

A Numerical Model for Flash Boiling of Gasoline-Ethanol Blends in Fuel Injector Nozzles

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ABSTRACT

Fuels are formulated by a variety of different components characterized by chemical and physical properties spanning a wide range of values. Changing the ratio between the mixture component molar fractions, it is possible to fulfill different requirements. One of the main properties that can be strongly affected by mixture composition is the volatility that represents the fuel tendency to vaporize. For example, changing the mixture ratio between alcohols and hydrocarbons, it is possible to vary the mixture saturation pressure, therefore the fuel vaporization ratio during the injection process.

This paper presents a 1D numerical model to simulate the superheated injection process of a gasoline-ethanol mixture through real nozzle geometries. In order to test the influence of the mixture properties on flash atomization and flash evaporation, the simulation is repeated for different mixtures characterized by different gasoline-ethanol ratio. The Homogeneous Relaxation Model (HRM) is used as non-equilibrium two-phase model. As equation of state, the Peng Robinson equation is considered. Non-ideal thermodynamic properties are considered for the gasoline-ethanol blends. About the gasoline, a binary surrogate is used. The thermodynamic saturation properties of the multi-component blends are calculated by using fugacity and standard mixing rules for the cubical equation of state. The proposed 1D model is validated against experimental data available in literature.

The simulation results reveal as the azeotropic behavior of the mixtures characterized by a medium-low ethanol concentration affected the mixture superheating degree influencing the flash evaporation and effervescent atomization outside the nozzle exit. These results can be used

to improve initial condition for 3D CFD Lagrangian spray simulations especially when the spray targeting plays a fundamental role as for the Gasoline Direct Injection (GDI) engine.

INTRODUCTION

Nowadays, the main focus about IC-Engine development is how to increase the overall engine efficiency reducing emissions and fuel consumption. From this point of view, the injection system plays a fundamental role for both Diesel and gasoline engines because the combustion efficiency strongly depends on penetration, diffusion, and break-up of the liquid jet. In particular, the relation between penetration and break-up influences the IC-Engine architecture, especially when the fuel is injected directly into the combustion chamber. At present, the formation of the spray in DI-engines is obtained by forcing the liquid fuel into the combustion chamber by using pressures of the order of 100 bar, through multi-hole or swirl atomizers. Aerodynamic interactions will eventually break up the liquid jet into a cloud of small droplets. The use of high pressure injectors confers high velocity to the droplets generating the risk of liquid fuel impingement on piston and cylinder wall, which leads, among other problems, to the formation of unburned hydrocarbon emissions.

The idea to promote the generation of a low penetrating and fast vaporizing fuel spray has driven the research toward the possibility to promote the thermodynamic break-up of the liquid jet during the injection [1,2,3]. Thermodynamic break-up happens when the liquid pressure inside the nozzle drops below its saturation pressure at injection temperature allowing the nucleation of bubbles into the liquid core that, growing rapidly, could produce the so called 'effervescent atomization' just outside the nozzle exit. As consistently reported in literature [4], by the thermodynamic break-up it is possible to generate smaller droplets as by the mechanical

break-up. Thermodynamic break-up is thermally driven and depend on the superheating degree of the fuel during the injection process.

Figure 1 shows a schematic representation of injection processes (from pressure P_0 to pressure P_1) through a short nozzle, simplified with a vertical straight line at constant temperature. A superheated fuel injection process ($b-b_1$) is compared to a sub-cooled injection process ($a-a_1$). During a superheated injection process, the fuel reaches a metastable state (b_1 in figure 1) that represents a non-equilibrium thermodynamic state for the liquid because it does not reside on the saturation pressure curve. If vapor phase is generated in this case, the velocity at which the fuel adjusts to its equilibrium temperature (same temperature between liquid and vapor phases) does not necessarily correspond to the velocity at which fuel is depressurized. Indeed, a time for nucleation and a time for bubble growth are required during this process. The sum of these two times represents the delay of the liquid in reaching its thermodynamic equilibrium, (b_2 in figure 1) and it is called relaxation time. The excess of liquid enthalpy is responsible for the bubble growth which takes place at constant pressure. The closer the point b_1 is to the spinodal limit, the more explosive the evaporation is. If the issuing time through the nozzle is comparable to the relaxation time of the fuel, this condition might trigger flash evaporation or flash boiling within the nozzle or just outside the nozzle exit section, influencing the overall flow and spray characteristics, thus affecting the mixture formation and the combustion performances.

Chang and Lee [1] suggested the idea of inducing thermodynamic break up during the fuel injection process in order to reach a greater liquid atomization by heating the fuel or increasing nucleation sites within the liquid. According to them, these approaches result in numerous practical problems, such as pyrolysis, which will lead to formation of carbon deposit within the nozzle or soot formation in the combustion chamber and through the exhausts. In order to reduce the environmental impact of the IC-engines, in recent years also numerous alternative fuels are being studied. For example, alcohol fuels such as ethanol, burn cleaner than standard gasoline, producing less CO and NO_x, and its use in conventional IC-engines requires minor modifications [6]. Ethanol can be used also as a blending component of the fuel, producing lean combustible mixtures which have higher octane number and can increase the engine efficiency compared to conventional hydrocarbon fuels. Alcohols are usually lighter and have higher volatility compared to most hydrocarbons. Ethanol is highly volatile compared to heptane or octane, but usually less volatile compared to other important gasoline components such as 2-methylbutane. Generally, the fuel volatility depends primarily on the boiling point and the saturation pressure of the constituents. Furthermore the volatility of a commercial gasoline is usually

controlled by additives, or by adjusting the components according to regulations and seasons. It is well known that blends of gasoline and ethanol in low percentages of ethanol (20 %) gives result to azeotropic mixtures, which vapor pressure can be higher than the vapor pressure of the pure components.

The present study proposes a multi-component 1D flash boiling model by which it is possible to model the thermodynamic break-up of mixtures between gasoline and ethanol. The modeling of such a process involves thermodynamic non-equilibrium for describing the phase-change. In the present work the Homogeneous Relaxation Model (HRM) in the form proposed by Downar-Zapolski is used. This approach was successfully employed by other authors [5]. The HRM is validated considering single-component conditions, using experimental data for water flashing flows available in literature. In this work, a gasoline surrogate based on two of the most important constituent for commercial gasoline is defined [7,8]: 2-methylbutane 64% and heptane 36%. The thermodynamic state of single and multi-component fluids is described by the Peng-Robinson Equation of State (PR-EOS). The saturation pressure of the non-ideal gasoline-ethanol blend is calculated using experimental activity coefficients from literature. The insurgence of flash evaporation within a cylindrical injector nozzle is investigated for different fuel blends, and the evaporation of the superheated atomized droplet is also discussed.

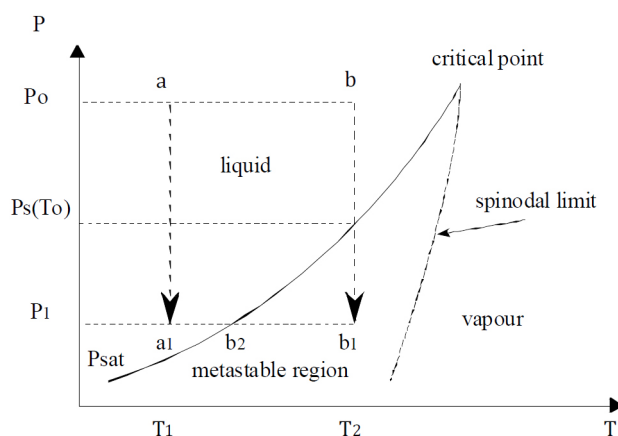


Figure 1. In a superheated injection process, $b-b_1$, the liquid is depressurized below the saturation curve and enters the metastable region.

FLASH EVAPORATION OF MULTI-COMPONENT FUEL

THERMODYNAMIC STATE CALCULATION

To calculate the fuel thermodynamic properties, the cubical Peng-Robinson Equation of State (PR-EOS) is considered. By [equation \(1\)](#), the pressure is expressed as the sum of a repulsive and an attractive term

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

The use of this cubic equation of state allows calculating the fluid densities in sub-critical, critical, and supercritical conditions, obtaining more satisfactory results dealing with hydrocarbon fuels rather than polar substances. Nevertheless, this equation is well suited for a wide variety of compounds and its popularity in petroleum calculations justifies its use in the present study. An analysis of PR-EOS errors in the evaluation of pure substance properties is proposed in this section as well. [Equation \(1\)](#) can be rewritten in terms of compressibility factor Z

$$Z^3 - (1 - B)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0 \quad (2)$$

where

$$A = \frac{aP}{R^2T^2} \quad (3)$$

$$B = \frac{bP}{RT} \quad (4)$$

$$Z = \frac{Pv}{RT} \quad (5)$$

[Equation \(2\)](#) generates either one or three roots depending on the number of phases in the system. Dealing with physical quantities only real roots are of interest. In the case of a two phase solution the largest root is the compressibility factor for the vapor phase while the smallest positive root is the compressibility factor for the liquid phase. The intermediate root is not computed as it is physically meaningless. The coefficients for [equations \(2, 3, 4, 5\)](#) are obtained applying [equation \(1\)](#) at the critical point

$$a(T) = a(T_c)\alpha(T_r, \omega) \quad (6)$$

$$a(T_c) = 0.45724 \frac{R^2T_c^2}{T_c} \quad (7)$$

$$\alpha(T_r, \omega) = \left(1 + k(1 - \sqrt{T_r})\right)^2 \quad (8)$$

$$k(\omega) = 0.37464 + 1.54226\omega - 0.26992\omega^2 \quad (9)$$

$$b = 0.7780 \frac{RT_c}{P_c} \quad (10)$$

where α is a dimensionless function of reduced temperature (T_r) and acentric factor (ω). α is equal to unity at the critical temperature. k is a characteristic constant of each substance and it was correlated to ω [9]. [Figure 2](#) shows the typical S-shaped sub-critical isotherm curve calculated by the cubic equation of state. [Table 1](#) shows the thermodynamic properties of the fluids that are used in the present work.

Table 1. Thermodynamic parameters for the Peng-Robinson equation of state

	heptane	2-methyl-butane	ethanol
Formula	C7H16	C5H12	C2H6O
Boiling T @ Patm [K]	371.6	300.9	351.5
Triple point T [K]	182.6	113.3	159.1
Critical Pressure Pc [MPa]	2.740	3.381	6.360
Critical Temperature Tc [K]	540.1	461.0	515.8
Critical Compressibility Factor Zc [-]	0.262	0.272	0.240
Molar Weight [kg/mol]	100.2e-3	72.15e-3	46.07e-3
Acentric Factor w [-]	0.349	0.229	0.644

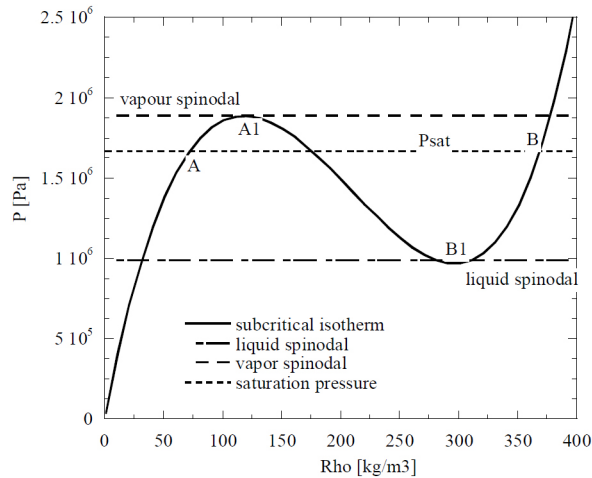


Figure 2. Example of subcritical isotherm obtained with the Peng-Robinson cubical equation of state.

Physically, in any isothermal process the changes in fluid pressure and density must have the same sign, thus the following mechanical stability condition must be respected

$$\left(\frac{\partial P}{\partial \rho}\right)_T > 0 \quad (11)$$

Considering the isotherm curve of [Figure 2](#), this requirement is met by the gas branch up to point A as well as the liquid branch starting from point B. In the two-phase region, this criteria is satisfied as well within the vapor saturation point A and the relative maximum A₁, and from the relative minimum B₁ and the liquid saturation point B. The section included between the relative maximum A₁ and the relative minimum B₁ of the pressure is regarded as meaningless and unphysical, while portions of vapor above and portion of liquid below the saturation pressure can be experimentally obtained for metastable states. The latter aspect is important because allows the model to calculate the density from pressure for a superheated fuel, assuming local metastable equilibrium. The saturation pressure is constrained between the two relative extremes, A₁ and B₁.

The fugacity approach is used to calculate the saturation pressure. For pure substances the formulation proposed by Peng and Robinson [9] is adopted

$$\ln \frac{f}{P} = Z - 1 - \ln(Z - B) - \frac{A}{2\sqrt{2}B} \ln \left(\frac{Z + 2.414B}{Z - 0.414B} \right) \quad (12)$$

where f is the fugacity of the considered phase, Z is the compressibility factor, and the coefficients A and B are obtained by [equations \(3\) and \(4\)](#). At equilibrium, the fugacity of the vapor phase must be equal to the fugacity of the liquid phase.

$$f^L = f^V \quad (13)$$

This relation is satisfied by using a convergence criterion [9], iterating from the critical point to the triple point. The pressure corresponding to this condition is the vapor pressure.

In the present work the calculation of thermodynamic extensive property of real fluids is considered. The enthalpy departure function is here used to calculate the difference between the real fluid enthalpy and the ideal gas enthalpy (identified by a star superscript) [9]

$$h - h^* = RT(Z - 1) + \frac{T \frac{da}{dT} - a}{2\sqrt{2}b} \ln \left(\frac{Z + 2.414B}{Z - 0.414B} \right) \quad (14)$$

The enthalpy per mass unit H can be obtained multiplying the molar enthalpy h by the number of moles per mass unit, which is the inverse of the molar weight M_w ,

$$H = \frac{1}{M_w} \left[h^*(T) + RT(Z - 1) + \frac{T \frac{da}{dT} - a}{2\sqrt{2}b} \ln \left(\frac{Z + 2.414B}{Z - 0.414B} \right) \right] \quad (15)$$

The ideal molar enthalpy is calculated as a function of the temperature by using a polynomial function as proposed by McBride et al. [10]

$$\frac{h^*(T)}{RT} = a_1 + \frac{1}{2}a_2T + \frac{1}{3}a_3T^2 + \frac{1}{4}a_4T^3 + \frac{1}{5}a_5T^4 + \frac{b_1}{T} \quad (16)$$

[Table 2](#) summarizes the coefficients used for [equation \(16\)](#) relative to the working fluids. The last row reports the enthalpy of formation at 298 K. [Figure 3](#) shows enthalpy for n-heptane calculated by using the PR-EOS at a pressure equal to 1 bar and the reference ideal enthalpy obtained by [equation \(16\)](#). Once the vapor and liquid saturated non-ideal enthalpies are calculated from the triple point to the critical point, the latent heat of vaporization can be simply obtained by difference of the two curves. This calculation is done for the whole subcritical range of temperatures and is plotted for 2-methylbutane and ethanol as well in [Figures 4 and 5](#). The difference in the latent heat of vaporization between the alcohol and the two alkenes appears evident from the plots. [Figure 6](#) shows the saturation pressure for the three single component fuels, in the temperature range of interest for the present study. In the same plot an horizontal line is traced in correspondence of the atmospheric pressure to help locate each boiling point reported in [table 1](#).

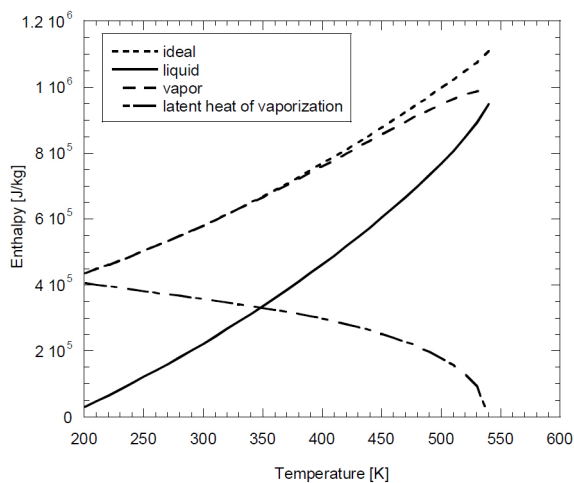


Figure 3. Ideal and real enthalpies, and latent heat of vaporization for n-heptane, calculated using the Peng-Robinson EOS.

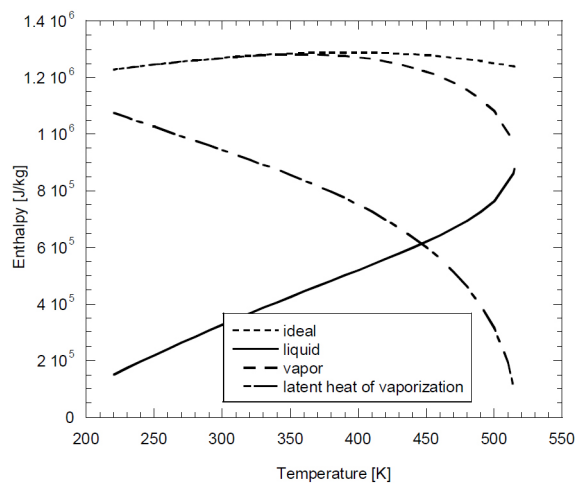


Figure 5. Ideal and real enthalpies, and latent heat of vaporization for ethanol, calculated using the Peng-Robinson EOS.

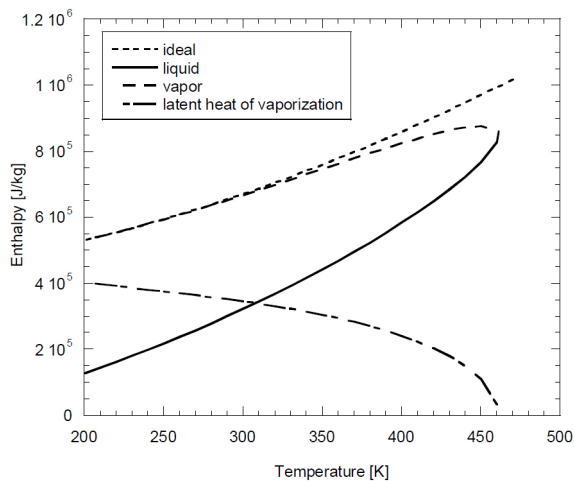


Figure 4. Ideal and real enthalpies, and latent heat of vaporization for 2-methylbutane, calculated using the Peng-Robinson EOS.

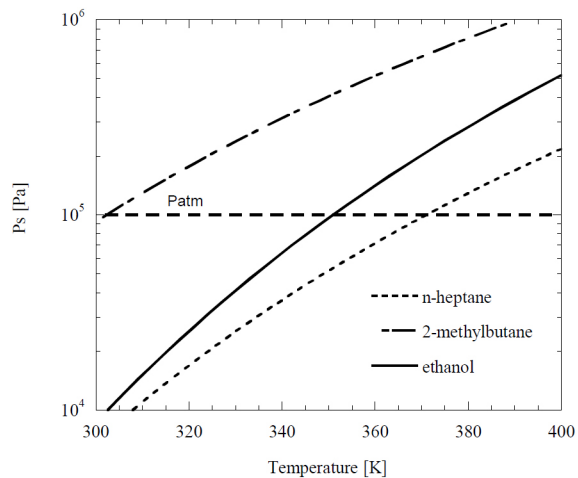


Figure 6. Saturation pressures in the temperature range of interest for n-heptane, 2-methylbutane and ethanol.

Table 2. Coefficients for the polynomial relation proposed by McBride et al. [10] for $T < 1000$ K.

	heptane	2-methylbutane	ethanol
a1	1.11532484e01	1.08328820	4.8586817
a2	-9.49415433e-03	4.45710760e-02	-3.74006740e-03
a3	1.95571181e-04	8.23899340e-06	6.95550267e-06
a4	-2.49752520e-07	-3.52580470e-08	-8.86541147e-08
a5	9.84873213e-11	1.57857620e-11	3.51684430e-11
b1	-2.67711735e04	-2.08075350e04	-2.99961309e+04
H298/R	-2.25870196e+04	-1.84859760e04	-2.82578288e+04

ACCURACY OF PREDICTIONS USING THE PR-EOS

Saturation pressure and latent heat of vaporization for heptane, 2-methylbutane, and ethanol are compared with experimental data, mainly from National Institute of Standard and Tehnology (NIST) [11] using statistical tools. Defining the percentage deviation between the calculated and the experimental value as

$$d_i = 100 \frac{i_{exp} - i_{eq}}{i_{exp}} \% \quad (17)$$

the average absolute deviation (AAD), the bias (BIAS), the standard deviation (SDV), and the root mean square deviation (RMS) can be calculated respectively as

$$AAD = \frac{1}{n} \sum |d_i| \% \quad (18)$$

$$BIAS = \frac{1}{n} \sum d_i \% \quad (19)$$

$$SDV = \sqrt{\frac{\sum (d_i - BIAS)^2}{n-1}} \% \quad (20)$$

$$RMS = \sqrt{\frac{1}{n} \sum (d_i)^2} \% \quad (21)$$

where n is the number of data points. Values from the PR equation are calculated every 10 K, from the triple point to the critical temperature. Values corresponding to saturation

pressures below 100 Pa were neglected because too close to the arbitrary convergence criterion used in the fugacity numerical approach. Only 4 useful data points were found instead to compare ethanol's latent heat of vaporization. Nevertheless, deviations from experimental data are found to be contained and uniform. Overall results are shown in tables 3 and 4. Table 3 shows an overall good agreement about the predictions of vapor pressure, being the deviations for 2-methylbutane, heptane, and for ethanol respectively 3.15 %, 3,62 % and 5,20 %.

Table 3. Comparison between vaporpressure predictions versus experimental data from literature.

		AAD%	BIAS%	RMS%	SDV%
Substance	data points	PR	PR	PR	PR
C5H12	27	3.15	-1.31	6.33	6.31
C7H16	31	3.62	-3.62	7.73	6.94
C2H6O	27	5,20	-2,72	5,75	5,16

Table 4. Comparison between latent heat of vaporization predictions versus experimental data from literature.

		AAD%	BIAS%	RMS%	SDV%
Substance	data points	PR	PR	PR	PR
C5H12	33	1.87	1.07	4.54	4.46
C7H16	31	1,58	0,52	1,95	1,94
C2H6O	4	11,90	11,90	13,98	8,46

Table 4 shows very accurate predictions for latent heat of vaporization for the alkenes, which errors are below 1,9%, but wider errors for ethanol, also due to the lack of experimental data.

A further analysis of these thermodynamic parameters is proposed within a typical working temperature range of a GDI fuel injection system. Variables are plot in the temperature range 260 K - 400 K. Errors on calculations of saturation pressure and latent heat of vaporization are analyzed as function of temperature in the selected range and plotted in Figure 7 and 8. It can be seen that the PR-EOS performs better with increasing T for the hydrocarbons while the alcohol present a variable error. It must be pointed out also that even if only few points were found to evaluate latent heat of vaporization for ethanol, results have been found comparable to other fuel libraries such as the one implemented in KIVA. Overall errors become particularly low in our sub-range of interest, which is $300 \text{ K} < T < 380 \text{ K}$.