



Transient behavior near liquid-gas interface at supercritical pressure

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ABSTRACT

Numerical heat and mass transfer analysis of a configuration where a cool liquid hydrocarbon is suddenly introduced to a hotter gas at supercritical pressure shows that a well-defined phase equilibrium can be established before substantial growth of typical hydrodynamic instabilities. The equilibrium values at the interface quickly reach near-steady values. Sufficiently thick diffusion layers form quickly around the liquid-gas interface (e.g., 3–10 μm for the liquid phase and 10–30 μm for the gas phase in 10–100 μs), where density variations become increasingly important with pressure as mixing of species is enhanced. While the hydrocarbon vaporizes and the gas condenses for all analyzed pressures, the net mass flux across the interface reverses as pressure is increased, showing that a clear vaporization-driven problem at low pressures may present condensation at higher pressures. This is achieved while heat still conducts from gas to liquid. Analysis of fundamental thermodynamic laws on a fixed-mass element containing the diffusion layers proves the thermodynamic viability of the obtained results.

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1. Introduction

Liquid fuel injectors are present in many combustion applications. These injectors are designed to optimize the liquid breakup process or atomization, where droplets form and then vaporize and mix with the surrounding gas (i.e., oxidizer), allowing the combustion chemical reaction to occur. Therefore, understanding how this liquid disruption process develops is crucial to obtain a good performance of combustion chambers and engineering applications (e.g., diesel engines, rocket engines).

These combustion chambers often operate at very high pressures, since combustion efficiency is improved and a higher specific energy conversion can be obtained. These pressures can be above the critical pressure of the injected fuel. When this supercritical situation occurs, the thermodynamics and fluid dynamics of the injection phenomena are drastically modified. Since gas readily dissolves in the liquid at high pressures, a new solution is formed typically with a much higher critical pressure than the original liquid. At subcritical pressures, a clear distinction between the liquid and the gas phase exists and the liquid breakup is mainly driven by capillary forces and hydrodynamic instabilities, depending on the fluid properties and configuration of the problem. How-

ever, at high-pressure regimes close or above the critical pressure of the new liquid solution, diffusion can become one of the main drivers of the mixing process and a well-defined liquid-gas interface may not be easily identified [1].

In fact, liquid injected into an environment exceeding its critical properties will undergo a transition to a supercritical thermodynamic state. In this process, the liquid goes through a near-critical state where liquid-like densities and gas-like diffusivities will be present. Consequently, the classical liquid-gas interface seems to disappear even before supercritical conditions are achieved. Furthermore, as the critical point is reached, the liquid-gas density ratio reduces and surface tension approaches zero, increasing the aerodynamic effects on the liquid breakup [2,3]. This situation has often been described with the wrong assumption that the liquid fuel simply transitions to a supercritical gas-like state in a single-phase manner. Experimental results from Mayer et al. [4] show the behavior, but no emphasis is made on whether the observed results correspond to an actual transition of the injected liquid to a supercritical gas-like state or if rapid disruption of the liquid stream due to enhanced aerodynamic effects cause the formation of small droplets, which in turn could not be easily seen in experimental setups.

Recent works from Jarrahbashi et al. [5,6], and Zandian et al. [7,8] present results for the liquid disruption process of incompressible round jets and planar sheets, respectively, when injected into a gas. Simulations with varying Reynolds number and Weber number show that high-speed flows not only can induce a fast breakup process generating small droplets, but also similar

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densities for the liquid and gas phases (i.e., high-density or high-pressure environments) and reduced surface tension can cause a similar behavior. In this scenario, the formation of certain structures is slowed down in favor of another formation process for droplets and an enhanced radial development of the two-phase mixture. These works do not include any treatment of the energy equation or species mixing, but show results likely to be seen in supercritical pressure injection. These results suggest that when the gas-like appearance of the jet is observed, it may still be in a liquid state, instead of a supercritical state of the fuel. Therefore, it becomes necessary to determine the characteristic times of each process (i.e., analyze whether the transition to a supercritical state occurs faster than the liquid disruption cascade or not).

On the other hand, several chemical species are present in real combustion applications, thus modifying completely the fluid behavior. Under supercritical pressure conditions, not only the mixing of vaporized fuel and surrounding gas must be accounted for, but also the gas dissolving into the liquid phase due to phase-equilibrium conditions. This diffusion of species generates a liquid solution and a gas mixture with varying composition around the liquid-gas interface which modifies the fluid properties. That is, mixture critical properties will differ from pure species critical properties. Precisely, critical pressure of the liquid solution will increase close to the interface, even above the chamber pressure in some configurations. In this situation, the transition of the injected liquid to a supercritical state is delayed and a distinguishable two-phase behavior can be maintained. Some experimental results also provided in [4] show that, for configurations including different species, the liquid-gas interface can be restored depending on the local mixture composition, temperature and pressure. Moreover, numerical results provided by Jordà-Juanós and Sirignano [9] show that phase-equilibrium laws together with a real-gas equation of state are able to reproduce the coexistence of two phases at supercritical pressures.

Thus, the modeling of fluid behavior at high pressures becomes the main issue. At this pressure regime, thermodynamic non-idealities should be considered [3,10]. The use of a real-gas equation of state together with fundamental thermodynamic principles to compute fluid properties is suggested. Although a cubic equation of state may not provide the same accuracy as other methods, its use is recommended because of its easy manageability and its capability to predict the liquid-phase solution. Then, transport properties should be computed using high-pressure models, always ensuring that low-pressure solutions can be recovered. It becomes important not to mix non-ideal and complex models with simpler ones, since better accuracy in these fluid states can be lost. For instance, He et al. [11] show the effects of non-idealities on the diffusion process, where the so-called diffusion barrier can be identified.

Phase-equilibrium laws have to be satisfied at the liquid-gas interface and can be combined with an equation of state to predict mixture composition on each side of the interface. However, works by Dahms and Oefelein suggest that phase-equilibrium results should be carefully used at supercritical pressures [1,12,13]. They propose that traditional phase equilibrium can only be applied far enough of the critical point. In the transcritical region, where temperature is approaching its critical value, the liquid-gas interface enters a continuum region. Under this consideration, fluid properties do not experience a discontinuity across the interface, but they evolve continuously. Then, temperature does not become the same on both sides of the interface. Nevertheless, interface thicknesses of the order of a few nanometers are shown, which could be considered as a discontinuity, similar to the practical treatment of shock waves.

The present paper proposes a numerical study of liquid-gas dynamics at high pressures using a non-ideal equation of state

and different models to compute transport properties. Particularly, phase-equilibrium laws are imposed at the liquid-gas interface and the development of a diffusion layer on each side is analyzed to infer if a well-established phase equilibrium exists before typical hydrodynamic instabilities, such as the Kelvin-Helmholtz instability, grow sufficiently to disrupt the liquid jet. That is, if fluid properties vary considerably around the interface, the liquid disruption process may be modified.

The rest of this document is structured as follows. First, the problem configuration and the governing equations, as well as different fluid properties models, are presented in Section 2. Then, the numerical methodology to solve the governing equations and the matching conditions at the liquid-gas interface is introduced in Section 3. An analysis of the obtained results, based on reference mixtures of oxygen (O_2) and *n*-octane (C_8H_{18}) or oxygen and *n*-decane ($C_{10}H_{22}$), is shown in Section 4. Finally, a summary of the main findings concludes the paper in Section 5.

2. Problem statement and governing equations

2.1. Problem definition

A 1-D domain is defined where a liquid composed of pure species B is suddenly introduced into a gas composed of pure species A (see Fig. 1). Pressure is constant throughout the domain and temperature is higher in the gas phase, but without exceeding the critical temperature of the pure liquid species. This temperature difference across the interface can drive the vaporization of the liquid phase. Because of phase equilibrium, gas species A will dissolve in the liquid phase and vapor of species B will mix with the gas. This situation will generate diffusion layers composed of both species; that is, a binary mixture will exist on both sides of the interface. To capture these layers, the domain has to be defined large enough to include them at all times. In other words, it should become numerically infinite.

When supercritical pressures for the liquid are considered, the mixing of species around the interface allows the coexistence of both phases, as the mixture critical pressure becomes higher than the pure liquid critical pressure and may rise above the chamber pressure.

2.2. Governing equations

The governing equations to be solved are the continuity equation, Eq. (1), the species continuity equation, Eq. (2), and the energy equation, Eq. (3). The momentum equation is not needed under the assumptions taken in this and other works [14]. The problem is mainly driven by diffusion forces and fluid velocity becomes very small. Then, momentum flux is negligible compared to the studied high pressures and, together with the constant-pressure assumption, it becomes unnecessary to solve the momentum equation. Only in low-pressure situations this assumption may need to be reconsidered.

The one-dimensional equations in Cartesian coordinates are, in both phases,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0 \quad (1)$$

$$\frac{\partial}{\partial t}(\rho Y_i) + \frac{\partial}{\partial x}(\rho u Y_i) + \frac{\partial}{\partial x}(J_i) = 0 \quad (2)$$

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x}(\rho u h) = \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) - \sum_{i=1}^N \frac{\partial}{\partial x} (J_i h_i) \quad (3)$$

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