



# Non-equilibrium gas–liquid interface dynamics in high-pressure liquid injection systems

Rainer N. Dahms\*, Joseph C. Oefelein

*Combustion Research Facility, Sandia National Laboratories, Livermore, CA 94551, USA*

Available online 26 June 2014

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## Abstract

The transition of classical spray atomization processes to single-phase continuous dense-fluid mixing dynamics with diminished surface tension forces is poorly understood. Recently, a theory has been presented that established, based on a Knudsen-number criterion, that the development of such mixing layers is initiated because the multicomponent two-phase interface becomes much wider than the mean free molecular path. This shows that the transition to mixing layers occurs due to interfacial dynamics and not, as conventional wisdom had suggested, because the liquid phase has heated up to supercritical temperatures where surface tension forces diminish. In this paper we focus on the dynamics of this transition process, which still poses many fundamental questions. We show that such dynamics are dictated by substantial statistical fluctuations about the average interface molecule number and the presence of significant interfacial free energy forces. The comprehensive analysis is performed based on a combination of non-equilibrium mean-field thermodynamics and a detailed modified 32-term Benedict–Webb–Rubin mixture state equation. Statistical fluctuations are quantified using the generally accepted model of Poisson-distributions for variances in systems with a small number of molecules. Such fluctuations quantify the range of pressure and temperature conditions under which the gradual transition to dense-fluid mixing dynamics occurs. The interface begins to deteriorate as it broadens substantially. The related interfacial free energy forces do not instantly diminish only because vapor–liquid equilibrium conditions do not apply anymore. Instead, such forces along with the present interfacial statistical fluctuations are shown to gradually decrease as the interface transitions through the molecular chaos regime and to diminish once the interface enters the continuum regime. Then, the interfacial region becomes a continuous gas–liquid mixing layer with diminished free energy forces that is significantly affected by single-phase real-fluid thermodynamics and transport properties.

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*Keywords:* Direct injection; Diesel engine; Supercritical flow; Real fluid model; Nonequilibrium thermodynamics

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## 1. Introduction

Mayer et al. [1,2] were one of the first to show that under certain high-pressure conditions, the presence of the widely recognized spray atomization and evaporation process is replaced

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\* Corresponding author. Address: Sandia National Laboratories, Combustion Research Facility, 7011 East Avenue, MS9051, Livermore, CA 94550, USA.

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

by diffusion-dominated dense-fluid mixing layers. Past research into multiphase flows has provided additional insights into the physics of high-pressure fluid dynamics [3–19]. Despite these prior contributions, modern theory has lacked a first principle explanation for the observed phenomena. To address this, Dahms et al. [20] and Dahms and Oefelein [21] have recently presented such a theory that explains and quantifies the conditions under which a multicomponent mixture transitions from classical spray atomization processes to dense-fluid mixing. They developed a system of models which coupled real-fluid thermodynamics in multicomponent and multiphase mixtures with vapor–liquid equilibrium and Linear Gradient Theory. The vapor–liquid equilibrium calculations provided the compositions and mixture states of the respective vapor and liquid phases. Linear Gradient Theory provided the detailed spatial distribution of these compositions across the two-phase interfacial region.

Gradient Theory was established by van der Waals [22,23] in 1893 and reformulated later by Cahn and Hilliard [24] in 1958 to compute the physical and continuous variation of fluid properties across a thin molecular vapor–liquid interface. The capability of Gradient Theory to calculate the physical mean molecular structure across such interfaces has recently been confirmed by statistical analysis of molecular dynamic simulations [25–27]. The analysis showed that the enthalpy contained in hot unburnt ambient gases is usually not sufficient to heat up the multicomponent gas–liquid interface to its critical temperature where surface tension forces diminish. Instead, the theory indicated that the transition to dense-fluid mixing layers occurs through combination of broadening two-phase interfaces, reduction in mean free path, and a reduction in surface tension. The broadening of the interface was mainly attributed to high subcritical gas–liquid interface temperatures, while the reduction of the mean free path was mainly attributed to high pressure. This showed, based on an interface Knudsen-number criterion, that at certain high pressure and temperature conditions, the multicomponent two-phase interface becomes much wider than the mean free molecular path. Then, the transition to dense-fluid mixing layers occurs due to interfacial dynamics which distinctively differ from classical molecular behavior.

In this paper, the formerly presented theory is extended to quantify the non-equilibrium dynamics of the transition process. The analysis shows that the initiation of this transition is determined by substantial statistical fluctuations about the average interface molecule number. Such variations are shown to decrease with increasing pressure and temperature conditions. The resulting probability of departing from vapor–liquid equilibrium conditions quantifies the range of pressure

and temperature conditions under which the gradual transition to dense-fluid mixing dynamics occurs. When this happens, the interface begins to broaden substantially. Non-equilibrium mean-field thermodynamics, based on the Cahn–Hilliard equation [24], in combination with a detailed mixture state equation, are adopted to calculate corresponding interfacial free energy forces. The analysis shows that these forces do not instantly diminish only because the two-phase interface departs from classical molecular behavior. Instead, such forces along with present interfacial statistical fluctuations are shown to gradually decrease as the interface transitions through the molecular chaos regime and to diminish once the interface enters the continuum regime. To illustrate the framework, we focus on conditions typical of diesel engine injection. The analysis, however, is quite general and applies to a wide range of modern propulsion and power systems.

## 2. Model formulation

The coupled system of models employed is based on the theoretical-numerical framework developed by Oefelein [28,29]. It provides a detailed mixture state equation for the evaluation of thermodynamic and transport processes in a hydrocarbon mixture. This framework is combined with non-equilibrium mean-field thermodynamics of two-phase interfaces. The formulation is based on the Cahn–Hilliard equation and is shown to converge to the equations of Gradient Theory in the limit of thermodynamic equilibrium.

### 2.1. Thermodynamic and transport properties

A modified 32-term Benedict–Webb–Rubin (BWR) equation of state is applied in conjunction with the extended corresponding states model and non-linear mixing rules to calculate the  $p$ - $v$ - $T$  behavior of multicomponent mixtures [30,31]. This framework has been shown to provide accurate results over a wide range of pressures, temperatures and mixture states, especially at saturated liquid conditions. The thermodynamic properties of real-fluid mixtures 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 pressure correction is then applied using departure functions of the form given by Reid et al. [32, chapter 5]. These functions are exact relations derived using Maxwell's relations (see for example VanWylen and Sonntag [33, 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

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