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Investigation of the evaporation and fuel property effect on Liquid Jets in Supersonic Crossflow

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Abstract: Due to the longer auto-ignition time with liquid fuels compared with hydrogen, the understanding of interaction of shock waves with sprays and the subsequent vapor mixing is significant to design ramjets/scramjets with liquid fuel sprays. In this study, an Eulerian-Lagrangian framework is developed based on the OpenFOAM platform. In this solver, detailed multi-component transport models for Eulerian gas-phase species properties are included. In addition, Lagrangian spray break-up, atomization and evaporation models are added to simulate liquid phase. In addition, an equilibrium wall function is added to model the near-wall properties. The newly developed solver is used to conduct large eddy simulations (LES) on non-reactive liquid jets in supersonic crossflow (JISCF) with liquid sprays. The liquid penetration length are compared with the experimental data, showing a very good agreement. Effects of evaporation and fuel properties (e.g., heat capacity and enthalpy of evaporation) on penetration length, temperature, Sauter mean diameter (SMD) and volumetric parcel flux are discussed in this study. It is shown that evaporation effects primarily show up in the temperature field. For n-heptane sprays, such impact could be conducted to other properties of the flow field like spray plume size, particle size distribution and volumetric flux, which is caused by the smaller enthalpy of evaporation and heat capacity comparing to water. Full version of this paper has been published as a journal article: Shufan Zou, Dezhi Zhou, Suo Yang, "Effects of Evaporation and Fuel Properties on Liquid Jets in Supersonic Crossflow: a Computational study using a compressible Eulerian-Lagrangian solver", Atomization and Sprays 30 (9) (2020) 675-696. https://doi.org/10.1615/AtomizSpr.2020034860
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1. Introduction

The combustion chamber of scramjet engines in hypersonic vehicles have to work under supersonic conditions to get rid of the great loss in energy and the heavy thermal load introduced by the gas deceleration to subsonic conditions [1]. Direct fuel injection into the supersonic crossflow has extremely limited residence time to allow fuel-air mixing at the molecular level. The liquid fuel sprays even deteriorate the combustion efficiency comparing to gaseous fuels, because they require more residence time for liquid atomization and evaporation. As a result, considering the fuel delivery manner in such high-speed air-breathing propulsion systems, a fundamental understanding of the physics of a liquid jet injected to a supersonic air flow is of significant practical importance and stimulating theoretical interests as well ([2]).

To simulate liquid jet sprays in supersonic flows, a fully compressible computational fluid dynamics (CFD) solver with multi-phase flow capability is needed. For liquid-gas phase simulation in CFD, two strategies (i.e., Eulerian-Eulerian and Eulerian-Lagrangian) are typically used in the

literature (such as [3–5]). The development of such a robust simulation tool is very challenging, especially when both sprays and chemical reactions are involved (see [6]), due to the complexity of simulating two-phase interaction, chemistry and turbulence. First of all, accurate fuel spray modeling is crucial, because liquid fuel spray, fuel droplet atomization, evaporation and mixing determines the following combustion process. myColorWhen reaction is not involved in the configuration of interest, the development of a robust multi-phase solver is still challenging. The detailed Eulerian-Eulerian framework such as the volume of fluid (VOF) method is believed to accurately resolve both the gas and liquid phases. However, these methods could incur strict requirement on the resolution of the mesh to resolve all small droplets and easily cause prohibitive computation cost (see [7]). It is reasonable to set a size threshold and use Lagrangian particle tracking method for liquid droplets smaller than the threshold but still use the Eulerian-Eulerian VOF framework for liquid droplets larger than the threshold. One can also further simplify it to a pure Eulerian-Lagrangian model, which is reported by [8] to be able to capture the averaged flow field properties well.

Tthere are several recent investigations on liquid spray in supersonic cross flows (such as [5, 9, 10]) which focus on the shock-spray interaction effectsmyColor, droplet size distribution and jet plume trajectory. To our best knowledge, the effects of evaporation and liquid fuel properties on the JISCF are missing in the literature. Hence, the second objective of this study is to study the effects of evaporation and fuel properties on liquid plume trajectory and droplet size distribution via employing the new solver developed in this paper. It is shown that without tuning any Lagrangian model parameters, good agreements in terms of penetration length and liquid plume trajectory are achieved, compared with the experimental data measured by [11]. Subsequently, effects of evaporation and liquid thermophysical properties on the liquid plume and penetration length are discussed and analyzed.

2. Methods

2.1 Governing equations for gas phase

Governing equations for gas phase include transport equations of mass, momentum, species and energy expressed by enthalpy:

$$\frac{\partial \rho_g}{\partial t} + \nabla \cdot (\rho_g \boldsymbol{u_g}) = \dot{S}_m, \tag{1}$$

$$\frac{\partial \rho_g \boldsymbol{u_g}}{\partial t} + \nabla \cdot (\rho_g \boldsymbol{u_g} \otimes \boldsymbol{u_g}) = -\nabla p_g + \nabla \cdot \boldsymbol{\tau_g} + \dot{\boldsymbol{S}}_{\boldsymbol{F}}, \tag{2}$$

$$\frac{\partial \rho_g Y_s}{\partial t} + \nabla \cdot (\rho_g Y_s \boldsymbol{u_g}) = -\nabla \cdot \boldsymbol{j_s} + \rho_g \dot{\omega}_s + \dot{S}_{Y_s} \qquad s = 1, ..., n_s, \tag{3}$$

$$\frac{\partial \rho_g h_g}{\partial t} + \nabla \cdot (\rho_g h_g \boldsymbol{u}_g) + \frac{\partial \rho_g K_g}{\partial t} + \nabla \cdot (\rho_g K_g \boldsymbol{u}_g) - \frac{\partial p_g}{\partial t} = \nabla \cdot (\boldsymbol{\tau}_g \cdot \boldsymbol{u}_g) + \nabla \cdot \boldsymbol{q} + \dot{S}_h, \tag{4}$$

where t is time and x is spatial coordinate, ρ_g is the density of the gas mixture, $\boldsymbol{u_g}$ is the gas velocity vector, p_g is the pressure, τ_g is the viscous stress tensor, h_g and K_g are the enthalpy and kinetic

energy of the gas, respectively, $\boldsymbol{q}$ is the heat flux, Y_s is the mass fraction of species s, and $\dot{\omega}_s$ is the net reaction rate of species s. $\boldsymbol{j_s}$ is the diffusion flux of species s with an expression of

$$\boldsymbol{j_s} = -\rho Y_s \left(D_s \frac{\nabla X_s}{X_s} + \boldsymbol{u_c} \right).$$

Due to the coupled liquid phase, an additional source term is added on the right-hand-side of each equation in terms of the inter-phase exchanges in mass, momentum, species and energy/enthalpy. These terms are estimated on the droplets in the cells (see [12]):

$$\begin{cases} \dot{S}_m = \dfrac{1}{V_{\text{cell}}} \sum_i \dot{m}_{i,d}, \\ \dot{\boldsymbol{S}}_{\boldsymbol{F}} = -\dfrac{1}{V_{\text{cell}}} \sum_i \boldsymbol{F}_{i,d}, \\ \dot{S}_{Y_s} = \begin{cases} \dot{S}_m \text{ for liquid phases species,} \\ 0 \quad \text{for others,} \end{cases} \\ \dot{S}_h = -\dfrac{1}{V_{\text{cell}}} \sum_i \left(\dot{Q}_{conv} + \dot{Q}_{evap} \right), \end{cases} \tag{5}$$

where myColorsubscripts d and i denote droplets and the i-th droplet, respectively, the summation over i means the summation over all the Lagrangian particles within this cell, $\dot{Q}_{conv}$ is the rate of heat exchange by convection between gas phase and liquid phase, and $\dot{Q}_{evap}$ is the evaporation-induced heat transfer. Since in this study, there is no chemical reaction involved and the temperature of the flow field is considerably low, the radiation effects are not considered.

2.2 Governing equations for liquid phase

For Eulerian-Lagrangian method, dispersed liquid phase is modeled by a large number of spherical droplets tracked by a Lagrangian model. In this study, although we neglect the primary break-up and replace the integrated liquid jet by some dispersed droplets, we can still assume the spray is diluted (see [13]) and hence the interaction between droplets can be neglected. Based on this assumption, we could model the Lagrangian particles by:

$$\frac{dm_{i,d}}{dt} = \dot{m}_{i,d}, \tag{6}$$

$$\frac{d\boldsymbol{u}_{i,d}}{dt} = \frac{\boldsymbol{F}_{i,d}}{m_{i,d}}, \tag{7}$$

$$c_{p,i,d} \frac{dT_{i,d}}{dt} = \frac{\dot{Q}_{conv} + \dot{Q}_{evap}}{m_{i,d}}, \tag{8}$$

where $m_{i,d}$, $\boldsymbol{u}_{i,d}$, $c_{p,i,d}$ and $T_{i,d}$ are the mass, velocity, heat capacity at constant pressure and temperature of the i-th droplet, respectively. Both density and heat capacity are expressed as functions of droplet temperature T_d to handle the thermal expansion of droplets as in [14]:

$$\rho_d \left(T_d \right) = \frac{a_1}{a_2^{1+(1-T_d/a_3)^{a_4}}}, \tag{9}$$

$$c_{p,d}(T_d) = \frac{b_1^2}{\tau} + b_2 - \tau\left\{2.0b_1b_3 + \tau\left\{b_1b_4 + \tau\left[\frac{1}{3}b_3^2 + \tau\left(\frac{1}{2}b_3b_4 + \frac{1}{5}\tau b_4^2\right)\right]\right\}\right\}, \tag{10}$$

where a_1, a_2, a_3, a_4 and b_1, b_2, b_3, b_4 are model constants, T_d is the droplet temperature, $\tau = 1 - T/T_0$, $T_0 = min(T_d, T_{ref})$ and T_{ref} is a reference temperature as a function of species: for water $T_{ref} = 647.13$K and for n-heptane $T_{ref} = 540.2$K.

2.3 Secondary break-up modeling

[15–17] proposed the break-up model basing on the competition between bag break-up modeled by

$$We = \rho_d u_r^2 r_d/\sigma > 6.0 \tag{11}$$

with unstable droplets life time

$$t_{bag} = C_{bag}\left[\frac{\rho_1 r_d^3}{2\sigma}\right]^{1/2} \tag{12}$$

and stripping modeled by

$$We/\sqrt{Re} > 0.5 \tag{13}$$

with unstable droplets life time

$$t_{strip} = C_{strip}\frac{r_d}{u_r}\left(\rho_d/\rho_g\right)^{1/2}, \tag{14}$$

where We is Weber number, σ is the surface tension coefficient and Re is the Reynolds number, $C_{bag} = 2.22$ and $C_{strip} = 20$ are model constants. To account for the residence time here, the diameter of the unstable droplets here is modeled by

$$d_d(t) = \frac{d_{stable}t + t_{stable}}{t + t_{stable}}, \tag{15}$$

where d_{stable} is the stable criterion diameter satisfying stability criterion (11) or (13), and t_{stable} indicates the corresponding life time for the mode. Here, the child droplets are assumed to be located at the center of parent droplet.

3. Results and Discussion

3.1 Configuration and conditions

The flow conditions for the JISCF in this study follow the set-up of [18], with liquid flux $\dot{m} = 6.415$ g/s (i.e., the gas-liquid momentum ratio $q_0 = 7$) and injector diameter $d_0 = 0.5$ mm. The injector located at the center of the bottom floor and 25 mm downstream from the free stream inlet. The inlet condition is set as a free stream inlet condition with a supersonic air flow at Mach number $M = 1.94$, static pressure $p_\infty = 2.9$ kPa and static temperature $T = 303.2$ K. To utilize the experimental data measured by [18] for our solver validation, the spray liquid is firstly selected as water. To further study the effects of liquid fuel properties (e.g., viscosity, heat capacity, and

enthalpy of evaporation), n-heptane is also selected as the liquid fuel in this study. While injecting n-heptane, all the other flow features are kept the same as the water spray case.

The simulation is performed in the domain with the size: 160 mm streamwise, 62 mm spanwise and 50 mm height-wise. The domain is discretized into approximately 6 million grid cells ($346 \times 116 \times 149$). Since WMLES is conducted by the newly developed solver with the equilibrium wall function, the grid cells are clustered towards the wall. To better capture the near-wall and near-injector spray, the finest cell (0.14 mm) is near the injection due to the limit of the Eulerian-Lagrangian method (i.e., the grid cells should be larger than the Lagrangian particles). Under such a setting, the first layer of grid cells near the bottom wall is scaled by: $\delta x = \delta y = \delta z \approx 50y^+$, which is reasonably good for the implementation of log-layer modeling wall function($> 50y^+$). myColor Considering the maximum size of the spray droplet is at the order of magnitude of 0.1 mm, the current grid with the 0.14 mm finest cell is considered to be the finest grid that can be used to resolve the gas flow field. All the simulation cases in this study have been run for about 15 flow-through times to obtain statistically stationary time-averaged data, after the initiation transition.

3.2 Effects of evaporation

Most of the investigations in the literature (such as [19] and [10]) neglect the evaporation effects in liquid JISCF, due to the short residence time of the droplet in the domain of interest. However, as stated by [9], due to the shock-spray interaction, the gas-liquid interface would be heated up, although the core of the spray plume stays cold. As a result, it is clear that droplet phase change could have effects on the spray plume trajectory and droplet size distribution. In this section, we analyze the effects of evaporation on the gas flow and spray properties of JISCF in detail by switching on/off the evaporation model. Sprays with both water and n-heptane are investigated and compared.

3.2.1 N-heptane

Water is widely used in liquid JISCF experiments due to its well-known properties and ease of access. With the validation of the newly developed solver by comparing to the water JISCF measured data, we further extend the liquid to more realistic liquid fuel, n-heptane (one of the main components of gasoline). N-heptane has approximately one order of magnitude larger viscosity than water, while its heat capacity is almost half of the water counterpart and its enthalpy of evaporation is approximately 75% of the water counterpart The difference in physical properties hints the potential difference in response to evaporation. Due to the short residence time of the liquid spray in JISCF, most of the numerical studies ignore the evaporation effects, which, as seen in our water spray simulations, is valid. However, as will be shown in this section, the evaporation effects on n-heptane are not negligible and can significantly affect the spray droplet size distribution.

Acknowledging the obvious difference in temperature fields, we would expect significant difference in terms of spray properties with evaporation. Figure 1 shows the time-averaged volumetric flux on the slice at $x/d = 100$, in which the half on the left-hand-side of the yellow dashed line is calculated without evaporation and the half on the right-hand-side is calculated with evaporation. Noticeable extension of the size of spray plume is observed, which could also be clearly illustrated in Fig. 2(b). From Fig 2, it is observed that near the spray core and near the wall, the spray plume is extended by evaporation at different axial locations. Such effect is naturally conducted to the

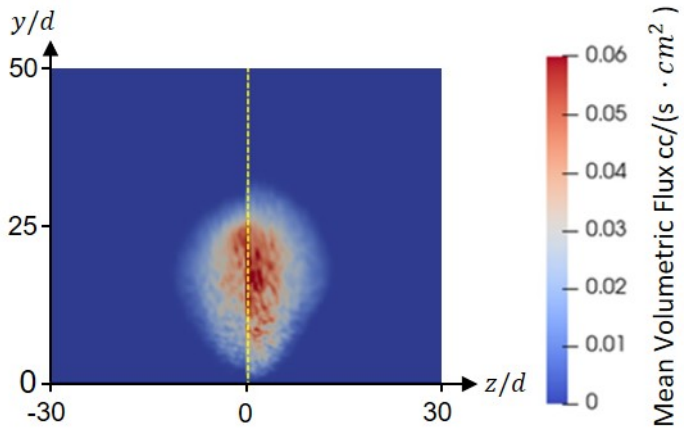

Figure 1: Time-averaged streamwise volumetric flux at the $x/d = 100$ slice.

increase in penetration height of the spray. The size distribution of the droplets, characterized by SMD, are plotted in Fig. 3. We can observe that the evaporation effects start to manifested at downstream locations, where the longer residence time allows the evaporation to take effect. At $x/d = 100$ and 150, evaporation decreases the SMD of the droplets near the core of the spray, indicating that the increase of the mean volumetric flux near the top surface and the wall is caused by the further break-up of the droplets in the core of the spray. In other words, evaporation is able to enhance the secondary droplet break-up in the spray core and drive them expand the spray plume. To explain this observation, we firstly shows the re-distribution of streamwise velocity U_x of gas flow on the spray side at $x/d = 100$ in Fig. 5, compared with no evaporation case. The case with evaporation shows higher velocity near the interior region which enhance the secondary droplet break-up, but lower velocity near the wall. The increase of gas flow velocity near the spray core will accelerate the droplets and increase the volumetric flux in the core region of the spray. As the dominant criterion $We \sim U^2$, the break-up is highly velocity-dependent, the difference in velocity here (see also Fig.4) is amplified and finally resulting in the great difference in size distribution.

Therefore, the relative low temperature of the incoming supersonic gas flow does not mean that we can neglect the evaporation effects. Whether we can neglect evaporation should depends on the properties of the injected liquid. Neglecting evaporation effects may underestimate the size of spray plume, significantly overestimate the mean volumetric flux and downstream size distribution.

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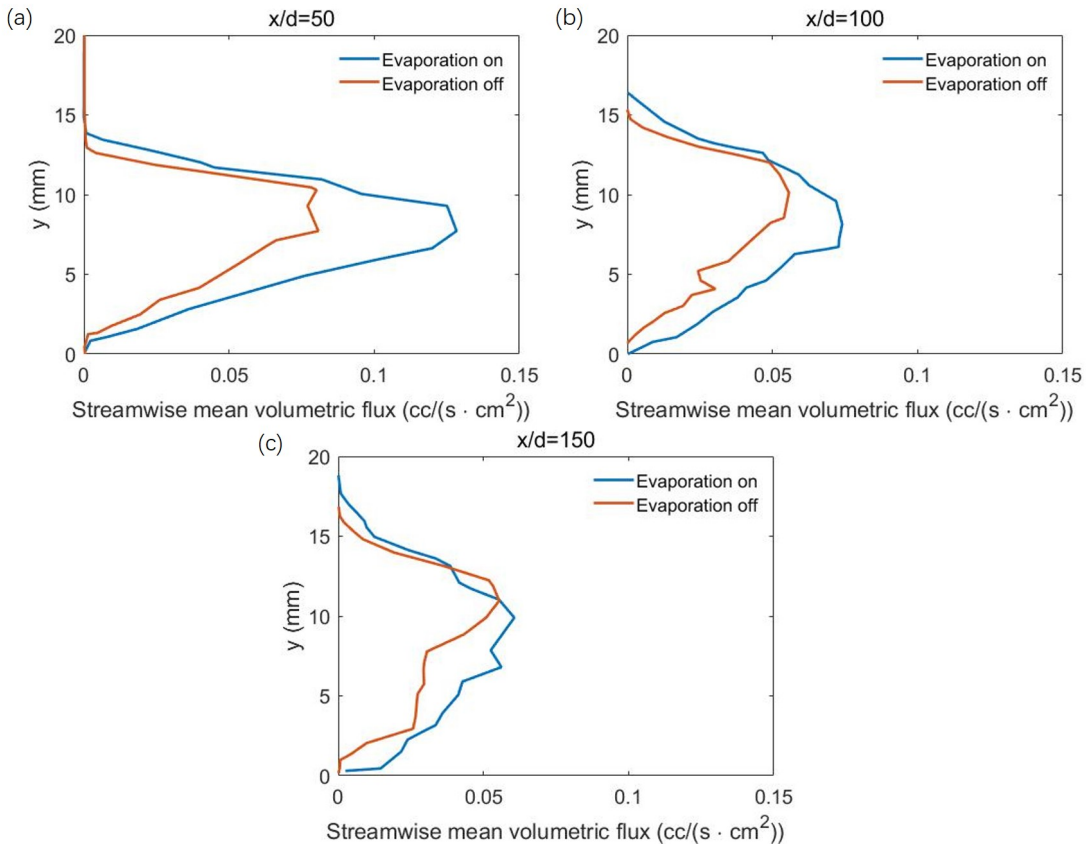

Figure 2: Streamwise mean volumetric flux at (a) $x/d = 50$, (b) $x/d = 100$ and (c) $x/d = 150$ on the center plane in n-heptane cases.

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4. Conclusions

In this paper, we first developed a fully compressible Eulerian-Lagrangian solver (sprayRCSFoam) based on the OpenFOAM platform with a newly implemented wall function. By simulating a liquid jet in supersonic flow with wall-modeled large eddy simulations (WMLES), the predicted penetration length by sprayRCSFoam was compared with the experimental data and showed good agreement. myColorWith the newly developed solver, we conducted water and n-heptane JICSF simulations. For water spray, although evaporation could lead to obvious temperature difference, the overall spray difference due to evaporation is negligible. For n-heptane, evaporation could have significant effects on both the gas-phase flow field and spray plume properties at downstream locations. It is also found that the n-hetapne evaporation could enhance the secondary break-up at the spray core due to the larger droplet velocity, which significantly changes droplet distribution in the interior spray plume. Finally, This study validates our fully compressible solver with sprays, which suggests its potential to simulation and investigate supersonic spray combustion of liquid fuels for future study.

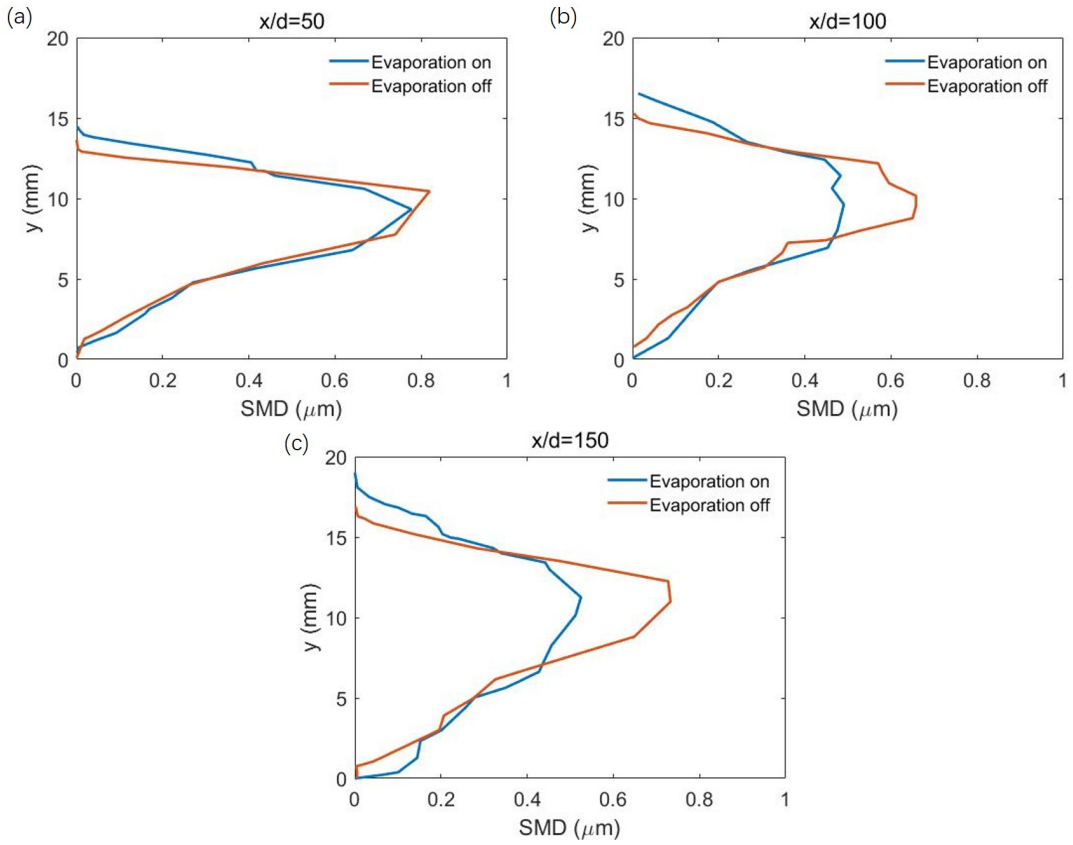

Figure 3: Sauter mean diameter (SMD) distribution at (a) $x/d = 50$, (b) $x/d = 100$ and (c) $x/d = 150$ on the center plane in n-heptane cases.

5. Acknowledgements

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Page Limits: The total length of the paper including references should be limited to 10 pages.

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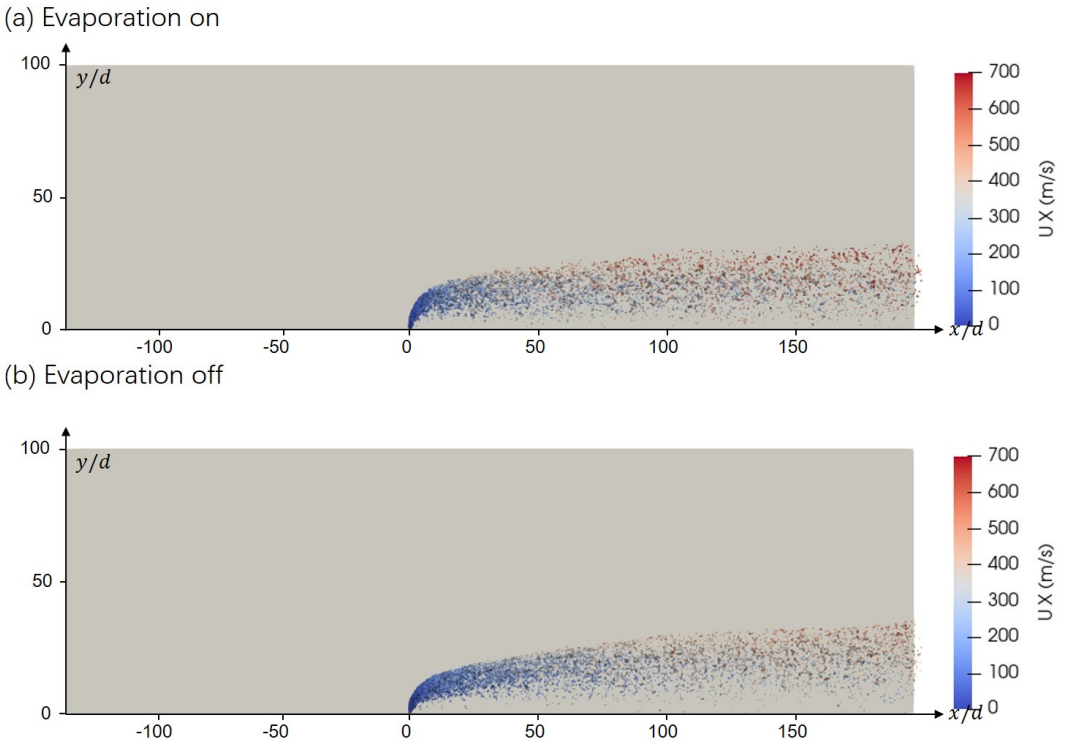

Figure 4: Instantaneous velocity U_x of n-heptane droplets: (a) evaporation on; (b) evaporation off.

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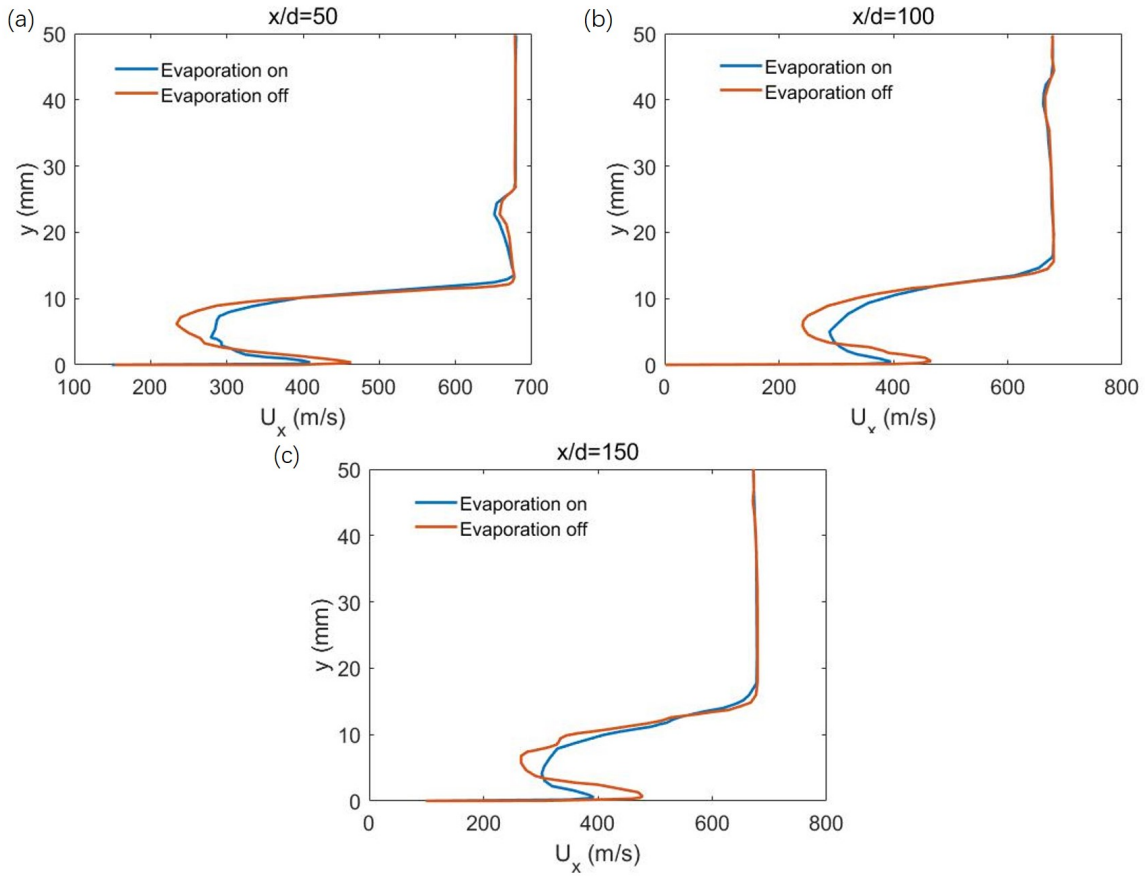

Figure 5: Mean streamwise gas velocity U_x distribution at $x/d = 100$ on the center plane in n-heptane cases.

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