



# Liquid jet breakup regimes at supercritical pressures



Rainer N. Dahms\*, Joseph C. Oefelein

Combustion Research Facility, Sandia National Laboratories, P.O. Box 969, MS 9051, Livermore, CA 94551, USA

## ARTICLE INFO

### Article history:

Received 26 August 2014

Revised 29 June 2015

Accepted 2 July 2015

Available online 23 July 2015

### Keywords:

Supercritical

Multiphase

Liquid

Injection

Real-fluid

Breakup regimes

## ABSTRACT

Previously, a theory has been presented that explains how discrete vapor–liquid interfaces become diminished at certain high-pressure conditions in a manner that leads to well known qualitative trends observed from imaging in a variety of experiments. Rather than surface tension forces, transport processes can dominate over relevant ranges of conditions. In this paper, this framework is now generalized to treat a wide range of fuel–oxidizer combinations in a manner consistent with theories of capillary flows and extended corresponding states theory. Different flow conditions and species-specific molecular properties are shown to produce distinct variations of interfacial structures and local free molecular paths. These variations are shown to occur over the operating ranges in a variety of propulsion and power systems. Despite these variations, the generalized analysis reveals that the envelope of flow conditions at which the transition from classical sprays to diffusion-dominated mixing occurs exhibits a characteristic shape for all liquid–gas combinations. For alkane–oxidizer mixtures, it explains that these conditions shift to higher pressure flow conditions with increasing carbon number and demonstrates that, instead of widely assumed classical spray atomization, diffusion-dominated mixing may occur under relevant high-pressure conditions in many modern devices.

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## 1. Introduction

Liquid injection of multicomponent fluids at elevated operating pressures is not well understood. Imaging from a variety of experiments have long shown that under some conditions, when the pressure of the working fluid approaches or exceeds the thermodynamic critical pressure of the liquid phase, the presence of discrete two-phase flow dynamics may become diminished. Then, the characteristic processes of primary and secondary atomization, multicomponent evaporation, and liquid ligament and droplet formation do not occur. As a consequence, the widely acknowledged drop deformation and breakup regimes of two-phase flows [1,2] do not apply anymore. Instead, the classical gas–liquid interface is replaced by a single-phase diffusion dominated dense-fluid mixing layer, which is substantially affected by non-ideal thermodynamics and transport. Such phenomena have been demonstrated to occur in various systems, such as those that involve the injection of liquid nitrogen or oxygen into environments composed of nitrogen, helium, hydrogen, or argon [3–5]. Many works have served to corroborate these observations [6–36].

Modern theory has long lacked a first-principle explanation for the observed phenomena. In contrast to pure fluids, discrete vapor–liquid interfaces in multicomponent mixtures along with their surface tension forces do not necessarily diminish only because the

thermodynamic critical pressure of the liquid phase is exceeded. In recent years, experimental evidence of substantial surface tension forces in various hydrocarbon mixtures at high pressures ( $p > 500$  bar) was provided in the literature [37–39]. It is generally accepted, however, that surface tension forces in multicomponent mixtures diminish once the temperature of the injected liquid phase approaches its critical value. Previous research into gas–liquid interfaces during diesel engine fuel injection processes has shown, however, that those interfaces are generally not heated to their critical temperature due to the lack of enthalpy contained in the unburned ambient gases [40,41].

Recent studies quantified the conditions under which a specific *n*-dodecane–nitrogen mixture (relevant for diesel engine fuel injection) transitions between classical spray atomization and diffusion-dominated dense-fluid mixing dynamics [42–44]. It was established that the breakdown of the classical non-continuum two-phase interface and the consequent development of dense-fluid mixing layers is initiated because the multi-component two-phase interface becomes much wider than the mean free molecular path. This showed that the transition to mixing layers occurs due to interfacial dynamics and not, as conventional wisdom had suggested, because the liquid phase has heated to supercritical temperatures where surface tension forces diminish.

The findings outlined above have most recently been corroborated by Manin et al. [45] by applying long-distance microscopic imaging using an ultra-fast LED source with a diffuser background behind the *n*-dodecane jet. When the jet is injected at lower temperatures but

\* Corresponding author.

E-mail address: [Rndahms@sandia.gov](mailto:Rndahms@sandia.gov) (R.N. Dahms).

supercritical pressures, classical droplet and ligament stretch and breakup dynamics were observed. At the high pressure and higher temperature conditions predicted by Dahms et al. [42–44], such dynamics become diminished and no droplets could be detected anymore. Furthermore, the transition from liquid to gaseous state appeared much smoother compared to observations made at lower temperature and pressure conditions. Falgout et al. [46] have also provided evidence of dense-fluid mixing layers using ballistic imaging of the same diesel fuel injector at the same chamber conditions. A thickened turbulent *n*-dodecane–nitrogen mixing layer was found to evolve with a cellular structure characteristic of gas jets.

While the findings outlined above support the theory presented in previous works [42–44,47], the consequence of these observations and implications with respect to other propulsion and power systems is not clear. Thus, the objective of this paper is to now apply the theory to gain a clearer understanding regarding the regimes present in other practical systems. This is accomplished by performing a generalized analysis over a wider range of propellant combinations (e.g., liquid-fuel–air in gas turbines and reciprocating engines, and liquid oxygen–hydrogen for cryogenic rocket applications). A series of representative interface profiles are calculated over a wide range of flow and mixture conditions. Substantial differences are demonstrated in species specific molecular properties, which result in distinct variations of two-phase interfacial structures and local mean free pathways. The systematic analysis leads to the derivation of a more general regime diagram for liquid jet breakup that demonstrates when classical drop atomization and breakup regimes are being replaced by diffusion-dominated interfacial mixing for a range of conditions relevant in modern power and propulsion systems.

## 2. Model formulation

Details related to implementation of the theory to derive the regime diagrams of interest here are explained in detail by Dahms and Oefelein [43]. Thus, only a brief description is given here for brevity. The starting point of the model is based on the framework developed by Oefelein [48], which provides a generalized treatment of the thermodynamics and transport processes for hydrocarbon mixtures at near-critical and supercritical conditions. This scheme is combined with the theoretical framework developed by Dahms et al. [42] and Dahms and Oefelein [43], which facilitates vapor–liquid equilibrium and gas–liquid interface structure calculations to compute both surface tension forces and the local two-phase interface thicknesses. Deriving the regime diagrams then involves the implementation of thermodynamics and transport properties coupled with linear gradient theory to model respective interfacial structures. Following is a description of both of these frameworks.

### 2.1. Thermodynamic and transport properties

The development of equations of state has evolved in recent decades from simple cubic and virial equations to Beattie–Bridgeman and Benedict–Webb–Rubin equations, and then to modified Benedict–Webb–Rubin and Helmholtz energy equations of state [49]. In this study, the extended corresponding states model [50,51] is employed using a modified Benedict–Webb–Rubin (*BWR*) equation of state to evaluate the  $p$ – $v$ – $T$  behavior of the inherent dense multicomponent mixtures. Use of modified *BWR* equations of state in conjunction with the extended corresponding states principle has been shown to provide consistently accurate results over the widest range of pressures, temperatures and mixture states, especially at saturated conditions. Having established an analytical representation for real mixture  $p$ – $v$ – $T$  behavior, thermodynamic properties are obtained in two steps. First, respective component properties are combined at a fixed temperature using the extended corresponding states methodology to obtain the mixture state at a given reference pressure. A pres-

sure correction is then applied using departure functions of the form given by Reid et al. [52, Chapter 5]. These functions are exact relations derived using Maxwell's relations (see for example VanWylen and Sonntag [53, Chapter 10]) and make full use of the real mixture  $p$ – $v$ – $T$  path dependencies dictated by the equation of state. Standard state properties are obtained using the databases developed by Gordon and McBride [54] and Kee et al. [55]. Chemical potentials and fugacity coefficients are obtained in a similar manner. Likewise, viscosity and thermal conductivity are obtained using the extended corresponding states methodologies developed by Ely and Hanley [56,57]. Mass and thermal diffusion coefficients are obtained using the methodologies outlined by Bird et al. [58] and Hirschfelder et al. [59] in conjunction with the corresponding states methodology of Takahashi [60].

### 2.2. Vapor–liquid equilibrium theory

The real-fluid model for multicomponent mixtures is applied to obtain vapor–liquid equilibrium conditions. Assuming that the liquid is in thermodynamic equilibrium with its vapor, the equilibrium conditions are prescribed by the equality of temperature, pressure, and species chemical potentials between the vapor and liquid phases. Then, the critical point of a multicomponent mixture can be obtained as the point where the mixture compositions of the vapor and liquid phase become equal at supercritical pressures.

### 2.3. Linear gradient theory for gas–liquid interface structures

Gradient theory provides a widely accepted methodology to calculate detailed interface structures between gases and liquids [61,62]. At equilibrium, as applied in this paper, the model has been shown to be equivalent to mean-field molecular theories of capillarity. The foundation of this theory was established by van der Waals in 1893 [63,64] and reformulated later by Cahn and Hilliard in 1958 [65]. Over past decades, gradient theory has been successfully applied to a wide variety of fluids: hydrocarbons and their mixtures, polar compounds and their mixtures, polymer and polymer melts, vapor–liquid and liquid–liquid interfaces. Recently, gradient theory has also been successfully compared to Monte Carlo molecular simulations of vapor–liquid and liquid–liquid interfaces [66–68]. There, gradient theory proved successful in capturing both surface tension and details of subcritical vapor–liquid molecular interfacial structures. It is worth pointing out that, for the simulation of molecular vapor–liquid interfaces, fundamental thermodynamic quantities such as pressure and chemical potential remain meaningful in gradient theory. Linear gradient theory has been derived from gradient theory by assuming a linearized minimization function of the Helmholtz free energy density distribution across the vapor–liquid interface for the calculation of the interfacial density profiles. Linear gradient theory has proven successful in calculating binary and multicomponent interface states of the kind considered here [69,70].

The interfacial profile of a planar multicomponent gas–liquid interface is obtained by minimizing the Helmholtz free energy, which is expanded as a Taylor series and truncated at lower spatial derivatives [61,62]. The influence parameter, which determines the response of the density gradient to local variations of the species chemical potentials from their bulk value, is assumed to be density-independent [71] and is calculated based on the prior works of Lin et al. [61]. For temperatures higher than the critical temperature of the vapor component, the corresponding reduced temperature is set to a single value, consistent with suggestions from Zuo and Stenby [70]. This method has found wide acceptance and has also been adopted here [69] even though more suitable and generalized methods have also been most recently proposed [72]. Using gradient theory, the surface tension and spatial interface dimension can then be calculated once the species density profiles within the interface have been obtained. In the limit of thermodynamic equilibrium, these profiles can

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