

LAGRANGIAN TECHNIQUES FOR PARTICLE FLUX AND CONCENTRATION

BY

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THESIS

Submitted in partial fulfillment of the requirements
for the degree of Master of Science in Aerospace Engineering
in the Graduate College of the
University of Illinois at Urbana-Champaign, 2010

Urbana, Illinois

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ABSTRACT

A new technique is proposed for computing Eulerian particle concentration and fluxes based on Lagrangian particle trajectories. In particular, a Lagrangian concentration differential equation is solved along a particle path using Eulerian derivatives for the particle velocity divergence field. This is referred to as the Lagrangian Concentration Differential Equation (LCDE) technique and is shown to provide efficient and accurate results for steady flows. It is compared to other Lagrangian techniques using high order trajectory simulations for particle with a linear drag law. Steady two-dimensional flows in a corner and past a cylinder are considered as the fundamental flows while the MS317 airfoil is considered as an industrial application. For all these flows, the concentration or flux fields are predicted for both tracer particles (which follow the flow) and for particles of finite inertia, as characterized by Stokes numbers. The LCDE approach is found to capture the accuracy of area-based Lagrangian methods (which are limited to steady flows) but may also be used in unsteady flows. In future work, this approach may be investigated with respect to unsteady and three-dimensional flows.

ACKNOWLEDGEMENTS

This work was funded by NASA Glenn Research Center's icing branch for their Icing Research Tunnel with Colin Bidwell as the technical manager.

I would like to thank my adviser, Professor Eric Loth, for his guidance, insight, and support throughout my graduate studies. To members of Professor Loth's research group, Albert Lee and Jason Mickey, thank you for sharing your knowledge.

I would also like to thank my parents for everything they have done. For all the opportunities they have given me. For making my education a priority and giving me everything needed to attain it. For believing in me, especially when I am struggling.

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CHAPTER 1 INTRODUCTION

1.1 Motivation

A natural approach when simulating individual particle interactions (with the fluid, with another particle, or with a wall) is to follow particle trajectories, i.e. the Lagrangian dispersed-phase representation. In this case, particle path-lines are defined based on the center of mass of a single particle (or for a cloud of particles) along which Ordinary Differential Equations are used to update particle position, velocity, mass, temperature, etc. This provides high accuracy with respect along a particle path, including particle-wall and particle-particle reflections. However, determination of volume or area-averaged quantities, such as particle concentration or mass flux per unit area, on an Eulerian grid requires summation of several Lagrangian trajectories. Because the statistical sample size used is limited by the number of particles used for the spatial averaging, this can lead to uncertainty and/or inaccuracy, especially for unsteady flows. Numerical errors associated with concentration predictions with an insufficient number of Lagrangian particles per cell can lead to substantial non-physical oscillations when two-way coupling is important (Sivier *et al.* 1996).

To avoid this problem, Eulerian dispersed-phase representations are often used when particle concentrations are important, especially when two-way coupling phenomenon is important. Such an approach employs Partial Differential Equations (PDEs) for the particle characteristics (e.g. velocity and concentration) which are discretized as cell-averages on an Eulerian grid. These quantities are integrated in time based on discrete spatial and temporal gradients and assumptions of continuity. However, this can lead to

non-physical diffusion of particle mass and momentum during advection. Furthermore, reflecting boundary conditions are difficult to treat within an Eulerian approach.

Therefore, it is desirable to develop a method which can incorporate the trajectory accuracy of the Lagrangian approach and the concentration accuracy of the Eulerian approach. A recent hybrid concept termed the Full Lagrangian method was developed by Healey & Young (2005) based on a linear drag force and a Jacobian system of equations. The present approach seeks to use elements of this approach while preserving the simplicity of conventional Lagrangian approaches, e.g. allowing for generalized surface forces and trajectory ODE's. The latter is accomplished by employing a Lagrangian Concentration Differential Equation (LCDE) along the particle path. To solve this equation, the particle velocity divergence is obtained by discretizing the spatial derivatives from nearby particle paths in the Eulerian domain. The use of these Eulerian spatial derivatives combined with the LCDE equation can be referred to as the Globally Eulerian Locally Lagrangian (GELL) approach. The present technique is evaluated by comparison to conventional techniques for different flowfields. This includes fundamental flowfields for which there is an analytical solution for the fluid flow (and for the particle concentration for certain inertia limits).

The performance of numerical methods with respect to droplet impact on airplane surfaces is the primary application motivation. In particular this project aims to support simulations of ice accretion and a numerical equivalent of an Icing Research Tunnel. Ice accretion is the process by which a layer of ice builds up on solid objects that are exposed to freezing precipitation or to super-cooled fog or cloud droplets. For this particular work, ice accretion is aircraft icing on a one element airfoil. Icing on airfoils form during the

descent of aircraft before landing and is extremely dangerous because it can change the characteristic of the control surfaces of an airplane and decrease the aerodynamic performance i.e. increase drag and decrease lift. The liquid water content is a quantity used to measure the available liquid which may lead to accretion and is the mass of liquid per unit volume (usually in g/m^3). A quantity that is used to measure the ice accretion on airplane elements is the impact efficiency (β) also known as the impingement efficiency. The impact efficiency is defined as the droplet flux rate at the body surface normalized to the freestream flux rate.

The Icing Research Tunnel (IRT) for NASA Glenn Research Center (GRC) is a facility which can measure impact efficiency on various aerodynamic surfaces. It can produce continuous airspeeds from 50 to 350 knots and temperatures as low as $-25 \pm 1^\circ\text{F}$ year-round. Super-cooled water droplets between 15 and 50 microns with liquid water content (LWC) controllable between 0.2 and 2.5 g/m^3 can be produced to form an icing cloud. The 6 ft. high, 9 ft. wide, 20 ft long test section can accommodate many full-sized aircraft components as well as large-scale models and an 8.6 ft diameter turntable in the test section can rotate horizontally for various angles of attack. A good example of an icing test is that of the MS317 airfoil of Papadakis *et al.* (2003). As such, this case will be used herein for numerical computation and compared with the experimental impact efficiency data.

1.2 Particle Momentum Equations

Both Lagrangian and Eulerian approaches are derived from the overall particle translational equation of motion which specifies that the product of particle mass and

acceleration is equal to the net sum of the forces acting on the particle. This mass (m_p) can be expressed in terms of the particle volume (∇_p) and density (ρ_p), or in terms of the particle diameter (d):

$$m_p = \nabla_p \rho_p = \frac{\pi d^3 \rho_p}{6} \quad 1$$

If one assumes negligible contact interactions (i.e. particle concentrations are small enough such that particle-particle collisions are not significant), the Lagrangian equation for particle velocity ($\mathbf{v}$) is given by

$$m_p \left(d\mathbf{v} / dt \right) = m_p \mathbf{g} + \mathbf{F}_{\text{surf}} \quad 2$$

The left hand side (LHS) includes the particle path temporal derivative of the particle velocity while the right hand side (RHS) includes the body force based on gravity ($\mathbf{g}$) and fluid dynamic surface forces ($\mathbf{F}_{\text{surf}}$). Conventionally, the components of the surface force include drag, lift, virtual mass, history, and fluid stress forces. Similarly, ordinary differential equations (ODEs) can be written for particle position ($\mathbf{x}_p$) and mass as

$$d\mathbf{x}_p / dt = \mathbf{v} \quad 3a$$

$$dm_p / dt = \dot{m}_p \quad 3b$$

As in equation (Eq.) 2, the LHS of equations (Eqs.) 3a and 3b include particle-path temporal derivatives. The RHS of Eq. 3b is the mass transfer from the surrounding fluid to the particle, which is a function of the difference between vapor species fractions on the particle surface and that in the far-field in the case of droplet evaporation.

The RHS expressions of Eqs. 2 and 3b include $\mathbf{F}_{\text{surf}}$ and $\dot{m}_p$ which are the surface integrated fluid dynamic force and mass flux to the particle. One may simulate the detailed flow and species around the particle to obtain these, but this is typically computationally prohibitive if there are many small particles. The point-force approach avoids this problem by employing theoretical and empirical models for $\mathbf{F}_{\text{surf}}$ and $\dot{m}_p$ based on relative differences between particle characteristics and that of the surrounding fluid. The dominant contribution of the surface force is typically the drag component which is non-zero in the presence of finite viscosity of the surrounding fluid (μ_f). For a spherical solid particle surrounded by a uniform continuum flow of with constant density (ρ_f), this force can be represented by the Stokes drag and a Stokes correction (f) as:

$$\mathbf{F}_D = -3\pi d \mu_f \mathbf{w} \quad 4a$$

$$\text{Re}_p \equiv \frac{\rho_f |\mathbf{w}| d}{\mu_f} \quad 4b$$

$$\mathbf{w}(t) \equiv \mathbf{v}(t) - \mathbf{u}_{@p}(t) \quad 4c$$

The drag force of Eq. 4a acts in the direction opposite of the particle relative velocity ($\mathbf{w}$), which is based on the “unhindered” continuous-fluid velocity ($\mathbf{u}_{@p}$), extrapolated to the particle centroid ($\mathbf{x}_p$). The “unhindered” velocity neglects local flow disturbances caused by the particle, i.e. it is the velocity that would occur if the particle was not present. The Stokes correction factor is unity for a particle Reynolds number which is small ($\text{Re}_p \ll 1$) and otherwise can be modeled with the Schiller-Naumann (1935) empirical expression to extend the drag to finite Reynolds numbers:

$$f = 1 + 0.15 \text{Re}_p^{0.687} \quad \text{for } \text{Re}_p < 1000 \quad 5$$

The temporal response to the restoring drag force can be used to define a particle response time as

$$\tau_p \equiv \frac{m_p |\mathbf{w}|}{F_D} = \frac{\rho_p d^2}{18\mu_f f} \quad 6$$

This expression assumes that the particle density is large compared to that of the surrounding fluid ($\rho_p \gg \rho_f$, e.g. water droplet in air) so that the virtual mass is negligible and the effective mass is equal to the particle mass. In addition, the high density ratio limit indicates that the other surface force components are generally small compared to the drag as long as particle spin and fluid shear effects are weak (Maxey & Riley, 1983) so that

$$\mathbf{F}_{\text{surf}} \approx \mathbf{F}_D \quad 7$$

Herein, this simple surface force will be employed with Eq. 4a, but the LCDE approach may be extended to a more complex surface force, e.g. to include lift, history force, fluid stress and added mass force terms using the techniques discussed by Loth & Dorgan (2009).

The Stokes number (St) is also called the Modified Inertia Parameters and is the ratio of the particle response time (τ_p) and the continuous-fluid velocity changes (τ_f)

$$St \equiv \frac{\tau_p}{\tau_f} \quad 8$$

This is a general expression with different τ_p and τ_f for different flowfields. The continuous-fluid velocity changes can be defined using a ratio of characteristic of the flowfield length-scale (corner length for the corner flow, diameter for the cylinder flow and chord length for the airfoil) to velocity-scale (the incoming velocity for the corner flow and the freestream velocity for the cylinder and airfoil flows).

1.3 Previous Numerical Techniques

1.3.1 Lagrangian methods for Particle Trajectories

The momentum and position ODE's (Eqs. 2 and 3a) may be integrated in time for a discrete time increment (Δt) assuming constant τ_p and $\mathbf{u}_{@p}$ to yield:

$$\mathbf{v}^{n+1} = \mathbf{v}^n e^{-\Delta t/\tau_p^n} + \left(1 - e^{-\Delta t/\tau_p^n}\right) \left[\mathbf{u}_{@p}^n + \mathbf{g}\tau_p^n\right] \quad 9a$$

$$\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \tau_p^n \left[\mathbf{w}^n - \mathbf{g}\tau_p^n\right] \left(1 - e^{-\Delta t/\tau_p^n}\right) + \left[\mathbf{u}_{@p}^n + \mathbf{g}\tau_p^n\right] \Delta t \quad 9b$$

Scheme 1

This one-step exponential scheme is popular as it is inherently stable and “exact” for linear particle drag ($f=1$) with uniform flow ($\nabla \mathbf{u}=0$). The former assumes small particle Reynolds number, but it has been shown that explicitly updating the particle response times with the most recently calculated relative velocity ($\mathbf{w}^n$) and employing relatively small time-steps (ca. $\Delta t < 0.1\tau_p$), allows reasonable temporal accuracy (to within 1% accuracy) for $Re_p < 40$ in uniform flows by Lee V. & Loth (2007). To incorporate effects

of non-uniform flow along the particle path, Barton (1996) assumed the fluid velocity varied linearly along the particle path to obtain:

$$\mathbf{v}_p^{n+1} = \mathbf{v}_p^n e^{-\Delta t/\tau_p^n} + \mathbf{u}_{@p}^n \left(1 - e^{-\Delta t/\tau_p^n}\right) + \left(\mathbf{u}_{@p}^{n+1} - \mathbf{u}_{@p}^n\right) \left\{1 - \frac{\tau_p^n}{\Delta t} \left(1 - e^{-\Delta t/\tau_p^n}\right)\right\} \quad 10a$$

$$\begin{aligned} \mathbf{x}_p^{n+1} = & \mathbf{x}_p^n - \tau_p^n \left(\mathbf{u}_{@p}^n - \mathbf{v}_p^n\right) \left(1 - e^{-\Delta t/\tau_p^n}\right) + \mathbf{u}_{@p}^n \Delta t \\ & + \left(\mathbf{u}_{@p}^{n+1} - \mathbf{u}_{@p}^n\right) \left\{\frac{\Delta t}{2} - \tau_p^n + \frac{(\tau_p^n)^2}{\Delta t} \left(1 - e^{-\Delta t/\tau_p^n}\right)\right\} \end{aligned} \quad \begin{array}{l} \text{Scheme 2} \\ 10b \end{array}$$

Barton (1996) also introduced a higher-order scheme that assumed quadratic variation of the fluid velocity in time by additionally considering an earlier time-step value to estimate the first and second time derivatives of the fluid velocity along the particle-path as:

$$\mathbf{A} = \frac{\mathbf{u}_{@p}^{n+1} - \mathbf{u}_{@p}^{n-1}}{2\Delta t} \approx \left(\frac{d\mathbf{u}}{dt}\right)^n \quad 11a$$

$$\mathbf{B} = \frac{\mathbf{u}_{@p}^{n+1} - 2\mathbf{u}_{@p}^n + \mathbf{u}_{@p}^{n-1}}{2\Delta t^2} \approx \left(\frac{1}{2} \frac{d^2\mathbf{u}}{dt^2}\right)^n \quad 11b$$

These two terms can be used to put forward an exponential scheme as:

$$\begin{aligned} \mathbf{v}_p^{n+1} = & \mathbf{v}_p^n e^{-\Delta t/\tau_p^n} + \mathbf{u}_{@p}^n \left(1 - e^{-\Delta t/\tau_p^n}\right) + \mathbf{A} \left\{\Delta t - \tau_p^n \left(1 - e^{-\Delta t/\tau_p^n}\right)\right\} \\ & + \mathbf{B} \left\{\Delta t^2 - 2\tau_p^n \Delta t + 2(\tau_p^n)^2 \left(1 - e^{-\Delta t/\tau_p^n}\right)\right\} \end{aligned} \quad 12a$$

$$\begin{aligned} \mathbf{x}_p^{n+1} = & \mathbf{x}_p^n - \tau_p^n \left(\mathbf{u}_{@p}^n - \mathbf{v}_p^n\right) \left(1 - e^{-\Delta t/\tau_p^n}\right) + \mathbf{u}_{@p}^n \Delta t \\ & + \mathbf{A} \left\{\frac{\Delta t^2}{2} - \tau_p^n \Delta t + (\tau_p^n)^2 \left(1 - e^{-\Delta t/\tau_p^n}\right)\right\} \\ & + \mathbf{B} \left\{\frac{\Delta t^3}{3} - \tau_p^n \Delta t^2 + 2(\tau_p^n)^2 \Delta t - 2(\tau_p^n)^3 \left(1 - e^{-\Delta t/\tau_p^n}\right)\right\} \end{aligned} \quad \begin{array}{l} \text{Scheme 3} \\ 12b \end{array}$$

Note that Schemes 2 and 3 revert to Scheme 1 in a uniform flow since both **A** and **B** would go to zero.

1.3.2 Ensemble-Average Methods for Concentration and Surface Flux

Perhaps the simplest and most common approach to determine Eulerian concentration from Lagrangian particle trajectories is the ensemble-average bin method. At a given instant of time, a summation over a computational cell volume (Fig. 1) can be used to express concentration as:

$$\alpha_i = \frac{1}{\forall_{\Delta,i}} \sum_{j=1}^{N_{p\Delta}} \forall_{p,j} \quad 13$$

In this expression, $\forall_{\Delta,i}$ is the volume associated with node $\mathbf{x}_i$ which contains $N_{p\Delta}$ number of particles, each of which has a volume $\forall_{p,j}$. This can be extended to parcels which have N_{pP} particles per parcel and $N_{p\Delta}$ parcels per cell as:

$$\alpha_i = \frac{1}{\forall_{\Delta,i}} \sum_{j=1}^{N_{p\Delta}} N_{pP} \forall_{p,j} \quad 14$$

The parcel volume is assumed to be much less than the computational cell volume.

Parcels are more computationally efficient than tracking individual particles if there are many particles in the domain. However, both Eqs. 13 and 14 are subjected to statistical averaging if the control volume is independent of the particle spacing. In particular, the statistical uncertainty of the particle concentration ($\mathcal{U}\alpha$) for a random

distribution of particles is inversely proportional to the square root of the sampling frequency:

$$\frac{\mathcal{U}\alpha}{\alpha} \sim \frac{1}{\sqrt{N_{p\Delta}}} \quad 15$$

Based on this, a frequency of 100 particles per cell translates into an uncertainty of 10%, while 10^4 particles would be needed to ensure an uncertainty of 1%. For an ordered distribution of particles, the error is inversely proportional to the sampling frequency:

$$\frac{\mathcal{U}\alpha}{\alpha} \sim \frac{1}{N_{p\Delta}} \quad 16$$

In either case, a large number of particles per cell are needed for accurate predictions of Eulerian concentration gradients, i.e.:

$$N_{p\Delta} \gg 1 \quad \text{for accurate cell-averaged concentration} \quad 17$$

As a result, the number of particles required for convergence can greatly exceed the number of fluid nodes in a domain (DeAngelis *et al.* 1997).

To obtain particle mass flux per unit time ($\dot{M}_p$) for a given discrete area ($A_{\Delta,i}$) with the same bin approach, a flux summation through a discrete computational area over a time average can be used:

$$\dot{M}_{p,i} = \frac{1}{\tau_{avg}} \sum_{j=1}^{N_{p\Delta,i}} m_{p,j} \quad 18$$

In this expression, τ_{avg} is the time used for integration and $N_{p\Delta,i}$ is total number of particle trajectories crossing the discrete area in this averaging time. Often the discrete mass flux per area is of interest, which may then be obtained for bin i as:

$$\left(\frac{\dot{M}_p}{A} \right)_{\Delta,i} = \frac{1}{A_{\Delta,i} \tau_{\text{avg}}} \sum_{j=1}^{N_{p\Delta,i}} m_{p,j} \quad 19$$

In either case, statistical uncertainty requires that the number of particles (or parcels) used in the summation be large per Eq. 18.

For a 2-D flow with a vertical surface, the incremental area along the y -axis is based on the location of the bin centroid (y_i) and the neighboring bin centroids:

$$\Delta y_i = \frac{1}{2}(y_{i+1} + y_i) - \frac{1}{2}(y_i + y_{i-1}) \quad 20a$$

$$\frac{1}{2}(y_i + y_{i-1}) < y_p \leq \frac{1}{2}(y_{i+1} + y_i) \quad 20b$$

Eq. 20b specified the collection range for which a particle impact will be collected in the bin whose centroid is y_i . For uniform spacing, this simplifies to a constant bin length. A representation of the 2-D bin with particles impacting the bin can be seen in Fig. 2a with a weighting function

$$\Phi_{i,j} = \begin{cases} 1 & \text{if } |y_p - y_i| \leq \Delta y \\ 0 & \text{if } |y_p - y_i| > \Delta y \end{cases} \quad \text{for ensemble-average} \quad 21$$

The above expression gives uniform contribution for each particle hitting the collection bin.

One may define the impact efficiency (β) of particles through a plane (e.g. segment of an airfoil) by defining the injection area (A_{inj}) by assuming that the injection velocity and concentration are both uniform. Taking the injection plane to be normal to the particle velocity, the impact efficiency is equal to the mass flux per surface area normalized by the mass flux per unit area at the injection plane:

$$\beta_i \equiv \frac{(\dot{M}_p/A)_{flux}}{(\dot{M}_p/A)_{inj}} = \frac{A_{inj} \sum_{j=1}^{N_{p\Delta,i}} m_{p,j}}{A_{\Delta,i} \sum_{j=1}^{N_{p,inj}} m_{p,j}} \quad 22$$

The injection mass flux is computed using $N_{p,inj}$ particles injected over an area A_{inj} . In order to compute the particle concentration, one may employ Reynolds Transport Theorem (RTT) for an arbitrary quantity q :

$$\oint_{\forall} \frac{\partial q}{\partial t} d\forall = - \oint_A q(\mathbf{v} \cdot \mathbf{n}) dA + \oint_{\forall} \dot{q} d\forall \quad 23$$

In this equation $\mathbf{v}$ is the velocity of the transported quantity, $\mathbf{n}$ is the outward normal to the surface, and $\dot{q}$ is the source strength within the volume. If $\mathbf{q}$ and $\mathbf{v}$ are finite and continuously differentiable in space, then the first term on the RHS of this equation is the inward flux to the control volume. The opposite of this term is the outward flux. The quantity $\mathbf{q}$ can then be substituted with mass of particles per mixed-fluid volume ($\alpha\rho_p$). In addition, the first term on the RHS represents the particle mass flux through a control surface. Applying this relation to the particle injection cross-sectional area which has uniform properties and averaging over time yields:

$$\dot{M}_{p, \text{inj}} = \oint_{A_{\text{inj}}} \overline{(\alpha \rho_p)(\mathbf{v} \cdot \mathbf{n})} dA = \alpha_{\text{inj}} \rho_p v_{\text{inj}} A_{\text{inj}} \quad 24$$

Applying this relation to a downstream discrete flux location area yields:

$$\dot{M}_{p, \text{flux}} = \oint_{c.s} \overline{(\alpha \rho_p)(\mathbf{v} \cdot \mathbf{n})} dA = \frac{1}{\tau_{\text{avg}}} \sum_{j=1}^{N_{p\Delta}} m_{p,j} \quad 25$$

In this expression $N_{p\Delta}$ is the number of particles that flux through the area A_{Δ} .

Note that the dot product effectively modifies this surface area to be the area perpendicular to the particle velocity. The mass flux at any two parallel planes is thus conserved if there is no mass transfer between the particle and fluid phases (as is assumed herein).

Assuming constant density for each particle the integral of Eq. 25 can be expressed as:

$$\overline{(\alpha \rho_p)} A_{\Delta} \overline{\mathbf{v} \cdot \mathbf{n}} = \frac{1}{\tau_{\text{avg}}} \sum_{j=1}^{N_{p\Delta}} m_{p,j} \quad 26$$

Then averaging the velocity over all particles, the expression for particle concentration at a node becomes:

$$\bar{\alpha}_i = \frac{N_{p\Delta,i}}{\rho_p A_{\Delta,i} \tau_{\text{avg}}} \frac{\sum_{j=1}^{N_{p\Delta,i}} (m_{p,j})}{\sum_{j=1}^{N_{p\Delta,i}} (\mathbf{v}_j \cdot \mathbf{n}_i)} \quad 27$$

A similar summation can be used for $N_{p\Delta}$ parcels for a parcel approach. The normalized concentration for the ensemble bin-average method can then be expressed as:

$$\alpha^* \equiv \frac{\bar{\alpha}_i}{\bar{\alpha}_{inj}} = \frac{\rho_p A_{\Delta, inj}}{\rho_p A_{\Delta, i}} \frac{\sum_{j=1}^{N_{p\Delta, i}} (m_{p,j})_{flux}}{\sum_{j=1}^{N_{p\Delta, i}} (\mathbf{v}_j \cdot \mathbf{n}_i)_{flux}} \frac{\sum_{j=1}^{N_{p\Delta, i}} (\mathbf{v}_j \cdot \mathbf{n}_i)_{inj}}{\sum_{j=1}^{N_{p\Delta, i}} (m_{p,j})_{inj}} \quad 28$$

For a steady flow with $N_{p, inj}$ particles of constant density injected over an area A_{inj} at uniform $\mathbf{v}_j \cdot \mathbf{n}_i$, this ratio simplifies to:

$$\alpha^* = \frac{A_{\Delta, inj} N_{p\Delta, i} (\mathbf{v} \cdot \mathbf{n})_{inj}}{A_{\Delta, i} \sum_{j=1}^{N_{p\Delta, i}} (\mathbf{v}_j \cdot \mathbf{n}_i)} \quad 29$$

If the particles are injected over a vertical plane whose normal is in the x-direction, then $\mathbf{v}_j \cdot \mathbf{n}_j = v_{x,j}$ and for particles which simply follow the fluid streamlines (i.e. $\mathbf{v}=\mathbf{u}$), $\alpha^*=1$.

1.3.3 Weighted Average Methods for Concentration and Surface Flux

A variant of the above ensemble bin method is to use a shape function to weight the contribution from each particle (or each parcel). The shape functions may be quadratic or higher-order, but linear variations are typical and easy to implement. For a 2-D flow, the discrete flux area per unit depth is simply a line segment. If one considers a vertical surface discretized into segments of length Δy with junctions y_i , the linear shape function over two neighboring segments can be described as:

$$\Phi_{i,j} = \begin{cases} 1 - |y_p - y_i| / \Delta y & \text{if } |y_p - y_i| \leq \Delta y \\ 0 & \text{if } |y_p - y_i| > \Delta y \end{cases} \quad \text{for weighted-average} \quad 30$$

A 2-D linear shape function with particles impacting the collection plane is shown in Fig.

2b. For the weighted-average bin approach, the mass flux through an incremental area (between two neighboring junctions) becomes:

$$\dot{M}_{p,i} = \frac{1}{\tau_{\text{avg}}} \sum_{j=1}^{N_{p\Delta,i}} (\Phi_{i,j} m_{p,j}) \quad 31$$

For a 2-D flow with a vertical surface, the incremental area along the y-axis is centered at the junction value and can be expressed as:

$$\Delta y_{i,w} = \frac{1}{2}(y_{i+1,w} + y_{i,w}) - \frac{1}{2}(y_{i,w} + y_{i-1,w}) \quad 32$$

Note that the junction values are not the same as the centroid values used in the ensemble-average method. The discrete mass flux per area per weighted bin becomes:

$$\left(\frac{\dot{M}_p}{A} \right)_{\Delta,i} = \frac{1}{A_{\Delta,i} \tau_{\text{avg}}} \sum_{j=1}^{N_{p\Delta,i}} (\Phi_{i,j} m_{p,j}) \quad 33$$

Note that the incremental areas overlap between adjoining nodes so that the mass flux for a particle between two nodes is distributed to the associated discrete area for each node.

For impact efficiency at a collection location:

$$\beta_i = \frac{A_{\text{inj}} \sum_{j=1}^{N_{p\Delta,i}} (\Phi_{i,j} m_{p,j})}{A_{\Delta,i} \sum_{j=1}^{N_{p,\text{inj}}} m_{p,j}} \quad 34$$

The mean volume fraction at an Eulerian junction node can be expressed as a flux sum through a discrete area over the number of particles. For a steady flow with $N_{p,\text{inj}}$

particles of constant particle mass injected over an area, the concentration ratio for the weighted method is:

$$\bar{\alpha}_i = \frac{N_{p\Delta,i}}{\rho_p A_{\Delta,i} \tau_{avg}} \frac{\sum_{j=1}^{N_{p\Delta,i}} (\Phi_{i,j} \mathbf{m}_{p,j})}{\sum_{j=1}^{N_{p\Delta,i}} (\Phi_{i,j} \mathbf{v}_j \cdot \mathbf{n}_i)} \quad 35$$

The only difference between the ensemble and weighted bin formulation is the existence of a linear shape function for the numerator and denominator.

To apply these methods, particles must be injected at an upstream inflow plane and then collected at the flux plane of interest. If the inflow particle concentration is uniform, this can be represented by the following homogenous particle spacing:

$$(\Delta x_p = \Delta y_p = \Delta z_p)_{inj} = (\forall_p / \alpha)_{inj}^{1/3} \quad 36$$

If the time-step is fixed between particle injections as Δt_{inj} and injection velocity is in the x-direction, the initial streamwise particle spacing $(\Delta x_p)_{inj}$ will be equal to $(v\Delta t)_{inj}$. As such, the particle spacing for a rectangular y-z initialization plane is related to the injection volume fraction and injection particle mass flux by:

$$(\Delta y_p^2 = \Delta z_p^2)_{inj} = \left(\frac{\forall_p}{\alpha v \Delta t} \right)_{inj} = \left(\frac{\rho_p \forall_p \Delta A \tau_{avg}}{\dot{M}_p \Delta t} \right)_{inj} \quad 37$$

If the flow is also steady and the inflow particle velocity is uniform, the mass flux may be computed by releasing a single set of particles at the inflow plane with this spacing and determining the mass fluxes over discrete downstream areas based on $\tau_{avg} = \Delta t_{inj}$.

1.3.4 Area Methods for Surface Flux

The area-based technique employs the steady uniform inflow assumptions needed for Eq. 22, to relate the change in the stream-tube area to the change in mass flux perpendicular to that area. This technique has been developed by NASA and is implement in their LEWICE code by Ruff and Berkowitz (1990) and is efficient for simple geometries, e.g. where trajectories do not cross. It notes that the discrete mass flux through a particle stream-tube is constant:

$$\dot{M}_{p, \text{inj}} = \dot{M}_{p, \text{flux}} \quad 38$$

It further assumes that the stream-tube is defined by a set of particle paths. A 2-D representation of the stream-tube and trajectories and the associated areas are shown in Fig. 3a. From this, the mass flux per unit area can be based on Eq. 19 (and specifically for 2-D flows with $N_{p\Delta}=2$ as:

$$\left(\frac{\dot{M}_p}{A_\Delta} \right)_i = \frac{(m_{p,1} + m_{p,2})}{A_{\Delta,i} \tau_{\text{avg}}} \quad 39$$

The equation for the discrete area and stream-tube center are:

$$A_\Delta = \sqrt{(x_{p,1} - x_{p,2})^2 + (y_{p,1} - y_{p,2})^2} \quad 40a$$

$$x_i = (x_{p,1} + x_{p,2}) / 2 \quad 40b$$

$$y_i = (y_{p,1} + y_{p,2}) / 2 \quad 40c$$

Note that three-dimensional (3-D) flows may require three or four paths. For the area approach, the impact efficiency of Eq. 22 becomes:

$$\beta_i(x_i, y_i) = \frac{A_{\Delta, \text{inj}}}{A_{\Delta, i}} \frac{m_{p,1} + m_{p,2}}{m_{p,1, \text{inj}} + m_{p,2, \text{inj}}} \quad 41$$

The mean volume fraction for a stream-tube between trajectories in 2D can be expressed as a flux through a discrete area:

$$\bar{\alpha}_i(x_i, y_i) = \frac{2}{\rho_p A_{\Delta, i} \tau_{\text{avg}}} \frac{m_{p,1} + m_{p,2}}{\mathbf{v}_1 \cdot \mathbf{n}_i + \mathbf{v}_2 \cdot \mathbf{n}_i} \quad 42$$

The area method obtains the discrete area for a fixed and small pre-selected number of particles and is not subjected to statistical uncertainty that constrains the ensemble average method. The concentration ratio for a 2D flow with no mass transfer $m_p = m_{p, \text{inj}}$ is given by:

$$\alpha_i^*(x_i, y_i) = \frac{2A_{\text{inj}}(\mathbf{v} \cdot \mathbf{n})_{\text{inj}}}{A_{\Delta, i}(\mathbf{v}_1 \cdot \mathbf{n}_i + \mathbf{v}_2 \cdot \mathbf{n}_i)} \quad 43$$

Since the number of particles required for the stream-tube for each discrete region is much less than the ones for the ensemble method and its variant, the computational cost for the area-based method is substantially lower. When particle trajectories cross or bounce, the area-based method is still valid as long as the particle trajectories remain nearby each other after crossing or bouncing.

1.3.5 Full Lagrangian Methods for Local Concentration

An alternate method that reduces the number of particles or parcels required is the “full Lagrangian” method introduced by Osipov (1998). In this approach, particle concentration is carried along as an additional characteristic (along with velocity,

temperature, position, etc.) which can be determined base on a differential equation along the particle trajectory. This equation can be derived from the Eulerian particle concentration PDE (assuming constant particle density):

$$\frac{\partial \alpha}{\partial t} + \frac{\partial (\alpha v_j)}{\partial x_j} = \frac{\alpha \dot{m}_p}{\nabla_p \rho_p} \quad 44$$

Though differentiation the above formulation is rearranged as:

$$\frac{1}{\alpha} \left(\frac{\partial \alpha}{\partial t} + v_j \frac{\partial \alpha}{\partial x_j} \right) + \frac{\partial v_j}{\partial x_j} = \frac{1}{\alpha} \left(\frac{d\alpha}{dt} \right) + \frac{\partial v_j}{\partial x_j} = \frac{\dot{m}_p}{\nabla_p \rho_p} \quad 45$$

This can be rearranged to yield a Lagrangian ODE for concentration change:

$$\frac{d \ln(\alpha)}{dt} = -\nabla \cdot \mathbf{v} + \frac{\dot{m}_p}{m_p} \quad 46$$

A key for this method is to obtain the divergence of the particle velocity field in terms of a path derivative of the Jacobian tensor ($\mathcal{J}_{ij}$) of the Eulerian-Lagrangian transformation. The determinant of this Jacobian gives the change in volume of a differential parcel volume along the parcel path over a time shift of Δt . If there is no mass transfer (as will be the case for all the simulations herein), this change is inversely proportional to the change in the volume fraction which allows a discretized change in the parcel volume for a given time-step:

$$|\mathcal{J}| = \frac{\alpha^n}{\alpha^{n+1}} \quad 47$$

To compute the LHS determinant, all the components of the Jacobian must be determined. If the particle surface force consists only of a linear drag force, Healy & Young (2005) noted that these components can be obtained from a set of coupled ODEs:

$$\frac{d\mathcal{J}_{ij}}{dt} = \dot{\mathcal{J}}_{ij} \quad 48a$$

$$\frac{d\dot{\mathcal{J}}_{ij}}{dt} = \frac{1}{\tau_p} \left(\mathcal{J}_{kj} \frac{\partial u_i}{\partial x_k} - \dot{\mathcal{J}}_{ij} \right) \quad 48b$$

Since the Jacobian is not generally symmetric, this pair of equations yields eight ODEs in 2-D flows and eighteen ODEs in 3-D flows. These simultaneous equations can be integrated along the particle path using a predictor-corrector technique. For monodisperse particles, the volume fraction in a cell can then be averaged using a cell-based summation:

$$\alpha_i = \frac{1}{N_{p\Delta,i}} \sum_{j=1}^{N_{p\Delta,i}} \alpha(x_{p,j}) \quad 49$$

Note that a reasonable volume fraction can be obtained with just one representative particle per cell. As such, the “full Lagrangian” approach is often worthwhile since the overall number of particle trajectories will be much less than that with traditional Lagrangian concentration methods. For example, Healy & Young (2005) found that the total number of parcels in the domain can be reduced by a factor of 20-50 in 2-D flows (indicating substantial improvement in overall efficiency) and the savings are even more dramatic for 3-D flows.

1.4 Objectives of the Present Study

The ultimate goal for the development of Eulerian-Lagrangian techniques is to aid the NASA Glenn Research Center engineers to improve the numerical accuracy on the prediction of ice forms at different conditions in their Ice Research Tunnel. In order to improve the computational efficiency for the prediction of ice accretions on airplane elements, both Lagrangian and Eulerian approaches will be into a Lagrangian Concentration Differential Equation (LCDE) method. A key attribute of this approach is that the aerodynamics and droplet impingement can be directly computed using a low number of particle trajectories and alleviate the computational intensity for numerical studies for concentration and fluxes. This method will also be able to handle complex unsteady flowfields without the loss of accuracy. Ultimately, it will serve as a replacement of traditional area methods to aid the NASA engineers for their IRT studies.

CHAPTER 2 METHODOLOGY

2.1 Globally Eulerian Locally Lagrangian Approach

2.1.1 Lagrangian Concentration Differential Equation

The present method generalizes the Full Lagrangian method for non-linear drag and other surface forces. It also avoids the numerical integration of a Jacobian system by instead sampling the local particle velocity gradient field for a stream-tube (based on two particle trajectories that are closely spaced to each other) and a modified concentration equation from the “full Lagrangian” method without the added mass effect:

$$\frac{d \ln(\alpha)}{dt} = -\nabla \cdot \mathbf{v} \quad 50$$

The differential equation above is integrated along the particle path along with the particle position and velocity. The common treatment for divergence uses a stream-tube which is similar to the area-based method that utilizes the two particle trajectories to avoid extremities in different directional divergences. It also avoids the assumption that the drag force is linear. Hence, the concentration ratio at different locations can be defined as:

$$\alpha_i^* \equiv \frac{\alpha_i}{\alpha_{inj}} \quad 51$$

Since the concentration is of individual particles, there is no averaging needed to express the concentration ratio. The treatment of obtaining the concentration at different time-steps will be discussed in section 2.1.2.

Utilizing the Eq. 21 ($N_{p\Delta,i}=1$), the impact efficiency can be written as:

$$\beta_i = \frac{A_{inj}}{A_{\Delta,i}} \quad 52$$

The discrete area is defined by the distance between the two adjacent particles in the stream-tube at the measuring plane (Eq. 40a). Applying concentrations from Eq. 29, this expression can be extended as

$$\beta_i = \frac{A_{inj} N_{p\Delta,i} (\mathbf{v} \cdot \mathbf{n})_{inj} (\mathbf{v}_j \cdot \mathbf{n}_i)}{A_{\Delta,i} (\mathbf{v}_j \cdot \mathbf{n}_i) (\mathbf{v} \cdot \mathbf{n})_{inj}} = \frac{\alpha_i (\mathbf{v}_j \cdot \mathbf{n}_i)}{\alpha_{inj} (\mathbf{v} \cdot \mathbf{n})_{inj}} \quad 53$$

Simplifying in terms of the concentration ratio the impact efficiency for the method becomes:

$$\beta_i \equiv \alpha_i^* \frac{(\mathbf{v}_j \cdot \mathbf{n}_i)}{(\mathbf{v} \cdot \mathbf{n})_{inj}} \quad 54$$

The method uses the same number of particles as the area-based method for a 2-D fluid and may use less in 3-D. Although this method requires one more ODE than the area-based method, it requires no computation of the normal velocity for local concentration.

2.1.2 Discretization of Concentration Equation

From Eq. 50, the concentration of particle trajectory can be computed by integration. The relationship can be expressed in exponential finite difference form for a discrete time increment (Δt) to yield:

$$\alpha^{n+1} = \alpha^n \exp(-\Delta t \nabla \cdot \mathbf{v}^{n+1/2}) \quad 55a$$

$$\alpha^{n+1} = \alpha^n \left[1 - \Delta t (\nabla \cdot \mathbf{v}^{n+1/2}) \right] \quad 55b$$

For each $n+1$ time-step, the previous time concentration is needed to for the computation. Both schemes were tested and Eq. 55a was chose for this study because it avoids the approximation for the exponential and gives a more accurate result. The concentration is computed along with particle trajectory and velocity when marching the particle trajectory forward in time using the exponential methods in 1.3.1. The treatment of the particle velocity divergence will be discussed in the next section.

2.1.3 Discretization of the Particle Velocity Divergence

Particle velocity divergence is of critical importance for the numerical treatment of the GELL method. In order to compute this divergence, a simple finite difference method for a single particle path was first considered:

$$(\nabla \cdot \mathbf{v})_i^{n+1/2} = \frac{v_{x,i}^{n+1} - v_{x,i}^n}{x_i^{n+1} - x_i^n} + \frac{v_{y,i}^{n+1} - v_{y,i}^n}{y_i^{n+1} - y_i^n} \quad 56$$

This method worked well for the corner flow, but was not appropriate for the cylinder or airfoil flows. Once the trajectories become horizontal or vertical, one of the denominators of Eq. 56 would become zero and thus will give unphysical results.

To avoid such problems, a stream-tube approach is used with neighboring particles. This approach allows isoperimetric formulations that express the element coordinates and element velocity in the form of interpolations using the natural coordinate system of the elements (Fig 4b). For 2-D flows with particles released along an inflow line segment with index i , quadrilateral elements are used where the four corners of a quadrilateral element are computed using two neighboring trajectories. These trajectories are denoted as x_{i-1} and x_{i+1} at two times: t^n and t^{n+1} as shown in Fig. 3b. The trajectory values are used to compute the velocity divergence for particle i using the following formulations. The general two dimensional element coordinate interpolations are:

$$x = \sum_{i=1}^4 \Phi_i x_i \quad 57a$$

$$y = \sum_{i=1}^4 \Phi_i y_i \quad 57b$$

Where x and y are the coordinates at any point of the element, and $x_i, y_i, i = 1, \dots, 4$, are the coordinates of the 4 element nodes. Quantities Φ_i are the interpolation functions in the natural coordinate system with variables ξ and η that each varying from +1 to -1. The variables ξ and η are the direction coordinates in natural coordinates that are equivalent to x and y in the Cartesian coordinate system. The same interpolation can be applied to element velocities:

$$v_x = \sum_{i=1}^4 \Phi_i v_{x,i} \quad 58a$$

$$v_y = \sum_{i=1}^4 \Phi_i v_{y,i} \quad 58b$$

The interpolation functions are the same for both the velocities and coordinates and this places the four points in natural coordinates in respect of ξ and η as (1, 1), (-1, 1), (-1, -1), and (1, -1). The interpolation functions associated with each point are:

$$\Phi_1 = \frac{(1+\xi)(1+\eta)}{4} \quad 59a$$

$$\Phi_2 = \frac{(1-\xi)(1+\eta)}{4} \quad 59b$$

$$\Phi_3 = \frac{(1-\xi)(1-\eta)}{4} \quad 59c$$

$$\Phi_4 = \frac{(1+\xi)(1-\eta)}{4} \quad 59c$$

To evaluate the displacement derivatives, the following can be used:

$$\begin{bmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \end{bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{bmatrix} \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{bmatrix} \quad \text{or} \quad \frac{\partial}{\partial \mathbf{r}} = J \frac{\partial}{\partial \mathbf{x}} \quad 60$$

In the above expression, $\mathbf{r}$ and $\mathbf{x}$ are the principle directions in natural and Cartesian coordinate system. Then invert the Jacobian from Eq. 59 to get

$$\begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{bmatrix} = J^{-1} \begin{bmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \end{bmatrix} \quad 61$$

Where the inverse of the Jacobian in 2D can be expressed as:

$$J^{-1} = \frac{1}{\frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} - \frac{\partial y}{\partial \xi} \frac{\partial x}{\partial \eta}} \begin{bmatrix} \frac{\partial y}{\partial \eta} & -\frac{\partial y}{\partial \xi} \\ -\frac{\partial x}{\partial \eta} & \frac{\partial x}{\partial \xi} \end{bmatrix} \quad 62a$$

$$\frac{\partial x}{\partial \xi} = \frac{1}{4} \left[(1+\eta) x_{i+1}^{n+1} - (1+\eta) x_{i+1}^n - (1-\eta) x_{i-1}^n + (1-\eta) x_{i-1}^{n+1} \right] \quad 62b$$

$$\frac{\partial x}{\partial \eta} = \frac{1}{4} \left[(1+\xi) x_{i+1}^{n+1} + (1-\xi) x_{i+1}^n - (1-\xi) x_{i-1}^n - (1+\xi) x_{i-1}^{n+1} \right] \quad 62c$$

$$\frac{\partial y}{\partial \xi} = \frac{1}{4} \left[(1+\eta) y_{i+1}^{n+1} - (1+\eta) y_{i+1}^n - (1-\eta) y_{i-1}^n + (1-\eta) y_{i-1}^{n+1} \right] \quad 62d$$

$$\frac{\partial y}{\partial \eta} = \frac{1}{4} \left[(1+\xi) y_{i+1}^{n+1} + (1-\xi) y_{i+1}^n - (1-\xi) y_{i-1}^n - (1+\xi) y_{i-1}^{n+1} \right] \quad 62e$$

Assume the desired path is in the middle of the two paths computed the value for ξ and η are (0, 0) respectively. Where the position x and y are related to the points in Fig. 3b of the stream-tube. The divergence between the particle stream-tube can be obtained via:

$$(\nabla \cdot \mathbf{v})^{n+1/2} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} \quad 63a$$

$$\left[\left(\frac{\partial v_x}{\partial x} \right)^{n+1/2} \right] = \frac{1}{4} J^{-1} \left[(1+\eta_1) v_{x,i+1}^{n+1} - (1+\eta_2) v_{x,i+1}^n - (1-\eta_3) v_{x,i-1}^n + (1-\eta_4) \right. \\ \left. (1+\xi_1) v_{x,i+1}^{n+1} + (1-\xi_2) v_{x,i+1}^n - (1-\xi_3) v_{x,i-1}^n - (1+\xi_4) \right] \quad 63b$$

$$\left[\left(\frac{\partial v_y}{\partial y} \right)^{n+1/2} \right] = \frac{1}{4} J^{-1} \left[(1+\eta_1) v_{y,i+1}^{n+1} - (1+\eta_2) v_{y,i+1}^n - (1-\eta_3) v_{y,i-1}^n + (1-\eta_4) \right. \\ \left. (1+\xi_1) v_{y,i+1}^{n+1} + (1-\xi_2) v_{y,i+1}^n - (1-\xi_3) v_{y,i-1}^n - (1+\xi_4) \right] \quad 63c$$

Eq. 62b-e and 63b-c and be further simplified when using the four corner points as:

$$\frac{\partial x}{\partial \xi} = \frac{1}{4} \left[x_{i+1}^{n+1} - x_{i+1}^n - x_{i-1}^n + x_{i-1}^{n+1} \right] \quad 64a$$

$$\frac{\partial x}{\partial \eta} = \frac{1}{4} \left[x_{i+1}^{n+1} + x_{i+1}^n - x_{i-1}^n - x_{i-1}^{n+1} \right] \quad 64b$$

$$\frac{\partial y}{\partial \xi} = \frac{1}{4} \left[y_{i+1}^{n+1} - y_{i+1}^n - y_{i-1}^n + y_{i-1}^{n+1} \right] \quad 64c$$

$$\frac{\partial y}{\partial \eta} = \frac{1}{4} \left[y_{i+1}^{n+1} + y_{i+1}^n - y_{i-1}^n - y_{i-1}^{n+1} \right] \quad 64d$$

$$\begin{bmatrix} \left(\frac{\partial v_x}{\partial x} \right)^{n+1/2} \\ \left(\frac{\partial v_x}{\partial y} \right)^{n+1/2} \end{bmatrix} = \frac{1}{2} \mathcal{J}^{-1} \begin{bmatrix} v_{x,i+1}^{n+1} - v_{x,i+1}^n - v_{x,i-1}^n + v_{x,i-1}^{n+1} \\ v_{x,i+1}^{n+1} + v_{x,i+1}^n - v_{x,i-1}^n - v_{x,i-1}^{n+1} \end{bmatrix} \quad 64e$$

$$\begin{bmatrix} \left(\frac{\partial v_y}{\partial x} \right)^{n+1/2} \\ \left(\frac{\partial v_y}{\partial y} \right)^{n+1/2} \end{bmatrix} = \frac{1}{2} \mathcal{J}^{-1} \begin{bmatrix} v_{y,i+1}^{n+1} - v_{y,i+1}^n - v_{y,i-1}^n + v_{y,i-1}^{n+1} \\ v_{y,i+1}^{n+1} + v_{y,i+1}^n - v_{y,i-1}^n - v_{y,i-1}^{n+1} \end{bmatrix} \quad 64f$$

The above treatment of divergence uses two particle trajectories and will resolve the unphysical result from the finite differencing.

2.2 Flowfield Conditions

2.2.1 Corner Flow

The corner flow is a simple 2-D flow given by the velocity potential:

$$\phi_f = \frac{A(y^2 - x^2)}{2} \quad 65$$

In this expression, A is a positive constant. The velocity components and their derivatives for the fluid flowfield are:

$$u_x = \frac{\partial \phi_f}{\partial x} = -Ax, \quad \frac{\partial u_x}{\partial x} = -A, \quad \frac{\partial u_x}{\partial y} = 0, \quad 66a$$

$$u_y = \frac{\partial \phi_f}{\partial y} = Ay, \quad \frac{\partial u_y}{\partial x} = 0, \quad \frac{\partial u_y}{\partial y} = A, \quad 66b$$

For simplicity the constant A is set to be 1. The equations then become:

$$u_x = \frac{\partial \phi_f}{\partial x} = -x, \quad \frac{\partial u_x}{\partial x} = -1, \quad \frac{\partial u_x}{\partial y} = 0, \quad 67a$$

$$u_y = \frac{\partial \phi_f}{\partial y} = y, \quad \frac{\partial u_y}{\partial x} = 0, \quad \frac{\partial u_y}{\partial y} = 1, \quad 67b$$

If we consider the domain with $x < 0$ and $y > 0$, the flow enter the domain through the left boundary turns upward. The stagnation-point is at the origin. The streamlines of the corner flow can be seen in Fig. 4a.

The particle trajectories can be obtained analytically by solving the differential equations of position from Healy and Young (2005):

$$\frac{dV_x}{dt} = \frac{1}{\tau_p} (u_x - v_x) \quad 68a$$

$$\frac{dV_y}{dt} = \frac{1}{\tau_p} (u_y - v_y) \quad 68b$$

The relationship $v_x = \partial x / \partial t$, $v_y = \partial y / \partial t$ and Eq. 67 can be substituted into Eq. 68,

$$\tau_p \frac{d^2 x}{dt^2} + \frac{dx}{dt} + x = 0 \quad 69a$$

$$\tau_p \frac{d^2 y}{dt^2} + \frac{dy}{dt} - y = 0 \quad 69b$$

The above expression may be solved with the initial condition $x(0) = -1$, $v_x(0) = 1$, $y(0)$

$= y_0$ and $v_y(0) = y_0$ as:

$$x(t) = -\frac{1}{2} \frac{(-1 + 4\tau_p - \sqrt{1 - 4\tau_p} + 2\sqrt{1 - 4\tau_p} \tau_p) e^{\left[\frac{1}{2} \frac{(-1 + \sqrt{1 - 4\tau_p})t}{\tau_p} \right]}}{-1 + 4\tau_p} + \frac{1}{2} \frac{(-\sqrt{1 - 4\tau_p} + 1 - 4\tau_p + 2\sqrt{1 - 4\tau_p} \tau_p) e^{\left[\frac{1}{2} \frac{(1 + \sqrt{1 - 4\tau_p})t}{\tau_p} \right]}}{-1 + 4\tau_p} \quad 70a$$

$$y(t) = \frac{1}{2} \frac{y_0 (1 + 4\tau_p + \sqrt{1 + 4\tau_p} + 2\sqrt{1 + 4\tau_p} \tau_p) e^{\left[\frac{1}{2} \frac{(-1 + \sqrt{1 + 4\tau_p})t}{\tau_p} \right]}}{1 + 4\tau_p} - \frac{1}{2} \frac{y_0 (\sqrt{1 + 4\tau_p} - 1 - 4\tau_p + 2\sqrt{1 + 4\tau_p} \tau_p) e^{\left[\frac{1}{2} \frac{(1 + \sqrt{1 + 4\tau_p})t}{\tau_p} \right]}}{1 + 4\tau_p} \quad 70b$$

Differentiating the above expressions yields the analytical solution for velocity at different particle response times:

$$v_{x,\text{exact}}(t) = \frac{1}{4} \frac{(-1 + 4\tau_p - \sqrt{1 - 4\tau_p} + 2\sqrt{1 - 4\tau_p}\tau_p)(-1 + \sqrt{1 - 4\tau_p})e^{\left[\frac{1}{2} \frac{(-1 + \sqrt{1 - 4\tau_p})t}{\tau_p}\right]}}{(-1 + 4\tau_p)\tau_p} - \frac{1}{4} \frac{(-\sqrt{1 - 4\tau_p} + 1 - 4\tau_p + 2\sqrt{1 - 4\tau_p}\tau_p)(1 + \sqrt{1 - 4\tau_p})e^{\left[\frac{1}{2} \frac{(1 + \sqrt{1 - 4\tau_p})t}{\tau_p}\right]}}{(-1 + 4\tau_p)\tau_p} \quad 71a$$

$$v_{y,\text{exact}}(t) = \frac{1}{4} \frac{y_0(1 + 4\tau_p + \sqrt{1 + 4\tau_p} + 2\sqrt{1 + 4\tau_p}\tau_p)(-1 + \sqrt{1 + 4\tau_p})e^{\left[\frac{1}{2} \frac{(-1 + \sqrt{1 + 4\tau_p})t}{\tau_p}\right]}}{(1 + 4\tau_p)\tau_p} + \frac{1}{4} \frac{y_0(\sqrt{1 + 4\tau_p} - 1 - 4\tau_p + 2\sqrt{1 + 4\tau_p}\tau_p)(1 + \sqrt{1 + 4\tau_p})e^{\left[\frac{1}{2} \frac{(1 + \sqrt{1 + 4\tau_p})t}{\tau_p}\right]}}{(1 + 4\tau_p)\tau_p} \quad 71b$$

The above analytical solutions for the corner flow particle trajectories can be used to evaluate the accuracy of the particle trajectories for different numerical Schemes.

2.2.2 Cylinder Flow

An inviscid, incompressible two-dimensional flow over a cylinder is used to incorporate non-linear velocity gradients effects for a fundamental flowfield. It is unphysical because there are no boundary layers, but it is still a useful test because the existence of an analytical solution for the velocity field. The fluid flowfield is given by the velocity potential with the streamlines of flow in Fig 4b:

$$\phi_f = U_\infty x \left(1 + \frac{R^2}{x^2 + y^2} \right) \quad 72$$

In this expression, U_∞ is the freestream velocity of the flowfield, and R is the radius of the cylinder. The velocity components for the fluid flowfield are consequently as:

$$u_x = \frac{\partial \phi_f}{\partial x} = U_\infty \left[1 + \frac{(y^2 - x^2)R^2}{(x^2 + y^2)^2} \right] \quad 73a$$

$$u_y = \frac{\partial \phi_f}{\partial y} = -\frac{2U_\infty xyR^2}{(x^2 + y^2)^2} \quad 73b$$

For simplicity the constant U_∞ and R are both set to 1. The equations thus become:

$$u_x = 1 + \frac{y^2 - x^2}{(x^2 + y^2)^2} \quad 74a$$

$$u_y = -\frac{2xy}{(x^2 + y^2)^2} \quad 74b$$

The flow is from left to right and considered from $-1.5D$ to $1.5D$ where D is the diameter of the cylinder.

2.2.3 Airfoil Flow

The MS(1)-0317 airfoil is representative of modern medium speed airfoils. It was designed in the mid 1970's for general aviation aircraft (McGhee and Beasley, 1980). A grid of MS317 generated in GRIDGEN is shown in Fig. 5a. The Mach number contours with the streamlines are shown in Fig 5b. The numerical flowfield is computed using a Reynolds Averaged Navier-Stoke (RANS) simulation in WIND-US. The fluid flowfield is then used by WIND-US's multiphase feature to compute particle trajectories. These trajectories are the bases of different numerical methods for the calculation of impact efficiency on the airfoil surface using MATLAB. The computational domain is from $-3C$ to $+3C$ where C is the chord length of the airfoil.

2.2.4 Velocity Interpolation

In order to compute the particle velocity vector at different time, interpolation schemes are needed. If the surrounding fluid properties are available on an Eulerian grid, $\mathbf{u}_{@p}$ can be interpolated from the Eulerian nodes of the continuous-phase based on the shape functions Φ computed from the particle position, i.e.

$$\mathbf{u}_{@p} = \sum_{j=1}^{N_\Phi} \mathbf{u}_j(t) \Phi_j(\mathbf{x}_p) \quad 75$$

This interpolation was simplified by using the value the velocity interpolated to the cell center (instead of the particle location). Such a result is consistent with $\xi=0$ and $\eta=0$. In this equation, N_Φ is all the number of computational cells associated with a particle location, which is four for a two dimensional element. Use of the shape function allows the velocity of all surrounding nodes to be included in the evaluation of $\mathbf{u}_{@p}$. This is shown schematically in Fig. 6 for a two-dimensional grid.

CHAPTER 3 RESULTS

3.1 Particle Trajectory Accuracy

The analytical trajectories of the corner and cylinder flows can be used to evaluate the accuracy of the particle trajectories for different numerical methods, and the max error along a particle trajectory (ϵ) in the horizontal velocity can be defined as:

$$\epsilon = \max \left(\frac{|v_{x,\text{exact}}^i - v_x^i|}{v_{x,\text{exact}}^i} \right)_{\text{for } i=1,\text{max}} \quad 74$$

In this expression, $v_{x,\text{exact}}$ is the analytical particle x velocity, v_x is the numerical particle horizontal velocity from the different numerical schemes, and i is the time-step index.

The accuracy of the trajectories was first tested using the analytical solutions at time-steps (Δt) ranging from 10^{-1} to $10^{-2.5}$ non-dimensionalized by the ratio of domain length and maximum velocity which is unity. With the collection plane at $x = 0$ and releasing from $x = -1$, a number of particles were released for Stokes number of 0.1 using three exponential methods from Barton (1996) to compute their trajectories. The maximum error for this particular case can be represented by considering a loop over all N particles trajectories:

$$\epsilon = \max \left(\frac{|v_{x,\text{exact},i}(t) - v_{x,i}(t)|}{v_{x,\text{exact},i}(t)} \right) \text{ for } i=1, N_p \quad 75$$

The exact solution was based on Eq. 71 and the results of the maximum error plotted as a function of time-step can be seen in Fig. 7a. The velocity error decreases roughly

linearly with decreasing time-steps. The differences of the velocity error were negligible at small time-steps for all three methods.

The cylinder flow was also tested where particles are released from $x/D = -1.5$ and then collected at $x/D = 1.5$ for the zero-inertia case where the particle velocity is equal to the flow velocity. For the cylinder case, the maximum error is therefore:

$$\varepsilon = \max \left(\frac{|u_x(x_i, y_i) - v_{x,i}(x_i, y_i)|}{u_x(x_i, y_i)} \right) \text{ for } i=1, N_p \quad 76$$

An analytical solution for the particle velocity can be obtained from the zero-inertia case using the analytical flowfield velocities evaluated at the particle positions. The results are in Fig. 5b. As the time-step decreases, the error of Scheme 3 decreases consistently with first-order accuracy for particle velocity even when the fluid velocity along the particle path is non-linear. In contrast, Schemes 1 and 2 do not show improvement of accuracy as the time-step decreases. This is caused by the nonlinear velocity field, Schemes 1 and 2 does not account for the nonlinear velocity changes. Hence, Scheme 3 was used for all subsequent studies.

3.2 Particles in a Corner Flowfield

The ensemble, weighted averaging, area-based, and LCDE methods are investigated to evaluate the concentration ratio (α^*) for a simple steady two-dimensional corner flow in the second quadrant where the fluid velocity for the x and y direction are described in Eq. 67. The particles are released from $x=-2$, and for a range $y= [0 \ 1]$. The particle trajectories in the corner flowfield are shown in Fig. 8 for different Stokes numbers with

the flow streamlines in the background. In each case, the particle initial velocities are set equal to that of the surrounding fluid ($v_x=u_x$, $v_y=u_y$).

For $St=0$, the particle velocities are also equal to the flow velocities throughout the domain so the trajectories would follow the fluid streamlines (Fig. 8a). It can be seen that no particles hit the vertical wall. For $St=0.5$ (Fig. 8b), the particle trajectories indicate reduced turning due to more inertia. For $St=10$, (Fig. 8c) there is little turning and the particles continue along their initial velocity angles and impact the wall accordingly.

The ensemble, weighted averaging, and LCDE methods are selected to see the effect of particle resolutions on concentration ratio. The particles are released from the $x=-2$ and then collected at $x=-1$ (marked in Fig. 8a) with the same Stokes number ($St = 0$) for zero-inertia. The same release range of $y = 0$ to $y = 1$ and bin size of $0.1y_{\max@inj}$ are used for all three methods. The concentration ratio (α^*) results are plotted against the final vertical location ($y/y_{\max@inj}$) of the particles or bins in Fig. 9.

Fig. 9a shows that increasing the number of particles collected per bin results in α^* converging to the analytical result ($\alpha^*=1$). For the case with only 5 particles (distributed over 20 bins), α^* has substantial errors since the particle number per bin is low and some bins do not get any contribution from the particles. When the particle number released is increased to 50 particles (roughly 4-5 particles per bin) the errors in α^* have decreased to roughly $\pm 20\%$ (or 40% overall variations) consistent with Eq. 16. When the particle number reaches 500, α^* is close to the analytical solution, i.e. within 2%, also consistent

with Eq. 16. This qualitative trend is thus consistent with Eq. 17, i.e. the bin based method requires a large number of particles to provide consistently accurate result for α^* .

Similar results can be seen for the weighted averaging method in Fig. 9b. As the number of particles collected per weighted bin increase the concentration ratio distributions become smoother and converge to that of the numerical analytical solution. For the 5 particles case, α^* behaves similarly to that of the ensemble method. As N_p goes to 50, α^* has improved greatly and is within 5-10% of the analytical result. The effect of shape function inclusion allows a smoother and more diffused profile. For the 500 particles case, the profile is within 1% of the exact solution ($\alpha^*=1$), consistent again with Eq. 17.

In Fig 9c, the LCDE method is tested for the same conditions as the previous two numerical methods. However, there is a weak impact of the number of particles used. The results for α^* are very similar for 5, 50, and 500 particles collected. This high accuracy of the LCDE method occurs because α^* is computed directly. As such, it does not rely statistical convergence and only depends on the trajectory accuracy of the particles. Since the area-based method also uses two particle trajectories, it provides the same level of accuracy.

Based on the above particle resolution study, $N_p=50$ gives a reasonable and representative result for the bin based methods and is therefore used for the remaining studies. For the area-based and LCDE methods a particle number of 10 is used. For the following cases, the particles are injected at $x=-2$, and collected at $x=-1$ with a bin size of $0.1y_{\max@inj}$ and with the same injection range from $y = 0$ to $y = 1$. The concentration ratio

results are plotted against the vertical bins centers for the ensemble and weighted bin methods and against the vertical location impact location for the area and LCDE methods. For $St=0$, there should be no change in concentration consistent with incompressibility for the fluid flow, as shown in Fig. 10a. All four methods have reasonable agreement with the analytical result. However, the bin based methods have significant fluctuations compared to the other methods. This is particularly noticeable for the ensemble method because only 2-3 particles hit per bin. For the weighted averaging method, the shape functions distribute the contributions resulting in less error. However, there are errors for the first and last bin of the weighted averaging method and ensemble bin methods because the bins are not getting consistent contributions. For the area-based and LCDE method, the values of the concentration are almost identical to the analytical solution.

The numerical methods are further investigated for $St = 1$ in Fig. 10b with otherwise the same conditions used for Fig. 8a for which similar trends for all four methods were observed. The ensemble bin method has the largest errors because of variations in the number of particles hitting each bin. In this particular case, the weighted averaging method gives relatively small errors compared to the ensemble method by its use of the linear shape function. The area-based and LCDE methods give a constant distribution at the collection plane and provides good agreement with the weighted averaging method.

The next case considers $St = 10$ where the particle trajectories generally follow the initial trajectory angles and the concentration ratios are shown in Fig. 10c. In this case, one would expect that the particle concentration will be reduced due to the increase in impact area (compared to injection area). The ensemble bin method yields spurious fluctuations because of the low number of particles hitting per bin. The weighted

averaging method reduces the fluctuation by the use of the shape functions but has spikes at the initial and final bins. The area-based and LCDE methods give constant concentration ratios that agree with the weighted method.

To consider the potential performance of these techniques on angled surfaces, a collection plane set as a simple ramped surface with a uniform slope of 1 was placed around the corner to test the behavior of various methods. For the ensemble and weighted averaging bin methods, 500 particles are injected with a collection bin size of $0.08y_{\max@inj}$ to ensure accuracy. For the area-based and LCDE methods, 20 particles were used. For $St=0$ and $St = 1$, the trajectories are plotted in Fig. 11. For the zero-inertia ($St=0$) case, the particle trajectories follow the flowfield. For the finite inertia case, the particle trajectories are not affected by the corner. Hence the trajectories are relatively straight.

The concentration ratios are plotted against the vertical collection plane location in Fig. 12a for the zero-inertia case ($St = 0$). Theoretically, $\alpha^*=1$ where the trajectories hit, but is otherwise zero. The various methods are approximately consistent with this result. Non-physical fluctuations again exist for the ensemble bin and weighted averaging methods because certain bins do not have a high number of particles hitting to give accurate results. The area-based method and LCDE method gives a smooth concentration ratio that closely follows unity despite a small number of trajectories.

A finite-inertia case is also considered for the ramped corner flow. The same conditions are plotted in Fig. 12b as Fig. 12a with $St = 1$. The four methods agree with each other. The bin-based methods (ensemble and weighted) only show minor

differences of concentration along the collection plane because of there are more particles hitting each bin and the accuracy of α^* is increased. The area-based and LCDE methods do not show such problems.

3.3 Particles in a Cylinder Flow

For the incompressible, inviscid two-dimensional flow described by Eq. 74, the various methods are investigated to evaluate concentration ratio (α^*) for vertical collection planes. Trajectories for particles entering at the left boundary of the computational domain ($x=-1.5D$) and exiting through the right boundary of the domain ($x=1.5D$) are plotted for different Stokes numbers in Fig. 13. The initial velocities of the particles are set as the fluid velocity and the particles are marched with a time-step of 10^{-2} . For zero-inertia ($St=0$), all of the particles go around the cylinder as the particle velocity is the same as the flowfield velocity. For $St = 1$, the particles around the edge of the cylinder do not return to the centerline leaving a void wake. For $St = 10$, the particles are not significantly influenced by the flowfield and exhibit little turning.

The zero-inertia case can be used as a reference to test the accuracy of different methods since its zero divergence characteristic leads to uniform concentration ratio throughout the flowfield. In Figure 14a, variable bin sizes were investigated for a constant number of particles ($N_p=101$) collected at the plane where $x/D = 0$. When the bin size is $y/D = 0.05$, the ensemble and weighted averaging bin methods give α^* with substantial spatial diffusions near the particle field edges. In contrast, the area-based and LCDE methods are consistent with the analytical result except near the edge of the cylinder. This is due to the time-step induced numerical error in the position at the

collection plane. If the time-step is reduced by 100 fold, the error in α^* is negligible. When the bin-size is halved, the area-based and LCDE methods are unaffected but again show an error near the discontinuity at $y/D = 1/2$. This problem does not appear in the bin-based methods though non-physical fluctuations remain indicating that such methods are more accurate as bin resolution decreases.

Next, a study for the number of particles used was conducted for the ensemble and weighted averaging bin methods with zero-inertia and a uniform bin size of $\Delta y/D=0.05$. The particles are again collected at the top of the cylinder ($x=0$) to compute α^* . For the ensemble method, Fig. 15a shows that for a low number of particles released the numerical prediction is greatly lower than the analytical solution. As the number of particles released from the injection plane increases, the prediction using the ensemble method converges to that of the analytical solution. This result is consistent with the particle resolution study for the corner flow and shows that the ensemble bin method need a high number of particles per bin to obtain accurate results.

For the weighted averaging method, α^* predictions give similar trends to that of the ensemble bin method but with improved convergence. In Fig. 15b, when a low number of particles are released, α^* is significantly lower than the analytical solution. As the number of particles released increases, the numerical results of α^* approach the analytical solution value. The results for the LCDE and area-averaged methods are not shown, but the predictions from these techniques were not sensitive to the number of particles (similar to the result of Fig. 9c).

The impact of finite inertia cases is next considered. For the case $St = 1$, α^* results are shown in Fig. 16a. Because some of the particles hit the upstream surface of the cylinder, a fraction of the released particles do not reach the collection plane at the top of the cylinder. This also leads to an increased concentration of particles near the cylinder surface at this location. This explains the peak in α^* near $y/D=0.5$. As usual, the weighted method gives a smoother behavior because of the shape function weighting. The area-based method gives results almost identical to that of the LCDE method and captures the sharp discontinuity at $y/D=0.5$. At this location, the concentration is high just above the surface as the particles trajectories become quite close. All of the methods are consistent with the far-field solution ($\alpha^* \rightarrow 1$) at larger y/D values away from the cylinder.

For $St=10$, the concentration ratio at the collection plane tends back to unity (Fig. 16b) as there is little trajectory curvature. For the ensemble bin method, approximately 10 particles hit the collection plane which results in greater statistical error. For the weighted averaging method, because only a few bins getting concentration at the collection plane there is significant diffusion. The area-based method once again closely agrees with the LCDE method and yields almost constant concentration values at the impact plane.

The collection plane is next moved to the wake of the cylinder ($x/D=1.5$). The zero-inertia case is first tested with the analytical solution. The results are displayed in Fig. 17a. For bins close to $y/D = 0$, the ensemble and weighted averaging bin methods give errors near the centerline but tend to the analytical solution away from the centerline of the cylinder. The deviations of concentration ratio for the area-based and LCDE methods

near the centerline of the cylinder are an artifact of the errors introduced by the time-step in the trajectories. As the impact locations get away from the centerline, all the methods approach the analytical solution, though the edge of the field is diffused in the case of the ensemble and weighted averaging bin methods.

For $St = 1$, the α^* results are in Fig. 17b. Because some of the particles are hitting the surface of the cylinder, only a fraction of the particles released are being collected at the collection plane. This leaves a void region closely associated with a high concentration region. The ensemble and weighted averaging bin methods will have fewer particles hitting each bin and hence explains great fluctuation in α^* for the ensemble method. The weighted method gives a more smooth behavior because of the smoothing effect from the shape function weighting. The area-based method gives results almost identical to that of the LCDE method with a smooth transitional profile.

For $St = 10$, the results of α^* plotted against the collection location normalized by the cylinder diameter can be seen in Fig. 17c. The ensemble-average bin method has only a few collected particles due to a large amount of particles hitting the surface of the airfoil and this gives a big variation in α^* compared to the area-based and LCDE methods. The weighted averaging method has the same behavior as the ensemble method with shape function smoothes out the results. The area-based and LCDE method shows good agreement with each other and tend to the unity concentration analytical solution appropriate for infinite Stokes number.

It is also interesting to investigate the impact efficiency (β) on the surface of the cylinder since it resembles particles hitting the leading-edge of an airfoil. Fig. 18 gives the result of the impact efficiency (β) for different Stokes numbers. In order to obtain accurate result for all of the numerical methods, a N_p of 1000 is used for the bin based methods but a N_p of 20 was found to be sufficient for the area-based and LCDE methods. The variable s is the surface distance from the left of the cylinder which acts as the leading edge. At the centerline ($s=0$), the impact efficiency near unity and falls off for the high inertia case ($St = 100$) can be seen in Fig. 18a. The analytical solution is obtained using the ratio of the surface distance on the cylinder to the corresponding release y differences. All methods agree well with the analytical solution. As a high number of particles are being used, the bin based methods' error is greatly reduced. For the bins near the top of the cylinder, the values deviate from the analytical result because of numerical diffusion. The area-based and LCDE methods exhibit good agreement. However, area-based and LCDE methods uses an averaging method of the last two particle locations to compute the intersection location instead of interpolation for the intersection location on the surface of the cylinder.

For $St = 1$, Fig. 18b gives the impact efficiency on the surface of the cylinder. As the collection location moves always from the centerline of the cylinder, the impact efficiency decreases. The ensemble and weighted averaging bin methods yield some fluctuations but are generally quite reasonable. The area-based and LCDE method agree with each other. The impact efficiency contains no data for the area-based and LCDE methods for the edge of the cylinder because the sparse injection prevents neighboring

trajectories from hitting the surface of the cylinder at the edge. The same behavior can be seen in the study for the MS317 airfoil.

Further decreasing the Stokes number to 0.5, the impact efficiency on the surface of the cylinder is displayed in Fig. 20c. Similar trend for the impact efficiency is observed when compare to $St = 1$, the impact efficiency decreases as the collection locations move away from the center of the cylinder. The ensemble and weighted averaging bin methods give variations away from the centerline of the cylinder since fewer particles are hitting each bin. The area-based and LCDE methods show good agreement. Note that there should be no impact efficiency for $St=0$.

3.4 MS317 Airfoil

The MS317 airfoil using the Shear Stress Transport (SST) $k-\omega$ turbulence model (Menter, 1993) with a viscous boundary layer was simulated with a chord Reynolds number of 4.77×10^6 based on a chord of 0.9144 meter (36 inches) and a flow speed of 0.2 Mach (78.25 m/s). The angle of attack with respect to the chord lines was set as 0 which corresponds to an angle of 6 with respect to the zero-lift-line. The code WIND-US (Bush 1998) was used to compute the flowfield conditions. The particles are released uniformly upstream of the airfoil from -3C with an initial horizontal velocity of 199 ft/s (60.65 m/s) and no vertical velocity. A particle number of $N_p = 401$ was released for the bin based methods and $N_p = 50$ was used for the area-based and LCDE methods. Particle trajectories for different droplet diameters thus produce different Stokes numbers as plotted in Fig. 19. The zero-inertia case is shown in Fig. 19a, the particles are following the flowfield and do not impact the surface of the airfoil. In Figs. 19b-d, it can be seen

that increasing the particle inertia reduces the trajectory curvatures and increases the likelihood of impact.

For $St = 0.04$ ($r_p = 21 \mu m$), β is plotted against the surface distance (s) in meters from the leading edge in Fig. 20a. The numerical results from the ensemble, weighted averaging, area-based, and LCDE methods are plotted along with the experimental results obtained from Papadakis *et al.* (2003) and the numerical results from Lee, S & Loth (2008). All methods have errors when compared with the experimental result. The ensemble average and weighted averaging methods under-predict the experimental but gives good agreement with the LCDE method. The area-based method gives scatter results within the experimental and numerical results which are caused by the boundary conditions in WIND-US which stops the particle before it accurate impacts the surface and results in inaccurate particle impact locations. The LCDE method gives the best agreement with the experimental data.

For $St = 0.31$ ($R_p = 79 \mu m$) in Fig 20b, all numerical methods over-predict β values because splashing is not accounted for by the simulations (the measurements were for collection efficiency while the prediction are for impact efficiency). The ensemble average and weighted averaging methods gives good agreement with each other. The area-based and the LCDE methods give smooth distributions that are generally consistent with the numerical results from Lee & Loth (2008). There are some differences at the edge due to not considering splashing.

CHAPTER 4 SUMMARY

4.1 Conclusion

Simulations were conducted for particle trajectories, concentrations, and impact efficiency for two flows and an airfoil for several particle Stokes numbers. The particle trajectory approach was first investigated with respect to accuracy as a function of time-step. For linear flowfield of a corner, the error in velocity does not affect the integrity of the numerical methods. For the nonlinear flowfield around a cylinder, velocity error is substantial and higher-order methods with small time-step are needed for high accuracy.

For the predictions of particle concentration and mass flux, the bin-based methods yielded statistical error when the particles per bin were not high. The ensemble-average is the simplest to implement but yielded the highest errors while the weighted averaging method required less number of particles per bin to obtain accurate results. However, both methods yielded numerical diffusion at the edges of particle laden regions.

The area-based method is the most efficient method in computing the particle concentration ratio for the present flows. It requires only a few particles' trajectories to the flux plane. However, it is sensitive to numerical errors in trajectory computation, especially near particle concentration discontinuities and cannot be applied to unsteady flows.

The LCDE method has similar efficiencies and accuracy to the area-based method though it does require integration of an additional ODE (beyond the four required for

position and velocity in two dimensions). It computes the particle concentration accurately with the use of only a few particles in flows with either linear or nonlinear flow velocity variations. Further study for unsteady and three-dimensional flowfields (unsteady, with added mass effects, etc.) is recommended to test the integrity of all the methods.

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CHAPTER 5 FIGURES

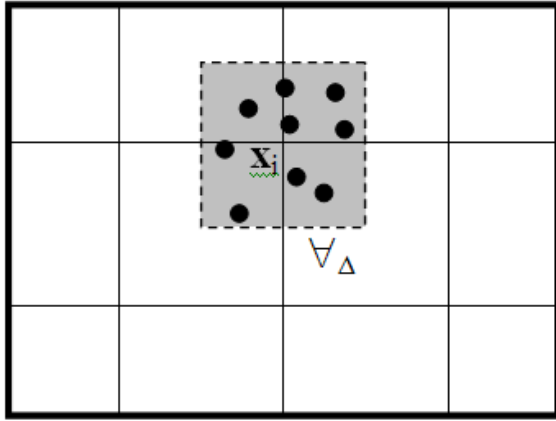


Figure 1. Schematic of a two-dimensional Eulerian continuous-phase grid showing summation of particle volumes in a computational volume to compute volume fraction associated with a node x_i .

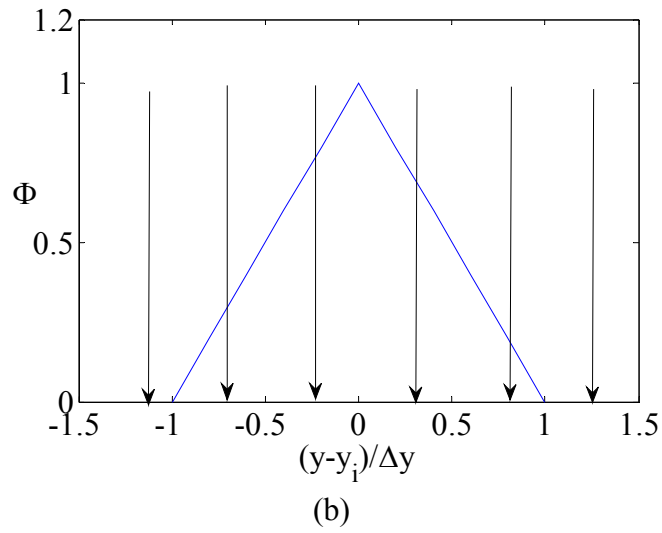
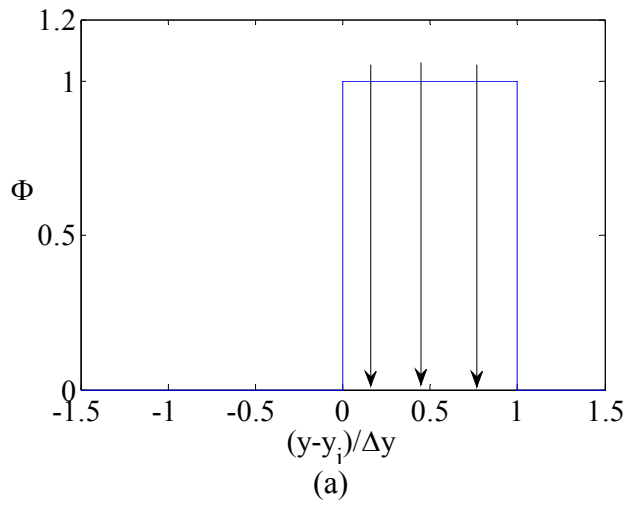
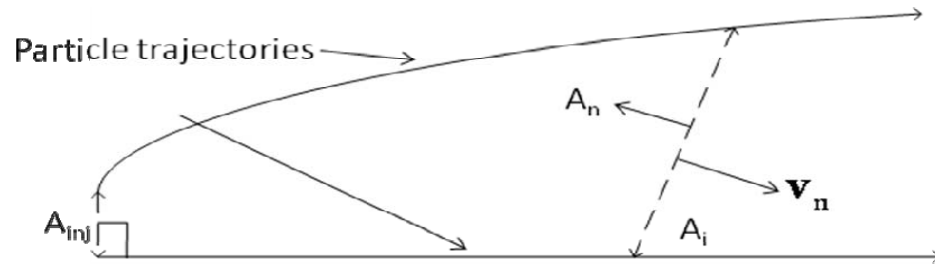
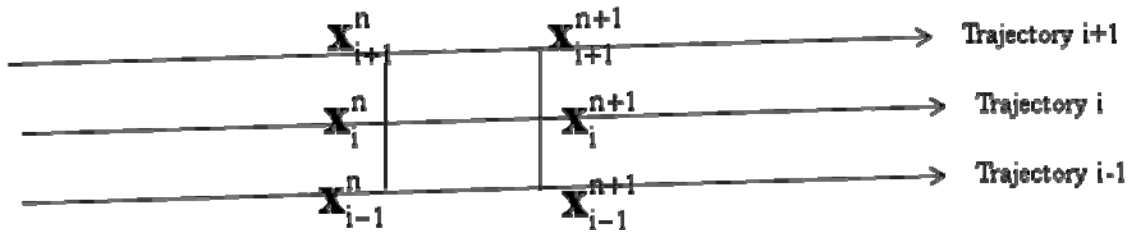


Figure 2. Shape functions for a) Ensemble Averaging and b) Weighted Averaging



(a)



(b)

Figure 3. Stream-tube for a) the area-based technique where $\Delta A = \Delta y$ for a two-dimensional flow and b) the 2-D LCDE technique

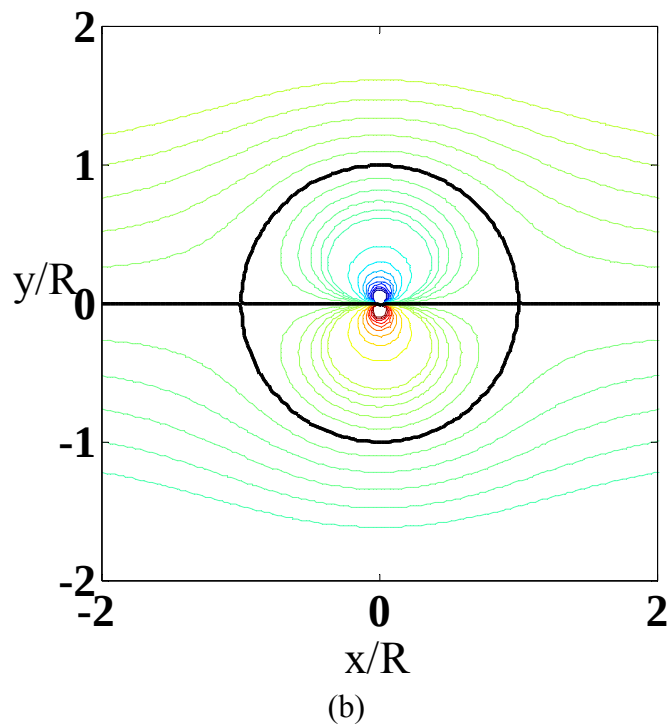
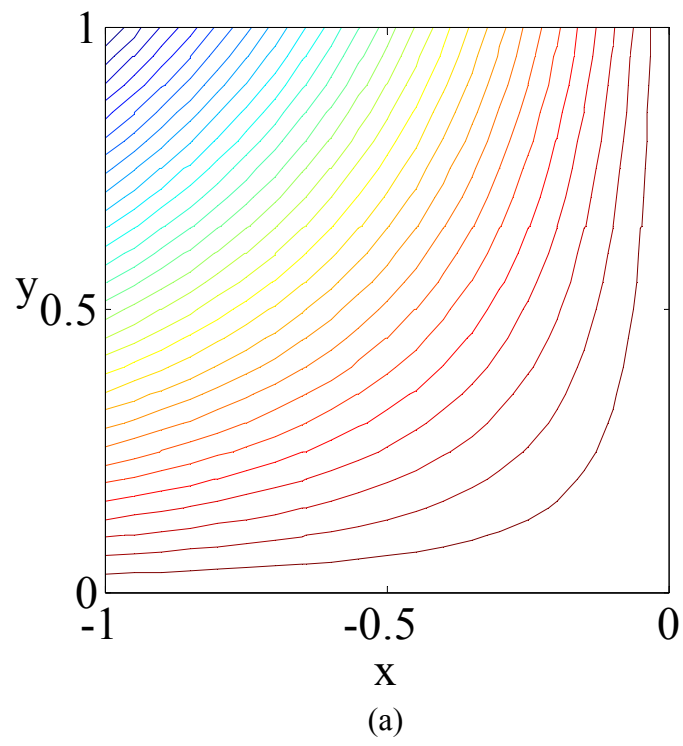
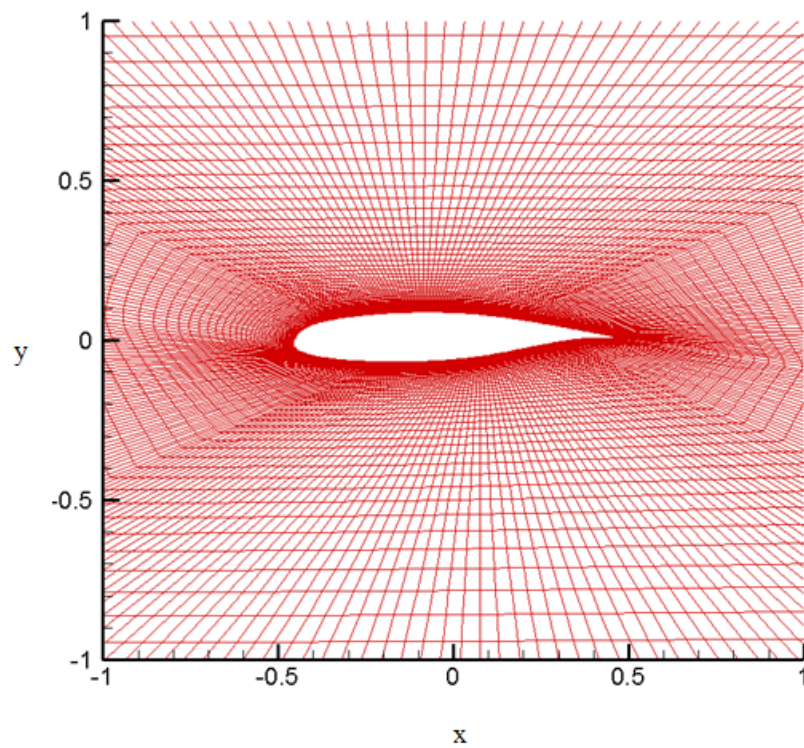
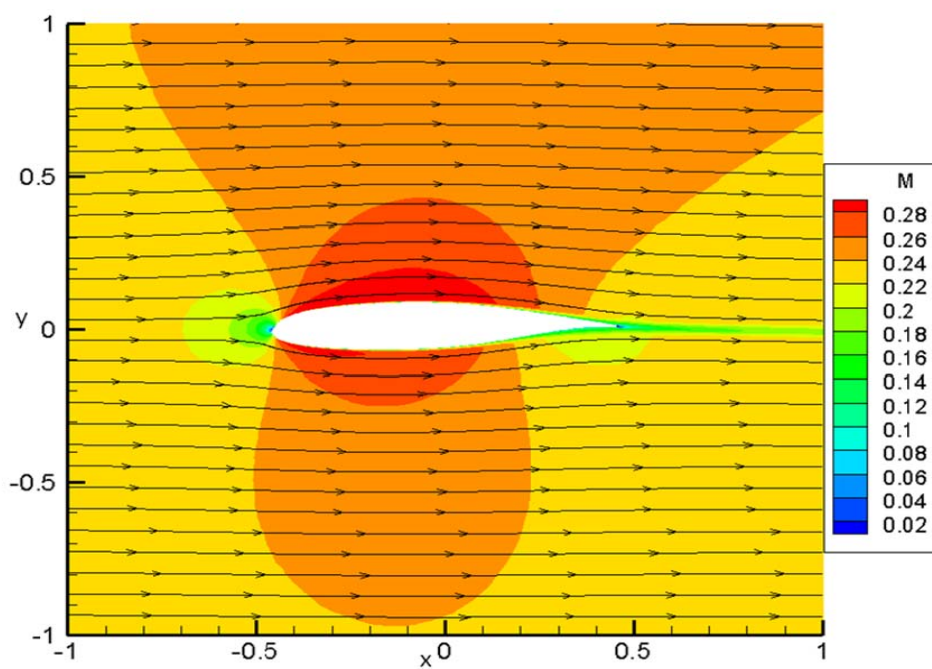


Figure 4 Streamline of a) corner flow, and b) cylinder flow



(a)



(b)

Figure 5. MS317 a) Grid, b) RANS Mach number contours with streamlines in meters (m)

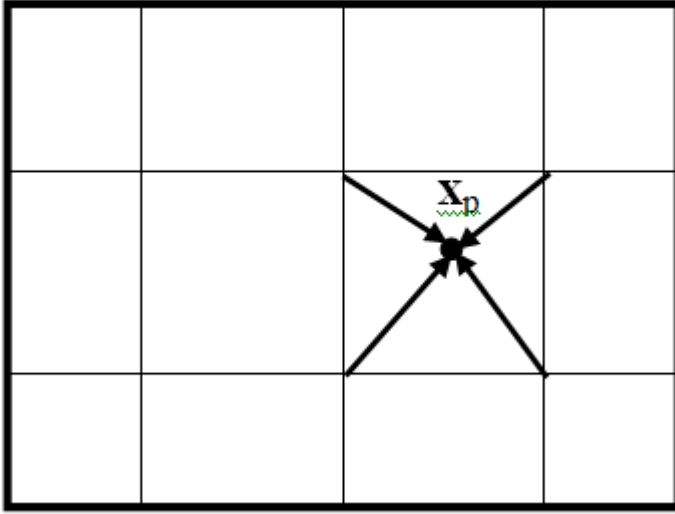


Figure 6. Interpolation of continuum-phase fluid velocity of the surrounding nodes to the particle position at x_p for a 2-D grid

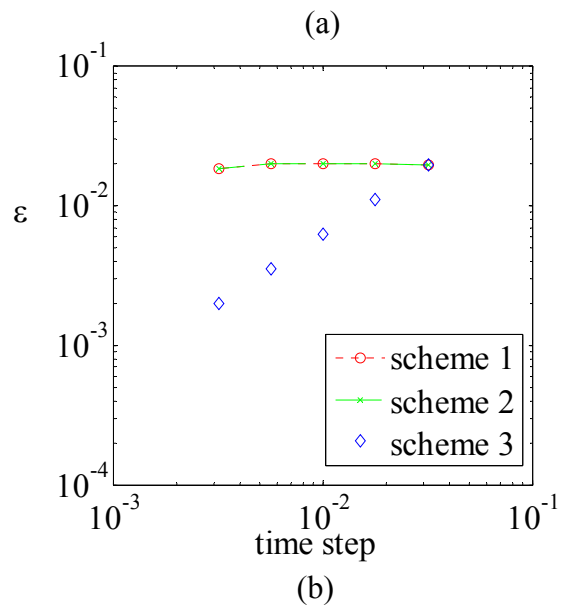
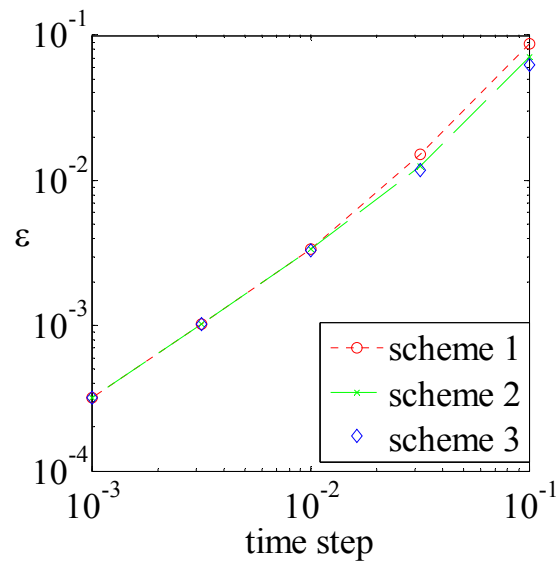


Figure 7. Prediction of x-velocity errors for: a) corner flow with $St = 0.1$ and b) cylinder flow with $St = 0$.

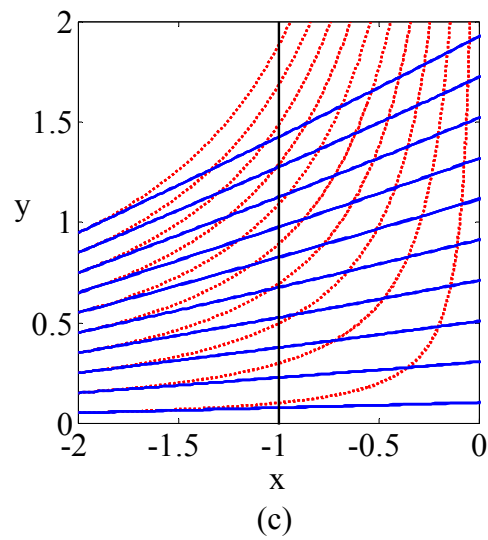
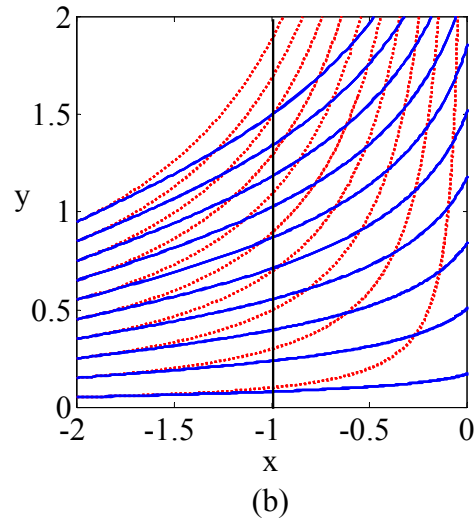
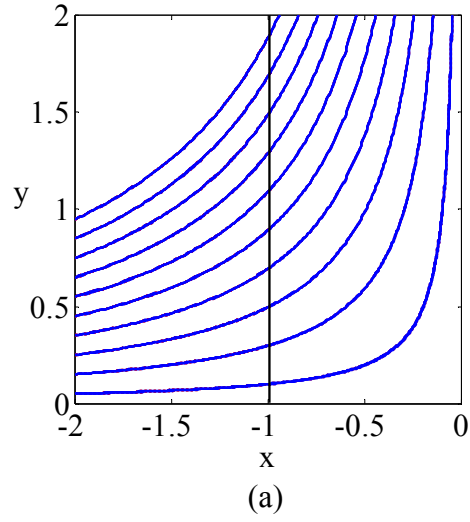
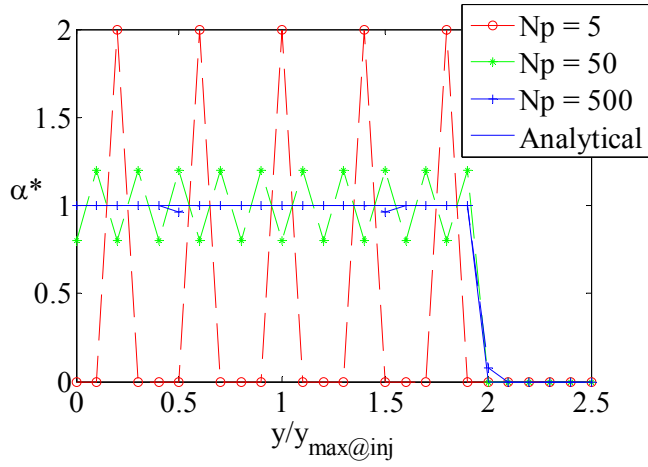
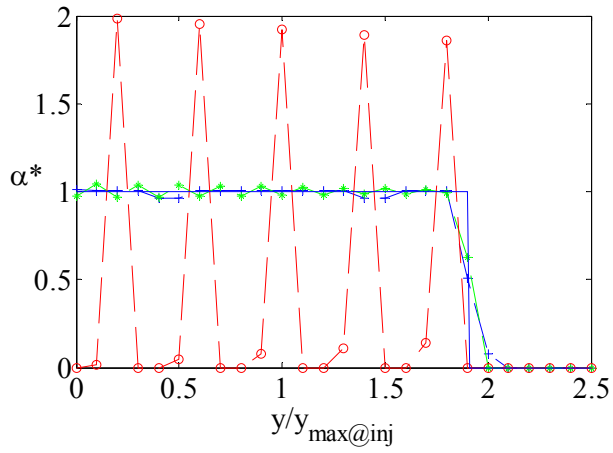


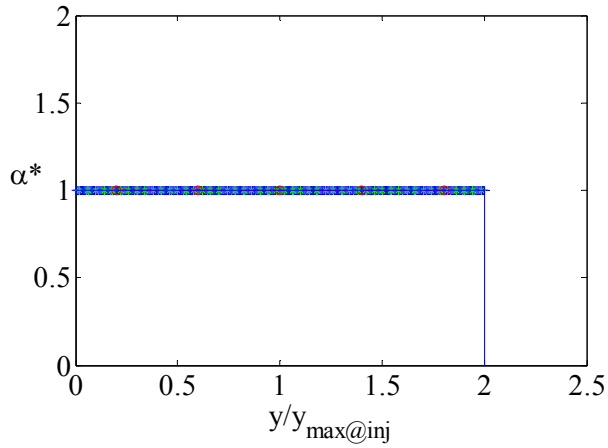
Figure 8. Particle Trajectory with streamline on the base for $N_p=10$ at a) $St=0$, b) $St = 0.5$, and c) $St = 10$



(a)



(b)



(c)

Figure 9. Effect of N_p 5, 50, 500 on concentration ratio for $St=0$ for: a) ensemble-method (different symbols for 5,50 and 500), b) weighted method, c) LCDE method (all with analytical results)

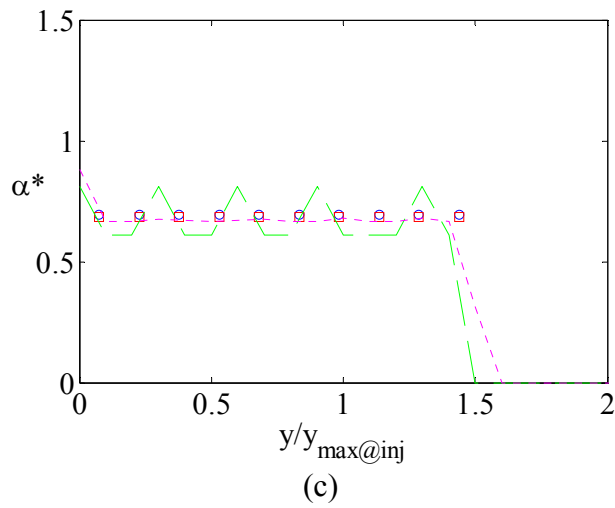
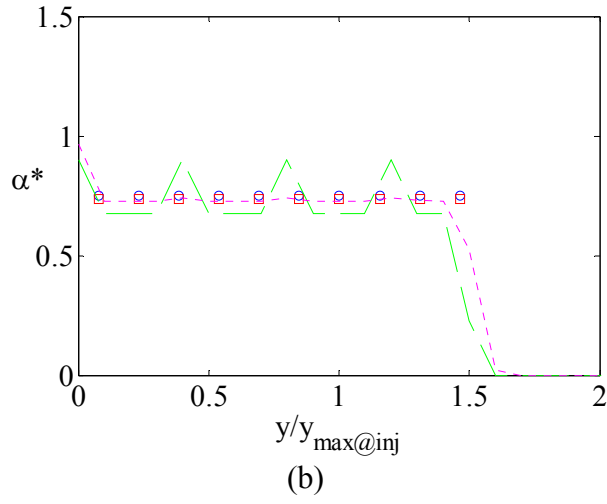
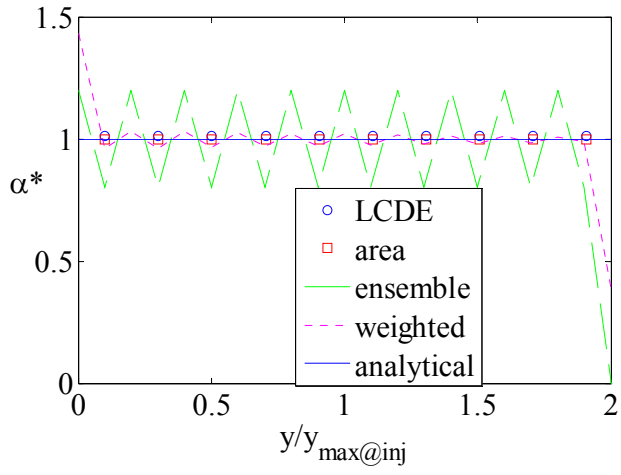


Figure 10. Concentration ratio at vertical wall of corner flow for $\Delta x=0.1$, $N_p=50$ for ensemble and weighted bin $N_p = 10$ for area-based and LCDE, a) $St=0$, b) $St = 1$, c) $St = 10$

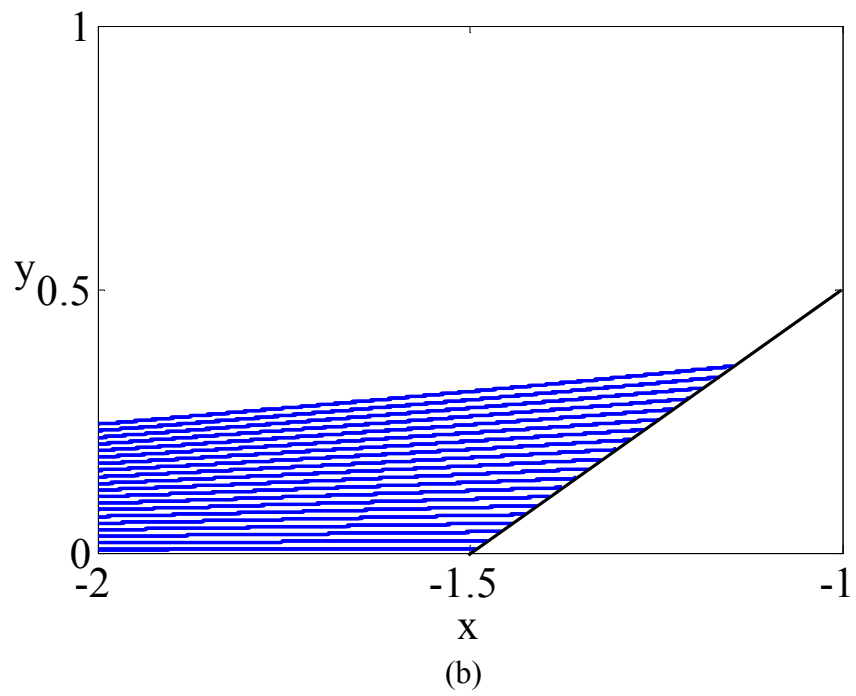
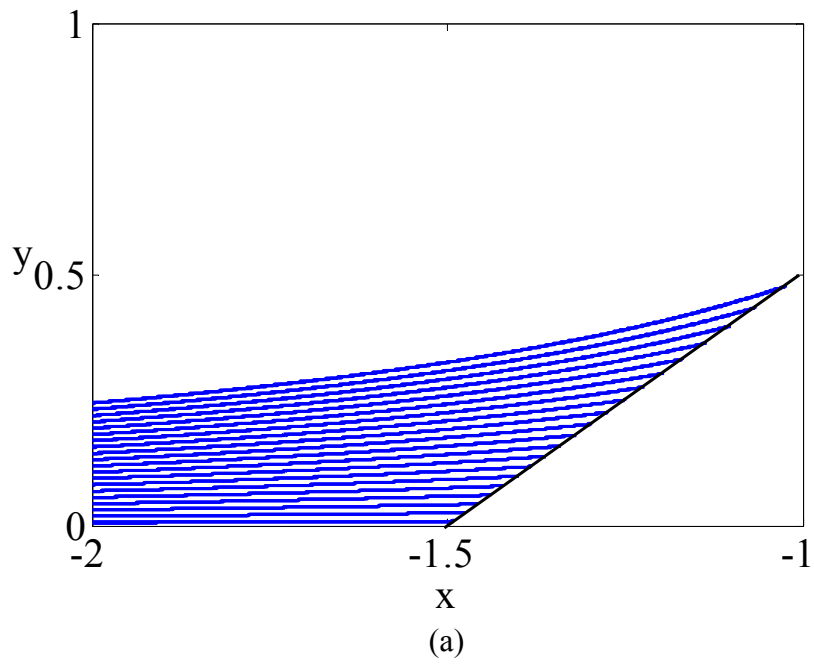


Figure 11. Trajectories for a ramped surface with ramp slope = 1 a) $St = 0$ and b) $St = 1$

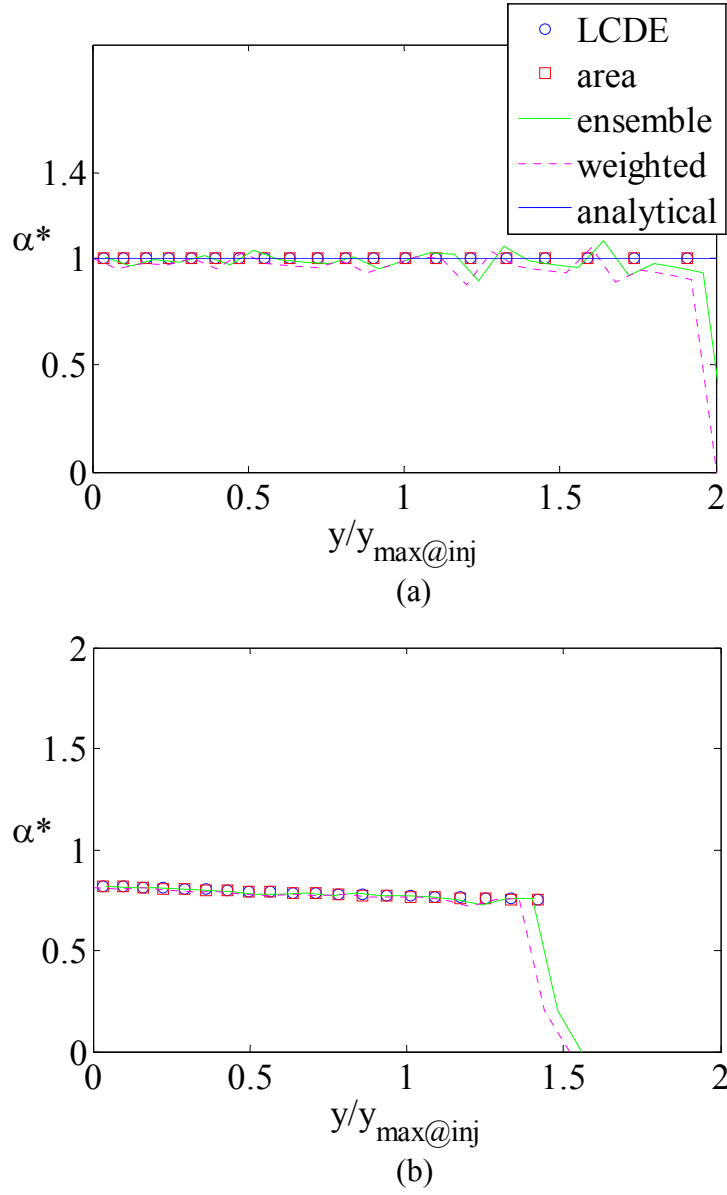


Figure 12. Concentration ratio for a ramped surface with ramp slope = 1 a) $St = 0$ and b) $St = 1$

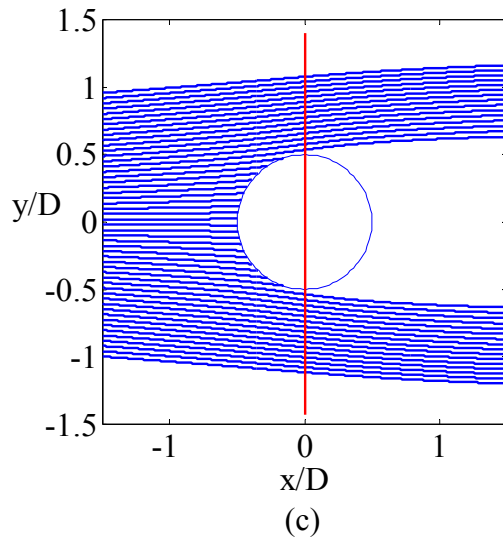
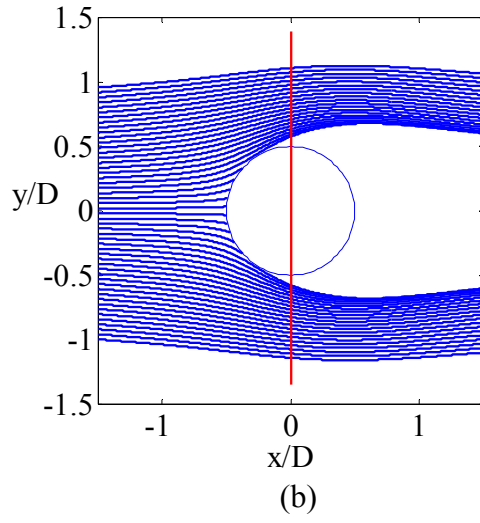
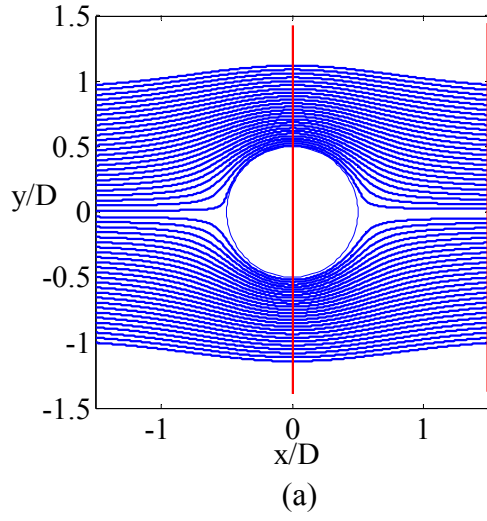


Figure 13. Particle trajectories for $St=1$ and two flux planes at $x/D=0$ and $x/D=1.5$ at a) $St=0$, b) $St = 1$, and b) $St = 10$ all for $y_{\max@inj}=D$

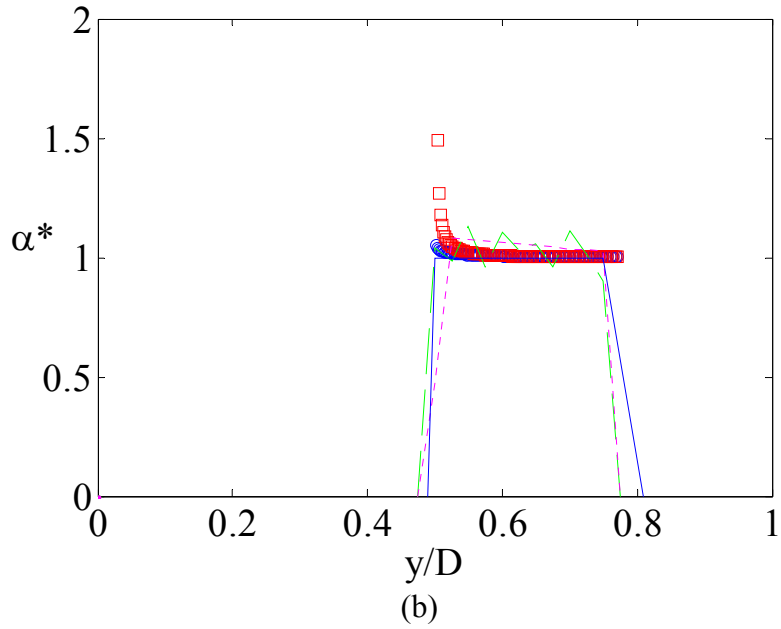
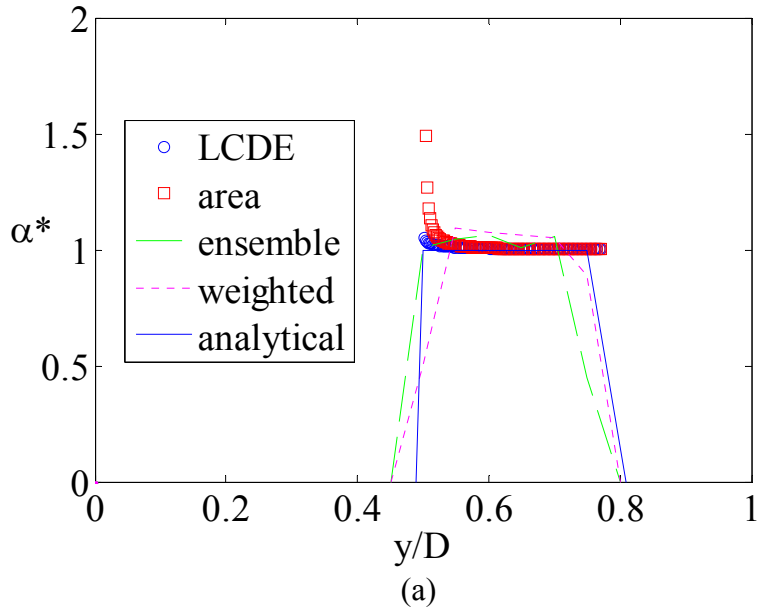


Figure 14. Bin resolution study of concentration ratio for $x/D = 0$, $N_p = 101$, $St = 0$, and $\Delta y/D =$ a) 0.05 and b) 0.025

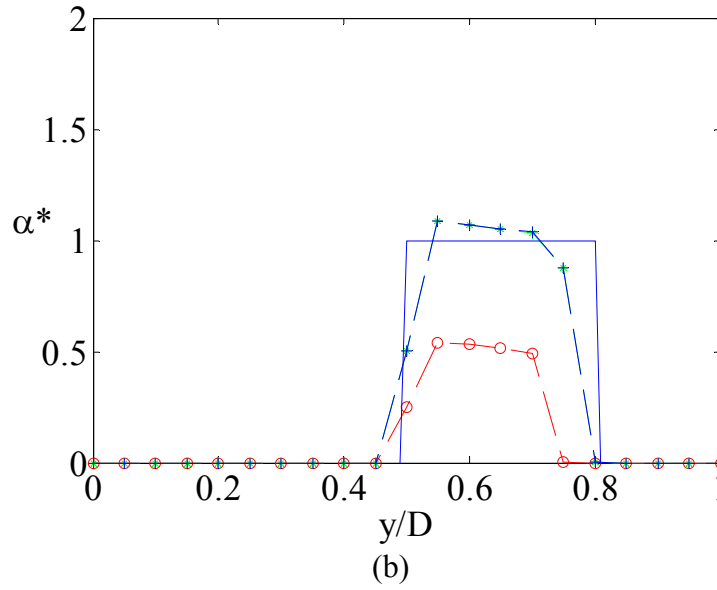
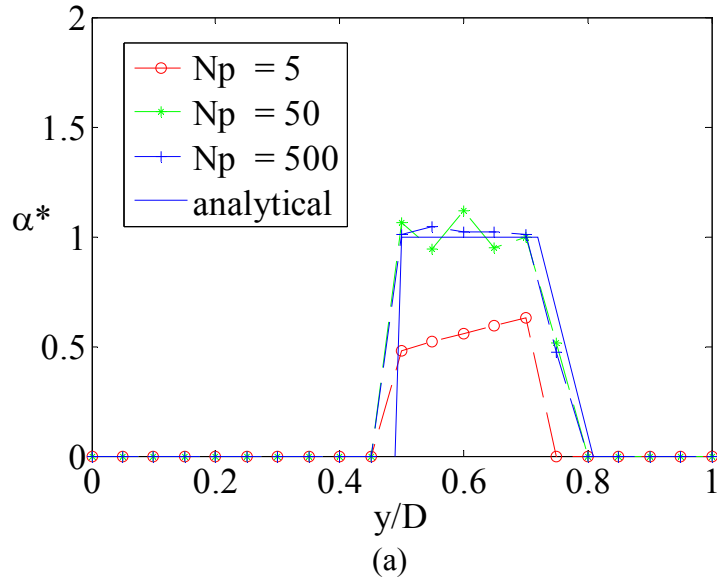


Figure 15. Particle resolution study of concentration ratio for $x/D = 0$ $\Delta y/D = 0.05$, $St = 0$, and $N_p = 5, 50, 500$ a) ensemble bin method and b) weighted averaging bin method

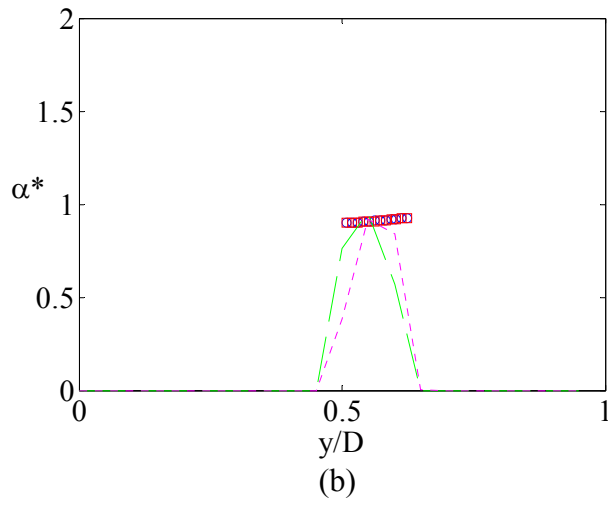
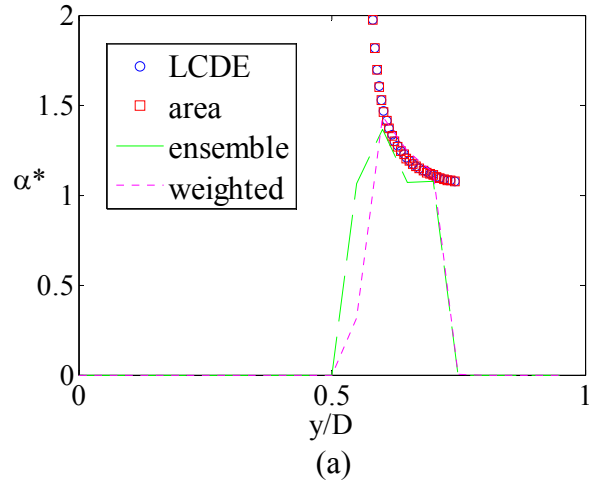
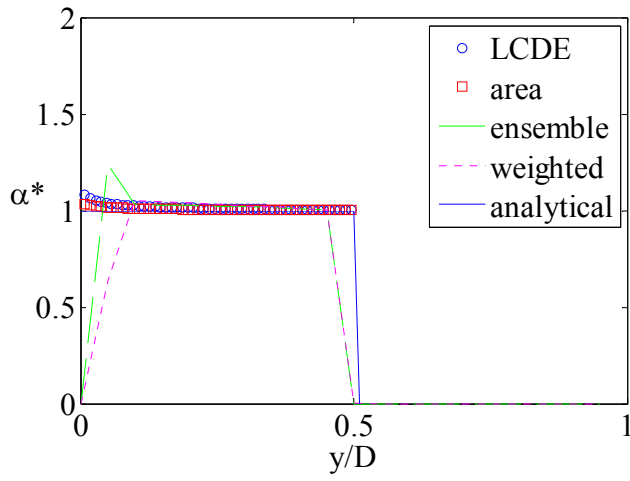
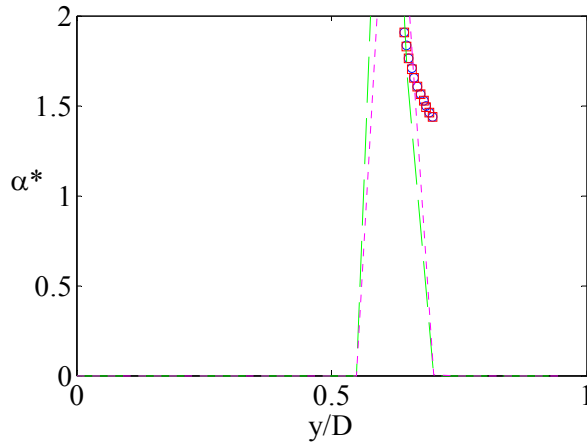


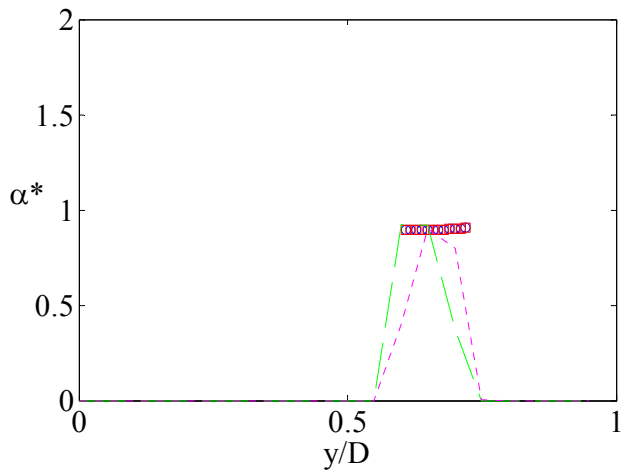
Figure 16. Concentration ratio for $\Delta y/D = 0.05$, $N_p = 50$ at $x/D=0$, a) $St = 1$, and b) $St = 10$



(a)

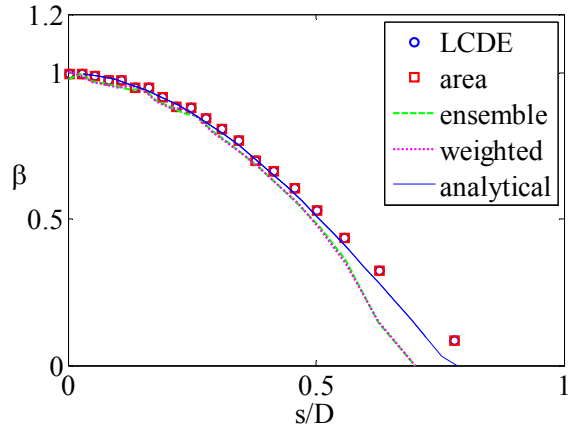


(b)

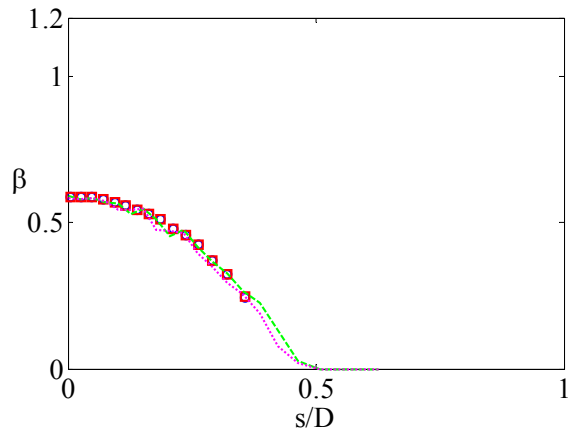


(c)

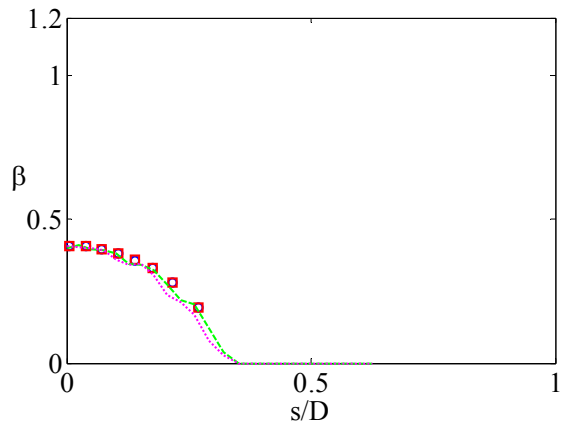
Figure 17. Concentration ratio for $\Delta y/D = 0.05$, $Np = 50$ at $x/D=0$, a) $St = 1.5$ b) $St = 1$, and c) $St = 10$



(a)



(b)



(c)

Figure 18. Impact Efficiency a) $St = 100$ (no initial vertical particle velocity), b) $St = 1$, and c) $St = 0.5$ on cylinder surface for different techniques ($N_p=20$ for LCDE and area and $N_p=1000$ for bin methods)

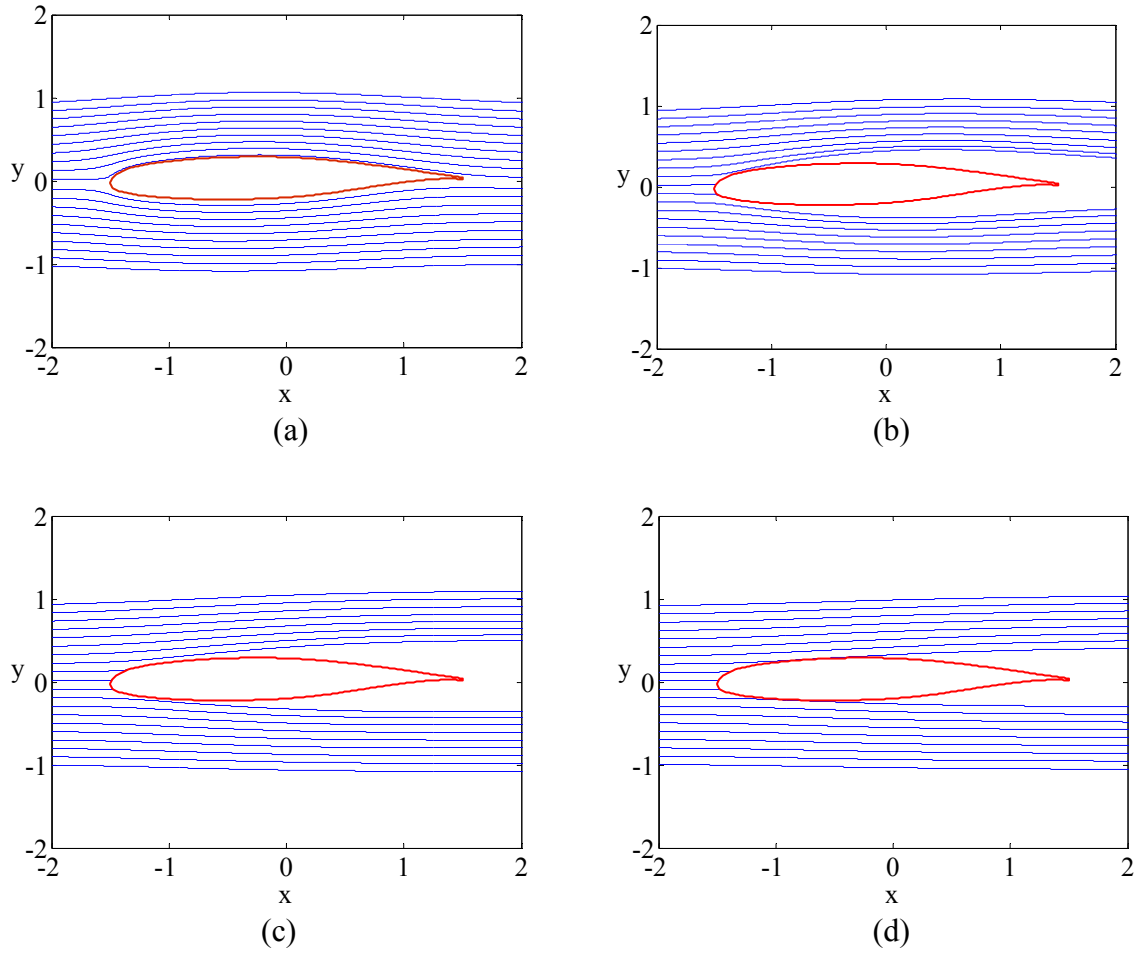


Figure 19 Particle trajectories in meters for a) $St=0.0$, b) $St=0.04$, c) $St=0.31$ and d) $St=100$ all for $y_{\max@inj}=D$

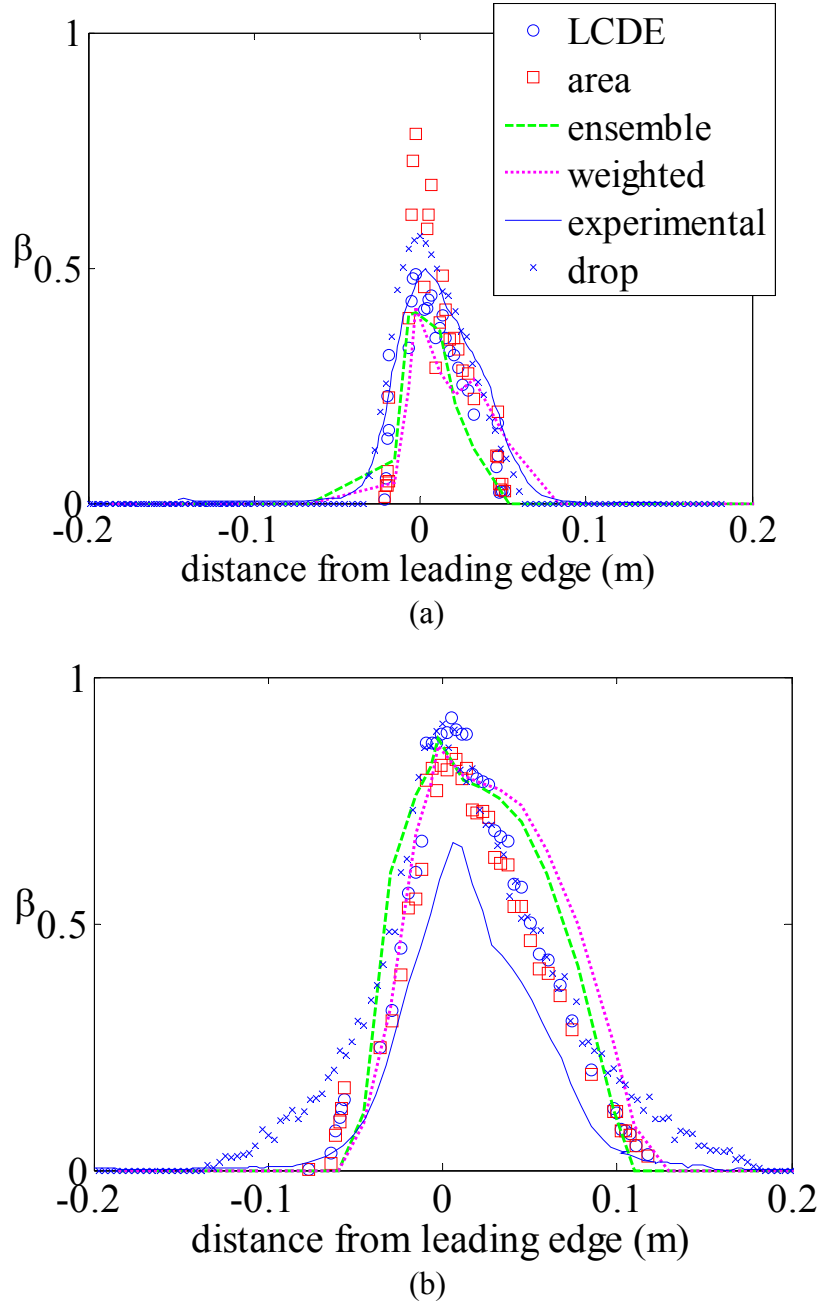


Figure 20 Impact Efficiency for $N_p=401$ for ensemble & weighted averaging $N_p = 50$ for LCDE & area-based a) $St = 0.04$ ($r_p = 21 \mu m$), and b) $St = 0.31$ ($r_p = 79 \mu m$)