

Validation of Mesh- and Timestep- Independent Spray Models for Multi-Dimensional Engine CFD Simulation

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ABSTRACT

Resolution of droplet-scale processes occurring within engine sprays in multi-dimensional Computational Fluid Dynamics (CFD) simulations is not possible because impractically refined numerical meshes or time steps would be required. As a result, simulations that use coarse meshes and large time steps suffer from inaccurate predictions of mass, momentum and energy transfer between the spray drops and the combustion chamber gas, or poor prediction of droplet breakup and collision and coalescence processes. Several new spray models have been proposed to address these deficiencies, including use of an unsteady gas jet model to improve momentum transfer predictions in under-resolved regions of the spray, a vapor particle model to minimize numerical diffusion effects, and a Radius of Influence drop collision model to ensure consistent collision computations on different meshes. The present work combines these models with improved KH-RT models to improve the consistency of drop breakup predictions. A modified mean collision time model is also proposed to reduce timestep dependency of droplet collision prediction. The models have been implemented into the KIVA CFD code and are demonstrated to achieve independency with respect to both mesh sizes and time steps. The code was validated for non-evaporating and evaporating sprays, and also for diesel engine simulations with variations of larger than one order of magnitude in mesh cell volume and around two orders of magnitude in time steps. The numerical results were found to match available experimental measurements very well, including spray tip penetration, local drop velocity and Sauter mean diameter (SMD) and averaged mean diameter (AMD) of non-evaporating diesel sprays. The new spray models were also applied to simulate evaporating sprays and good agreement was found with measured liquid and vapor

penetration lengths. Finally, the engine simulations were also found to agree well with experimental engine data.

INTRODUCTION

The impact of automotive technology on climate change and environment protection, stresses the need to improve fuel economy and meet stringent emission regulations. Design and optimization of internal combustion engines are expected to be conducted with rapid and productive R&D cycles. Multidimensional engine Computational Fluid Dynamics (CFD) simulation has become more-and-more important as a tool of prediction and analysis, mainly because of its efficiency, low cost, and the ability to get insights about in-cylinder physics without constraints on costly apparatus and specialized measurement techniques.

One of the key aspects of engine CFD is to simulate spray processes. For Direct Injection (DI) diesel and spark-ignited direct-injection (SIDI) engines, the spray processes include injection of liquid fuel and its subsequent break-up, collision between liquid droplets, evaporation from liquid into vapor and mixing with the combustion chamber gas. An accurate prediction of the fuel vapor distribution is one of the prerequisites for realistic modeling of the in-cylinder combustion process and the prediction of engine work output and emissions.

Despite its importance spray modeling is still very challenging for engine CFD researchers [1]. The typical size of the injector nozzle is much smaller than other characteristic dimensions such as intake port sizes, and a wide range of length scales need to be resolved to fully understand the in-cylinder physics. In addition, typical fuel injection velocity is several hundred m/s, compared to only a few m/s in the chamber gas, resulting in a jet boundary/shear

layer with very strong gradients between the two phases. Abraham [2] investigated the mesh size required for adequate resolution of a spray, and found that the near-nozzle mesh size should be at least of the same magnitude as the nozzle diameter to obtain accurate results.

However, such refined mesh resolution is impractical for engine optimization since many simulations have to be run with multiple permutations of parameters to find optimized designs, and the computational cost of running simulations on a refined mesh is prohibitive. As a result, accuracy has to be compromised with efficiency, and in a typical optimization study [3] using the KIVA CFD code [4] and detailed chemistry, the mesh size is nearly 17 times the nozzle diameter.

One of the most popular approaches to simulate spray is the “Lagrangian-Drop Eulerian-Fluid”(LDEF) method, in which liquid fuel is treated as Lagrangian drop and ambient gas is treated as a continuum and is discretized into cells. The two phases are coupled by adding spray source terms to the gas phase conservation laws. In order to save computational cost on tracking droplets, Dukowicz [5] proposed a particle-fluid approach, in which droplets with similar properties are grouped into “parcels” and the spray is solved statistically. These methods have been implemented into the KIVA code [4], and are widely adopted in commercial CFD codes. As pointed out by McKinley and Primus [6], when the mesh resolution is inadequate, the LDEF approach does not accurately capture strong gradients of velocity, temperature and fuel vapor concentration in the gas phase.

Béard [7] proposed a “Couplage Lagrangien-Eulérien” model with a sub-grid “gaseous particle” approach. In order to account for numerical diffusion effects, he suggested that the parcel should not couple with a gas phase cell until its spreading “radius of influence” reaches the mesh scale. Before that, vapor mass and momentum were transported together with the liquid parcel as a gaseous particle. The spreading rate of influence was determined by molecular diffusivity or molecular viscosity, depending on whether it was the influence of vapor mass or momentum. Their results showed mesh-independency of vapor penetration. However, droplet collision was not considered in the simulation, and no results were shown demonstrating the predictions of drop size distribution or liquid penetration are mesh-independent.

The attempts of using adaptive meshes were reported by Lippert et al. [7] and Xue and Kong [9]. In their studies, the spray resolution was dynamically refined locally. The advantage of an adaptive mesh in engine application has not been known.

Abraham and Magi [10] proposed a “Virtual Liquid Source” approach to replace the near-nozzle liquid drops with a liquid core. Liquid was assumed to be moving at the injection

velocity within the core, and spray source terms were added in the cells adjacent to the core surface. In this way, the two-way coupling between drop and gas was avoided. A similar approach was studied by Versevel et al. [11]. A common issue of these two studies is that the spray is assumed to evaporate at a very fast rate, and the break-up and collision of droplets outside the liquid core are neglected. This is not necessarily true for early injection, low temperature engine conditions. Also, the model could not be applied in the case of spray-wall impingement.

Wan and Peters [12] used a one-dimensional model for the liquid spray and coupled it with a three-dimensional Eulerian gas simulation. Since the spray was modeled instead of two-way coupled with the gas phase cell, the mesh-dependency of the spray source terms was removed. However, the near-nozzle break-up physics was not well captured and the simulation was sensitive to the choice of initial droplet diameter.

Instead of modeling the spray, Abani et al. [13] modeled the gas velocity with unsteady turbulent round jet theory [14], and used it to correct the spray-axial gas phase cell velocity. The mesh-dependency of the gas-to-liquid coupling was eliminated when the modeled “gas jet” velocity is applied in the drag calculation. The predictions of liquid penetration in non-evaporating chamber conditions were mesh-independent. However, Abani did not address the mesh-dependency of break-up models, and notable inconsistent drop size predictions could be seen in his results [13].

Unlike mesh-dependency, the investigation of timestep-dependency of spray models is rarely reported in the literature. The physical processes in engines have different time scales that vary according to engine conditions. Munnannur [15] reported a “Mean Collision Time” (MCT) approach to reduce the timestep-dependency for droplet collisions. The MCT was estimated and compared with the CFD timestep. The simulation used the MCT if it was smaller than the CFD timestep to better resolve the collision process.

In this study, the unsteady gas jet model [13] is applied in the KIVA code to obtain mesh-independent drag predictions. The gas jet model is also applied with an improved Kelvin-Helmholtz, Rayleigh-Taylor (KH-RT) hybrid break-up model [16] to remove the mesh-dependency of droplet break-up process. A sub-cycle approach is adopted to remove timestep-dependency of the KH-RT model. In terms of droplet collisions, a mesh-independent Radius of Influence (ROI) collision model [17] is used. The Mean Collision Time approach is investigated and a sub-cycle model is proposed as further improvement. A Vapor Particle Model [18] is also applied to improve the prediction of mass and energy coupling between droplet and gas.

The models were validated in three steps: first, non-evaporating sprays were studied and the predictions of liquid penetration, droplet Sauter mean diameter (SMD) and Averaged mean diameter (AMD) and droplet velocity were compared with available experimental data. Both mesh- and timestep- dependency were evaluated and compared to the performance of the standard KIVA code with KH-RT break-up model. Second, an evaporating spray was studied and the predictions of liquid and vapor penetrations were investigated. Finally, the models were validated in a diesel engine case with available liquid penetration data.

DIESEL SPRAY MODELS

[1]. UNSTEADY GAS JET MODEL

The unsteady gas jet model was originally proposed by Abani et al. [13] to remove the mesh-dependency of liquid drop-ambient gas coupling. The model is based on unsteady gas jet theory [14], in which the jet tip develops with respect to time according to:

$$\frac{dx}{dt} = \frac{3}{K} \frac{U_{inj,eff}(x,t) d_{eq}}{x} \quad (x \geq x_0) \quad (1)$$

where x is jet tip penetration, K is an entrainment constant, $U_{inj,eff}$ is the “effective injection velocity”, d_{eq} is the equivalent diameter which is related to nozzle diameter d_{noz} and liquid-gas density ratio by:

$$d_{eq} = d_{noz} \sqrt{\frac{\rho_l}{\rho_g}}$$

The downstream spray-axial location x_0 marks the start of jet velocity decay and is calculated as:

$$x_0 = \frac{3d_{eq}}{K}$$

The theory assumes the effective injection velocity is an integral of the response to changes of the injection speed from start of injection t_0 to the current time t :

$$U_{inj,eff}(x,t) = U_{inj}(t_0) + \int_{t_0}^t R(x,t-\tau) \left(\frac{dU_{inj}(\tau)}{d\tau} \right) d\tau \quad (2)$$

in which the response function R takes the form:

$$R(x,t-\tau) = 1 - \exp\left(-\frac{t-\tau}{\tau_v(x,\tau)}\right) \quad (3)$$

where τ_v is a response time scale, which is related to the local flow time scale τ_f by a Stokes number St :

$$\tau_v(x,\tau) = St \cdot \tau_f(x,\tau) = St \cdot \frac{x}{U_{inj}(\tau)} \quad (4)$$

This assumption is justified by the fact that a fluid particle responds to a change in the surrounding gas velocity exponentially [19]. The time scale of the response is determined by how long the local fluid particle has resided in the flow. Notice that, in the case of a steady injection, the effective injection velocity equals to the actual injection velocity and Eq. (1) yields the steady jet theory proposed by Abraham [20].

Abani et al. [13] did not mention how particles at different axial locations within the jet should behave with respect to time. In other words, should the effective injection velocity $U_{inj,eff}(x,t)$ be valid for all the particles at time t no matter where they are, or they should have their own local effective injection velocities? Intuitively, far-downstream particles should respond to injection change more slowly than near-nozzle particles. Consequently, the response time scale in Eq. (4) is suggested to be determined by the local spray-axial location of the particle (denoted as y), instead of the spray tip penetration x :

$$\tau_v(y,\tau) = St \cdot \tau_f(y,\tau) = St \cdot \frac{y}{U_{inj}(\tau)}$$

Thus, the response function takes the form:

$$R(y,t-\tau) = 1 - \exp\left(-\frac{t-\tau}{\tau_v(y,\tau)}\right)$$

and the effective injection velocity for each axial location is written as:

$$U_{inj,eff}(y,t) = U_{inj}(t_0) + \int_{t_0}^t R(y,t-\tau) \left(\frac{dU_{inj}(\tau)}{d\tau} \right) d\tau \quad (5)$$

The local gas jet speed at spray axis is correspondingly calculated as:

$$U_{jet,ax}(y,t) = \frac{3}{K} \frac{U_{inj,eff}(y,t)d_{eq}}{y} \quad (y \geq x_0) \quad (6)$$

Assuming axi-symmetry, the gas jet velocity at any radial location r within the jet cross-section can be calculated as [13]:

$$U_{jet}(y,r,t) = \frac{3U_{inj,eff}(y,t)d_{eq}}{Ky \left(1 + \frac{12r^2}{K^2 y^2}\right)} \quad (y \geq x_0) \quad (7)$$

The present unsteady gas jet model corrects the drop-gas relative motion with:

$$\frac{d\vec{u}_d}{dt} = \frac{3}{8} C_D \frac{\rho_l}{\rho_g} \frac{1}{d} |\vec{V}_{jet} + \vec{V}'_{turb} - \vec{u}_d| (\vec{V}_{jet} + \vec{V}'_{turb} - \vec{u}_d) + \vec{g} \quad (8)$$

where $\vec{u}_d$ is droplet velocity vector, C_D is drag coefficient, ρ_g is local gas phase density, $\vec{V}_{turb}$ is local gas phase turbulent fluctuating velocity vector, and $\vec{g}$ is gravity acceleration. $\vec{V}_{jet}$ is the gas phase mean flow velocity with the axial component corrected by Eq.(7). Notice that the radial and azimuthal components are kept, so that other flow velocity components are not influenced. Equation (5) should be used to calculate the effective injection velocity $U_{inj,eff}(y,t)$ for every parcel. However, the integral in Eq. (5) is very expensive if used for all particles, especially when the parcel number is large (e.g., under non-evaporating conditions). Therefore, it is proposed in this study that at every time t^n , the effective injection velocity is calculated only at a limited number of axial locations, $\mathcal{Y}_i$:

$$U_{inj,eff}(y_i, t^n) = U_{inj}(t_0) + \int_0^{t^n} R(y_i, t^n - \tau) \left(\frac{dU_{inj}(\tau)}{d\tau} \right) d\tau \quad (i = 1 \dots N) \quad (9)$$

where N is taken as 40 and $\mathcal{Y}_i$ was uniformly distributed across the spray penetration length at time t^n . These effective injection velocities were used as interpolation points to get the effective injection velocity at any location $\mathcal{Y}$ where the particle resides.

[2]. IMPROVED KH-RT BREAKUP MODEL

Modeling spray atomization a Kelvin-Helmholtz/Rayleigh-Taylor hybrid breakup model [21, 16] was used in this study. The Kelvin-Helmholtz (KH) model is based on linear stability analysis of a liquid jet [22] and is used to model its primary breakup [23]. From the linear stability analysis any perturbation applied to a liquid-gas interface can be expanded as a Fourier series, with its fastest growing mode contributing to the eventual breakup and generation of new droplets. The growth rate and wave length of the fastest growing mode was found numerically [23] as:

$$\frac{\Lambda_{KH}}{r_p} = 9.02 \frac{(1 + 0.45Z^{0.5})(1 + 0.4T^{0.7})}{(1 + 0.87We_g^{1.67})^{0.6}} \quad (10)$$

$$\Omega_{KH} \left[\frac{\rho_l r_p^3}{\sigma} \right]^{0.5} = \frac{(0.34 + 0.38We_g^{1.5})}{(1 + Z)(1 + 1.4T^{0.6})} \quad (11)$$

in which Λ_{KH} is the wave length of the fastest growing wave, Ω_{KH} is its growth rate, r_p is the jet radius, σ is surface tension, the dimensionless gas Weber number We_g is defined as:

$$We_g = \frac{\rho_g U_{rel}^2 r_p}{\sigma}$$

with U_{rel} being the magnitude of liquid-gas relative velocity:

$$U_{rel} = |\vec{V}_{gas} + \vec{V}'_{turb} - \vec{u}_d| \quad (12)$$

in which $\vec{V}_{gas}$ is the CFD gas phase velocity. Similarly, the liquid Weber number is defined as:

$$We_l = \frac{\rho_l U_{rel}^2 r_p}{\sigma}$$

and the dimensionless Ohnesorge number is:

$$Z = \frac{\sqrt{We_l}}{Re_l}$$

with the Reynolds number being:



$$\text{Re}_l = \frac{\rho_l U_{rel} r_p}{\mu_l}$$

μ_l is the dynamic viscosity of the liquid. The last dimensionless number is the Taylor number:

$$\text{T} = Z\sqrt{\text{We}_g}$$

Reitz [23] proposed that the radius of new drops (denoted as r_c) created during the primary breakup process could be related to the wave length Λ_{KH} by:

$$r_c = B_{KH} \Lambda_{KH} \quad (13)$$

where B_{KH} is a constant. With the concept of “blob injection” [24], which models the liquid jet injection with parcels of blobs that have their initial characteristic sizes equals to the effective nozzle diameter, the primary breakup is modeled as a process where new drops (with radius r_c) are formed from parent drops (with radius r_p). The radius change of the parent drop due to mass loss to its “child” drops is described by the rate equation [24]:

$$\frac{dr_p}{dt} = -\frac{r_p - r_c}{\tau_{KH}} \quad (14)$$

in which the breakup time scale τ_{KH} is calculated as:

$$\tau_{KH} = \frac{3.726 C_{KH} r_p}{\Lambda_{KH} \Omega_{KH}} \quad (15)$$

where C_{KH} is a constant.

With the limitation of computational power, it is impractical to track each droplet formed from the parent drop. Following the “droplets in parcel”, Reitz [23] suggests that new droplets could not leave their parent parcel until their mass reaches or exceeds 3% of the average injected parcel mass. The new droplets are then grouped into a “shed parcel” (or child parcel) that is separated from its parent. This parcel-shedding process helps to predict realistic a drop size distribution in the primary breakup region. Also, as the number of parcels is increased, the local statistical resolution could also be improved.

Thus the KH breakup model takes two steps: the first step is to gradually reduce the parent drop size by the rate equation

(14); the second step is to create a new parcel from the parent. Su et al. [21] pointed out that the second step was a numerical regrouping of droplets and not an actual breakup event, therefore aside from mass conservation of parent-child parcels, the original SMD should also be conserved. This approach is referred as “SMD conservation” and has been included in the present mesh- and time step-independent spray models.

The KH break-up model strips small droplets off the jet (represented by parent parcels/blobs), but the jet still maintains itself as a dense liquid core. Beyond a certain distance from nozzle, the Rayleigh-Taylor (RT) model is applied to all parcels together with the KH model to predict secondary break-up [21, 16]. This distance is called the “breakup length” and is predicted by Levich' theory [22] as:

$$L_{brk} = C_b d_{noz} \sqrt{\frac{\rho_l}{\rho_g}} \quad (16)$$

in which C_b is a constant. The RT model considers the instability generated when two fluids with different densities accelerated perpendicular to their interface. The frequency and wavelength of the fastest growing wave are given by Bellman [25] as:

$$\Omega_{RT} = \sqrt{\frac{2}{3\sqrt{3}\sigma} \frac{[-a(\rho_l - \rho_g)]^{3/2}}{\rho_l + \rho_g}} \quad (17)$$

$$\Lambda_{RT} = 2\pi \sqrt{\frac{3\sigma}{-a(\rho_l - \rho_g)}} \quad (18)$$

In the case of a high-speed droplet moving in air, a is the deceleration due to drag. As in the KH model, this fastest growing wave is assumed to lead to the breakup of droplets. Su et al. [21] suggested predicting the radius of the newly-formed droplet and the time of breakup as:

$$r_c = B_{RT} \Lambda_{RT} \quad (19)$$

$$\tau_{RT} = \frac{C_{RT}}{\Omega_{RT}} \quad (20)$$

in which B_{RT} , C_{RT} are two constants. Unlike the KH model, the standard implementation of RT model does not strip small

child drops off from their parent; instead, a catastrophic breakup of the parent drop into small drops is assumed, and the liquid column is eventually disintegrated and dispersed into the ambient gas.

To implement the RT model, Beale and Reitz [16] assumed that RT waves grow on the droplet surface if their wavelength Λ_{RT} is smaller than the droplet diameter, and the drop is not assumed to break-up until the waves have been growing for a time greater than the break-up time τ_{RT} . In other words, the drop instantly breaks-up when time exceeds τ_{RT} . But in reality, droplets experience not only break-ups but also collisions within the spray. A successful collision would disturb (or even merge) the surfaces of its two participants and disrupt the growth of RT waves. Since break-up and collision occur at each time step, this treatment introduces timestep dependency: if the timestep is smaller than τ_{RT} , RT wave growth might be interrupted by a collision; if the timestep is larger than τ_{RT} , no interruption due to collision routine is expected. As a result, running the simulation with large and small time steps might produce completely different drop size distributions.

Accordingly, in this study the RT breakup process was modeled by a rate equation similar to that of the KH model, Eq. (14):

$$\frac{dr_p}{dt} = -\frac{r_p - r_c}{\tau_{RT}} \quad (21)$$

in which r_c is predicted by Eq. (19). The parent drop breaks up continuously at each time step, and the timestep dependency mentioned above is avoided. If assuming r_c and τ_{RT} does not change with time, Eq. (25) can be solved analytically as:

$$r_p = r_c + (r_{p,0} - r_c) \exp\left(-\frac{t}{\tau_{RT}}\right) \quad (22)$$

in which $r_{p,0}$ is the radius of parent drop at the start of break-up. Thus, τ_{RT} is the characteristic time required to break the parent drop; while in Beale and Reitz's approach, τ_{RT} is the final breakup. This requires different choices of the constant C_{RT} in Eq. (20).

In practice, neither rate equation (18) nor (25) can be solved analytically, since both r_c and τ_{KH} (or τ_{RT}) change with time, r_p and U_{rel} can change significantly. Therefore, we

propose a sub-cycle approach to solve the rate equation (18). Take the KH model as an example, at every timestep $t^n \rightarrow t^{n+1}$, Δt is compared with the predicted breakup time scale τ_{KH}^n . If $\Delta t \leq f \cdot \tau_{KH}^n$, in which f is a fraction smaller than 1, an Euler scheme is used to predict r_p^{n+1} and no sub-cycle is needed. If $\Delta t > f \cdot \tau_{KH}^n$, a sub-cycle time step $\Delta t_{KH}^{(1)} = f \cdot \tau_{KH}^n$ is used (superscript (1) means the first sub-cycle). The change in drop velocity during the sub-cycling is calculated using Eq. (8), with the assumption that the local gas velocity does not change significantly. The magnitude of the drop-gas relative velocity is then updated as $U_{rel}^{(1)}$. For simplicity, the properties μ_l, ρ_l, σ and ρ_g are assumed to be unchanged throughout the sub-cycling, and $f \leq 0.02$ was sufficient to eliminate timestep dependency with negligible increase of computational time.

The mesh-dependency of the KH-RT breakup model mainly comes from the calculation of U_{rel} in Eq. (12), in which CFD cell gas velocity $\vec{V}_{gas}$ is used. Since Abani et al. [13] did not use the gas jet-corrected relative velocity U_{rel} in the breakup model, notable mesh-dependent SMD results were observed in spite of mesh-independent prediction of the drag force and the collision process. Note that the gas jet-corrected relative velocity U_{rel} :

$$U_{rel} = \left| \vec{V}_{jet} + \vec{V}_{turb}' - \vec{u}_d \right| \quad (23)$$

only applies beyond x_0 from nozzle, and Abani et al. [13] assume the jet speed at spray axis is:

$$U_{jet,ax}(y,t) = \begin{cases} U_{inj,eff}(y,t) & (y < x_0) \\ \frac{3}{K} \frac{U_{inj,eff}(y,t) d_{eq}}{y} & (y \geq x_0) \end{cases} \quad (24)$$

In the near nozzle region where the droplet velocity is very close to the injection velocity, using Eq. (24) for $y < x_0$ significantly under-predicts the drop-gas relative velocity, and hence under-predicts drag and KH break-up. Therefore, it is proposed in the present study to use a parabolic profile within $y < x_0$, which merges with the profile for $y > x_0$ (see Figure 1), such that the jet velocity is:

$$U_{jet,ax}(y,t) = \begin{cases} \gamma U_{inj,eff}(y,t) \cdot \left[1 - \left(\frac{x}{x_0}\right)^2\right] & \text{if } y \leq x_0 \\ \gamma U_{inj,eff}(y,t) \cdot \left[1 - \frac{1}{8} \left(\frac{x}{x_0}\right)^2\right] & \text{if } x_0 < y < x_{cvg} \\ \frac{3U_{inj,eff}(y,t)d_{eq}}{Ky} & \text{if } y > x_{cvg} \end{cases} \quad (25)$$

in which γ is a constant taken as 0.6. It should be noted that either (24) or (24) are difficult to validate with existing experimental data since measuring the drop velocity and size distribution in the near-nozzle dense spray region is very difficult. For the blob-based KH-RT break-up model, to resolve the real and complicated near-nozzle physics is not possible, and its outcomes can only be validated with downstream measurements. In this sense, the primary objective of current near-nozzle modeling is to eliminate mesh-dependency with reasonable physics, such that the models maintain generality on different meshes. In this sense, assuming the parabolic entrained gas jet velocity profile at the spray axis not only provides mesh-independent break-up outcomes, but also solves the problem of under-predicting near-nozzle breakup, as seen in the original model.

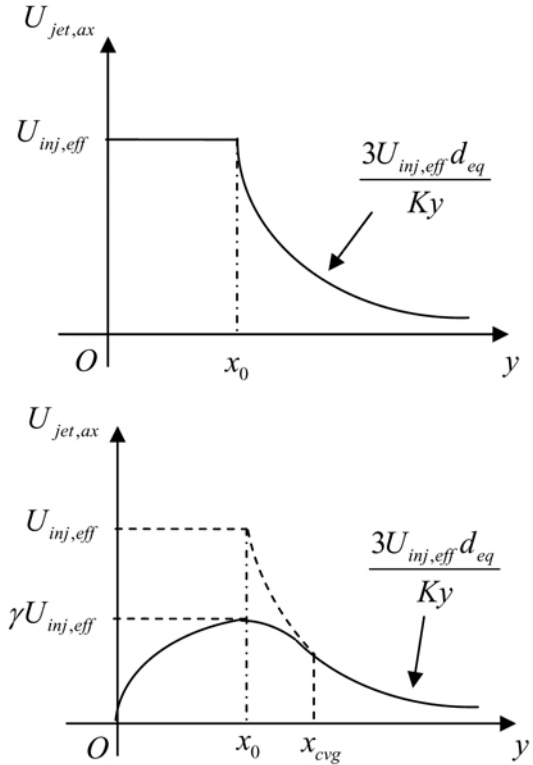


Figure 1. Unsteady Gas Jet Model; original (Top); in this study (Bottom).

[3]. MESH AND TIMESTEP-INDEPENDENT COLLISION MODELS

The Radius-of-Influence (ROI) collision model of Munnannur and Reitz [17] removes mesh-dependency of the droplet collision process. Collision partners of a certain parcel are searched for within a “sphere of influence” centered at the parcel's location. All parcels within this sphere are possible partners to collide with the centered parcel. The prediction removes the dependency on gas phase mesh size (as seen in O'Rourke's original model [4]), or the dependency on collision mesh size if a separate collision mesh is used [26]. The probable number of collisions of the two colliding drop parcels is:

$$\nu = \frac{N_1 N_2}{V_{col}} \pi (r_1 + r_2) |\vec{u}_{d,1} - \vec{u}_{d,2}| \quad (26)$$

in which N_1 and N_2 are the numbers of droplets within the two parcels, r_1 and r_2 are the droplets radii, and V_{col} is the volume of the sphere of influence. The new collision outcomes suggested by Munnannur and Reitz [17], i.e., bounce, stretching and reflexive separation, have been used in this study together with coalescence and grazing [4] to better predict the results of a successful collision.

The issue of timestep dependency was also investigated by Munnannur [15] in light of Reiffel's argument for the "particle in cell" approach in Direct Simulation Monte Carlo method [27]. Reiffel suggested that the timestep should be properly chosen such that the average distance traveled by a particle in this timestep is some fraction of the average cell length. Basing on his ROI approach, Munnannur estimated the "mean collision time" (MCT) for each cell as:

$$\Delta t_{col} = \frac{C_{col}}{u_{d,max,cell}} \cdot \frac{R_{inf}}{N_{cell}^{1/3}}$$

in which $u_{d,max,cell}$ is the maximum droplet velocity magnitude in the cell, R_{inf} is the Radius of Influence, N_{cell} is number of parcels in the cell, and C_{col} is a constant. The global MCT is then taken as the minimum of the cell MCTs. To fully implement the ROI approach and eliminate mesh dependency, the MCT is calculated in this study for each parcel based on the ROI concept:

$$\Delta t_{col} = \frac{C_{col}}{u_d} \cdot \frac{R_{inf}}{N_{ROI}^{1/3}}$$

in which u_d is the average droplet velocity magnitude, and N_{ROI} is number of parcels in the sphere of influence. The global MCT is taken as the minimum of all parcels' MCTs. Similar to Reiffel's argument, within the timestep for the collision routine, parcels should not traverse too many ROIs, otherwise the predictions of collision probability and outcomes would be inaccurate. On the other hand, too small a timestep results in excessive computational cost, since the cost is proportional to square of total number of droplet parcels. Therefore, Munnannur [15] proposed dynamically controlling the timestep, such that if Δt_{col} is smaller than the computational timestep, Δt_{col} is chosen as the computational timestep; if Δt_{col} is greater than the timestep, collisions are carried on only when accumulated time of Δt_{col} is reached.

However, if $\Delta t_{col} < \Delta t$, taking Δt_{col} as the timestep for an entire engine simulation imposes the timestep on other physical process that might occur at very different time scales. Therefore in this study, instead of replacing Δt with Δt_{col} , it is proposed to sub-cycle the collision routine with Δt_{col} if it is smaller than Δt . After each sub-cycle, all the droplet properties except their spatial locations are updated to reflect the collision outcomes, and these updated properties are used to predict the collision process in the next sub-cycle.

[4]. VAPOR PARTICLE MODEL

The liquid-to-gas coupling where cells receive transported momentum from drop parcels is still dependent on mesh size; and this problem is not addressed with the above models. In addition, the two-way coupling of mass and energy is still mesh-dependent. As a result, on a coarse mesh where the jet is under-resolved, numerical diffusion effects significantly under-estimate the transport of vapor fuel and thus under-predicts vapor penetration.

To address this issue, Abani and Reitz [18] proposed a Vapor Particle Model as a combined Lagrangian and Eulerian approach for vapor-air mixing. In this model, in the region where the jet is under-resolved, a portion of the vaporized fuel travels with the liquid particle as a vapor cloud. Depending on the local resolution of the jet, the cloud gradually releases its vapor to the local cells, until the liquid particle becomes fully vaporized and then the vapor cloud becomes a vapor particle. The vapor particle continues downstream until a critical distance is reached, where the local mesh size is sufficient to resolve the spreading jet and the remaining fuel vapor is released to the cells. This model was found effective for reducing the mesh-dependency of vapor fuel transport, and has been included in the present study. Unlike the model of Béard [7], momentum coupling is considered by the unsteady gas jet model. In addition, the coupling of vapor particle and gas phase cell is based on the comparison of the local jet radius and mesh size, instead of molecular diffusion. More details can be found in [18].

RESULTS AND DISCUSSION

[1]. MODELS FOR COMPARISON

The above mentioned models have been implemented in the KIVA code, and will be denoted hereafter as "New Spray Models". Results from the standard KIVA code with the original KH-RT model [16] (denoted as "Old Spray Models") will be compared to those from the new spray models. Details of the model differences are summarized in Table 1. The standard KIVA k-e turbulence model was used in the computations with the standard initializations.

<table 1 here>

[2]. NON-EVAPORATING SPRAYS

The new spray models were firstly studied under non-evaporating chamber conditions. Experimental validation data were taken from PDA measurements of Mitroglou et al. [28]. In their experiments, the spray characteristics of a 6-hole injector for a Direct-Injection (DI) gasoline engine were investigated with Iso-octane fuel. Details of the experiment and case setup are summarized in Table 2.

<table 2 here>