

## Effects of ambient vapor concentration on ethanol evaporability

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### Keywords

Ethanol, Droplet evaporation, Ambient vapor concentration, Lagrangian model, Numerical simulation.

## 1. INTRODUCTION

In 2012, fossil fuels accounted for 84 % of worldwide energy consumption. In 2040, even with the increase in renewable and nuclear energy, predictions have shown that fossil fuels will still account for 78 % of energy use (IEA, 2016). However, there is a huge concern over greenhouse-gas emissions and petroleum scarcity that motivates a search for alternative fuels. In this context, ethanol is considered a clean, efficient, and affordable energy source solution. Ethanol may be considered the most widely used biofuel in the world, concentrating its largest production in the U.S.A., followed by Brazil. In 2017, these two countries accounted for about 84% of the total global fuel ethanol production, which was approximately 87 billion liters (RFA, 2017).

Droplet evaporation plays a crucial role in liquid-fueled combustion devices. Basically, the liquid fuel jet is injected and atomizes into several droplets to generate a polydisperse spray, which evaporates in the hot gaseous medium. Then, the fuel vapor mixes with the oxidant and burns. In this context, accurate droplet evaporation prediction is essential to correctly model spray combustion. Therefore, the purpose of this study is to investigate the ambient mass fraction of fuel vapor impacts in the ethanol evaporability, mimicking the usual in certain practical situations, by means of numerical simulations. First, the predictions of the evaporation model are validated by comparison with experimental measurements, and, then, the ambient vapor concentration is varied in the ranges of 0.0-0.75 to investigate the effects of ambient conditions on the droplet evaporation for low and high temperatures.

## 2. DIFFERENTIAL-ALGEBRAIC MATHEMATICAL MODEL

Mass and thermal energy transfer processes are described by differential equations, which express the temporal changes of droplet size and temperature:

$$\frac{dm_d}{dt} = -\dot{m}_d, \quad (1)$$

where  $m_d$  is the droplet mass and  $\dot{m}_d$  is the droplet mass evaporation rate that leads directly to droplet size reduction:

$$\frac{dD_d}{dt} = -\frac{2\dot{m}_d}{\pi\rho_l D_d^2}, \quad (2)$$

where  $D_d$  is the droplet diameter,  $\rho$  stands for density and the subscript  $l$  refers to the liquid phase, and:

$$m_d c_{p,l} \frac{dT_d}{dt} = Q_s, \quad (3)$$

where  $c_p$  is the specific heat capacity and, as previously mentioned,  $Q_s$  is the power transferred to promote the droplet thermal energy variation per unit of time, which is transferred as heat. The Abramzon-Sirignano evaporation model (ASM), which was proposed by Abramzon & Sirignano (1989), was adopted to represent the mass and energy transfers between the liquid and gaseous phases.

## 3. NUMERICAL AND COMPUTATIONAL MODELS

The evaporation models presented were implemented in the in-house code MFSim and it was used for the computations conducted. The 4<sup>th</sup> order Runge-Kutta method is used in time discretization to predict the temporal advancement of droplet size and temperature (Eqs. 2 and 3). Additionally, all the thermodynamic and transport properties used during the simulations are computed with the open source package Cantera.

## 4. RESULTS AND DISCUSSION

### 4.1. Validation

The ASM predictions are compared with the experimental measurements of Saharin et al. (2012) for anhydrous ethanol droplets. The fuel droplets with initial diameter between 430 and 609  $\mu\text{m}$  were supported in a cross-fiber system. In all experiments the ambient pressure was kept atmospheric and under normal gravity condition, while the temperature varied from 473 to 673 K. In Figure 1, comparisons of the normalized squared droplet diameter temporal evolution obtained with the numerical simulations and the experimental data are compared. This figure does not exhibit the droplet heat-up period for any ambient temperature due to limitations of the experimental procedure, only presenting the well-known  $D^2$  law, in which the droplet surface area varies linearly with time.

Experimental data presented in Fig. 1 exhibits a deviation from the linear  $D^2$  as the droplet diameter decreases due to the interference of water vapor from the ambient in the anhydrous ethanol droplet evaporation, which is caused by the hygroscopic nature of this short carbon chain alcohol. However, this effect gradually decreases as the ambient temperature is increased. Therefore, considering only the initial curve slope that actually represents pure ethanol evaporation, it can be concluded that the numerical results are in good agreement with the measurements for the whole range of temperature studied. The deviation between the numerical and experimental results might be justified by the simplifications assumed in the mathematical model and uncertain factors associated to the experimental data, as the calculation error in determining the droplet diameter by analyzing images, which is of the order of  $\pm 3\%$ , and the fact that the droplet initial temperature is not clear stated by Saharin et al. (2012).

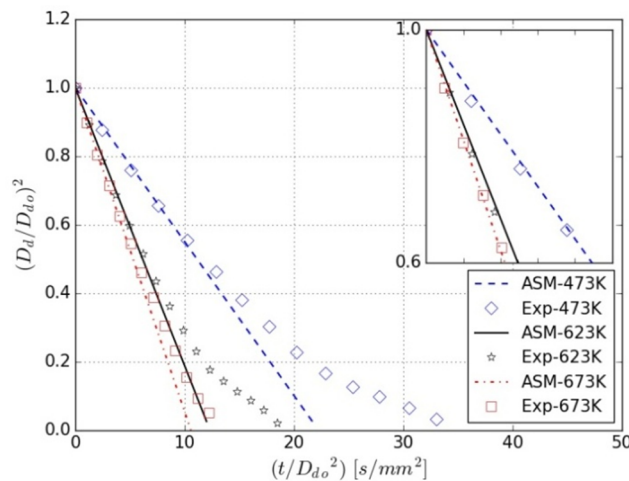


Figure 1: Comparison between numerical and experimental results for droplet diameter temporal variation.

### 4.2. Effects of ambient vapor concentration

It is already known from previous investigations that the evaporation process is highly influenced by ambient conditions, as vapor concentration and temperature (Abarham & Wichman, 2011). These two parameters should be analyzed together to determine the evaporation characteristics of a certain fuel. The results for ethanol droplet evaporation under atmospheric pressure, with initial temperature and diameter of 300 K and 500  $\mu\text{m}$  are shown in Figs 2 and 3.

From Figure 2 it is observed that when ambient fuel vapor mass fraction is non-null, condensation effects is observed as an increase in the droplet diameter before its evaporation. Even though for the high-temperature case the condensation effect is attenuated, one can still detect that those effects became more important as the ambient fuel vapor mass fraction increases.

Investigations based on the results presented in Fig. 3 have shown that there is a threshold ambient temperature that determines whether the area reduction rate, as well as the droplet evaporation time, will increase or decrease as the ambient vapor concentration is enhanced. This behavior can be explained by the existence of two competing factors that influence the evaporation process.

First, increasing the ambient vapor concentration reduces the mass transfer, more specially due to mass diffusion reduction, decreasing the Spalding mass transfer number and, consequently, the area reduction rate is reduced, causing the evaporation time increase. Second, increasing the ambient vapor concentration might enhance the energy transfer depending on the ambient temperature, increasing the Spalding energy transfer number and, as a result, the area reduction rate is augmented, causing the evaporation time reduction.

Hence, the way the area reduction rate of pure fuel droplets is influenced by the ambient vapor concentration is determined by the net result of those two factors. For ambient temperatures below the threshold temperature, the first factor predominates. However, when the ambient temperature is higher than the threshold temperature, the second factor has a stronger impact on the area reduction rate. As can be observed in Fig. 3, the first factor predominates for ambient temperature equals to 400 K, since the area reduction rate decreases as the ambient vapor concentration increases. However, for 1000 K the behavior is actually the opposite.

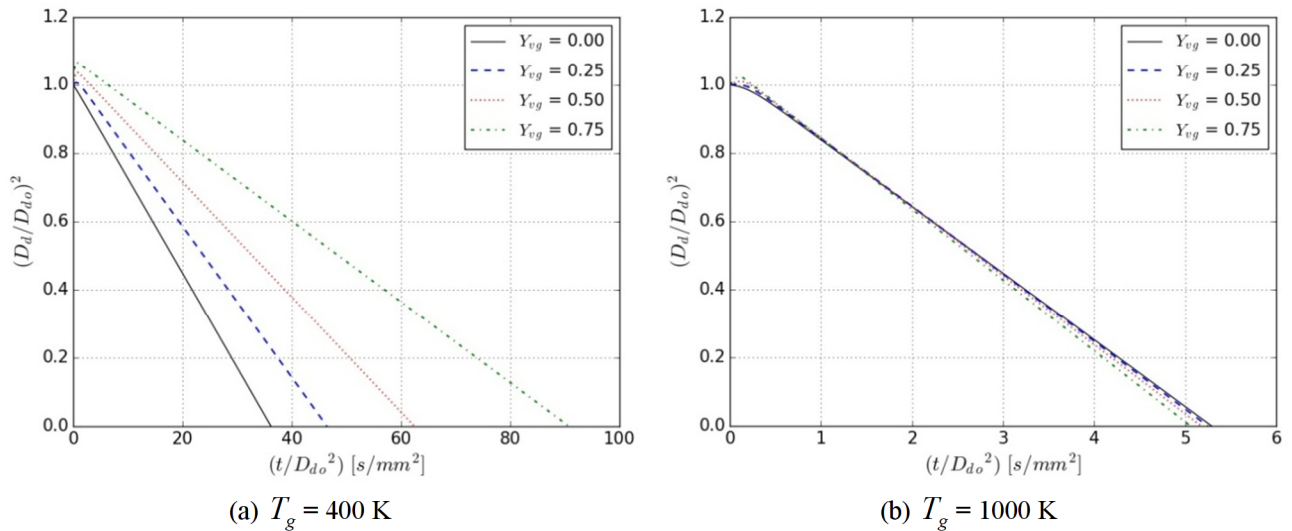


Figure 2: Comparison of droplet diameter temporal variations for several ambient mass fraction of fuel vapor.

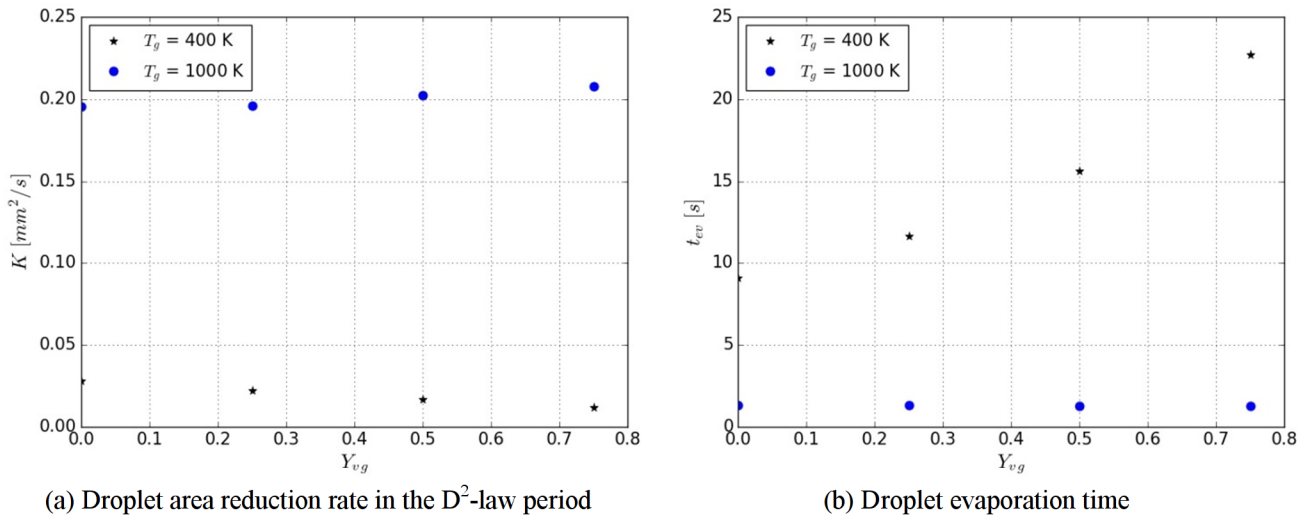


Figure 3: Droplet parameters for several ambient mass fraction of fuel vapor under different ambient temperatures.

## 5. CONCLUSION

The effects of ambient vapor concentration on ethanol evaporability depend on the ambient temperature.

## 6. ACKNOWLEDGEMENTS

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