Joint Velocity-Scalar PDF Modeling of Turbulent Spray Flows

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1 Introduction

The probability density function (PDF) method for turbulent flows has been studied for several decades. Lundgren [1] derived, modeled and solved a transport equation for the joint PDF of velocity, and Dopazo and O'Brien [2] for the joint PDF of composition. The transported PDF method became very popular since Pope's work [3]. It has been proved to be a successful tool for the simulation of turbulent single-phase flows, and in particular for reactive flows. The PDF method provides a computationally tractable way of calculating the statistics of inhomogeneous turbulent flows of practical importance. The major advantage of the PDF method is, that convection, body force, mean pressure gradient, and chemical reactions can be treated without assumptions. The most important closure problem, the modeling of the molecular diffusion, has been overcome. PDF methods describe the turbulent flow in a more complete way than the conventional turbulent models. All the moments of the considered quantities can be evaluated from the resulting PDF. Additionally, the Lagrangian PDF method takes full account of the long memory of turbulence. The past history of all the fluid particles' properties can be completely described by the multi-time Lagrangian PDF.

The PDF method has reached the level of maturity, and it has become a very active and fruitful research area [3][4][5]. PDF methods were applied to simulate multi-phase flows since 1990's. Raju [6] and Taut *et al.* [7] describe the gas phase in turbulent two-phase flows with the PDF transport equation. Rumberg and Rogg [8], Zhu *et al.* [9] deduced and solved the joint PDF transport equation of all liquid-phase and gas-phase dependent variables. Liu *et al.* [10] deal with the joint PDF transport equation of the properties of droplets and gas eddies seen by droplets. Ge and Gutheil [11] deduced, modeled, and solved the transport equation of the PDF of mixture fraction in turbulent spray flows. Ge and Gutheil [12][13] further developed a joint scalar PDF model and applied it to simulate spray flames. Kung and Haworth [14] applied the transported PDF to internal engine simulation. These studies demonstrate that PDF methods are very attractive to simulate turbulent multi-phase flows. However, there are still signification areas requiring careful research in this field.

In the present work, a new joint velocity-scalar PDF is introduced into the turbulent spray flows. The transport equation of the joint velocity-mixture fraction PDF of the gas phase in turbulent spray

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flows is derived, modeled, and solved. The numerical results are compared with the experimental data [15] and with the results of the extended κ−ε model [16].

2 Mathematical Modeling

Here we define a one-point one-time Eulerian, mass-weighted joint velocity-mixture fraction probability density function $\tilde{f}(\vec{V},\zeta_c;\vec{x},t)$ for the gas phase of turbulent spray flows:

$$\tilde{f}(\vec{V},\zeta_c;\vec{x},t) = \rho_g(\zeta_c)\left\langle \delta(\vec{U}-\vec{V})\delta(\xi_c-\zeta_c)\right\rangle / \overline{\rho_g}\,. \tag{1}$$

Here $\vec{V}$ and ζ_c denote the velocity and mixture fraction in sample space, respectively, and $\vec{U}$ and ξ_c are the corresponding velocity and mixture fraction in physical space. According to the transport equation of the momentum and mixture fraction in a turbulent spray flow, the PDF transport equation of the joint PDF $\tilde{f}$ can be deduced following Pope [3]:

$$\begin{aligned}\overline{\rho_g}\frac{\partial \tilde{f}}{\partial t} + \overline{\rho_g} V_i \frac{\partial \tilde{f}}{\partial x_i} + \left(\overline{\rho_g} g_i - \frac{\partial \overline{p}}{\partial x_i} + \overline{S}_{l,U_i}\right)\frac{\partial \tilde{f}}{\partial V_i} + \frac{\partial\left(\overline{S}_{l,1}\tilde{f}\right)}{\partial \xi_c} = \\ \frac{\partial}{\partial V_i}\left[\left\langle -\frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial p'}{\partial x_i}\middle| \vec{V},\zeta_c\right\rangle \tilde{f}\right] - \frac{\partial}{\partial \xi_c}\left[\overline{\rho_g}\left\langle \frac{\partial}{\partial x_j}\left(D_M \frac{\partial \xi_c}{\partial x_j}\right)\middle| \vec{V},\zeta_c\right\rangle \tilde{f}\right]\end{aligned} \tag{2}$$

The terms on the left-hand-side appear in closed form, they include the terms of convection, body force, mean pressure gradient, and spray sources $\overline{S}_{l,1}$, $\overline{S}_{l,U_i}$ due to mass and momentum transfer from the liquid to the gas. The terms on the right hand side must be modeled. They include the viscous stress tensor, the fluctuating pressure gradient, and the molecular diffusion fluxes. Due to the high-dimensional space in which the joint PDF evolves, it is infeasible to solve the modeled PDF transport equation using a finite-difference or finite-volume method. Monte-Carlo particle methods are widely used to solve the PDF transport equation because their computational time increases only linearly with the number of dimensions. The Monte-Carlo particle method requires the gas flow equations to be discretized with respect to mass rather than time or space. The Lagrangian particle methods are more popular compared to the Eulerian methods because it is easier to construct the physical model in Lagrangian frame, and the history of the turbulence is fully captured. From a Lagrangian viewpoint, the flow is discretized into a large number of particles [11]. Each particle has a set of properties $\{m_g^*, \vec{x}_g^*, \vec{U}_g^*, \xi_c^*\}$ (superscript '*' denotes the particle property). The PDF transport equation is transformed into a set of stochastic differential equations (SDE). The particle properties evolve by the SDEs. The evolution of the gas particles in the velocity-sample space is usually modeled with Langevin models [3][17]. In the present work, the simplified Langevin model is extended to model the gas velocity in the turbulent spray flow:

$$dU_i^*(t) = \frac{1}{\overline{\rho_g}}\left(\overline{\rho_g} g_i - \frac{\partial \overline{p}}{\partial x_i} + \overline{S}_{l,U_i}\right)dt - \left(\frac{1}{2}+\frac{3}{4}C_0\right)(U_i^*(t)-\tilde{U}_i)\frac{\tilde{\varepsilon}}{\tilde{k}}dt + (C_0\tilde{\varepsilon})^{\frac{1}{2}}dW_i\,. \tag{3}$$

The diffusion process is represented by a Wiener process $W(t)$, where $dW_i(t) = W_i(t+dt) - W_i(t)$ is Gaussian distributed with $\langle dW_i(t)\rangle = 0$ and $\langle dW_i(t)dW_j(t)\rangle = dt\delta_{ij}$. Effects of molecular diffusion are modeled using the extended interaction-by-exchange-with-the-mean (IEM) model [11]:

$$\frac{d\xi_c^*(t)}{dt} = -\frac{1}{2}\frac{\tilde{\varepsilon}}{\tilde{k}}C_\phi\left[\xi_c^*(t) - \hat{\xi}_c\right] + \frac{\overline{S}_{l,1}}{\overline{\rho_g}} \tag{4}$$

The model constants are set to $C_0 = 2.1$ [17] and $C_\phi = 2.0$ [11].

For the closure of the PDF transport equations, the conservation equations of gas flow including the extended k-ε model [16] are solved. The mean density, mean pressure, and the turbulent time scalar appearing in the Eqs. (3) and (4), are computed from the mean conservation equation of the gas flow. Considering a steady, two-dimensional, axi-symmetric, turbulent liquid jet with no swirl, the Favre-averaged governing equations of a gas flow can be written as

$$\frac{\partial(\overline{\rho}\tilde{U}_i\tilde{\Phi})}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\Gamma_{\Phi,eff}\frac{\partial\tilde{\Phi}}{\partial x_i}\right) = \overline{S}_{g,\tilde{\Phi}} + \overline{S}_{l,\tilde{\Phi}}. \tag{5}$$

The conserved variables $\tilde{\Phi}$ and the source terms of the gas phase $\overline{S}_{g,\tilde{\Phi}}$ and the liquid phase $\overline{S}_{l,\tilde{\Phi}}$ are described in detail in [16].

Assuming a dilute spray, both droplet-droplet interaction and coalescence are neglected. Only drag force and gravity are considered here:

$$\frac{d\vec{U}_d}{dt} = \frac{3}{8}\frac{\overline{\rho_g}}{\rho_l}C_d(\mathrm{Re})\frac{|\vec{U}_r|}{r_d}\vec{U}_r + \vec{g}. \tag{6}$$

The effect of gas-phase turbulence on droplet velocities is modeled using the stochastic-separated-flow model [18]. The instantaneous gas velocity is computed by a Monte-Carlo method according to the turbulent kinetic energy. The distribution of the velocity fluctuating is assumed to be Gaussian distributed [16]. Methanol droplet heating is modeled using the infinite-conductivity model [19]:

$$\frac{4}{3}\pi\rho_l C_{p,l} r_d^3\frac{dT_d}{dt} = \dot{m}_d\left(\frac{\hat{C}_{p,F}(T_\infty - T_d)}{B_T} - L_v(T_d)\right) \tag{7}$$

This model is appropriate for the small droplet size and the fuel methanol with its relatively high volatility at atmospheric pressure. The Abramzon-Sirignano model [19] is used to calculate convective droplet heating and evaporation in a convective flow field:

$$\dot{m}_d = 2\pi\rho_F D_F r_d \breve{\mathrm{Sh}}\ln(1+B_M). \tag{8}$$

The subscript F denotes properties in the gas film surrounding the droplet that are determined according to the 1/3 rule [20]. $\breve{\mathrm{Sh}}$ is the modified Sherwood number [16].

Equation (5) is solved by a finite-volume method based on SIMPLE algorithm. It provides the mean variables that appear in the evolution equations of droplets and gas particles. The joint velocity-mixture fraction PDF transport equation is solved by a Lagrangian Monte-Carlo particle method. The one-point PDF is represented by a finite number of gas particles. Each gas particle has a set of properties $\{m_g^*, \vec{x}_g^*, \vec{U}_g^*, \xi_c^*\}$. The gas particle with the coordinate $\vec{x}^*$ evolves according to

$$\frac{d\vec{x}^*}{dt} = \vec{U}^*. \tag{9}$$

The value of $\hat{\tilde{\xi}}_c$ in Eq. (4) is determined using the particle cloud-in-cell method [21]. A second-order algorithm [21] is used to solve Eq. (6). At each time step, new gas particles are supplied at the inlet. At the axis of symmetry the particles are reflected. If particles move out of computational domain, they are discarded. To reduce the statistical error in the result of the Monte-Carlo method, a time-averaging scheme is implemented [21].

Equations (6)-(9) are solved by a Lagrangian stochastic droplet parcel method. The spray is represented by a finite number of droplet parcels. Each parcel contains a number of droplets with the same location, size, velocity, and temperature [16]. The spray source terms $\overline{S}_{l,\tilde{\Phi}}$ are calculated using the particle-source-in-cell model [22]. They are fed back to the finite-volume method code and gas-phase PDF code. The Favre-averaged variables $\tilde{U}$, $\tilde{k}$, and $\tilde{\varepsilon}$ appearing in Eqs. (3), (4), and (6), are computed by the finite-volume method and then linearly interpolated to the gas particle and droplet positions.

3 Results and Discussion

A steady, two-dimensional, axi-symmetric, non-reacting turbulent liquid jet without swirl is modeled. A dilute methanol spray is injected into turbulent air. The experiments were performed by McDonell and Samuelsen [15], and their results are available for comparison with the simulations. The geometry of the liquid injector is described in [15]. The position of the fuel injector's exit is marked as x = 0 mm. The gas and droplet velocities, droplet size distribution, liquid flux and concentration of methanol vapor are measured at the axial locations x = 7.5 mm, 25 mm, 50 mm, 75 mm, and 100 mm. The experimental data at x = 7.5 mm are taken as inlet profiles for the simulations. The mass flow rate of the liquid fuel is 1.32 g/s. The airflow results in a pressure drop of 3.73 kPa. At the inlet, the top-hat profile is prescribed for the particles' mixture fraction, and a Gaussian profile for the velocity.

Figure 1 shows the radial profiles of gas-phase mean axial velocities at four different cross sections x = 25 mm (top left), x = 50 mm (top right), x = 75 mm (bottom left), and x = 100 mm (bottom right). Symbols denote experimental data [15]. Solid lines indicate the results of the present PDF method and dashed lines show former results using the extended κ–ε model [16]. The results of the PDF method are in very good agreement with experimental data. The PDF method improves the results of the moment closure model. This is true in particular for the velocity near the centerline, c.f. Fig. 2. The RHS of Fig. 2 shows that the Sauter mean radius is hardly affected by the gas-phase model.

The present extended simplified Langevin model is suitable for use in turbulent spray flows. This model neglects the effects of the mean velocity gradient, which is main source of the discrepancies found in the current simulation. In the region close to the nozzle, the mean velocity gradient is large, which causes some discrepancies with experimental data in this region.

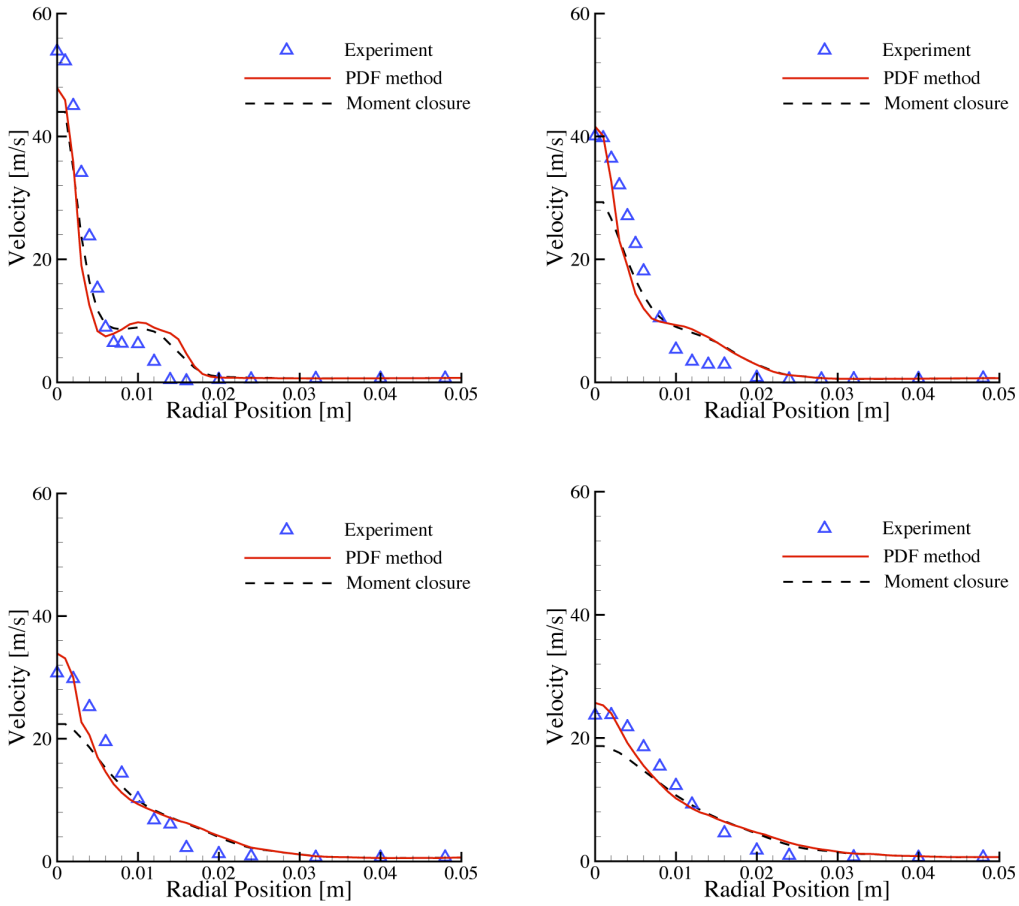

Fig. 1 Radial profiles of the gas-phase mean axial velocity at x = 25, 50, 75, and 100 mm.

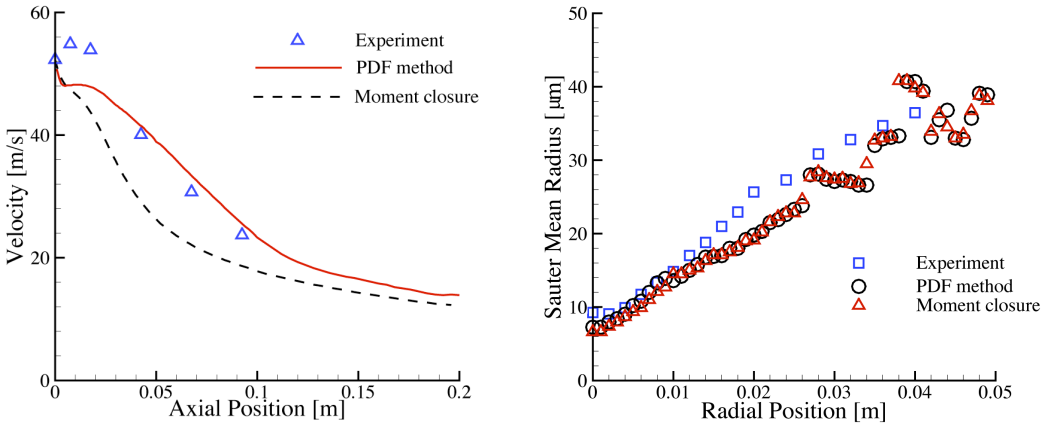

Fig. 2 Left: Axial profile of the gas-phase mean axial velocity along the centerline. Right: Radial profile of the Sauter mean radius at x = 100 mm.

Excellent agreement is found further downstream where the mean velocity gradient is relatively smaller and its effect is negligible. The generalized Langevin model takes into account the effect of the mean velocity gradient. In this sense, the generalized Langevin model could offer better results of gas phase velocity.

4 Conclusions

In present work, a joint velocity-scalar PDF is introduced for turbulent spray flows. The joint velocity-mixture fraction PDF transport equation of the gas phase in turbulent spray flows is deduced. The velocity is modeled through an extended simplified Langevin model, and molecular mixing through an extended IEM model. The PDF transport equation is solved by a Lagrangian Monte-Carlo particle method. The droplet characteristics including heating, vaporization, and motion are solved by a Lagrangian droplet parcel method. To close the PDF transport equation and droplet evolution equation, the mean conservation equations of the gas flow are solved by a SIMPLE-algorithm-based finite volume method. A steady, two-dimensional, axi-symmetric, turbulent methanol/air dilute non-reactive spray flow without swirl is simulated. The results of the gas velocity are in very good agreement with experimental data, and they improve the simulation using the extended κ–ε model. The extended Langevin model is a very promising approach for the modeling of turbulent spray flows.

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