



Experimental and numerical analysis of iso-octane/ethanol sprays under gasoline engine conditions



P. Keller^{a,*}, T. Knorsch^b, M. Wensing^b, C. Hasse^a

^a Chair of Numerical Thermo-Fluid Dynamics, Department of Energy Process Engineering and Chemical Engineering, Technische Universität (TU) Bergakademie Freiberg, Germany

^b Department of Engineering Thermodynamics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

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ABSTRACT

High pressure sprays under gasoline engine conditions are studied in a high pressure/high temperature constant volume chamber using a combined experimental and numerical approach. Both pure iso-octane and ethanol as well as their mixtures are considered. The aim of this work is to investigate the differences between the single component sprays and to identify how the spray structure changes for multicomponent fuels. Especially the influence of the azeotropic behavior of iso-octane/ethanol mixtures on the differential evaporation and the resulting vapor formation is considered. Experimental techniques include Phase-Doppler Anemometry (PDA), shadowgraphy and Schlieren measurements and results are reported for the droplet size distribution, the liquid and the vapor distribution, respectively. The numerical investigations use both a single droplet model as well as 3D spray simulation. In both numerical approaches, the thermodynamic description of the vapor–liquid equilibrium (VLE) at the droplet surface takes into account non-ideal effects for multicomponent mixtures. Liquid activity coefficients are described using the non-random two-liquid (NRTL) approach.

First, the results for pure iso-octane and ethanol sprays for two operating points are presented with good agreement between numerical and experimental results. The differences in penetration between the two fuels are discussed. Afterwards, two binary iso-octane/ethanol mixtures, E10 and E85, respectively, are investigated for the same two operating points as for the pure component fuels. Starting from single droplet studies, the differential evaporation behavior is discussed especially with respect to the thermodynamic model. The influence of the azeotrope on droplet evaporation is investigated in detail and significant differences are found for the components' volatility. The resulting differences in the differential evaporation behavior are quantified using two factors, the differential evaporation and the separation factor, respectively. Using the same thermodynamic model, results from the full 3D simulation for the two mixtures are presented. The resulting fuel vapor distributions and the liquid compositions are analyzed and the influence of the azeotrope is discussed. The differential evaporation and separation factor are presented and it is shown that they are both suitable for quantitative analysis since their values are directly comparable between the single droplet and the 3D spray simulation.

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1. Introduction

In order to reduce emissions and to meet legislative requirements, direct injection is widely utilized in modern engines and its importance is still increasing. It was first introduced for diesel engines and now more and more gasoline engines are developed with direct injection replacing port fuel injection. Directly providing the fuel into the combustion chamber gives a number of opportunities to develop novel combustion concepts, which rely e.g. on mixture stratification. Thus, the combustion is not only influ-

enced by the overall stoichiometry or total mass of fuel injected but also by the fuel distribution inside the cylinder. The latter is directly influenced by the spray structure, the evaporation of the multicomponent fuel and the subsequent mixing in the gas phase. Understanding these processes from spray formation to start of combustion along the non-linear cause-and-effect chain has become crucial.

In the development and assessment of new combustion concepts, CFD has become an important tool to gain insight into these complex processes. Simulation techniques, often combined with advanced optical measurements, can provide information such as the local fuel distribution. However, the reliability of the numerical prediction directly depends on the employed submodels and their

* Corresponding author.

E-mail address: Peter.Keller@tec.tu-freiberg.de (P. Keller).

Nomenclature

Greek symbols

α	heat transfer coefficient [W/(m ² K)]
D_{eff}	effective thermal diffusivity [m ² /s]
α_{12}	separation factor –
τ_{ij}	NRTL binary coefficients –
σ	stress tensor [kg(m s ²)]
γ_i	activity coefficient of component i –
λ	thermal conductivity [W(m K)]
Ω_i	fractional evaporation rate $\Omega_i = \dot{m}_i/\dot{m}_F$ –
$\tilde{\rho}_i^s$	evaporation source term [kg(m ³ s)]
ρ_g	gas phase density [kg/m ³]
σ	surface tension [kg/s ²]
α_{ij}	NRTL binary coefficients –
θ_i	gas phase correction of component i –

Latin symbols

$\Delta h_{v,i}$	latent heat of vaporization of component i [J/kg]
Δt_d	droplet life time [s]
\dot{m}_F	overall fuel evaporation rate [kg/s]
\dot{m}_i	evaporation rate of component i [kg/s]
\dot{q}_l	inner droplet heat flux [W]
\mathbf{g}	specific body force [m/s ²]
\mathbf{u}_d	droplet velocity [m/s]
$\overline{Q^s}$	heat transfer source term [kg/(m s ³)]
$\overline{\mathbf{F}^s}$	spray momentum source term [kg/(m ² s ²)]
\overline{p}	pressure [kg/(m s ²)]
\overline{w}_i	differential evaporation factor of component i –
$\tilde{\mathbf{u}}$	Favre-averaged gas velocity [m/s]
\tilde{h}_s	sensible enthalpy [J/kg]
\tilde{k}	kinetic energy [m ² /s ²]
A_{ij}, \dots, D_{ij}	NRTL binary coefficients –
B_m	Spalding mass transfer number–
C_d	droplet drag coefficient –
c_p	heat capacity [J/(kg K)]
d	droplet radius [m]

α_{eff}	effective thermal diffusivity [m ² /s]
D_{im}^s	gas phase diffusion coefficient [m ² /s]
G_{ij}	NRTL binary coefficients –
K_i	equilibrium constant of component i –
L	latent heat of vaporization $L = \sum_i \Omega_i \Delta h_{v,i}$ [J/kg]
M_i	molar weight of component i [kg/mol]
N_p	number of droplets per parcel –
$p_{\text{vap},i}$	vapor pressure of component i [kg/(m s ²)]
r	radial coordinate $r_s \leq r < \infty$ [m]
r_s	droplet radius [m]
T	temperature [T]
V	cell volume [m ³]
$V_{m,l}$	liquid phase molar volum [m ³ /mol]
X_i	mole fractions –
$Y_{F,s}$	sum of fuel vapor mass fractions at the droplet surface –
$Y_{i,l}^0$	initial liquid phase mass fraction of component i –
$Y_{i,v}$	vapor mass fraction of species i –
Le	Lewis number $Le = \lambda_g / (c_{p,g} \rho_g D_{im}^s)$ –
We	Weber number $We = \rho_g u_{\text{rel}}^2 d / \sigma$ –

Subscripts

∞	gas, sufficiently far from surface
d	droplet
F	fuel
g	gas phase
l	liquid
m	mixture
s	surface
v	vapor
rel	relative
vap	vapor

Superscripts

(n)	time step
g	gas phase
s	source term

combination. Realizing that real fuels are multicomponent mixtures containing aromatics and iso-/n-alkanes among others, the accuracy of evaporation modeling strongly depends on the thermodynamic description of vapor–liquid equilibrium (VLE) [1–5]. With the introduction of biofuels, alcohols such as ethanol are now often mixed with gasoline. In the context of evaporation, this is particularly important since the real behavior of mixtures of alcohols, aromatics, iso- and n-alkanes is non-ideal and even azeotropes are observed. This does not only affect the boiling temperature but also the vapor composition [5]. Specifically looking at the liquid phase, non-idealities are often described either using equations of state (EOS) models to obtain the fugacity coefficients or with excess Gibbs energy models to determine the activity coefficients. For the latter, two popular choices are the Universal Quasi-chemical Functional Group Activity Coefficients (UNIFAC) or the non-random two-liquid method (NRTL), which is used in this work.

Despite the importance of non-ideal effects, many CFD studies of multicomponent sprays, based either on discrete components or continuous thermodynamics, use an ideal description of the VLE known as Raoult's law, see e.g. [6–10]. Recently, first detailed studies incorporating non-ideal effects into CFD were published [3,4,11–14].

The current study investigates the spray and mixture formation under gasoline engine conditions for pure iso-octane and ethanol as well as their mixtures in a combined numerical and experimen-

tal approach. The focus is to understand the difference between the single component sprays first. Following that, the influence of the thermodynamic modeling for the binary mixtures is studied. The simulations analyze single droplet evaporation and the 3D spray processes based on the Lagrangian model. The experiments provide important information about the macroscopic quantities vapor and liquid penetration as well as detailed information such as the droplet size distribution. This data is used for direct comparison with the numerical results.

The paper is structured as follows. In Section 2 the equations for the single droplet and the 3D CFD model using the Lagrangian approach are given including a short summary of the VLE approach. In Section 3 the experimental and numerical setup are described. The experimental and numerical results both for pure substances and different mixtures considering two operating conditions are presented in Section 4.

2. Model formulation

In this study, results both for single droplet calculations (called OD, since the droplet is assumed to have uniform temperature and composition) and full 3D simulation using the Lagrangian particle approach are reported in Section 4. Since the Lagrangian model is based on a single droplet point of view, we introduce the OD modeling approach first.

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