



# An investigation of thermodynamic states during high-pressure fuel injection using equilibrium thermodynamics



Lu Qiu\*, Rolf D. Reitz

Department of Mechanical Engineering, University of Wisconsin-Madison, 1500 Engineering Drive, Madison, WI 53706, USA

## ARTICLE INFO

### Article history:

Received 29 November 2014

Received in revised form 22 January 2015

Accepted 31 January 2015

Available online 9 February 2015

### Keywords:

Phase stability

Critical point

Supercritical

Phase transition

Condensation

Multiphase

High-pressure injection

Phase equilibrium

Thermodynamics

## ABSTRACT

A numerical investigation of mixing processes between an injected fuel (an *n*-alkane) and a chamber inert gas (nitrogen) was carried out for high-pressure fuel injection. The objective is to determine conditions for the coexistence of both liquid and gas phases under the typical ambient conditions encountered in diesel engines. A phenomenological investigation was built by coupling phase stability analysis with the energy conservation equation. Phase changes (including separation and combination) are predicted to occur so as to yield the lowest Gibbs free energy. It is also shown that predicted states without considering phase transitions can be very different from the corresponding thermodynamically correct states. By comparing four *n*-alkane/nitrogen mixtures it is shown that the lower limit of the two-phase region occurs at similar temperatures. However, heavy *n*-alkane/nitrogen mixtures have a larger upper limit, and phase separation occurs at higher temperatures. The present model predicts the existence of multiple phases locally in the dense spray jet under high temperature and pressure ambient conditions due to the significant reduction of the mixture temperature caused by vaporization and cooling.

© 2015 Elsevier Ltd. All rights reserved.

## Introduction

Thermodynamic analysis is useful to investigate the state of a mixture, whether in one, two or more phases. Classical equilibrium thermodynamics is founded on the First and Second Laws of thermodynamics. While the First Law is similar to the conservation of energy in fluid mechanics, the importance of the Second Law is often overlooked. Specifically in thermodynamic equilibrium calculations the Second Law plays a crucial role as it presents the one and only criterion that every global stable equilibrium system must obey. For a closed thermodynamic system at specified temperature, pressure and composition, the equilibrium state has the minimum Gibbs free energy (Callen, 1985). Therefore, this principle provides a very crucial phase stability criterion (Gibbs, 1873; Baker et al., 1982; Michelsen, 1982). A number of research works (Li and Firoozabadi, 2012; Haugen et al., 2011; Nghiem and Li, 1984; Okuno et al., 2010) have used phase stability to investigate the complex phase behavior of mixtures, including liquid–liquid and vapor–liquid–liquid phase equilibria. Analogously, there is recent work studying the use of Helmholtz free energy minimization as an alternative phase stability test (Mikyška and Firoozabadi, 2011).

\* Corresponding author.

E-mail addresses: [lqiu4@wisc.edu](mailto:lqiu4@wisc.edu) (L. Qiu), [reitz@engr.wisc.edu](mailto:reitz@engr.wisc.edu) (R.D. Reitz).

One special case of phase stability is the determination of the critical point (CP) lying on the stability limit. Just like for pure species, the CP is defined as the condition at which differences between the vapor and liquid phases vanish so that they can be considered only as one phase. For most pure species CPs can be found from databases, such as the Design Institute for Physical Properties (DIPPR) Rowley et al., 2001. However, it is difficult to tabulate all critical properties for mixtures due to the indefinite mixture composition. Also, the thermodynamically true critical point of a mixture is not a simple linear function of those of its components, such as the pseudo-critical properties used in various empirical correlations (Kreglewski and Kay, 1969; Li, 1971). In fact, in general the CP cannot be presented by an analytical equation in terms of temperature, pressure, volume and composition (Sadus, 1994). Therefore, there is a need to develop robust and efficient methods to calculate critical properties.

Hicks and Young (1977) calculated of CPs for binary mixtures using a stepping method and the CP was identified when there was a sign change. This method was shown to be capable of finding mixture CPs, and the results for a few systems of both equal and unequal size molecules were found to agree well with previous calculations. However, the reliability of the method is questionable for mixtures with more than two components. The earliest work of Gibbs (1876) founded the theoretical basis for rigorous CP calculations. Peng and Robinson (1977) applied Gibbs free energy

minimization to determine the CPs of multicomponent systems with their equation of state (EOS) model. Heidemann and Khalil (1980) presented an alternative method using direct Helmholtz free energy minimization, which was shown to be computationally cheaper. Sadus (1994) presented a thorough review of current methods in calculating CPs, including the critical transition criterion and its formulation. It was concluded that current theories and models can adequately capture the critical behavior for binary mixtures at least qualitatively, but there are still some challenges for ternary and other multicomponent mixtures. A method that can reliably predict mixture CPs called interval analysis was proposed by Stradi et al. (2001).

In computational fluid dynamics (CFD) simulations, species densities, velocity and internal energy are solved from the governing equations of mass, momentum and energy in each numerical cell, while intensive properties like temperature and pressure are determined under the assumption of thermodynamic equilibrium (Amsden, 1989). For ideal gas simulations the calculation is simple since the internal energy is only a single-valued function of temperature, and pressure can then be calculated from the ideal gas law relation. However, the ideal gas law is only valid at very low pressures and cannot be extended to high pressure conditions. To mitigate this insufficiency, real gas EOS models have been applied in advanced CFD simulations (Zong and Yang, 2006; Kim et al., 2011; Park, 2012; Petit et al., 2013), and the internal energy depends on both temperature and pressure. However, the equilibrium state must have the minimum Gibbs free energy, and a single-phase solution may not be able to satisfy this requirement. Thus, extra phases may need to be introduced to lower the Gibbs free energy (Qiu and Reitz, 2014a,b; Qiu et al., 2014a,b). Due to the small sizes of drops in high pressure fuel injection, spray models are generally subgrid-scale formulations, which assume that single, isolated drop correlations can be used to model vaporization and condensation processes. Moreover, the volume occupied by the liquid phase is often neglected. However, the validity of these assumptions is questionable in dense sprays, particularly if the Gibbs free energy of the local system is not tracked.

Newman and Brzustowski (1971) first investigated supercritical injection of carbon dioxide into a supercritical nitrogen environment. Chehroudi (2012) reviewed experimental work in high-pressure injection in liquid rockets. Experiments have shown that when fuel is injected into a chamber with pressure higher than the critical pressure of the fuel, classical liquid jet breakup phenomena diminish as droplets are hard to observe near the jet surface. In contrast, the density gradient across the shear mixing layer is found to reduce significantly as surface tension effects are suppressed, and “finger-like” structures instead of droplets are observed in experiments (Bruno, 2006; Lin et al., 2006; Oschwald et al., 2006; Wu et al., 1996; Chehroudi et al., 2002). Planar laser induced fluorescence has been used to investigate supercritical injection and mixing with the formation of another liquid phase (Roy et al., 2013) and such experiments have been modeled by Qiu and Reitz (2014b). A number of works focus on modeling supercritical flows and fuel evaporation processes under transcritical conditions (Manrique and Borman, 1969; Faeth et al., 1969; Hsieh et al., 1991; Curtis and Farrell, 1992; Zhu and Aggarwal, 2000; Delplanque and Sirignano, 1993; Jia and Gogos, 1992; Sirignano, 2010; Meng and Yang, 2014). Yang (2000) presented a review of transcritical and supercritical vaporization and mixing in liquid-fueled propulsion systems. It has been pointed out that these processes are more difficult to analyze due to thermodynamic non-idealities and transport anomalies in mixing layer development under supercritical conditions (Bellan, 2000; Okong'o and Bellan, 2003; Bellan, 2006; Selle et al., 2007; Okong'o and Bellan, 2010; Masi et al., 2013).

Indeed, the existence of droplets in high-pressure sprays has been questioned (Dahms et al., 2013). In this work, fundamental thermodynamics analysis is applied to examine the thermodynamic states of mixtures during high-pressure fuel injection processes, with a special focus on exploring whether two phases can be present, as often assumed in CFD models.

## Model formulation

### Equation of state

The Peng–Robinson (PR) equation of state (Peng and Robinson, 1976) is used with

$$P = \frac{R_u T}{v - b} - \frac{a}{v(v + b) + b(v - b)} \quad (1)$$

where  $P$  is pressure,  $T$  is temperature,  $v$  is molar volume and  $R_u$  is the universal gas constant (8.314 J/mole K). The two model constants  $a$  and  $b$ , namely the attraction force and volume parameters, are calculated using:

$$\begin{cases} a = 0.457235 \frac{R_u^2 T_c^2}{P_c} \cdot \alpha \\ b = 0.077796 \frac{R_u T_c}{P_c} \\ \alpha = \left[ 1 + \kappa \left( 1 - \sqrt{\frac{T}{T_c}} \right) \right]^2 \end{cases} \quad (2)$$

with  $\kappa$  determined using (Robinson and Peng, 1978)

$$\kappa = \begin{cases} 0.37464 + 1.54226\omega - 0.26992\omega^2, & \omega < 0.5 \\ 0.3796 + 1.485\omega - 0.1644\omega^2 + 0.01667\omega^3, & \omega > 0.5 \end{cases} \quad (3)$$

$T_c$ ,  $P_c$  and  $\omega$  are the critical temperature, critical pressure and acentric factor, respectively. The dimensionless parameter named compressibility factor  $Z$  is calculated as

$$Z = (Pv)/(R_u T) \quad (4)$$

Therefore,  $Z$  can be considered as an indication of the departure from ideal gas behavior. Specifically,  $Z$  is unity for ideal gases, but not for real (non-ideal) gases. In the case of a mixture, the classical one-fluid mixing rule is used with

$$\begin{cases} a = \sum_i \sum_j x_i x_j a_{ij} \\ b = \sum_i x_i b_i \\ a_{ij} = (1 - \delta_{ij}) \sqrt{a_i} \sqrt{a_j} \end{cases} \quad (5)$$

where  $x_i$  is the mole fraction of species  $i$  in the mixture.  $\delta_{ij}$  is the binary interaction parameter between components  $i$  and  $j$ . For the PR EOS, the compressibility factor at the critical point for a pure species is 0.307 (Peng and Robinson, 1976).

### Phase stability

Phase stability analysis determines if a tested phase can stably exist. If not, phase separation occurs and the equilibrium compositions are determined through phase splitting calculations. The present phase stability analysis is based on the stability test of Baker et al. (1982) and Michelsen (1982), which is based on Gibbs' earlier work (Gibbs, 1873). The adopted method is called the tangent plane distance (TPD) method and is calculated using:

$$\text{TPD}(\vec{x}) = \sum_{i=1}^{N_c} x_i \cdot (\mu_i(\vec{x}) - \mu_i(\vec{z})) \quad (6)$$

where  $\vec{x}$  and  $\vec{z}$  are the mole fraction and feeding compositions, respectively.  $\mu$  is the chemical potential and  $N_c$  is the number of components. It has been shown in Ref. (Baker et al., 1982) that a

Download English Version:

<https://daneshyari.com/en/article/7060318>

Download Persian Version:

<https://daneshyari.com/article/7060318>

[Daneshyari.com](https://daneshyari.com)