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Numerical investigation of ethanol and acetone spray injection into gaseous environment

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ABSTRACT: In this paper, the effect of evaporating sprays of ethanol and acetone injected into a cylindrical gaseous environment is numerically investigated. To make this investigation the Eulerian gas phase equations together with the Lagrangian liquid phase equations are solved assuming a two-way coupling between the two phases. According to the results, after a certain time from the start of injection, the overall percentage of total evaporation of acetone becomes significantly higher than ethanol, but at the early spraying time, both alcohols had similar overall evaporation rates. Also, in terms of spray tip penetration, they have almost the same amount of progress and more or less the same behavior. Also due to the almost identical injection flow rate of the droplets, the effects on the velocity fields in the gas phase have been almost similar. The important point to compare is the gas phase temperature field for both sprays after 1.5 ms of injection. The ambient temperature becomes much lower in ethanol spray because ethanol's boiling temperature and latent heat are both much higher than acetone.

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1. Introduction

Numerous processes in the industry use sprays, including water spraying in cooling towers, etc [1]. Therefore, a better understanding and more accurate modeling of the spray phenomenon and the including processes are important [2]. To point out the importance of the evaporation problem, droplet evaporation modeling began in 1950 with d2law [3], and it is modified during these years by Borman and Johnson [4], Abramzon and Sirignano [5]. In the field of alcohol and ketone evaporation, several studies have examined the evaporation of a single droplet of alcohols and ketones as single-component or multi-components [6]. Other studies have been conducted by mixing these materials as additives or improvers to other types of material in order to achieve higher efficiency in premixing [7].

Numerical study of alcohol and ketones spray such as ethanol and acetone has not been studied independently. Therefore, in this paper, a numerical study and simulation of evaporating sprays of these two different materials are presented.

2. Governing Equations

In this part, the equations, which govern the gas-phase, the continuous phase, and the liquid phase, the discrete phase, are introduced briefly. The Navier-Stokes equations governing the gas phase are solved in the Eulerian approach using the Finite-Volume method. The general transport Eq. (1) includes and can be replaced by the parameters of Table 1 to get mass, momentum, energy, turbulent kinetic energy, turbulent dissipation energy, and fuel vapor mass fraction equations.

$$\frac{\partial(\rho\phi\theta)}{\partial t}+\frac{\partial}{\partial r}(\rho\phi u\theta)+\frac{\upsilon}{r}\frac{\partial}{\partial\gamma}(r\rho\phi\upsilon\theta)+\frac{\partial}{\partial z}(\rho\phi w\theta)= \frac{1}{r}\frac{\partial}{\partial r}(\theta\Gamma_r\frac{\partial\phi}{\partial r})+\frac{1}{r}\frac{\partial}{\partial\gamma}(\theta\Gamma_\gamma\frac{\partial\phi}{\partial\gamma})+\frac{\partial}{\partial z}(\theta\Gamma_z\frac{\partial\phi}{\partial z})+S_\phi+S_{\phi,d} \quad (1)$$

θ in the general transport equation is the void fraction of the gas-phase which must be calculated for each cell. The trajectory and momentum equations for the liquid phase are shown in Eqs. (2) to (5).

$$\frac{dx_{i,d}}{dt}=u_{i,d} \quad (2)$$

$$\frac{du_{i,d}}{dt}=K_d((u_{i,g}+u'_{i,g})-u_{i,d})-\frac{1}{\rho_d}(\frac{dp_i}{dx_i}) \quad (3)$$

$$K_d=\frac{3}{4}C_d(\frac{\rho_g}{\rho_d})\frac{1}{D_d}|u_i-u_{i,d}| \quad (4)$$

$$C_d=\begin{cases}0.44 & \mathrm{Re}>1000\\ (24+3.6\,\mathrm{Re}^{0.687})/\mathrm{Re} & \mathrm{Re}\le 1000\end{cases} \quad (5)$$

where Re_d is the droplet Reynolds Number which is calculated from Eq. (6).

$$\mathrm{Re}_d=\frac{\rho_g|u_g-u_d|D_d}{\mu_g} \quad (6)$$

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Droplet energy equation is given as:

$$\frac{d(mC_pT)_d}{dt} = -\pi D_d K (T_g - T_d)\{Z/(e^Z - 1)\}Nu + Q\frac{dm_d}{dt} \quad (7)$$

The evaporation model is developed based on the Borman and johnson model [4]. Besides, all correlations for droplets and air properties are changeable by temperature and pressure and all are given from [8].

The discretization and solution algorithms are shown and listed in Table 1. In this research, the finite volume method has been used for the framework of discretization. The algorithm which is used in this research is the implicit non-repetitive Pisso method [8].

3. Validation and Grid independency

The geometry of the computational domain is shown in Fig. 1.

For the grid study, 3 different meshes were used as shown in Table 2.

Table 1. Discretization of different parts of equations

Problems	Solution
Frameworks of discretization	Finite Volume method
Temporal approximation	Euler-First order
Convection approximation	Hybrid of upwind and central
Diffusion approximation	Central
The solution of equations set	ADI method

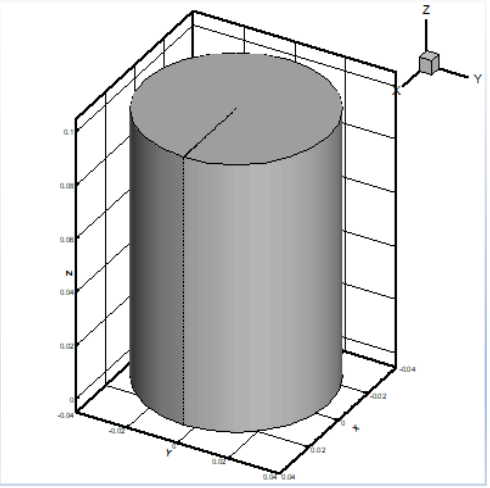

Fig. 1. The geometry of the study

Table 2. The number of grid

No.Mesh	No. Total nodes
Mesh 1	160000
Mesh 2	432000
Mesh 3	96000

The line that is used for study grid independency is the line with a high gradient, it is near the injection, and located 2 cm distance from the top and injector position. The results for grid independency are compared at after injection in Fig. 2.

After grid independency test, the independent time step is chosen as 3×10^{-6} . The spray droplet tip penetration is compared with the experimental results of Spray-A in Sandia [9]. The results of the simulation and experimental data are shown below in Fig. 3. It should be noted that the difference at the initial part of the result is regarding the atomization process which means that in the experimental study the droplets near the injector do not atomize at the first moments of injection and after a proper time when droplets break-up into the atomized droplet, the results get closer.

4. Results and Discussion

In this section, the comparison of the results of ethanol and acetone are presented. All thermophysical properties of these two hydrocarbons are considered as a function of temperature and pressure and given from [8]. The simulation conditions are shown in Table 3.

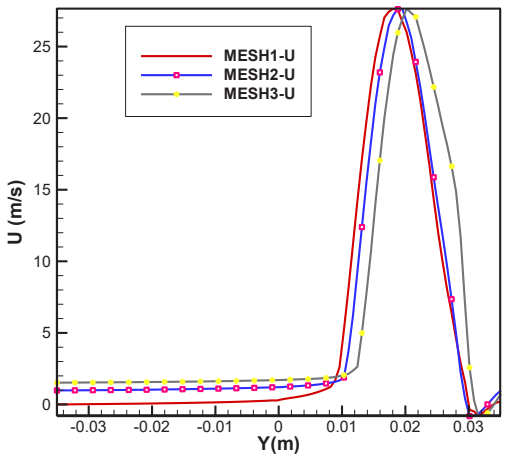

Fig. 2. comparison x-direction velocity for 3 different girds

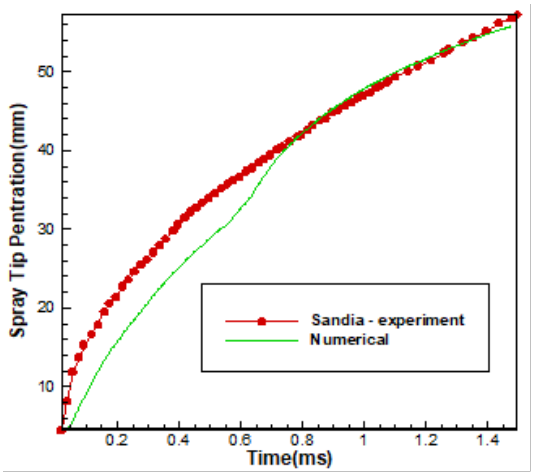

Fig. 3. Comparison between experimental data and numerical study

Table 3. Initial and environmental condition of the study

Parameter	Value(unit)	Parameter	Value(unit)
Ambient temperature	500 (K)	Injection angle	45
Wall temperature	500(K)	Injection time	1.5 (ms)
Ambient pressure	25. (bar)	Average Diameter	30(μm)
Initial droplet temperature	300(K)	Minimum diameter	0.5(μm)

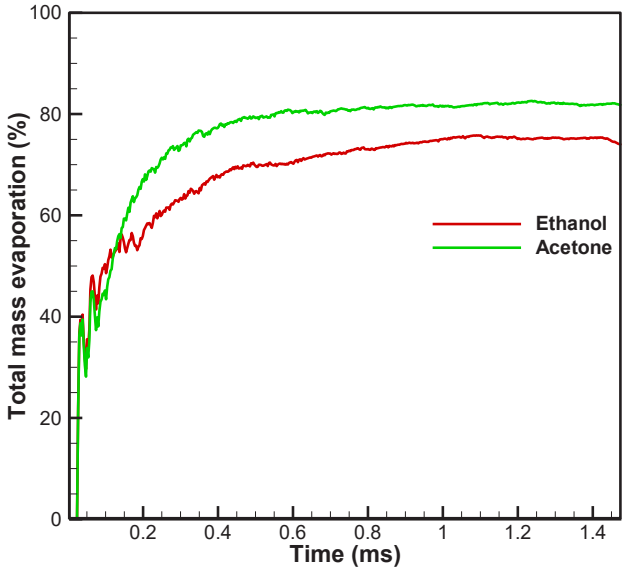

Fig. 4. comparison of total mass evaporation (%)

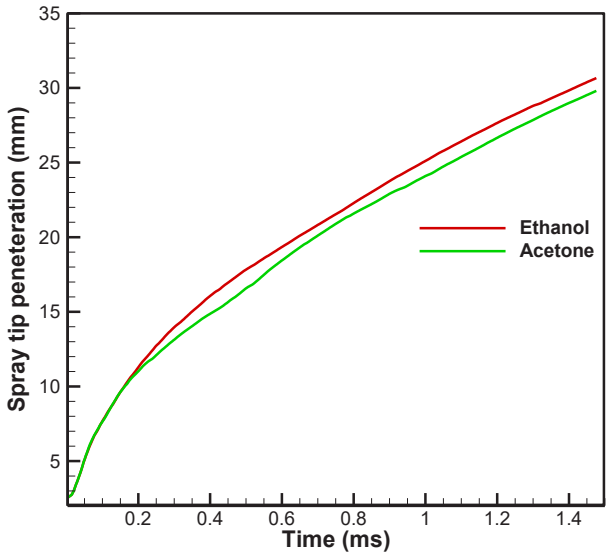

Fig. 5. comparison of spray tip penetration

The first results are regarding the comparison of spray tip penetration and total mass evaporation which are scaler parameters.

Due to chemical kinetics reasons, the total mass evaporation rate of acetone is higher than ethanol. In addition, because of the higher evaporation, the more little droplet might be in the environment, the spray tip penetration of acetone is lower than ethanol.

There are also differences in the effects of these two materials on the gas phase. Based on the higher presence of ethanol droplets in the environment and the higher evaporation temperature and the latent heat of vaporization of ethanol than acetone droplets, they have more effects on the gas phase temperature field which is shown in Figs. 6 and 7.

5. Conclusions

In this paper, the effect of evaporating sprays of ethanol and acetone injected into a cylindrical gaseous environment is numerically investigated. To make this investigation the Eulerian gas phase equations together with the Lagrangian liquid phase equations are solved assuming a two-way coupling between the two phases. According to the results, after a certain time from the start of injection, the overall percentage of total evaporation of acetone becomes significantly higher than ethanol, but at the early spraying time, both hydrocarbons had similar overall evaporation rates , the effects on the velocity fields in the gas phase have been almost similar. The important point to compare is the gas phase temperature field for both sprays after 1.5 ms of injection. Due to the fact that most of the evaporation occurs when the particles reach boiling temperature and the fact that all the heat required for evaporation is taken from the gas phase, the ambient temperature becomes much lower in ethanol spray because ethanol's boiling temperature and latent heat are both much higher than acetone.

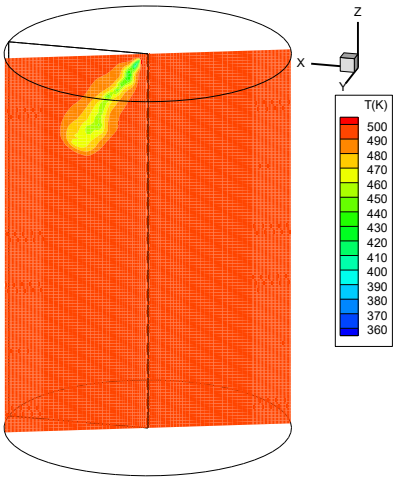

Fig. 6. Temperature field of ethanol spray injection

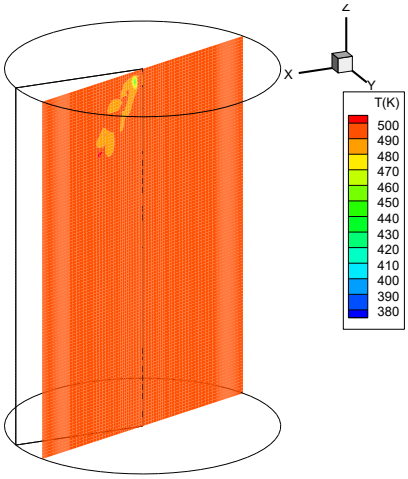

Fig. 7. Temperature field of acetone spray injection

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