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A PROBABILISTIC METHOD FOR MODELING THE SPRAYS

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Abstract: *Present paper presents a model for atomized non-evaporating liquid spray injected in diesel engine. The method consists of a fully interacting combination of Eulerian fluid and Lagrangian particle calculation.*

Key words: *spray, interaction, particle, probabilistic.*

1. Introduction

In this paper, we are interested in problems, such as high-pressure fuel injection in an internal combustion engine, in which the spray carries sufficient momentum to entrain and set into motion the surrounding gas. In turn, the motion of the gas in the vicinity of the particles reduces the resistance to their motion and allows the spray to penetrate much further than would otherwise be the case. It is important, therefore, to account for the interaction between the particles and the gas. This interaction is of course always present, but it is particularly significant whenever the total mass and momentum of the particles is comparable to that of the gas, and when the size of the particles is sufficiently small so that the coupling of a particle to the gas is strong.

The procedure is to represent the spray by discrete particles, rather than by continuous distributions. This amounts to a statistical (Monte Carlo) formulation of the problem, since the finite number of particles used represents a sample of the total population of particles.

Each computational particle is considered to represent a group of particles possessing the same characteristics such as size, composition, etc.

The use of discrete particles eliminates the problems of numerical diffusion and of resolution in the vicinity of the injector.

2. Application Description

It will be assumed that no particle coalescence or particle breakup occurs. This implies that the particles are sufficiently dispersed that particle collisions are infrequent. The initial breakup of liquid sprays or jets is not considered It is assumed that initial conditions for the particles are known. That is, the initial particle size distributions, positions, and velocities are independently specified.

This leads to two sets of equations, one set for the gas and the other for the particles. These equations will be coupled primarily by two mechanisms, the displacement of gas by the volume occupied by the particles and momentum interchange between particles and the gas. Because the particles are nonevaporating

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and nonburning, there is no mass exchange. Further, we assume that the gas or fluid containing the particles is compressible.

Spary equations:

$$\frac{\partial f}{\partial t}+\nabla_x\left(fu_p\right)+\nabla_{u_p}\left(fF_p\right)+ \frac{\partial}{\partial r_p}\left(fR_p\right)+\frac{\partial}{\partial T_p}\left(f\dot{T}_p\right)=\dot{Q} \tag{1}$$

where u_p, F_p, R_p and T_p is the velocity, force, rate of radius variation and the temperature of an arbitrary droplet in the spray at x position. $fdr_p dv_p dxdT_p$ is the probably number of droplets at x position, in the space dx, with u_p, F_p, R_p and $\dot{Q}$ is f rate of change, made by collision, and coalescention.

Continuity equation for the gas:

$$\frac{\partial \theta}{\partial t}+\nabla\cdot\theta u_g=0, \tag{2}$$

where θ is the void fraction, or the fraction of the volume occupied by the gas, and u_g is the gas velocity. The presence of the void fraction in this equation accounts for the displacement effect of the particles.

Momentum equation:

$$\frac{\partial}{\partial t}\theta u_g+\nabla\cdot\theta u_g u_g=\theta g-\frac{\theta}{\rho_g}\nabla p+ +\nabla\cdot\theta\mu_g\nabla u_g+\frac{1}{\rho_g}M_p \tag{3}$$

where g is the acceleration of gravity, p is the pressure, μ_g is the kinematic viscosity (or eddy viscosity if the flow is turbulent), and M_p is the term defining momentum exchange with the particles, per unit volume. An alternative form of this equation can be obtained by subtracting out the continuity equation:

$$\frac{\partial}{\partial t}u_g+u_g\cdot\nabla u_g= =g-\frac{1}{\rho_g}\nabla p+\frac{1}{\theta}\nabla\cdot\theta\mu_g\nabla u_g+\frac{1}{\theta\rho_g}M_p \tag{4}$$

This is the form of the equation used. The terms containing M_p, will be defined later.

In a turbulent flow, the gas equations of the previous section are written in terms of the mean velocity u_g. For particles, gas turbulence is important as a mechanism for diffusion; and it is convenient to write the instantaneous, rather than averaged, equations for the particles. To do this, we define the instantaneous gas velocity, $U_g=u_g+u_g'$, where u_g', is the turbulent component of the gas velocity.

Each particle, individually labeled by subscript *k*, is assumed to obey the following equations:

Particle velocity:

$$u_{pk}=dx_{pk}/dt \tag{5}$$

Particle momentum equation:

$$m_k\frac{d}{dt}u_{pk}=m_k g-\frac{m_k}{\rho_k}\nabla p+ +D_k[U_g](U_g-u_{pk}); \tag{6}$$

where x_{pk} is the particle position, u_{pk} is its velocity, m_k is its mass, and ρ_k is its density. The notation $D_k[U_g]$ is used to denote the drag function, evaluated using the velocity U_g, which is the coefficient in the force acting on the particle due to its motion through the gas. It will be convenient to abbreviate the notation to

D_k when referring to the drag function evaluated at the mean gas velocity u_g ($Dk \equiv Dk[u_g]$).

It is sometimes more convenient to consider the effect of turbulence on the particles to be due to a force f_{pk}, in which case the momentum equation is written:

$$f_{pk} = D_k[U_g](U_g - u_{pk}) - D_k(u_g - u_{pk}) \tag{7}$$

$$\Rightarrow m_k \frac{d}{dt} u_{pk} = m_k g - \frac{m_k}{\rho_k} \nabla p + D_k(u_g - u_{pk}) + f_{pk}; \tag{8}$$

The terms in the gas equations (eqs. 2 - 4) dependent on the particles have not yet been defined. Taking ensemble averages, we can write:

$$\theta = 1 - \sum_k \overline{4/3\pi r_k^3 \delta(x - x_{pk})} \tag{9}$$

$$M_p = -\sum_k \overline{D_k(U)(U_g - u_{pk})\delta(x - x_{pk})} \tag{10}$$

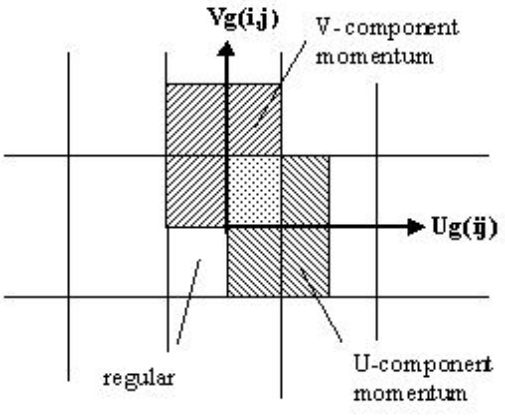

Fig. 1. *Typical cells.*

Velocities are defined in the middle of cell faces. Thus, there are two staggered meshes associated with the respective velocity components, and the corresponding cells, called momentum cells, are indicated by dashed lines in Fig. 1.

These computational cells act as control volumes for the dependent variables associated with the basic equations. The regular cells are the control volumes for the mass continuity equation. Variables associated with them are the pressure and the void fraction. The momentum cells are the control volumes for the momentum equations, and the associated variables are $u_{g,ij}$ and $v_{g,ij}$ and the components of the pressure gradient Δp. To a first approximation, these variables are assumed to be constant within their respective cells.

We shall also use a time-splitting procedure employing intermediate time levels denoted by superscripts such that:

$$t^n < t^T < t^{2T} < t^{3T} < t^{n+1} \tag{11}$$

For modeling purposes, it is not possible to deal with the large number of droplets, so that a sampling technique be employed in which each single particle represents a characteristic group of particles. This is equivalent to the following distributions function:

$$f(r,x,u_p,t) = \sum_k N_{pk} \delta(r - r_k) \cdot \cdot \delta(x - x_k)\delta(u_p - u_{pk}) \cong \frac{\Delta N}{\Delta r \Delta x \Delta u_p} \tag{12}$$

where N_{pk} is the number of identical particle by particle k, ΔN is the number of particles in the volume $\Delta r \Delta x \Delta u_p$.

The droplet size distribution is:

$$f_r(r) = \frac{6}{D_{32}} \exp\left(\frac{-6r}{D_{32}}\right) \tag{13}$$

where D_{32} is Sauter mean diameter which is consider to varying very little.

Eddy viscosity was estimated using a value appropriate to a turbulent gaseous jet:

$$\mu_g = 0.0161\sqrt{0.25\pi d^2 V^2}\,, \tag{14}$$

where d is the orifice diameter and V is the droplet injection velocity.

No attempt was made to calculate particle diffusion accurately. Particle turbulence was modeled using the assumption, that the fluid turbulence is isotropic and has a Gaussian distribution in velocity. Given the turbulent kinetic energy k, is $k = 0.1u_g u_g$, and turbulent velocity is:

$$u_g^{'} = k^{0.5}\,\mathrm{sgn}(X)\cdot erf^{-1}(|X|), \tag{15}$$

where, as before, *X* and *Y* are random variables selected for a uniform distribution in the range *-1 < X, Y < 1*. To complete the description, the relevant turbulence time scale τ is required. The velocity $u_g^{'}$ is assumed to act for a time equal to $\tau = \Delta t$. An elementary analysis suggests that the produces particle diffusion corresponding to:

$$D_T \approx 0.66\left(\frac{D_k}{m_k}\right)^2 q\tau^3\,. \tag{16}$$

The resulting particle concentration, which is Gaussian, forms a distribution function for the location of the particle. Particle positions are randomly selected from within this distribution, such that on each time step the diffusional increment in particle position is

$$\Delta x_{pk} = (4D_T\Delta t)^{0.5}\,\mathrm{sgn}(X)erf^{-1}(|X|) \tag{17}$$

This is equivalent to selecting the following random particle force on each time step

$$f_{pk} = m_k\frac{\Delta x_{pk}}{\Delta t^2}\,. \tag{18}$$

Each particle injected or entering the mesh must be assigned a velocity u_{pk}, a radius r_k, and the number of particles in the group N_{pk}. Let the number of computational particles injected per cell per time step be *K*. The radius of each particle is then chosen from a uniform random distribution that verified the relation.

$$\sum_{k=1}^{K} N_{pk}m_k = Q\Delta t\,. \tag{19}$$

If the pressure drop across the nozzle is known, then

$$V = C\left(\frac{2\Delta p}{\rho_p}\right)^{0.5}\,, \tag{20}$$

The transverse velocity is derived in terms of the initial spray angle using the relationship $0 < (u_{pk})_t \le Max(u_{pk})_t$ where

$$Max(u_{pk})_t = V\tan(\alpha/2), \tag{21}$$

$$\tan(\alpha/2) = C(\rho_g/\rho_p)^{1/2}\,. \tag{22}$$

Knowing the position of each particle at time t^{n+1} the void fraction is calculated using Eq. 9 where the summation is over all particles in regular cell *(ij)* and V_{ij} is the volume of that cell. The void fraction is assumed to be centered in the cell; values at cell faces are obtained by linear interpolation. For each regular cell the void fraction is:

$$\theta_{ij}^{n+1} = 1 - \frac{4\pi}{3V_{ij}} \sum_k N_{pk} r_k^3 , \qquad (23)$$

the continuity equation

$$\frac{\theta^{n+1} - \theta^n}{\Delta t} + \nabla \cdot \theta^{n+1} u_g^{n+1} = 0 . \qquad (24)$$

The equations that have to be solved next, simultaneously, are the gas and particle momentum equations over the momentum cell

$$\frac{u_g^{n+1} - u_g^n}{\Delta t} + F^n = g - \frac{1}{\rho_g} \frac{\partial p^{n+1}}{\partial x} + \\ + \left(g - \frac{1}{\rho_p} \frac{\partial p^{n+1}}{\partial x} \right) \Delta t S^{2T} - u_g^{n+1} S^{2T} + R^{2T} \qquad (25)$$

We shall employ a splitting procedure, which, while preserving the original equations, will solve them in a number of stages.

$$R^{2T} = \frac{1}{\rho_g \theta^{n+1} V_{mcel}} \sum_k \frac{N_{pk} D_k^{2T}}{1 + \Delta t \frac{D_k^{2T}}{m_k}} \left(u_{pk}^n - u_g^{'} \right), \\ S^{2T} = \frac{1}{\rho_g \theta^{n+1} V_{mcel}} \sum_k \frac{N_{pk} D_k^{2T}}{1 + \Delta t \frac{D_k^{2T}}{m_k}}, \qquad (26) \\ F^n = u_g^n \cdot \nabla u_g^n - \frac{1}{\theta^{n+1}} \nabla \cdot \theta^{n+1} \mu_g \nabla u_g^n .$$

We first calculate intermediate gas and particle velocities, accounting explicitly for all forces, except for particle interactions and turbulence, using the equations (27). Application of the present technique has been the modeling of fuel injection sprays. It would be desirable to compute sprays for which experimental data are available so that a direct comparison could be made.

$$\frac{u_{pk}^{n+1} - u_{pk}^n}{\Delta t} = g - \frac{1}{\rho_p} \frac{\partial p^{n+1}}{\partial x} + \\ + \frac{D_k^{2T} (U_g)}{m_k} \left(U_g^{n+1} - u_{pk}^{n+1} \right) \qquad (27)$$

The experiments of Hiroyasu and Kadota [3] come closest to providing such data and were therefore chosen to provide the basis for the following computations. For computational purposes these data had to be estimated, and in some cases drastic approximations had to be made. For computation purposes we used diesel fuel oil with density $\rho_p = 840\, kg/m^3$ injected in air, injector with 5 orifices $d = 0.25\, mm$ and open pressure $P_{in} = 215\ bar$.

The quadrilater generalized mesh used, was found necessary to refine near the spray axis because of the large velocity gradients. The computational programs were 2D and consider the injector in the middle of a chamfered bowl combustion chamber.

The Fig. 2, and 3 plot the velocity fields and particle motion computation for any representative crank angle in the cycle.

3. Conclusions

1. The numerical technique described has generally been well-behaved except under conditions when particles cluster locally so that the void fraction becomes negative in that cell. This is strictly unphysical
2. There are a number of possibilities for modifying the technique to prevent particles from packing closer together than the close-packed limit, for example.

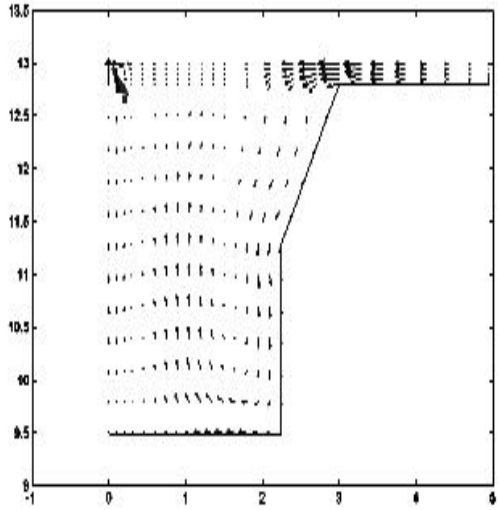

Fig. 2. *Crank angle 354.4*

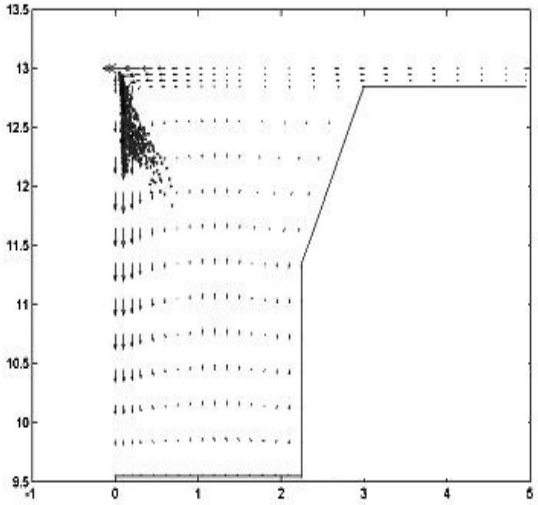

Fig. 3. *Crank angle 358.6*

3. The development of the technique is based on the assumption of noninteracting droplets. While this assumption is bound to fail in the vicinity of the injector.
4. Clearly, many other approximations are involved, such as the assumption of spherical droplets, as well as the numerical inaccuracies associated with a finite mesh.
5. Much better experimental data than currently available will be necessary to resolve these questions.

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