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Modeling of n-Hexane and n-Octane liquid fuel jets in gaseous crossflow for evaporation, combustion and breakup evaluation

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ABSTRACT

This paper investigates the phenomena of liquid fuel jets in gaseous crossflow for two types of fuels, namely n-Hexane and n-Octane. In this regard, a numerical model is developed to predict a droplet behavior including trajectory, velocity, evaporation and combustion, size degradation, breakup time and radius of produced child droplets. Therefore, the mass, concentration, energy and momentum conversation equations are derived to evaluate the droplet acceleration from initial conditions. The velocity distribution is then obtained through a numerical integration of the acceleration over time. A further integration is made to determine the droplet position. In addition, evaporation and combustion and Taylor Analogy Breakup (TAB) models are integrated to assess droplet evaporation, combustion rate, and breakup behavior during the injection process. The professional version of the Engineering Equation Solver (EES) software is used to solve the model which has the advantage of providing the thermodynamic properties of the different fluids involved through predefined functions. The behaviors of droplets are investigated for two injection cases: evaporation only and evaporation and combustion. The results obtained are presented in the variations in trajectories, velocities, droplet size and surface temperature corresponding to each case and type of fuel.

1. Introduction

The vast majority of our energy systems at present depends to some extent on a combustion process which involves a liquid fuel being injected into a combustion chamber especially within the transportation industry. Therefore, the development of these energy systems mandates deeper understanding of this problem in order to reduce emissions and fuel consumption and thereby improve efficiency and sustainability. Furthermore, the progressive advances in the computing capabilities allow the relatively complex numerical solution to become visible. This opens the horizon for scientists to explore further and validate experimental and simplified theoretical results of multiphase flow problems, in general, and for liquid fuel jets in crossflow, in particular.

The research studies conducted on the liquid jet atomization in a crossflow substantially motivated by the various industrial applications. For example, in airbreathing jet engines such as ramjet and scramjet, a liquid fuel is being injected into a turbulent gaseous crossflow for combustion. Moreover, a similar process also encountered in internal combustion engines. In these processes, an efficient atomization of the injected fuel considerably promotes efficient combustion process that yields less pollutant such as NO_x [1] and allows for a higher fuel utilization.

The problem of liquid jet injection into crossflow has been extensively investigated in the open literature, including jet penetration, trajectories, droplets size, velocities, and breakup. The comprehensive literature reviews have been reported in references [2–6]. Recently, Broumand and Birouk [7] have reviewed the liquid jet injection in a subsonic gaseous crossflow. They considered literature on the primary breakup, jet trajectory and penetration, breakup length, and droplets features. In addition, numerous experimental and numerical studies have considered droplet trajectory and liquid get in crossflow [8–10]. Pai et al. conducted investigated primary breakup of turbulent liquid jets in a crossflow [11]. Balasubramanyam and Chen [12] introduced the finite-conductivity evaporation in their CFD modeling study of liquid jet breakup in high-speed crossflow. The use of Taylor Analogy Breakup (TAB) model to simulate and predict droplet breakup has been reported by O'Rourke and Amsden [13]. Turner et al. [14] studied the breakup processes of diesel fuel sprays under transient condition. Rachner et al. [1] investigated the atomization of a plain jet of kerosene fuel in air crossflow to evaluate the combustion characteristics in gas turbines. Furthermore, Prakash et al. [15] considered the breakup processes of spray in gaseous cross-flow involving pressure swirl. The

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experimental setup was illustrated, and their results were reported along with visual photographs categorized based on the breakup regimes and Weber number. Another extensive study carried out by Kaushal [16] which has been dedicated to turbulent fuel injection in internal combustion engines. The study included a simulation in KIVA4-mpi where both primary breakup model and secondary, model (TAB), model are used. Furthermore, an experimental and numerical investigation of droplet breakup and atomization of diesel and bio-diesel fuels in a cross flow air was conducted by Kim et al. [17] where TAB model was considered for secondary diesel droplet breakup. Behzad et al. [18] reported simulation model developed to investigate the surface breakup of a non-turbulent liquid jet injected into high-pressure gas crossflow. They reported comparisons between the two fuels in terms of deformation and breakup regimes at different air flow rates.

In the current study, a circular liquid fuel jet injected into a gaseous crossflow is investigated for two fuels n-Octane and n-Hexane which have not been considered in earlier studies. The objective of this study is to predict the trajectory of these fuels droplet as a function of the position and the initial droplet diameter. In addition, the droplet velocity, surface temperature, and evaporation and combustion rates will be evaluated. Lastly, the number of droplets and the breakup time will also be predicted utilizing TAB model.

2. Problem formulation

The circular liquid fuel jet injecting normal to an air crossflow is shown in Fig. 1 with respect to the two Cartesian coordinates and the two corresponding velocity components. The schematic representation of the jet in crossflow problem illustrates how a gaseous flow moving at certain speed flows over a liquid jet causing atomization and deflection in the produced droplets' path.

The mathematical models are developed and numerically to be solved using Engineering Equation Solver (EES) [19]. The use of EES software enables an accurate assessment of the properties of the fluid due to the built-in functions that consider the instantaneous changes in the properties associated with temperature changes.

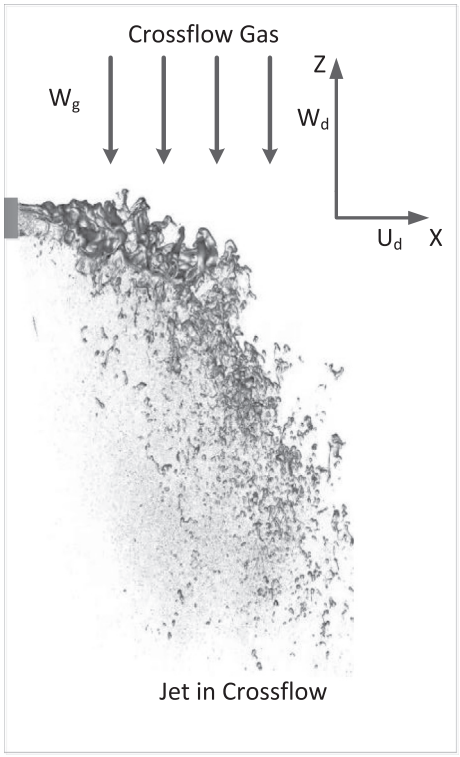

Fig. 1. Schematic representation of the liquid fuel injection into crossflow and atomization.

The numerical model is built based on three main sub-models. The first is a dynamic sub-model which determines the droplet acceleration, velocity, and instantaneous position. The second is an evaporation and combustion sub-model which evaluates the droplet evaporation/combustion rate, droplet size degradation, and droplet surface temperature. The third is the TAB breakup sub-model which predicts whether a droplet breakup or not. It also predicts the size of the produced droplets.

2.1. Dynamic sub-model

The droplet trajectory in X- and *Z*-directions can be determined using the Lagrangian reference frame as

$$x = x_0 + \int_0^t U_d\,dt \tag{1}$$

$$z = z_0 + \int_0^t W_d\,dt \tag{2}$$

where x_0 and z_0 are the initial droplet position components and U_d and W_d are the injection velocity components. The instantaneous droplet acceleration can be derived from the momentum equation (droplet motion equation) as follows

$$\frac{d(m_d \boldsymbol{v})}{dt} = \sum F = F_{surface} + F_{body} + F_{collisional} \tag{3}$$

where the body forces are F_{body} are only due to gravitational

$$F_{body} = m_d g = \forall_p\ \rho_f\ g \tag{4}$$

The surface forces $F_{surface}$ is given by

$$F_{surface} = F_{drag} + F_{lift} + F_{added\ mass} + F_{history} \tag{5}$$

In the analysis, we make some assumptions as follows:

- The flow is incompressible.
- The droplet has non-deformable spherical shape.
- The collision forces are negligible, thus ($F_{collisional} = 0$).
- The velocity is uniform ($F_{lift} = 0$).
- The history force is negligible ($F_{history} = 0$).

Furthermore, the drag force F_{drag} is calculated as

$$F_{drag} = F_{shear} + F_{pressure} \tag{6}$$

where

$$F_{drag} = -3\pi\ D\ \mu_f f\ V_{rel} \tag{7}$$

with

$$f = 1\ for\ Re \ll 1 \tag{8}$$

$$f = 1 + \frac{\frac{Re}{4}}{1 + \sqrt{Re}} + \frac{Re}{b} \tag{9}$$

While the shear force F_{shear} is equivalent to bouncy force and given as

$$F_{shear} = -\rho_f\ \forall_p\ g \tag{10}$$

Then, the momentum equation reduces to

$$\frac{\boldsymbol{dv}}{\boldsymbol{dt}} = \frac{-3\,\pi\,\boldsymbol{D}\,\boldsymbol{\mu_f f V_{rel}} + \forall_p\,(\boldsymbol{\rho_p} - \boldsymbol{\rho_f})\,\boldsymbol{g}}{\boldsymbol{m}} \tag{11}$$

The acceleration equation is then written for each component, according to the reference coordinate system shown in Fig.1, as a_x and a_z as