

Lagrangian Particle Tracking (LPT) - Two-Phase Flows

1.0 Introduction

Two-phase flow phenomena exist in a wide variety of engineering applications. The simulation of these particulate two-phase flows with simple or complex geometry is of special interest to many scientific and engineering endeavors. Examples include the design of power-generating devices such as internal combustion engines and liquid or solid rocket engines, pollution control, nozzle design, filter design, etc. In each of these applications the two-way coupling of the transportation of momentum, heat, and mass between continuous phase and particulate phase plays an important role in the nature of these flows.

During the past two decades, two-phase flows have been studied extensively. To date, two generally accepted methods have been used successfully in computer simulation of these two-phase problems: the Eulerian or Eulerian-Eulerian approach, and the Lagrangian or Eulerian-Lagrangian (particle tracking approach).

Description of Methodologies

Eulerian

The Eulerian method considers two fluids to exist as continuous phases. That is, both fluids are treated as though they are completely interpenetrating. This approach is suitable for simulating true two-fluid phenomena, such as the interaction of fuel and water. This method can also be employed in cases involving particulate flow where the particle phase can be assumed to behave as a continuum, such as dust or smoke in air. The advantage of this approach is its relatively high computational efficiency.

Lagrangian

The Lagrangian approach is a two-phase particle tracking method that allows for the calculation of the fluid-particle interaction between a dispersed phase and a continuous fluid.

Particles are tracked in a realistic manner by directly modeling the physics of the particle behavior in conjunction with the flow field. The Lagrangian model treats the particles as discrete entities in the flow field and calculates their relative trajectories. The continuous phase is simultaneously described and consequently solved with an Eulerian approach. The flow field can be laminar or turbulent in nature. With the Lagrangian approach, the solution of the dispersed phase is coupled to the continuous phase by representing the dispersed particles with a specified finite number of computational parcels. A random sampling technique is used to calculate the continuous phase flow properties based on the specified turbulence model. The resulting fluctuations in the continuous phase are used in a Lagrangian computation for particle motion. In turn, the exchanges of momentum, heat, and mass between the two phases are then computed. The main benefit of the Lagrangian approach is its flexibility and its ability to model poly-dispersed sprays.

Modeling Lagrangian Two-Phase Flows with STORM/CFD2000

CFD2000 employs an efficient Lagrangian methodology for simulation of two-phase flows and is applicable in both laminar and turbulent flow regimes. CFD2000 uses a modified non-iterative numerical technique known as PISO (Pressure Implicit with Splitting of Operators) [1,2] to solve the time dependent continuous phase equations using an Eulerian approach. The PISO method uses a predictor and multi-pressure corrector with an implicit density treatment to develop the coupling between the pressure and velocity fields. The discretized Navier-Stokes equations are formed on a non-staggered grid and are integrated implicitly in a time marching fashion.

The effects of the particle phase on the continuous phase are computed by adding the appropriate source term to the Navier-Stokes equations. The motion of the particle phase is simulated using a Lagrangian approach, in which a set of ordinary differential equations (ODE) are developed to describe the particle trajectories and velocities. In addition to the predictor and corrector steps of the solution procedure within the continuous phase, a global iterative process between the particulate phase and continuous phase is required to take into account the interaction between both phases.

Switch-on Physical Models

Sophisticated physical models have been included which can further describe specific particle behavior observed in nature, such as particle evaporation, particle breakup, particle combustion, and turbulent particle dispersion. Particle collision can also be taken into account in STORM/CFD2000 based on particles colliding with other particles and/or particles colliding with surface boundaries or blockages or blockages, including parameters for representing the effects of sticking and bouncing. The addition of these switch-on physical models allows for a more accurate description of the complex interactions between particulate phase and continuous phase to be modeled.

Particle Injection Modeling

The ability to prescribe detailed injection parameters is built into the Lagrangian scheme, which allows the investigator to describe how the particulate phase is injected into the computational domain. The injection parameters can be used to describe various planar or conical particle-injection patterns. Conical injection patterns can be described as being a solid cone or a hollow cone geometry and can be applied at any arbitrary angle. Injection parameters can also address non-uniform particle size distributions, which are often encountered in real world particulate-flow problems.

Summary

The two-phase flow capability in STORM/CFD2000 is a robust fully interacting solution methodology which employs the Lagrangian approach to describe particle motion while using an Eulerian method to model the continuous phase. Furthermore, the methodology accurately accounts for the constant interaction between the continuous and particulate phases.

The addition of switch-on models and boundary-interaction features allow more rigorous modeling of particulate flow phenomena. The general Lagrangian capabilities represent an enabling technology for the investigation of particulate flow behavior found in engineering applications across a broad range of industries.

2.0 Continuous Phase Flow Equation

In a general turbulent flow the Favre density weighted method of the flow variables is introduced into the governing equations.

It is helpful to use tensor notation in writing all governing equations [4]. The Stokes' hypothesis about the bulk viscosity will be used [5]. This assumption implies that the thermodynamic pressure p is equal to one-third of the invariant sum of normal stresses. Employing the density-weighted averaging procedure [3] along with the k - ϵ two equations model, the governing equations with the effect of particles for Newtonian flow are as follows:

Mass conservation:

$$\frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i}(pU_i) = S_{m,p} \quad (1)$$

Momentum conservation:

$$\frac{\partial pU_i}{\partial t} + \frac{\partial}{\partial x_j}(pU_iU_j) = \frac{\partial p}{\partial x_i} - \frac{\partial t_{ij}}{\partial x_j} + S_{U_i} + S_{U_i,p} \quad (2)$$

Energy conservation for static enthalpy:

$$\frac{\partial rh}{\partial t} + \frac{\partial}{\partial x_j}(rhU_j) = \frac{dp}{dt} + \frac{\partial}{\partial x_j} \left[\left(\frac{\mathbf{m}}{P_r} + \frac{\mathbf{m}_t}{P_{rt}} \right) \frac{\partial h}{\partial x_j} \right] + S_h + S_{h,p} + \dot{Q} \quad (3)$$

Species conservation:

$$\frac{\partial pY_i}{\partial t} + \frac{\partial}{\partial x_j}(pY_iU_j) = \frac{\partial}{\partial x_j} \left[\left(\frac{\mathbf{m}}{S_c} + \frac{\mathbf{m}_t}{S_{ct}} \right) \frac{\partial Y_i}{\partial x_j} \right] + \dot{\mathbf{w}}_i + S_{m,p} \quad i = 1, \dots, NS \quad (4)$$

Turbulent transport equation for kinetic energy k :

$$\frac{\partial pk}{\partial t} + \frac{\partial}{\partial x_j}(pkU_j) = \frac{\partial}{\partial x_j} \left[\left(\mathbf{m} + \frac{\mathbf{m}_t}{S_k} \right) \frac{\partial k}{\partial x_j} \right] + \mathbf{m}_t G - p\mathbf{e} + S_{k,p} \quad (5)$$

Turbulent transport equation for dissipation: e

$$\frac{\partial p e}{\partial t} + \frac{\partial}{\partial x_j} (p e U_j) = \frac{\partial}{\partial x_j} \left[\left(\mathbf{m} + \frac{\mathbf{m}_t}{\mathbf{s}_e} \right) \frac{\partial e}{\partial x_j} \right] + \frac{e}{k} (C_1 \mathbf{m}_t G - C_2 p e) + S_{e,p} \quad (6)$$

Equation of state for ideal gas:

$$p = \rho R T \quad (7)$$

The shear stress:

$$\tau_{ij} = (\mathbf{m} + \mathbf{m}_t) \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \quad (8)$$

Where, ρ is the ensemble averaged density of the mixture; U_i is the i -th component of the density-weighted mean velocity. In the three dimensional space, U_i has three components, $U_i = (U_1, U_2, U_3)$. h is the density –weighted mean static enthalpy, defined by

$$h = \sum_{i=1}^{NS} Y_i h_i \quad (9)$$

h_i is static enthalpy for each species, defined by

$$h_i = h_{ref} + \int_{T_{ref}}^T c_{pi} dT \quad (10)$$

Y_i ($i = 1, \dots, NS$) is density-weighted mean mass fraction of the i -th species; NS is total species number; h_{ref} is the reference enthalpy of the i -th species at reference temperature; c_{pi} is specific heat of the i -th species; p is mean pressure; \mathbf{m} is laminar viscosity; \mathbf{m}_t is turbulence eddy viscosity, defined by

$$\mathbf{m}_t = C_m p \frac{k^2}{e} \quad (11)$$

P_r is laminar Prandtl number; P_{rt} is turbulence Prandtl number; S_c is laminar Schmidt number; S_{ct} is turbulence Schmidt number; \dot{w}_i is species production rate. Q is the heat supply. The terms $S_{m,p}$, $S_{Ui,p}$ and $S_{h,p}$ are the source terms contributed by particles, which will be discussed later.

It should be mentioned that the turbulent Reynolds stress and scalar fluxes are modeled from the gradient transport model [6],

$$\overline{ru_i u_j} = -m_t \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) + \frac{2}{3} d_{ij} (rk + m_t \frac{\partial U_k}{\partial x_k}) \quad (12)$$

and

$$\overline{ru_i f} = -\frac{m_t}{s_t} \frac{\partial f}{\partial x_i} \quad (13)$$

In equation (5) and (6), the turbulent production term is

$$m_t G = m_t \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_j} - \frac{m_t}{p^2} \frac{\partial p}{\partial x_j} \frac{\partial p}{\partial x_j} - \frac{2}{3} (rk + m_t \frac{\partial U_i}{\partial x_i}) \frac{\partial U_j}{\partial x_j} \quad (14)$$

All constants in the equations above are listed in the following tables.

Turbulence model constants

C_1	C_2	C_m	s_k	s_e	s_t
1.45	1.92	0.09	1.0	1.3	0.9

Prandtl and Schmidt numbers

P_r	P_{rt}	S_c	S_{ct}
0.7	0.9	0.7	0.9

3.0 Continuous Phase Flow Equation

The Particle characteristics are governed by the equation of motion, the equation of evaporation and the equation of heat transfer. These ordinary differential equations will be integrated along the particle trajectories.

Particle Motion Equation

The equation of motion for a particle within a fluid continuum, was originally derived by Basset Boussinesq and Oseen for a fluid at rest, hence the B-B-O equation, and extended by Tchen [7] to the case of a fluid moving with variable velocity.

$$\frac{\rho}{6} d_p^3 \mathbf{r}_p \frac{dv_i}{dt} = \frac{\rho}{8} d_p^2 \mathbf{r} C_D |v_i - u_i| (v_i - u_i) \frac{\rho}{6} d_p^3 \frac{\partial p}{\partial x_i} + \frac{\rho}{12} d_p^3 \mathbf{r} \left(\frac{du_i}{dt} - \frac{dv_i}{dt} \right) + \frac{3}{2} d_p^2 \sqrt{\rho \mu} \int_{t_0}^t dt \frac{\frac{du_i}{dt} - \frac{dv_i}{dt}}{\sqrt{t - t_0}} + \frac{\rho}{6} d_p^3 \mathbf{r}_p F_{bi} \quad (15)$$

Where t_0 particle starting time, the sub-index r means the particle, v_i is the particle velocity and u_i is the fluid velocity, d_p is the particle diameter, t is time μ is the fluid laminar viscosity, ρ is the fluid density. The left hand side of the equation (15) is the initial force of the particle and the right hand side are drag forces on the particle, body force and other force on the particle. The fourth term is “Basset” which comes from the effect of the deviation of the flow pattern from steady state. Usually, the drag and gravity forces dominate the behavior of the particle; therefore, the approximate form of the B-B-O equation reduces to

$$\frac{dv_i}{dt} = \frac{U_i + u_i' - v_i}{\tau} + F_{bi} \quad (16)$$

Where, F_{bi} is the body force acting on the particle per unit mass in the i -direction, τ is the particle relaxation time and defined by

$$\tau^{-1} = \frac{3}{8} \frac{\rho}{\rho_p r_p} C_D |U_i + u_i' - v_i| \quad (17)$$

Where, u_i' is the fluid fluctuating velocity effect, C_D is the standard drag coefficient for where particle is usually given by [18] and [19]

$$C_D = \frac{24}{R_{ep}} \left(1 + \frac{1}{6} R_{ep}^{\frac{2}{3}}\right) \quad \text{if } R_{ep} \leq 1000$$

$$= 0.424 \quad \text{if } R_{ep} > 1000 \quad (18)$$

The particle Reynolds number R_{ep} is defined as

$$R_{ep} = \frac{|U_i + u_i' - v_i| \mathbf{r} d_p}{\mathbf{m}} \quad (19)$$

The particle position can be determined by integrating the following equation

$$\frac{dx_i}{dt} = v_i \quad (20)$$

Droplet Evaporation Model

If the particle is a liquid or droplet, the following equation set can describe the relation between its size and temperature:

$$\frac{dr_p}{dt} = -\frac{\dot{m}_{ev}}{4\pi r_p^2 \rho_p} \quad (21)$$

and

$$\frac{dT_p}{dt} = \frac{\dot{Q}_L}{m_p C_{pp}} \quad (22)$$

Where, \dot{m}_{ev} is the mass evaporation rate per unit area, \dot{Q}_L the heat transfer rate per unit area, C_{pp} the particle specific heat, m_p the particle mass, r_p the particle radii and T_p the particle temperature. It is assumed that the particle temperature is uniformed within that particle. The evaporation rate can be calculated by the Frosslin correlation [8]:

$$\dot{m}_{ev} = 2\pi d_p (pD_g) \left(1 + 0.3 R_{ep}^{\frac{1}{2}} S_c^{\frac{1}{3}}\right) \ln(1 + B_m) \quad (24)$$

The particle temperature can be found by introducing the latent heat of the particle (or droplet) L , and heat conduction rate at the particle surface per unit area \dot{Q}_c :

$$\dot{Q}_L = 4\pi r_p^2 \dot{Q}_c - \dot{m}_{ev} L \quad (25)$$

and

$$\dot{Q}_c = \frac{2K(T - T_p)}{d_p} (1 + 0.3R_{ep}^{\frac{1}{2}}P_r^{\frac{1}{3}}) \frac{\ln(1 + B_m)}{B_m} \quad (26)$$

Where, S_c , P_r and B_m are the Schmidt number, Prandtl number and mass transfer number, respectively. They are defined as

$$S_c = \frac{m}{rD_g} \quad (27)$$

$$P_r = \frac{mC_p}{K} \quad (28)$$

$$B_m = \frac{Y_s - Y_\infty}{1 - Y_s} \quad (29)$$

Where, D_g is the fluid diffusion coefficient, C_p the fluid specific heat and K is the fluid conductivity coefficient. It should be pointed out that D_g , C_p and K are highly dependent on the temperature and droplet vapor mass fraction at which they are evaluated. A “one third rule” [9] that utilizes a reference temperature equal to the droplet surface temperature plus one-third of the difference between the surrounding fluid and droplet surface temperature is used. Y_s can be calculated by the same procedure as follows:

$$Y_s = \left\{ 1 + \left(\frac{P}{P_v} - 1 \right) \frac{W_m}{W_f} \right\}^{-1} \quad (30)$$

Where, Y_s is the mass fraction for droplet, P_v the vapor pressure at the droplet surface, P the fluid pressure, W_f and W_m are the molecular weights of the droplet and mixture, respectively. They can be obtained by using a standard thermodynamics table, such as JANAF data bank [10].

The above physical model is only valid for dilute spray evaporation processes. Radiative heat transfer, and near critical and supercritical behavior are not included. A more sophisticated evaporation model, such as the “Group Evaporation” model [11] and/or the “Group Combustion” model [12] should be incorporated in the future to study the dense spray effect.

Particle Size Distribution Model

Generally, the sizes of particles are non-uniformed. The size distribution of particles, consist of a spectrum of different sizes. Overall particle size characteristics are represented by their distribution curve, which relates to the cumulative percentage of particle number N, surface area A or volume V as a function of size D. In many applications an average particle size is desirable instead of the complete size distribution, This average size is chosen as a mean diameter. The general definition of a mean diameter D_{ab} is

$$D_{ab} = \frac{\int_0^{\infty} D^a f(D) dD}{\int_0^{\infty} D^b f(D) dD} \tag{31}$$

where,

$$f(D) = \frac{dN}{dD} \tag{32}$$

Is a number distribution function, dN and N are the number of particles in the size range from D to $(D + dD)$ and the total particle number, respectively. Its corresponding cumulative function $F(D)$ is

$$F(D) = \int_0^{\infty} f(D) dD \tag{33}$$

In the particle tracking application, the so-called “Sauter Mean Diameter” SMD or D_{32} is commonly used, which is defined as the ration if particle volume to its surface area, etc.

$$SMD = \frac{\frac{1}{6} \overline{pD^3}}{\overline{pD^2}} = \frac{1}{6} \overline{D} \tag{34}$$

Where, \bar{D} is the average diameter. STORM/CFD2000 employs two different size distributions. They are the Rosin-Rammler Distribution [13] and c-squared Distribution [13].

Rosin-Rammer Distribution

$$\frac{dQ}{dD} = \frac{qD^{q-1}}{X^q} \exp[-(\frac{D}{X})^q] \tag{35}$$

$$\frac{X}{SMD} = \Gamma(1 - \frac{1}{q}) \tag{36}$$

Where, Q is the fraction of the total volume contained in particles of diameter less than D, X and q are correlation constants. The relationship among X, SMD and q is established through the Γ function. This model is mostly used in the two-phase flow applications.

c-Squared Distribution

The normalized number distribution function for X-squared distribution is defined as

$$f(D) = \frac{D^3}{3D^4} \exp(-\frac{D}{D}) \tag{37}$$

where,

$$\bar{D} = \frac{SMD}{6} \tag{38}$$

The corresponding cumulative distribution function is

$$F(D) = 1 - \exp(-\frac{D}{D}) [1 + \frac{D}{D} + \frac{1}{2}(\frac{D}{D})^2 + \frac{1}{6}(\frac{D}{D})^3] \tag{39}$$

It should be pointed out that the size distribution is a model to represent the whole particle size by a finite number of size ranges. None of these models is universally better than the other, but rather, each has particular benefits for a given application.

Particle Breakup Model

CFD2000 employs two breakup models. One is TAB (Taylor Analogy Breakup) model of O'Rourke and Amsden [14], the second is Reitz's wave instability model [15].

TAB Model

The TAB model is based on an analogy between an oscillating and distorting liquid droplet and a spring-mass system. The restoring force of the spring is analogous to the surface tension force. The external force on the mass is analogous to the gas aerodynamic force. The damping forces due to liquid viscosity are introduced to this analogy.

The equation for the acceleration of the liquid droplet distortion parameter is

$$\frac{d^2y}{dt^2} = \frac{2}{3} \frac{\mathbf{r}}{r_p} \frac{(U + u' - v)^2}{r_p^2} - \frac{8\mathbf{a}(T_p)}{\mathbf{r}_p r_p^3} y - \frac{5\mathbf{m}_l(T_p)}{\mathbf{r}_p r_p^2} \frac{dy}{dt} \quad (40)$$

Where the quantity y is proportional to the displacement of the droplet's surface from its equilibrium position, divided by the droplet radius. \mathbf{a} and \mathbf{m}_l are the liquid surface tension coefficient and viscosity respectively at the droplet temperature. After integrating equation (40), it gives

$$y(t) = \frac{W_e}{12} + \exp\left(-\frac{t}{t_p}\right) \left[(y(0) \frac{W_e}{12} \cos \mathbf{w}t + \frac{1}{\mathbf{w}} (\dot{y}(0) + \frac{y(0) - \frac{W_e}{12}}{t_p}) \sin \mathbf{w}t \right] \quad (41)$$

where,

$$W_e = \frac{\mathbf{r}(U + u' - v)^2 r_p}{\mathbf{a}} \quad (42)$$

is the Weber number,

$$t_p = \frac{2}{5} \frac{\mathbf{r}_p r_p^2}{\mathbf{m}_l} \quad (43)$$

is the viscous damping time and

$$\mathbf{w}^2 = 8 \frac{\mathbf{a}}{\mathbf{r}_p r_p^3} - \frac{1}{t_p^2} \quad (44)$$

is the square of the oscillation frequency.

The droplet oscillation and breakup computations require two normalized particle arrays (y for deformation and $\frac{dy}{dt}$ for oscillation), which can be determined by the above equations. Droplet breakup occurs if and only if $y(t)$ is greater than unity. Occurrence of breakup, the Sauter Mean Diameter (SMD) and oscillation velocity for the product drop depend on these two parameters and Weber number:

$$\text{SMD} = \frac{D/2}{\frac{7}{3} + \frac{1}{64} \frac{r_p D^3}{a} \left(\frac{dy}{dt}\right)^2} \quad (45)$$

Where D is the parent droplet diameter and a the droplet surface tension. Following breakup, the product drop has the same temperature with the parent drop and its deformation and oscillation parameters are set to zero.

Wave Instability Model

This model assumes that the atomization is described using injected “blobs”, which have the same size as the liquid nozzle exit diameter. The breakup of the blobs and the resulting droplets are modeled by the analysis of a wave stability for liquid nozzle. The wavelength of the fastest growing wave, Λ and the maximum wave growth rate Ω can be determined by the wave dispersion equation for a round jet:

$$\frac{\Lambda}{r_j} = 9.02 \frac{(1 + 0.45Z^{0.5})(1 + 0.40T^{0.7})}{(1 + 0.87W_e^{1.67})^{0.6}} \quad (46)$$

and

$$\Omega \left(\frac{r_p r_j^3}{a} \right) = \frac{(0.34 + 0.38W_e^{1.5})}{(1 + Z)(1 + 1.4T^{0.6})} \quad (47)$$

Where, $Z = \frac{\sqrt{W_{ep}}}{R_{ep}}$ is the liquid droplet Ohnesorge number, W_{ep} the liquid droplet Weber number, W_e the fluid Weber number, R_{ep} the liquid droplet Reynolds number, $T = Z\sqrt{W_e}$, r_j the liquid jet radius and a the liquid droplet surface tension.

The mean product droplet size and breakup rate are given by

$$\begin{aligned}
 r_p &= B_0 \Lambda && \text{if } B_0 \Lambda \leq r_j \\
 &= \min \left(\left(\frac{3pr_j^2}{2\Omega} \right)^{\frac{1}{3}}, \left(\frac{3r_j^2 \Lambda}{4} \right)^{\frac{1}{3}} \right) && \text{if } B_0 \Lambda > r_j
 \end{aligned} \tag{48}$$

and

$$\frac{dr_j}{dt} = -\frac{r_j - r_p}{3.726 B_1 r_j} \Lambda \Omega \tag{49}$$

Where, B_0 and B_1 are model constants. $B_0 = 0.61$, $B_1 = 10.0$ for atomization process and 1.73 for droplet secondary breakup [14],

Particle Collision Model

The Particle collision model, which was established by O'Rourke [16], is employed to calculate the collision and coalescence among the dispersed liquid phase. The collision will happen for a pair of particles if and only if they are in the same computational cell. The particles, associated with each computational parcel, are assumed to be uniformly distributed throughout the cell where they are located. A collision frequency between the parcel 1 with larger radius r_1 and parcel 2 with smaller radius r_2 is obtained from the following formula

$$\nu = \frac{N_2^n}{dV^n} P (r_1^n + r_2^n)^2 |v_1 - v_2| \tag{50}$$

Where, ν is the frequency, N_2 the number of particles of the parcel2, $|v_1 - v_2|$ is the relative velocity between two parcels and dV the volume of the cell, The probability P for n collisions is assumed to obey the Poisson distribution:

$$P_n = e^{-\bar{n}} \frac{\bar{n}^n}{n!} \tag{51}$$

where \bar{n} is the mean value $\bar{n} = \nu \Delta t$, Δt is the time step. The collision impact parameters are calculated stochastically with the probability information if the collision is coalescence. Otherwise, each collision is a grazing one. The critical impact parameter depends on the particle radius, the relative velocity and the surface tension coefficient.

Suppose the outcome of the collision is coalescence. For each collector particle n particles are subtracted from their associated parcel, and the size, velocity, etc. are appropriately modified. If there are not enough number of particles to take n coalescence with each collector, then n is recalculated so that all N_2^n particles coalesce, and the parcel associated with these particles is destroyed. If the outcome of each collision is a grazing one, only one collision is considered for each parcel. Grazing collisions which usually occur between particles of nearly equal size are calculated between N pairs of particles, where,

$$N = \min (N_1^n, N_2^n) \tag{52}$$

Turbulence Modulation Model

Turbulence Modulation effect appears with the presence of the dispersed particle phase. This effect comes into the governing equations (5) and (6) of turbulent kinetic energy and its dissipation rate through the source terms $S_{k,p}$ and $S_{e,p}$. Shuen [17] obtained the formula by using the momentum equation with the source term $S_{ui,p}$,

$$S_{k,p} = \overline{u_i S_{ui,p}} - U_i \overline{S_{ui,p}} \tag{53}$$

and

$$S_{e,p} = 2m \overline{\frac{\partial u_i'}{\partial x_j} \frac{\partial S_{ui,p}'}{\partial x_j}} \tag{54}$$

where, u_i' is the turbulence fluctuating velocity following the Gaussian distribution. The instantaneous properties of two phase interaction force $S_{ui,p}$, p are given

$$S_{ui,p} = \frac{1}{dV} \sum_{p=1}^{NP} [N_p \dot{m}_{ev,p} (v_i)_p - m_p N_p (\frac{U_i + u_i' - v_i}{t})_p] \tag{55}$$

Where, v_i is the instantaneous particle velocity, U_i the fluid velocity, t the particle relaxation time, \dot{m}_{ev} the liquid droplet evaporation rate, m_p particle mass, dV the cell volume, NP total number of particles and N_p the number of particles for each computational parcel.

The equation (2.53) and (2.54) can then be derived as

$$S_{k,p} = \frac{1}{dV} \sum_{p=1}^{NP} [N_p \dot{m}_{ev} \overline{u'_i(v'_i)_p} - m_p N_p \overline{u'_i \left(\frac{u'_i - v'_i}{t} \right)_p}] \quad (56)$$

and

$$S_{e,p} = 1.0 \frac{e}{k} S_{k,p} \quad (57)$$

Summary of Lagrangian Two-Phase Source Terms

$$S_{m,p} = \frac{1}{dV} \sum_{p=1}^{NP} N_p \dot{m}_{ev,p} \quad (58)$$

$$S_{ui,p} = \frac{1}{dV} \sum_{p=1}^{NP} [N_p \dot{m}_{ev,p} (v'_i)_p - m_p N_p \left(\frac{U_i + u'_i - v'_i}{t} \right)_p] \quad (59)$$

$$S_{h,p} = \frac{1}{dV} \sum_{p=1}^{NP} [N_p \dot{m}_{ev,p} (h-L) - m_p N_p (c_{p,p} \frac{dT_p}{dt} + \frac{dv'_i}{dt} v'_i)] \quad (60)$$

$$S_{k,p} = \frac{1}{dV} \sum_{p=1}^{NP} [N_p \dot{m}_{ev} \overline{u'_i(v'_i)_p} - m_p N_p \overline{u'_i \left(\frac{u'_i - v'_i}{t} \right)_p}] \quad (61)$$

$$S_{e,p} = 1.0 \frac{e}{k} S_{k,p} \quad (62)$$

$$\frac{dv'_i}{dt} = \frac{U_i + u'_i - v'_i}{t} + F_{bi} \quad (63)$$

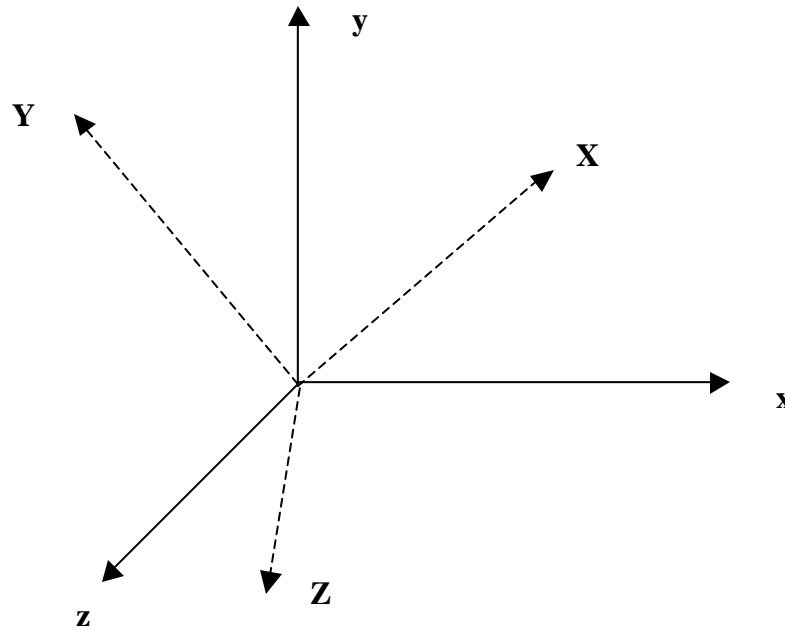
$$m_p = \frac{4}{3} \rho r_p^3 P_p \quad (64)$$

$$\dot{m}_{ev} = \frac{4}{3} \rho P_p \frac{(r_p^{n+1})^3 - (r_p^n)^3}{\Delta t} \quad (65)$$

$$t^{-1} = \frac{3}{8} \frac{\rho}{\rho_p r_p} C_D |U_i + u'_i - v'_i| \quad (66)$$

Coordinate Transformation of Particle Injection

If particle are injected into the computational domain by cone or wedge mode, the cone or wedge direction may be in any direction in the space. In the following figure, it is assumed that coordinate xyz is the fixed (or old) coordinate in space, XYZ is the cone coordinate (or new) with the main axis directing the injection direction.



If the direction cosine is known for XYZ to xyz, then the transformation of the coordinate takes the form:

$$\begin{aligned}
 x &= l_1 X + l_2 Y + l_3 Z \\
 y &= m_1 X + m_2 Y + m_3 Z \\
 z &= n_1 X + n_2 Y + n_3 Z
 \end{aligned}
 \tag{67}$$

Where, l_1, m_1, n_1 are the direction cosines of X axis to x,y and z axes, l_2, m_2, n_2 , the direction cosines of Y axis to x, y and z axes and l_3, m_3, n_3 the direction cosines of Z axis to x, y and z axes.

References

1. R.I. Issa, "Solution of the Implicitly Discretised Fluid Flow Equations by Operator-Splitting", J. of Comp. Phys., Vol. 62,pp 40-65, 1985.
2. R.I. Issa, B.Ahmadi – Defrui, K.R. Beshay and A.D. Gosman, "Solution of the Implicitly Discretised Reacting Flow Equation by Operator – Splitting", J.Comp. Phys., Vol. 93,pp 399-410,1991.
3. A. Favre, "Statistical Equations of Turbulent Gases, Problems of Hydrodynamics and Continuum Mechanics", SIAM, Philadelphia, 1969.
4. T.J. Chung, "Continuum Mechanics", Prentice –Hall Inc., Englewood, Cliffs, NJ, 1988.
5. H. Schlichting, "Boundary Layer Theory", 7th ed., McGraw – Hill, Translated by J.Kestin, 1979.
6. W.P. Jones, "Models for Turbulent Flows with Variables Density and Combustion", Prediction Methods for Turbulent Flows, Edited by W. Kollmann, Hemisphere Publishing Co., Washington, D.C., 1980.
7. S.L. Soo, "Fluid Dynamics of Multiphase Systems", Blaisdell Publishing Co., 1967.
8. N.Frossling, "On the Evaporation of Falling Droplets", Gerlands Beltrage Zur Geophysik, V.52, No. 170,1938.
9. G.L. Hubbard et al., "Droplet Vaporization:Effects of Transient and Variable Properties", In ternational Journal of Heat and Mass Transfer, V.18,p. 1003, 1975.
- 10.D.R. Stull and H. Prophet, "ANAF Thermochemical Table", 2nd edition, J. Phys. Chem. Ref.Data, V.3,p.311,1974.
- 11.J. Bellan and R. Cuffel, "A Theory of Nondilute Spray Evaporation Based Upon Multiple Drop Interaction", Combustion and Flame, V.51,p 55, 1983.
- 12.H.H. Chiu, H.Y. Kim and E.J. Croke, "Internal Group Combustion of Liquid Droplets", Presented at 19th Symposium (International) on Combustion. The Combustion Institute, pp. 971-980, 1982.
- 13.A.H. Lefebvre, "Atomization and Sprays", Hemisphere Publishing Corporation, 1989.
- 14.P.J. O'Rourke and A.A. Amsden, "The TAB Method for Numerical Calculation of Spray Droplet Breakup", SAE Technical Paper 970289 (1987).
- 15.R.D. Reitz and R. Diwakar, "Modeling Atomization Processes in High-Pressure Vaporizing Sprays in Atomization and Spray Technology", V.3
- 16.P.J. O'Rourke, "Collective Drop Effects on Vaporizing Liquid Sprays", Los Alamos Scientific Laboratory Report. LA-9069-T, 1981.
- 17.J.S. Suen, "A Theoretical and Experimental Investigation of Dilute Particulate Turbulent Gas Jet", Ph.D. Dissertation, Pennsylvania State University, May, 1984.
- 18.G.M. Faeth, "Spray Combustion Model A Review", Presented in Energy and Combustion Science,V.9,pp, 1-76, Pergamon Press, New York, 1983.
- 19.A. Putnam, ARS J.V.31, P. 1467,1961.