Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2016-0252

Vol. **23**, No. 4, pp. 1241-1262
April 2018

Liquid Fuel Evaporation under Supercritical Conditions

Guowei Xiao[1,2], Kai Hong Luo[1,3,*], Xiao Ma[2] and Shijin Shuai[2]

[1] *Center for Combustion Energy, Tsinghua University, Beijing 100084, P.R. China.*
[2] *State Key Laboratory of Automotive Safety and Energy, Tsinghua University, Beijing 100084, P.R. China.*
[3] *Department of Mechanical Engineering, University College London, Torrington Place, London WC1E 7JE, UK.*

Received 15 December 2016; Accepted (in revised version) 1 July 2017

Abstract. Molecular dynamics simulations are performed to study the supercritical mixing process of the n-dodecane/nitrogen binary system. Previous studies have shown the existence of supercritical phenomenon under certain conditions in modern propulsion systems such as diesel engines. However, the physical mechanisms and internal driving forces of this phenomenon are still not well understood. In this paper, we attempt to answer this question through simulating the diffusion and evaporation of gaseous nitrogen and liquid phase n-dodecane. It addresses under what conditions the supercritical transition phenomenon happens and what features the supercritical evaporation process have. A unique configuration is constructed to mimic the evaporation of an n-dodecane thin film in an open nitrogen environment under conditions ranging from subcritical to supercritical. The detailed structure of the liquid-vapor interface during the evaporating process is described and the evaporation rate and the interface thickness are estimated, which show differences between subcritical and supercritical evaporation. Results indicate that under relatively high pressure conditions, the liquid surface transitions into supercritical state, and the liquid-vapor interface expands significantly with vanishing surface tension, leading to a diffusion like mixing process. It is shown that the supercritical evaporation would happen under conditions that correspond to the in-cylinder conditions of a turbo-charged engine.

AMS subject classifications: 84-04

Key words: Molecular dynamics, n-dodecane, evaporation, supercritical.

*Corresponding author. *Email addresses:* prof.k.h.luo@outlook.com (K. H. Luo), xgw13@mails.tsinghua.edu.cn (G. Xiao), max@mail.tsinghua.edu.cn (X. Ma), sjshuai@mail.tsinghua.edu.cn (S. Shuai)

1 Introduction

It has long been recognized that in some modern propulsion systems powered by spray combustion, such as diesel engines and liquid rocket combustion chambers, the environmental pressure can be higher than the critical pressure of the injected fuel. Considering the high temperature in the combustion chamber, it is reasonable to expect that the injected fuel may undergo a transition from liquid phase to supercritical phase, which can only diffuse but not evaporate. Therefore, our conventional knowledge on the atomization and combustion of the spray may be not sufficient to describe those processes under such conditions. In fact, a number of studies focused on this issue have found fundamentally different phenomena. Experimental studies [1–8] relevant to the conditions of liquid rocket combustion chamber showed that under high pressure and temperature conditions, the non-reacting sprays exhibit some characteristics similar to a turbulent gas jet, rather than the conventionally recognized breakup and evaporation phenomena. Chehroudi et al. [1] reviewed and plotted the experimentally measured and theoretically derived results regarding the initial spreading angle of both single-phase gas jet and two-phase sprays, as a function of the environment-to-injectant density ratio. Quantitative agreement was confirmed between the measured results of two-phase sprays under near-critical conditions and the theoretical prediction for incompressible but variable-density gaseous jets by Dimotakis [9]. Besides that, smoothened liquid surface [10, 11] and the absence of ligaments or droplets [1, 4, 5, 12–14] were also observed and treated as signs of abnormal phenomena under supercritical conditions.

Despite these phenomenological descriptions and qualitative observations, our understanding of the supercritical injection process is still limited, due to the absence of effective quantitative measurement techniques. Most of the recent experimental studies have focused on the appearance and structural parameters of sprays, thus can provide little insight into the physical mechanism of these processes. In order to reveal the intrinsic features of this supercritical phenomena, especially the microscopic interfacial dynamics, more fundamental methods are desired.

Dahms et al. [15–18] made significant advances on this topic in their theoretical studies. A theoretical framework was presented to describe the thermodynamic structure of representative gas liquid interfaces under engine relevant conditions and predict the breakdown of classical two-phase spray atomization theory. A real-fluid model together with vapor-liquid equilibrium theory and gradient theory was used to reconstruct the detailed structure of the vapor-liquid interface. A Knudsen number criterion was developed to quantify the conditions under which the interface region was in the continuum regime, and thus transition from classical two-phase interface to one-phase mixing layer was initiated. In a recently published work [18], this framework was modified by applying the most modern form of the Helmholtz free energy equation of state and non-linear gradient theory and a generalized one-dimensional liquid injection model. The analysis showed that interfacial global thermal equilibrium is a prerequisite of vapor-liquid