) conditions are discussed with these compared to simulations where the far-field conditions are essentially invariant. It is observed that wet compression can significantly increase the rate of evaporation primarily due to the increase in droplet temperature and corresponding saturation pressure (fugacity); an increase in the density-weighted mass diffusivity is also beneficial in reducing the droplet consumption times. The QS model predicts substantially longer rates of evaporation relative to the TS model due to transient behavior associated with the initial evaporative cooling process, and the gas-phase compression heating process. Increases in the rate of volumetric compression can lead to more rapid droplet consumption, however there is a corresponding increase in spatial stratification in the gas- and liquid-phases which may not be advantageous for RCM applications. An ‘operating map’ has been developed based on parametric simulations of an *n*-dodecane droplet evaporating into nitrogen.

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1. Introduction

Wet compression is the process whereby droplet evaporation is achieved through compression heating of the gas-phase of a droplet laden aerosol. This phenomenon has received increasing attention in recent years with applications to internal combustion (IC) and gas turbine (GT) engines, as well as laboratory devices such as aerosol shock tubes (STs) and rapid compression machines (RCMs). In advanced IC engines non-conventional combustion strategies are being investigated in order to reduce soot, NO_x and unburned hydrocarbon (UHC) emissions while maintaining high energy conversion efficiencies [1–5]. In these, sometimes referred to as low temperature combustion (LTC) schemes, the fuel can be introduced very early in the compression stroke, in some cases well in advance of maximum piston compression. Under such conditions the in-cylinder gases are relatively cool, meaning they may be at or below the fuel’s boiling point (e.g., $T_b \sim 650$ K). During the piston’s compression stroke the liquid droplets are vaporized due to the gas-phase volumetric compression, and the fuel vapor is subsequently mixed with the gas-phase oxidizer. Droplet coalescence and wall wetting during compression, especially important

for highly involatile fuels or fuel components, can lead to extended evaporation times and the formation of unwanted emissions [6]. Wet compression is also important in IC engines that utilize “wet” ethanol, which is a minimally-processed ethanol-based fuel with high water content [7]. In these engines much of the ethanol readily evaporates during the induction stroke however, the water may not completely vaporize until well into the compression stroke.

In GT engines wet compression of water aerosols has been used to achieve “continuous cooling” in the compressor component of the engine [8–13]. In engines employing this process, water droplets with diameters on the order of ~ 15 μm are injected into the intake stream via fogging systems with high droplet output. The pressure-driven injectors used in these systems achieve very high relative droplet–air velocities and rapid mixing of the evolving water vapor with the air. This can result in significantly increased power densities along with cost and performance advantages relative to conventional inter-cooling units. However, it is only effective when the humidity ratio of the intake air is low and the residence time in the compressor is adequate to achieve complete evaporation.

In shock tubes (STs) and rapid compression machines (RCMs) wet compression has been proposed as a means of preparing test gases of high molecular weight (MW), involatile liquid fuels relevant to the transportation industry. Traditional charge preparation techniques use external mixing protocols based on partial pressure methodologies [14,15]. Diesel-representative fuels for example,

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Nomenclature

B	mass transfer number	<i>Greeks</i>	
c_p	specific heat at constant pressure	α	thermal conductivity
c_v	specific heat at constant volume	γ	ratio of specific heats, c_p/c_v
D	mass diffusion coefficient	κ	heat diffusivity
d	diameter	λ	second viscosity coefficient
D_{sm}	Sauter mean diameter	μ	dynamic viscosity
h	specific enthalpy	ρ	density
H	thermal energy supplied	ν	specific volume
I	specific internal energy	ϕ	fugacity coefficient
L	heat of vaporization		
Le	Lewis number (κ/D)	<i>Subscripts</i>	
\dot{m}	mass flow rate	avg	average
\bar{m}	non-dimensional mass flow rate, $\dot{m}/4\pi\rho_g D_g r_g$	b	boiling
N	total number of species in the mixture	c	critical point property
P	pressure	f	fuel
r	radial direction	g	gas-phase
\bar{r}	non-dimensional radius, r/r_s	i	i th species
R	ideal gas constant	ii	ii th cell
Re	Reynolds number, $\rho u D/\mu$	inst	instantaneous
t	time	j	j th species
\bar{t}	non-dimensional time, $\int \dot{\kappa}_1 dt/r_s^2$	k	k th species
T	temperature	l	liquid-phase
\bar{T}	non-dimensional temperature, T/T_{ref}	s	surface
u	velocity	0	initial condition
V	volume	∞	far-field condition
X	mass fraction, liquid phase		
Y	mass fraction, vapor phase		
z	compressibility factor		

have very low vapor pressures at standard conditions (e.g., <1 Torr) which make this option difficult or impossible. Heating the mixing tanks and equipment can lead to better fuel vaporization but this can result in seal degradation issues in RCMs, as well as concern for pre-test reactivity during the preparation process. Aerosols of suspended fuel droplets (Sauter mean diameter, $D_{sm} \sim 8\text{--}18 \mu\text{m}$) have been used to deliver liquid fuels to the machines where subsequent compression of the surrounding gas phase leads to evaporation of the liquid fuel droplets [16,17]. In shock tubes where test temperatures range from 900 to 2000 K the gas-phase compression event is achieved via a rapidly traveling shock wave (compression achieved in $\sim 30 \mu\text{s}$ to 600–700 K); the passing of the initial wave not only increases the pressure and temperature of the surrounding bath gases but it fragments the initial droplets and results in high convective velocities near the droplet surface (which enhances vaporization). The subsequent reflected wave compresses the evaporated mixture to the test conditions. In RCMs where test temperatures are generally between 600 and 1100 K the compression event is much slower (e.g., $\sim 15\text{--}60 \text{ms}$) and the bulk gas motion is often suppressed in order to minimize unwanted heat loss during the test period [17]. Droplet evaporation is much slower and is mainly diffusion-limited. Evaporation must also be achieved at lower temperatures, i.e., before the test temperature is reached.

2. Background

The design and operation of devices that can effectively utilize the wet compression process requires a fundamental understanding of droplet evaporation including vapor-phase mixing, diffusion, and saturation phenomena, along with a reasonably accurate means of simulating it with an integrated gas-phase compression model. Droplet evaporation models have a long history of development (e.g., see Refs. [18–20]) and include a number of approaches. Some assume that the bulk gas is stagnate with the gas-phase

transport diffusion/Stefan flow limited (i.e., $Re = 0$), while others assume a convective bulk gas flow with an associated Reynolds number (Re). Both quasi-steady (QS) [21–24] and fully transient (TS) [25–29] continuum models have been formulated, which generally utilize the assumption of liquid–vapor equilibria at the droplet–gas interface; other means of prescribing the interface conditions are also possible however (e.g., see Ref. [30]). The quasi-steady approach assumes that the gas-phase transport of heat, mass and momentum is sufficiently fast so that transients within the gas-phase can be ignored relative to the transients associated with the liquid-phase, including the rate of surface regression of the droplet. The fully transient approach does not make this assumption and has been demonstrated to be better suited to resolve evaporation within high pressure environments (e.g., $P > 10 \text{bar}$) where gas-phase heat and mass transport can be reduced relative to atmospheric conditions. Both approaches can incorporate various levels of complexity including an accounting of thermal gradients within the droplets, allowance of multiple constituents within the liquid phase, the use of real gas models for thermodynamic and transport properties, and the capability to transition between sub- and supercritical evaporation, among others.

The integration of droplet evaporation models with models for the gas-phase compression process has been attempted in a number of ways. Work to date has focused primarily on GT engine applications and has predominantly employed the quasi-steady approach; examples can be found in Refs. [31–38]. In these integrated models the droplets have been assumed to be uniform in temperature and composition, and the far-field (“mean-line”) gas-phase temperature has been modeled as homogeneous but unsteady. Effects of compression heating and bulk gas flow on droplet evaporation rates have been investigated, as have effects of evaporation on gas-phase cooling. Compressor operating maps accounting for ambient humidity and extent of liquid water injection have

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