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Development of a Model for Multiphase Turbulent Particle Dispersion in WIND-US*

V. Lee† and E. Loth‡

University of Illinois at Urbana/Champaign, Urbana, IL, 61801

D. Lankford§

Aerospace Testing Alliance, Arnold Engineering Development Center, Arnold AFB, TN, 37389

A simulation capability for turbulent dispersed multiphase flows was developed and implemented within WIND-US employing both structured boundary fitted meshes and unstructured meshes. The approach is based on a Reynolds-Averaged Navier-Stokes (RANS) Eulerian approach for the continuous fluid phase. A Continuous Random Walk (CRW) model was developed and implemented into WIND-US to model the turbulent velocity fluctuations seen by the dispersed phase as a stochastic process. The resulting code was then validated by simulations of a flow through a square duct section containing isotropic, homogenous turbulence consistent with measurements of turbulent particle diffusion by Snyder and Lumley. The simulations for both structured and unstructured meshes show good correlation between WIND-US and Snyder and Lumley's experimental data.

Nomenclature

a	Speed of sound
c_Λ	Eddy length scale coefficient
c_μ	Turbulence length scale coefficient
c_τ	Eddy time scale coefficient
d	Droplet diameter
f	Stokes correction factor
$\vec{g}$	Gravitational acceleration
k	Turbulent kinetic energy
M	Mach number
m	Mass
Re	Reynolds number
St	Stokes number
t	Time
$\vec{u}$	Fluid velocity
$\vec{v}$	Particle velocity
$\vec{w}$	Relative velocity
$\vec{x}$	Particle position
ϵ	Turbulent dissipation
γ	Random Gaussian number
Λ	Integral length scale

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†M.S. Student, Aerospace Engineering, AIAA member.

‡Professor,Aerospace Engineering, AIAA member.

§AIAA senior member.

μ Viscosity
ρ Density
τ Time scale
Subscript
D Domain
f Fluid
p Particle
σ Surface stress
$\forall$ Volume

I. Introduction

A. Motivations

Within the field of fluid dynamics, multiphase flows represent a large class of phenomena and problems where accurate simulation is of scientific and engineering interest. Aircraft wing and engine inlet icing is such a multiphase flow where a dispersed water "droplet" cloud interacts with a continuous gas phase. Here, particle dispersion due to turbulence is of great importance. Other multiphase flow problems involving gas-particle interaction in the area of space and missile systems include the propulsion systems of solid propellant rockets, where particles from the combustion process are produced and transported out the nozzle with the exhaust gases.

The addition of a multiphase capability to a CFD tool represents a great benefit to the variety of organizations and groups whose analysis and design work includes multiphase flows. The wide usage of the WIND-US platform by a large number of groups and its support by AEDC, Boeing, NASA-Glenn and the NPARC alliance makes the program a good choice upon which to add a multiphase model.

B. Background

The process of incorporating a multiphase solver into WIND-US means that a decision must be made as to whether this model will be Eulerian of Lagrangian. The Eulerian approach treats the dispersed particle phase in the same manner as the continuous fluid phase. The Lagrangian approach treats particles of the dispersed phase individually, tracking their positions and trajectories. For applications where the particles are small, turbulent diffusion is significant, and where there may be areas of the flow devoid of substantial particle concentrations, the Lagrangian model is generally more efficient.[6] The Lagrangian dispersed phase model was thus chosen to be incorporated into WIND-US.

A secondary consideration for the incorporation of a multiphase model pertains to whether the inter-phase interactions of mass, momentum, and energy between the fluid phase and dispersed phase are one-way coupled, (i.e., the surrounding fluid phase is not influenced and affected by the dispersed phase) or two-way coupled (i.e., the presence of the particle affects the continuous phase motion). For cases of low mass loading (lower than 1%), one-way coupling provides an adequate model of the inter-phase interactions. Furthermore, one-way coupling can be very computationally efficient, as it is often possible, especially with steady flows, to compute the converged solution of the continuous surrounding phase beforehand. It is unnecessary to then recompute the flow variables for the continuous phase during a multiphase simulation.

II. Overview of Physics and Modeling

A. Basic Terminology

To describe multiphase flow regimes, a few essential definitions are necessary. A "particle" will be defined herein as a relatively unattached body immersed in a flow. In terms of shape, often particles are spherical or can be reasonably approximated as such, so that the simple geometric diameter (d) can be used to describe their volume. In terms of size comparison, a macroscopic length of the continuous-flow domain (D) can be defined (e.g., a channel width or a jet diameter) and herein the particle size will be assumed to be small in comparison such that $d \ll D$.

Since each particle is assumed to be surrounded by a fluid which otherwise fills the domain, the particles

in general will be referred to as the "dispersed phase" and the surrounding fluid will be referred to as the "continuous-phase". Most of the analyses herein will assume a single dispersed-phase and a single continuous-phase, but they are generally extendable to multiple phases.

The continuous-phase surrounding the particle will always be a fluid (gas or liquid) so that it will be associated with the subscript "f". It will generally be assumed to behave as a continuum such that a dynamic fluid viscosity (μ_f) and density (ρ_f) of this phase can be defined (though some consideration will be given to the case where random molecular interactions are important). The subscript "p" will be used when referring to particle properties, e.g., the volume-averaged particle density is ρ_p. For a fluid particle (e.g. a gas bubble in liquid, or a liquid drop in a gas, or a liquid drop in another immiscible liquid), the viscosity of the particle (μ_p) becomes finite and may play a role in the particle dynamics. However, if the particle is composed of a solid substance (e.g., a coal particle), the viscosity of the particle is not defined or can be considered infinite.

A volume will generally be denoted as $\forall$, e.g., the entire (computational) domain will be denoted $\forall_D$ while an individual particle volume will be denoted as $\forall_p$. In the case when the particle is non-spherical, d will refer herein to the particle volumetric diameter, i.e., the diameter of a sphere which has the same net volume as that of the particle:

$$d = \left(\frac{6}{\pi}\forall_p\right)^{\frac{1}{3}} \tag{1}$$

The corresponding particle volumetric radius will be defined as $R = \frac{d}{2}$. The volume-averaged particle density is then simply based on the particle volume ($\forall_p$) and mass (m_p).

$$\rho_p = \frac{m_p}{\forall_p} \tag{2}$$

In comparing the particle mass to the mass of the surrounding fluid it displaces, a particle density ratio may be defined as:

$$\Psi = \frac{\rho_p}{\rho_f} \tag{3}$$

We may refer to "very high density" particles as having $\Psi \gg 1$. Examples of very high density particles include solid particles and droplets in a gas flow, which is the focus of this report.

In determining the fluid dynamics the forces and the velocities of the multiphase flow will need to be characterized. A force or a velocity will be represented as a vector quantity when given as $\vec{F}$ and as a scalar quantity when given with an index (e.g., F_i). The scalar magnitude of a vector will be represented by a regular typeface. With respect to the velocities of the different phases, the particle velocity ($\vec{v}$) is defined as the translational velocity of the particle center of mass ($\vec{x}_p$). The continuous-fluid velocity ($\vec{u}$) is defined in all areas of the domain unoccupied by particles. However, a hypothetical continuous-phase velocity can be extrapolated to the particle centroid and will be specially denoted as $\vec{u_{@p}}$ and termed the "unhindered velocity". The relative velocity of the particles ($\vec{w}$) is then based on the unhindered velocity, i.e., along a particle trajectory

$$\vec{w}\,(t) = \vec{v}\,(t) - \vec{u}_{@p}\,(t) \tag{4}$$

It is important to note that $\vec{u}_{@p}$ does not include the fluid dynamic effects resulting from the presence of the tracked particle itself (though, it can include the fluid dynamic effects of other particles).

B. Particle Equation of Motion

In general, the forces acting upon an isolated particle can be categorized into three types. These are body forces, surface forces, and collision forces. For the one-way coupled approach, the Lagrangian equation of motion (EOM) for an isolated particle can be given as

$$\frac{d\,(m_p\vec{v})}{dt} = \vec{F}_{body} + \vec{F}_{surface} + \vec{F}_{collision} \tag{5}$$

If it is assumed that the dispersed particle phase concentration is extremely small it may be assumed that the particle collision forces are negligible and can be neglected. The body forces are primarily gravitational. The surface forces may be further decomposed into drag, lift, particle surface stress force, added mass force, and history force.

$$\vec{F}_{surface} = \vec{F}_{drag} + \vec{F}_{lift} + \vec{F}_{\sigma} + \vec{F}_{\forall} + \vec{F}_{history} \tag{6}$$

The particle surface stress force arises from the particle/fluid surface interface. The added mass force arises from a portion of "added mass" that is carried along with the particle due to surface boundary conditions. This added mass force is expressed as

$$\vec{F}_{\forall} = -C_{\forall}\rho_f \forall_p \frac{d\vec{w}}{dt} \tag{7}$$

where the quantity $C_{\forall}$ is the added mass coefficient ($= \frac{1}{2}$ for a sphere). The Basset history force arises from the temporal development of the particle viscous boundary layer and wake as the particle accelerates through the continuous phase flow. If it is assumed that the particles are relatively heavy, that is

$$\Psi = \frac{\rho_p}{\rho_f} \gg 1 \tag{8}$$

which is true for the case of a solid particle immersed in a gas flow, the effects of lift and the Basset history force are secondary in comparison to drag and gravitational forces. DeAngelis et al.[4] showed that the lift and history force can be omitted while retaining the drag, added mass, and surface stress forces. Therefore, Eq. (6) is reduced to

$$\vec{F}_{surface} = \vec{F}_{drag} + \vec{F}_{\sigma} + \vec{F}_{\forall} \tag{9}$$

Combining the expressions for the drag, the added mass force, and the surface stress force[5] into eq. (5), the following expression is obtained:

$$\left(\rho_p + C_{\forall}\rho_f\right)\forall_p \frac{d\vec{v}}{dt} = -3\pi\mu_f d f \vec{w} + \forall_p \left(\rho_p - \rho_f\right)\vec{g} + \rho_f \forall_p \left(1 + C_{\forall}\right)\frac{\partial \vec{u}_{@p}}{\partial t} \tag{10}$$

where

$$f = 1 + \frac{Re_p/4}{1 + \sqrt{Re_p}} + \frac{Re_p}{60} \tag{11}$$

Several non-dimensional parameters arise in the analysis of turbulent particle diffusion. A particle response time, τ_p can be defined to be the response time of a particle to the surrounding fluid flow field.

$$\tau_p = \frac{m_{eff}|w|}{F_D} = \frac{\left(\rho_p + C_{\forall}\rho_f\right)d^2}{18\mu_f f} = \frac{4\left(\Psi + C_{\forall}\right)d}{3C_D|w|} \tag{12}$$

By normalizing the particle response time with some relevant timescale, the particle Stokes number can be defined as

$$St = \frac{\tau_p}{\tau_{\Lambda}} \tag{13}$$

Here, τ_{Λ} is the eddy integral timescale or eddy life time. The Stokes number then is a measure of how responsive a particle is to the surrounding fluid and of the particle inertia. A very small Stokes number ($St \ll 1$) indicates that the response time of the particle to a turbulent eddy structure is negligible and that the particle is very responsive to an integral scale turbulent structure. As the Stokes number grows, the response time increases and the particle velocities will begin to diverge from those of the continuous phase despite the continued influence of the continuous phase. For an extremely large Stokes number ($St \gg 1$), the particle's inertia is so great that it is negligibly affected by the surrounding fluid phase.

C. Turbulent Diffusion

Aside from a few specialized and simple cases, it is usually infeasible to attempt to resolve directly with a numerical solution the eddies in a turbulent flow. An unresolved-eddy simulation such as one done with the Reynolds Averaged Navier-Stokes equation (RANS), can be used to obtain turbulent statistics that can be used to obtain particle trajectories in a multiphase particle diffusion analysis.[2] The approach has the advantage of being extremely computationally efficient and can thus be applied to a large number of general problems. However, the disadvantage is that the handling of the unresolved eddy component using turbulence models introduces empiricism into the problem that must be addressed on a case by case basis.

Reynolds decomposition is used for the continuous fluid phase to separate the velocity field $\vec{u}_f$ into a mean component and an unresolved fluctuating component in the following manner:

$$\vec{u}_f = \bar{u}_f + u'_f \tag{14}$$

where the u'_f term denotes unresolved component.

The CRW model continuously correlates the turbulent velocity fluctuations with time. This is often accomplished through the use of a Markov process whereby the value of the velocity at some state (in time) is correlated to its value at the previous state (in time). This is done using the turbulent statistics from the continuous phase turbulence model to establish the correct length, time, and velocity scales and are used in conjunction with random number generators. The k-ϵ two equation turbulence model, which provides the turbulent kinetic energy and the dissipation can be used for this purpose.[1]

A Markov chain can, in general, be obtained from the Langevin equation.[1] The Langevin equation describes the motion of an object subjected to a linear retarding force and a random solution. In one dimension, the Langevin equation for the basis of the Markov chain for the simulation of turbulent velocity fluctuations is given here as:

$$\frac{du}{dt} = -\left(\frac{1}{\tau_{int}}\right) u(t) + \sqrt{\frac{2\overline{u(t)u(t)}}{\tau_{int}}}\gamma(t) \tag{15}$$

where the quantity τ_{int} represents some particle-eddy interaction timescale and $\gamma(t)$ is a continuous and uncorrelated random variable with a Gaussian distribution.

III. Numerical Implementation

A. Discretized Expressions for the EOM and CRW Model

By recasting eq. (10) in terms of τ_p, the particle equation of motion becomes

$$\frac{d\vec{v}}{dt} = -\frac{\vec{v} - \vec{u}_{@p}}{\tau_p} + \left(\frac{\rho_p - \rho_f}{\rho_p + C_\forall \rho_f}\right)\vec{g} \tag{16}$$

Eq. (16) can then be integrated to produce expressions for the particle velocities and positions.

Using Eq. (16), a discretized expression for the velocity can be obtained by taking a Taylor expansion about a mid-point time $\left(t + \frac{\Delta t}{2}\right)$ to produce a finite difference scheme where the drag coefficient is assumed to remain constant across the time interval. This expression is second order accurate.

$$v_i^{n+1} = \frac{\left[v_i^n + \frac{3\Delta t|\vec{w}^n|C_D^n u_{i@p}^n}{4d\left(\Psi+\frac{1}{2}\right)} + \frac{|\Psi-1|g\Delta t}{\left(\Psi+\frac{1}{2}\right)}\right]}{1 + \frac{3\Delta t|\vec{w}^n|C_D^n}{4d\left(\Psi+\frac{1}{2}\right)}} + O(\Delta t)^2 \tag{17}$$

A second order discrete expression for the particle position is simply obtained as:

$$\vec{x}_p^{n+1} = \vec{x}_p^n + \Delta t\frac{\vec{v}^{n+1} - \vec{v}^n}{2} + O\left(\Delta t\right)^2 \tag{18}$$

Equations (17) and (18) are used to advance the particle's position through the continuous phase in time.

The unresolved fluctuating velocity component from the RANS velocity decomposition needs to be acquired from the CRW model in order to acquire the $\vec{u}_{@p}$ term to solve Eq. (17). The implementation of the CRW model uses a Markov chain to perform the correlation of the velocity perturbations with time. Using the turbulent length and time scales computed from the kinetic energy and dissipation obtained from the continuous phase turbulence model, the discretized form of the Markov chain is obtained by solving the Langevin equation (Eq. (15)):

$$\vec{u}'_f\left(t + \Delta t\right) = \alpha\vec{u}'_f\left(t\right) + \left(1 - \alpha^2\right)^{\frac{1}{2}}\vec{\gamma}\left(t\right)\left(u'_{rms}\right) \tag{19}$$

The quantity $\vec{\gamma}$ is a random number from a Gaussian distribution, and α is the CRW correlation and is expressed as

$$\alpha = e^{\frac{-\Delta t}{\tau_{int}}} \tag{20}$$

For isotropic turbulence,

$$u'_{rms} = \left(\frac{2k}{3}\right)^{\frac{1}{2}} \tag{21}$$

The particle-eddy interaction timescale denotes the length of time in which a particle remains associated with an eddy structure before decorrelation. For the CRW model incorporated into WIND-US, τ_{int} is formulated as:

$$\tau_{int} = \min\left(\tau_{\Lambda}, \tau_{tra}\right) \tag{22}$$

where τ_{Λ} is the integral eddy timescale or eddy lifetime and τ_{tra} is the traversal time of the particle, or the length of time for a particle to travel through an integral eddy structure. This formulation is designed to capture a turbulent particle diffusion phenomenon known as the particle crossing-trajectory effect. The basis of this phenomenon involves particles whose relative or terminal velocity leads to an eddy traversal time shorter than the integral eddy timescale. In such a case, the particles are traversing through the turbulent structure and remaining entrained within it for a shorter period of time than the integral timescale. Thus, the particles effectively "cut" through the turbulent structures. The formulation of the effective interaction time as the minimum between the integral timescale and the traversal time captures the crossing-trajectory effect in the Markov chain by shortening the time of correlation.

The integral timescale and the traversal time are then calculated from the turbulence information provided by the turbulence model. Using the turbulent kinetic energy and dissipation, the integral timescale is:

$$\tau_{\Lambda} = c_{\tau}\frac{k}{\epsilon} \tag{23}$$

$$\Lambda = c_{\Lambda}c_{\mu}^{\frac{3}{4}}\frac{k^{\frac{2}{3}}}{\epsilon} \tag{24}$$

$$\tau_{tra} = \frac{\Lambda}{|\vec{w}|} \tag{25}$$

The quantities c_{τ} and c_{Λ} are empirical coefficients that must be experimentally determined. Bocksell[1] determined that for free shear flows, they are, respectively, .124 and .78. c_{μ} is the turbulence length scale coefficient and is 0.09. Note that the $\vec{u}$, ρ_f, k, and ϵ (used for $\vec{w}$, C_D, and $\vec{u}'$) are based on taking the average over a cell.

B. WIND-US Integration

Initial groundwork for the implementation, including data structures for the storage of multiphase data and processes and subroutines for the initialization of multiphase data was already laid in previous work to develop a multiphase solver using a discontinuous random walk model of turbulent diffusion.[4]

Two main data structures were created in the implementation of the WIND-US multiphase solver. These structures are derived type structures defined in the directory /source/modules in the file data_type_modules.f90. The "Drop" data type is a derived data type designed to contain the information of the dispersed phase particles during a simulation. This data type contains elementary real and integer variables and arrays which stores the particle identification, position, velocity, and the turbulent velocity fluctuation at the current time step as seen by the particle. Additionally, the data type can be modified to contain additional information specific to a particular analysis or simulation. The second data type defined in the directory source/modules is the "*Cpl_data*" data type. This derived type object is designed to store the zonal boundary and coupling data for each zone as it is being operated on by WIND-US. The data type contains fields that store a boundary node or cell's index or cell number, the boundary condition at that node or cell, and the identification of the adjacent zone and node/cell to which this node or cell is coupled. This data type then gives the multiphase subroutines a quick and powerful method to store and access all the pertinent information about the zone's boundaries by the multiphase solver.

For the permanent storage of the multiphase solution data, the WIND-US common file format was modified. The common file format produces binary grid and solution files that are accessed through the Common File Library, a set of I/O and manipulation subroutines. The Common File format produces files that are accessible through a UNIX styled path. The path root, represented as "/" is the root of the file's file structure. Further subnodes extending from the file root define the individual zones within the computational domain and subnodes underneath each zone path are used to store the zone's grid coordinates, flow solution variables, and boundary conditions. Modifications were made to the *.tda* file structure to allow the storage of dispersed phase data during multiphase simulations. Figure 1 shows a simplified diagram of the modifications to the .tda file structure. The modification inserts a subnode entitled *mphase* underneath each zonal subnode.

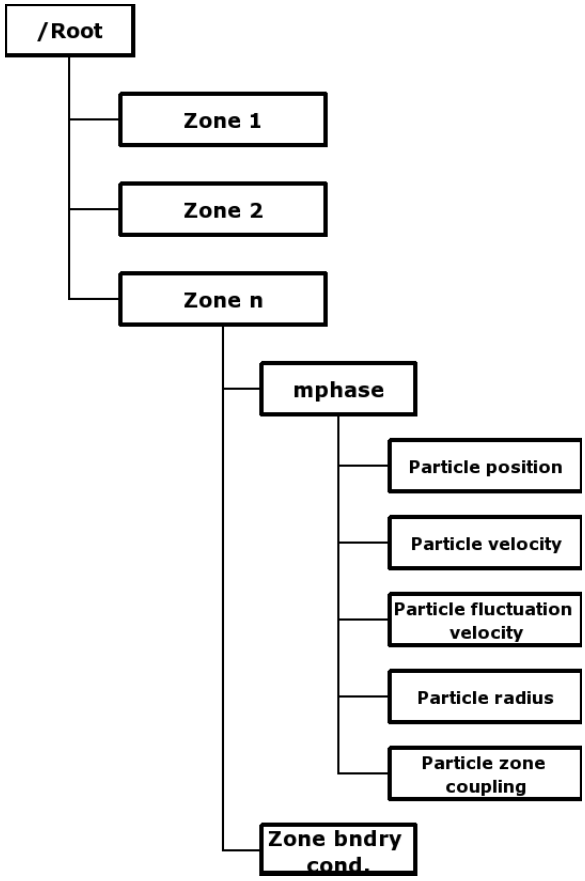

Figure 1. File structure modification for *.tda* file

This mphase node contains fields for storing particle position, particle velocity, fluctuation velocity, particle properties, boundary and zone coupling information for all the particles in the simulation.

A simplified subroutine calling tree of the multiphase solver is shown in Fig. 2. The main multiphase subroutine, *lpmphz.f90* for structured meshes and *Loop_Mphz.f90* is called from the WIND-US subroutine *rhssrc.f90* for a structured mesh and *Implicit110.f90* for an unstructured mesh where they are treated as source terms. The multiphase solver subroutines are called once for each iteration within a given cycle and for each zone.

The multiphase solver initializes by calling the subroutines *rwmphz*, *hybrid_scpl*, *rwglob*, and *pcplin* which are responsible for reading and initializing the dispersed phase data for the current zone from the *.tda* file into memory. These subroutine transfer the dispersed phase particle positions, velocities and properties from the *.tda* file into an array of Drop objects, sets up the zonal boundary condition and coupling information, returning an array of *Cpl_data* objects containing the coupled zone and coupled node/cell at each boundary node/cell in the current zone.

The *pinject* subroutine releases new particles into the current working zone provided that certain criteria are met. These criteria include having "nozzles" specified in the parameter input file for the current zone and an active particle count lower than the number of particles specified in the parameter input file. The pinject subroutine creates new Drop data type objects and initializes the property fields with conditions and values specified in the parameter input file.

The *pmove* subroutine advances the active particles in the current zone. The subroutine *psearch* is called from *pmove* to locate the host cell containing the particle. The host cell is used to extract the continuous phase fluid properties at the particle location. At present, the multiphase solver uses the cell center flow solution values in place of obtaining the actual fluid flow solution values at the exact particle location by interpolation. The *pmove* subroutine uses the fluid and particle velocities to calculate the relative velocity of the dispersed phase. The values of the turbulent kinetic energy and dissipation at the location of the

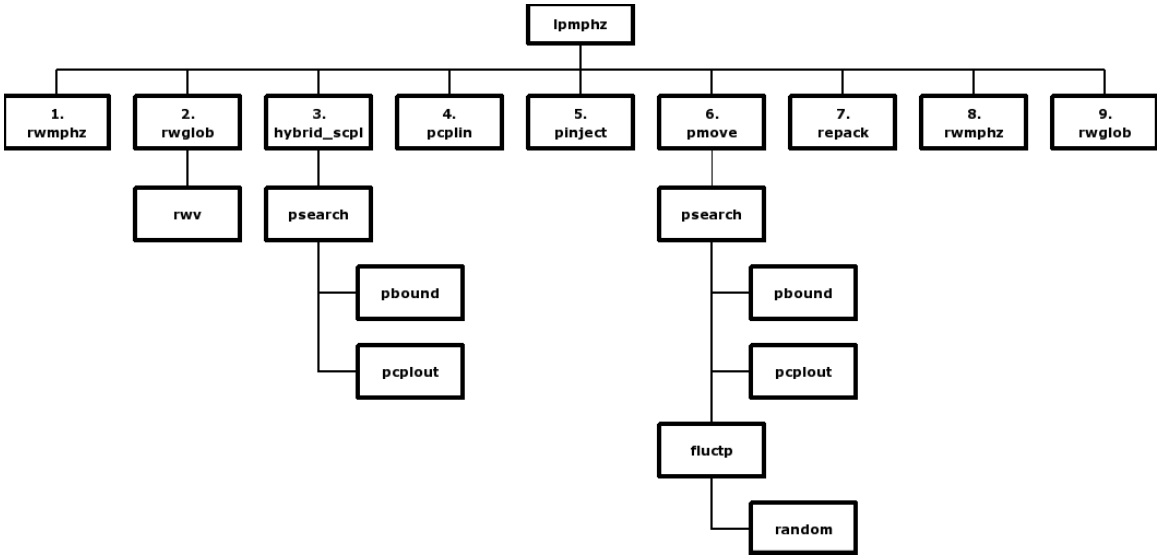

Figure 2. Multiphase calling tree

particle are then used by the subroutine fluctp to determine the $\vec{u}'_f$ fluctuation velocities experienced by the particle at that location.

The subroutine *fluctp* takes the previous timestep fluctuation velocity components as well as the turbulent kinetic energy and dissipation as input arguments and computes the turbulent velocity fluctuations in the continuous phase fluid using the Markov chain of Eq.(19). the *fluctp* subroutine also calls on the *gauss_random* subroutine to return a set of three random numbers from a Gaussian distribution with a mean of zero and a variance of one.

Pmove then uses Eq. (17) and Eq. (18) to update the particle velocities and advance the particle positions. The *repack* subroutine is then called to remove inactive particles from the zone and redistribute the active particles in the particle array.

Finally, the subroutines *rwmphz* and *rwglob* are called once more in write mode to write the particle data for the current zone back to the *.tda* file and the particles that need to be transferred to another zone to the proper *zcplb* nodes. Once this has been done, the main multiphase calling subroutine deallocates the memory used for the multiphase computations and advances to the next zone in the domain.

Implementation of the multiphase solver for unstructured grids is relatively straightforward and much of the details parallel that for a structured grid with the exception of the boundary conditions, where coupled cells replace coupled boundary nodes. The main issue of concern for hybrid grids with both structured and unstructured zones revolves around the passing of information between the two zone types and insuring that the data is interpreted correctly rather than any physical or numerical issue. For a structured zone, a coupled node on a boundary is referred to by its three indices whereas for an unstructured zone, a single number indicating the global cell number is referred to. The use of a single unified data type, the aforementioned *Cpl_data* data type insures that both structured coupling data and unstructured coupling data at the boundaries can be stored correctly and interpreted easily.

IV. Valdataion and Results

Validation of the WIND-US multiphase solver was done by simulating the experiment performed by Snyder and Lumley regarding the mean particle diffusion of different particles in a duct flow with grid generated turbulence in their 1971 paper.[8] In the original experiment, four types of particles, solid and hollow glass beads, copper particles, and corn pollen were released into a vertical wind-tunnel test section with a mean velocity of $21.49 ft/s$. Turbulence in the tunnel flow was generated by a 1" grid upstream of the test section. It was noted by Snyder and Lumley[8] that the decay of the turbulent kinetic energy and the dissipation was a function of the axial length of the tunnel with very little variation in the other directions

and could be represented with the following empirical forms:

$$k(x) = \frac{1}{2}\vec{u}_f^2 \left(\frac{1}{42.4\left(\frac{x}{M} - 16\right)} + \frac{2}{39.4\left(\frac{x}{M} - 12\right)} \right) \tag{26}$$

$$\epsilon(x) = \frac{1}{2}\vec{u}_f^3 \left(\frac{1}{42.4M\left(\frac{x}{M} - 16\right)^2} + \frac{2}{39.4M\left(\frac{x}{M} - 12\right)^2} \right) \tag{27}$$

where M represents the grid spacing, x is the distance from the grid and u is the mean velocity in the axial direction.

Each particle set was released at a down stream location 20 in. from the grid. The mean diffusion of each set was measured as a function of time. The properties of each group are summarized in Table 1.

Table 1. Particle properties used in Snyder and Lumley experiment[8]

Property	Hollow glass	Solid glass	Corn pollen	Copper
Diameter(μm)	46.5	87.0	87.0	46.5
Density (g/cc)	0.26	2.5	1.0	8.9
Term. vel. (cm/s)	1.67	44.2	19.8	48.3
Re	0.005	2.48	1.10	1.45

The WIND-US multiphase simulations were conducted using a 5x5x100 structured mesh, an unstructured mesh with approximately 4000 cells, and a hybrid structured/unstructured mesh containing a structured first half of the domain and an unstructured second half attached behind the structured zone. Figure 3 shows the grids for these three cases.

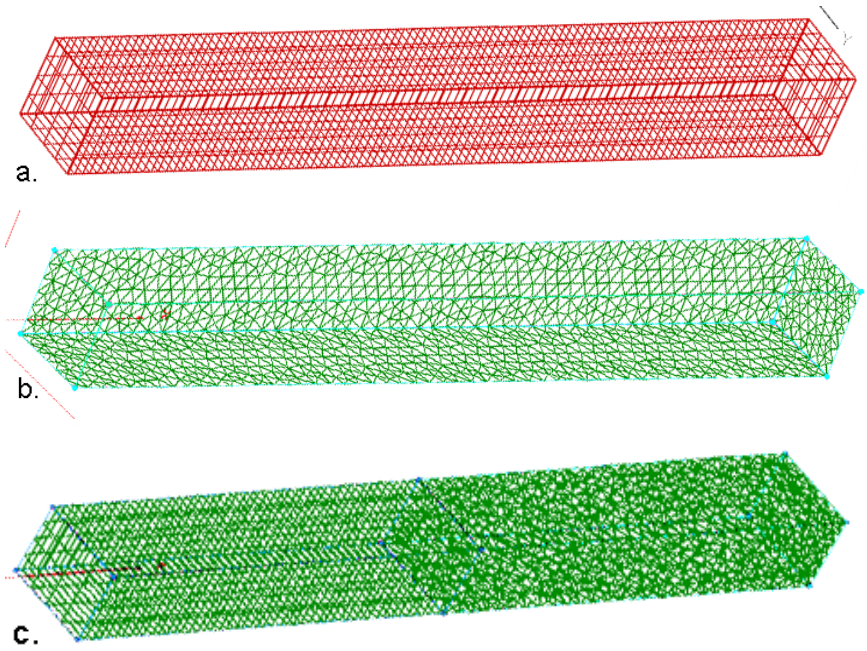

Figure 3. a: Structured mesh, b: unstructured mesh, c: hybrid mesh

The continuous phase solution was obtained by running WIND-US with the multiphase solver until a converged steady state solution for the continous phase was obtained. The boundary conditions on each of the three meshes were set such that the inflow condition would correspond to the inflow mean velocity of 21.49 ft/s. Since the mean velocity of the tunnel remains relatively constant through the length of the tunnel, the specified back pressure at the outflow boundary is set as 14.7 psi which is nearly the same as the inflow pressure of 14.6959 psi. To match the turbulence observed in the flow by Snyder and Lumley, the values of the turbulent kinetic energy and dissipation were extrapolated back from their empirical expressions to the

inflow plane ($x = 22$) of the domain. These values of k and ϵ were then set as part of the inflow conditions. The continuous phase solution was then run to convergence.

In the first simulation the four species of particles were released into a structured mesh. For the second and third simulations, the same was done for an unstructured and hybrid mesh, respectively. In all three simulations, the number of particles released into the flow was 800, a figure approximately equal to the quantity of particles in Snyder and Lumley's observations.

Figure (4) shows the mean diffusion of each of the four types of particles with respect to time for the simulation involving a structured grid. It can be seen that the "heavier" solid glass particles, which have a greater density ratio Ψ, diffuse less than the "lighter" hollow glass beads. This was expected since the heavier particles have a higher inertia. It can be observed that the correlation between the experimental results and the results from the WIND-US simulation appear to be extremely good especially in the case of the heavier particles including solid glass and copper. It can be noted that for the lighter particles of hollow glass and corn pollen, the WIND-US simulation seems to somewhat over-predict the mean diffusion initially.

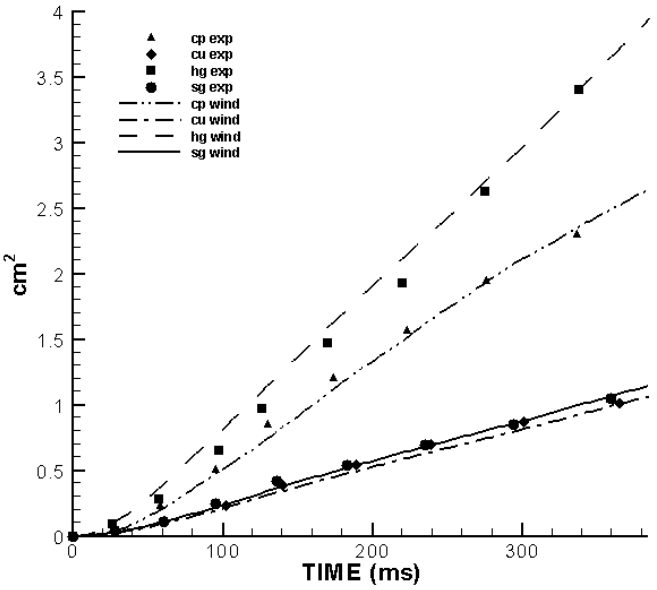

Figure 4. Snyder and Lumley simulation using structured mesh

Figure (5) shows the same mean diffusion data for a simulation performed with an unstructured mesh. Here it is readily apparent that there is good correlation between the experimental and simulated data as well. There tends to be some more discrepancies compared to the simulation performed using the structured mesh. This is attributed to the somewhat reduced spatial resolution for the unstructured mesh in the axial direction which can be observed in Fig. 3. For the Snyder and Lumley case, the decay of k and ϵ is a function of x, the axial direction and is mostly indifferent to change along y and z. Note that this difference may be eliminated if a linear interpolation within a cell was used instead of the present cell-averaged approach.

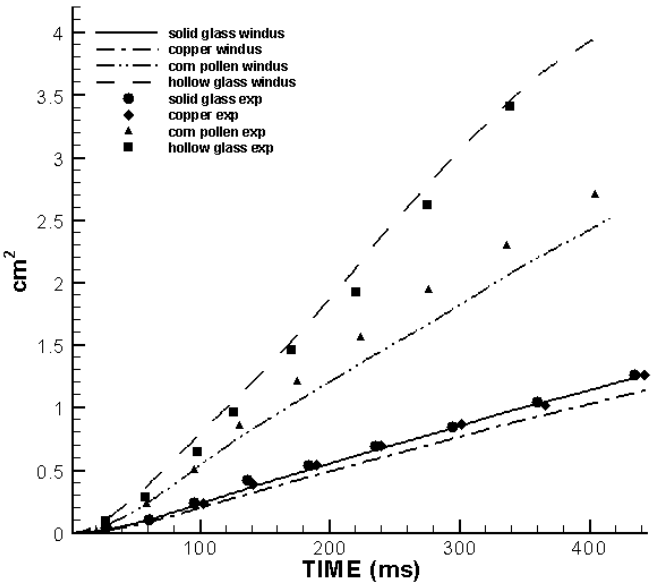

Figure 5. Snyder and Lumley simulation using unstructured mesh

Figure (6) shows the mean diffusion for the simulation using a hybrid mesh. With this simulation, it can be seen once again that there is good correlation in the case of the heavier particles. The mean diffusion of the hollow glass particles is slightly over-predicted as was the case with the other simulations. Overall, the correlation between the experimental results and WIND-US's multiphase simulations were very good.

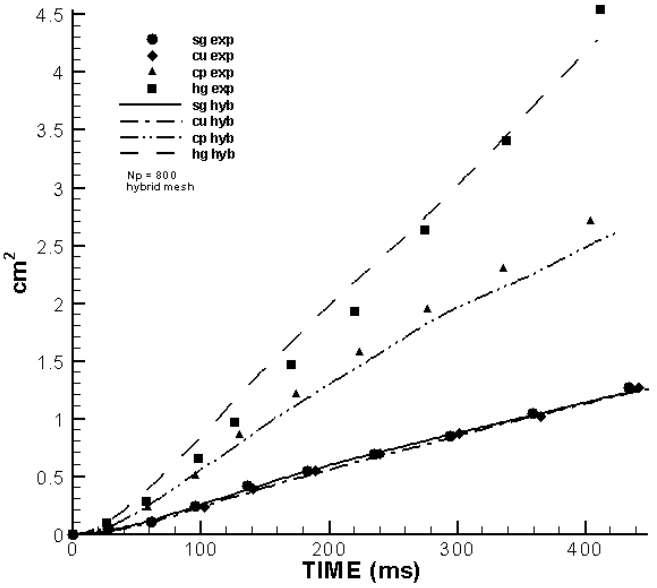

Figure 6. Snyder and Lumley simulation using hybrid mesh

V. Conclusion

A multiphase flow simulation capability was successfully incorporated into the WIND-US code. The resulting additions feature the capability to work with several types of meshes, including structured, un-

structured, and hybrid meshes. The modifications also feature the addition of a CRW model to handle the turbulent velocity fluctuations, giving the WIND-US code the ability to simulate multiphase flows with turbulent diffusion. The validation process for the WIND-US multiphase solver showed that there was good correlation between the experimental mean diffusion and the simulation values regardless of the mesh type. More importantly, the capability to capture the significant aspects of the physics of turbulent particle diffusion in multiphase flows has been demonstrated on structured, unstructured, and hybrid meshes. This represents a significant step toward achieving a capability in WIND-US to solve many general types of multiphase problems. The future incorporation of the capability to perform interpolation of fluid properties within a cell would further enhance the capability of WIND-US to resolve more details, increase the accuracy, and make the simulations less dependent on grid resolution.

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