

Abstract

OBEROI, ROSHAN C. Large-Eddy Simulation of Particulate Resuspension and Transport Under Influences of Human-Body Motion in an Indoor Setting. (Under the direction of Dr. Jack R. Edwards.)

A methodology is presented for simulating particulate resuspension and transport under influences of human-body motion in an indoor setting. The simulations in this study mirror experiments performed by the U.S. Environmental Protection Agency (EPA), which funded the present study, and the Research Triangle Institute (RTI) at the EPA test facility in Cary, NC.

A large-eddy simulation (LES) framework is implemented to obtain the time-dependent flow field within a room. An artificial compressibility method with low-diffusion upwinding and weighted essentially non-oscillatory (WENO) variable extrapolation is employed to obtain an incompressible Navier-Stokes solution. Unresolved fluctuations are accounted for by a Smagorinsky sub-grid scale stress model. A human body is modeled as an immersed boundary within the Cartesian grid domain. This body is comprised of several immersed components, representing separate body parts. Interpolation methods force the fluid and particle properties near the immersed surface to respond to the motion of the bodies, which is governed by prescribed rate laws.

The particle phase is assumed to be dilute, and thus, does not affect the solution of the carrier fluid. An Eulerian viewpoint is taken to model the particle fields, requiring separate solutions for each size of particle simulated. Size classes are determined by

taking sectional averages of a lognormal probability density function, extracted from experimental data. The motion of the particle fields, subject to hydrodynamic drag forces, is determined by solving mass and momentum conservation equations for each size class. A second-order TVD upwind scheme is used for the advection of particle fields, and a point-implicit sub-iteration method is used for time-advancement.

The present simulations involve a human body walking and stamping its feet for about 20 seconds – causing particles initially contained within a carpet to resuspend – then standing still for the remainder of the simulation. In order to account for the porous structure of the carpet, Darcy-type resistance terms are applied to the solution of the carrier fluid. Micro-scale surface effects acting on the particles, such as van der Waals and electrostatic forces, are modeled by applying a size-dependent sticking force to particles contained by the carpet. This sticking force is approximated in a parametric fashion by comparing simulated particle emission factors with those obtained experimentally. Effects of an HVAC system are also modeled by applying inflow boundary conditions of measured velocity at two known vent locations. These simulations are performed on a computational domain of approximately 5.4 million grid points and are mapped to 36 Intel Xeon processors on an IBM Blade Center Linux Cluster using the MPI message passing standard.

The simulations produced similar levels of particulate mass resuspension to those observed experimentally. Results indicated that a large majority of the particles resuspended originated from regions of the carpet very near where the immersed-body “feet” penetrated, while particles elsewhere in the room were mostly undisturbed. Despite the fact that most of the mass resuspended was due to large particles, much more

small-particle mass remained airborne over the duration of the 7-minute simulations due to much lower settling rates. A relatively “well-mixed” state was achieved in the room after about 3 minutes of physical time. This made it possible to identify steady particle-decay trends over the last few minutes of the simulations in order predict concentrations in the room beyond this extent of time.

**LARGE-EDDY SIMULATION OF PARTICULATE RESUSPENSION AND
TRANSPORT UNDER INFLUENCES OF HUMAN-BODY MOTION IN AN
INDOOR SETTING**

by
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Biography

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1 Introduction

Indoor air pollution can pose a variety of health risks, particularly in the home or daily work environment. Many different types of contaminants can pollute indoor environments. These may be gases; such as carbon monoxide, nitrogen dioxide, and radon; or particles; such as mold, asbestos, pollen, animal dander, lead dust, and chemical agents contained in household cleaning supplies. Short-term exposure can result in immediate reactions, such as irritation of eyes, nose, throat, and skin. Long-term exposure can have more serious implications, causing cancer, heart disease, and respiratory diseases. Reducing indoor pollution levels can be as simple as opening windows or using ventilation systems to filter and dilute contaminants. However, some household objects, such as carpets, rugs, and upholstery, act as a sink for settling particulate contaminants and can re-emit them when disturbed.

When emitted from a source, particles may stay airborne for short periods of time and affect local concentration levels or they may stay airborne for long periods of time and be transported throughout an entire building. In order to improve the quality of indoor environments, it is important to understand how different types of particle pollutants behave once emitted. Insight into this behavior can be gained by performing experimental or computational studies. Experimental methods allow precise measurement of particulate concentrations and fluid properties over long periods of time, but only at a limited number of locations. Computational methods, while difficult and time-consuming, are capable of predicting all relevant particle and flow quantities throughout an entire room or building at very closely spaced points.

The present paper focuses on a computational fluid dynamics (CFD) model for simulating the resuspension and transport of particles embedded in a carpet, under influences of human motion. This model is applied to the simulation of indoor air quality experiments performed by the United States Environmental Protection Agency (US EPA) and the Research Triangle Institute (RTI) at the EPA test house in Cary, North Carolina. Results of the experimental and computational studies are compared as a means of assessing the validity of the CFD model.

In the aforementioned experiments, particulate concentrations at various locations in a room were monitored over several minutes as a person walked forward and stamped in place in order to induce resuspension of particulates initially embedded in a carpet, then stood still for several minutes, allowing particles to be transported throughout the room and out of the doorways as dictated by hydrodynamic drag forces and gravity. A ventilation system was active during these experiments, imposing air inflow at two vent locations and outflow through the doorways. Particulate mass concentrations were monitored at several locations by Climet (4102) samplers, while particle size data were collected by Aerodynamic Particle Sizers (APS 3321).

In order to develop a CFD model that could simulate the experiments described, it is necessary to simulate the forcing experienced by the particle fields, namely, the time-dependent hydrodynamics induced by human-body motion and ventilation system activity within the room. A large-eddy simulation (LES) approach is used to obtain the hydrodynamic flow field. This technique involves solving a filtered set of the Navier-Stokes equations of fluid mechanics, such that only resolvable turbulent eddies are solved, and the effects of unresolvable fluctuations are modeled. Resolvability is

determined by the local spatial mesh resolution. Unresolvable effects are included as a sub-grid scale (SGS) model – in this case, a Smagorinsky SGS model [26].

The human body is represented as an ordered group of immersed components, each representing a different body-part, within a non-uniform Cartesian domain. The motion of the immersed components is coupled with the hydrodynamic flow field by an immersed boundary (IB) method similar to that proposed by Fadlun et al. [11]. Since the motion of the human predominates that of the fluid, prescribed rate laws were applied to the motion of each immersed component. The fluid field is then forced to adjust to the human-body motion, such that the velocity at the immersed-body surface is equal to that of the body itself.

The motion of the particle fields is solved from an Eulerian viewpoint, in which mass and momentum conservation equations are solved for each size class of particles represented. These size classes are extracted as sectional averages from a population density function, determined by experimental measurements. The particle fields are assumed to be dilute, and therefore, their solution does not affect that of the carrier fluid.

Of particular emphasis in this paper, is the solution of the particle fields near the surface of immersed bodies. Previously presented immersed boundary methods do not necessarily translate to aerosols, thus, special precautions are required to ensure mass conservation in the presence of moving immersed bodies. In the following sections, details of the CFD model and simulation results are presented.

2 Methods

While the present CFD model is applied to the simulation of resuspension experiments in a single room, it can be utilized for many other purposes. This model is intended to easily extend to other types of indoor particulate simulations, including networks of rooms, entire buildings, ventilation systems, and different types of human motion. An advantage of using computational simulations is that they can be applied in a design capacity, allowing detailed evaluation of building designs through accurate prediction of pollutant transport. Also, aspects of this model can be used in other types of CFD applications in which the representation of immersed boundaries without adaptive grids is desired. The model extends trivially to generalized coordinate systems, including unstructured meshes.

2.1 Overview of Experiments

The experiments were performed by the EPA and RTI at the EPA test house in Cary, North Carolina. Particle mass concentrations were measured by Climet (4102) samplers at five different locations within a 12.5 ft x 13.8 ft x 8.0 ft room, and size statistics were gathered by APS 3321 particle sizers. The room had two vents in the floor and two doorways – one to a hall, and one to a bathroom. The floor was covered with a 1-cm thick carpet. In order to determine the particle-mass loading within the carpet, a section was vacuumed and the particle matter weighed. Prior to the experiments, the room was evacuated and particle matter was allowed to settle such that only a very low “background” concentration remained airborne.

When the experiment commenced, a human subject walked forward from the hall doorway to a target location, stamped within a $1.5 \times 1.5 \text{ ft}^2$ source area for 20 seconds, then stood still while particle concentration and size measurements were recorded for several minutes. Size measurements allowed a size-based population density function to be generated, allowing mass concentration data to be converted to number concentrations. Time-averaged number concentrations were obtained at one-minute intervals at various locations.

2.2 Model Development

2.2.1 Governing Equations of Fluid Mechanics

The physical behavior of air in a residential setting is modeled by the incompressible Navier-Stokes equations of fluid mechanics. This system includes continuity and momentum equations, given by:

$$\begin{aligned} \frac{\partial u_i}{\partial x_i} &= 0 \\ \rho \frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i u_j + p \delta_{ij} - \tau_{ij}) &= f_{e,i} \end{aligned} \quad \text{Eq. 2-1}$$

where ρ is the constant fluid density, u_i is the local velocity, p is the local pressure, τ_{ij} is the viscous stress tensor, and $f_{e,i}$ is the net external force (per volume). Note that the continuity equation is not dependent on the local density because, for an incompressible

flow, $\frac{D\rho}{Dt} = 0$. For a calorically perfect gas in thermodynamic equilibrium, the viscous stress tensor is given by:

$$\tau_{ij} = \mu \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) - \frac{2}{3} \mu \left(\frac{\partial u_k}{\partial x_k} \right) \delta_{ij}, \quad \text{Eq. 2-2}$$

where μ is the molecular viscosity.

This form can be extended from the above Cartesian coordinate representation to a generalized (curvilinear) representation by the introduction of transformation derivatives. For the continuity equation, this is given by:

$$\frac{\partial}{\partial \xi} \left[\left(\frac{1}{J} \frac{\partial \xi}{\partial x_i} \right) u_i \right] + \frac{\partial}{\partial \eta} \left[\left(\frac{1}{J} \frac{\partial \eta}{\partial x_i} \right) u_i \right] + \frac{\partial}{\partial \zeta} \left[\left(\frac{1}{J} \frac{\partial \zeta}{\partial x_i} \right) u_i \right] = 0,$$

$$J = \xi_{x_3} \eta_{x_1} \zeta_{x_2} - \xi_{x_2} \eta_{x_1} \zeta_{x_3} + \xi_{x_1} \eta_{x_2} \zeta_{x_3} - \xi_{x_3} \eta_{x_2} \zeta_{x_1} + \xi_{x_2} \eta_{x_3} \zeta_{x_1} - \xi_{x_1} \eta_{x_3} \zeta_{x_2},$$

Eq. 2-3

where $\xi = \xi(x_i)$, $\eta = \eta(x_i)$, and $\zeta = \zeta(x_i)$ are the generalized coordinates, and J is the transformation Jacobian. A similar transformation may be performed on the momentum equation, but first, a compact form is introduced in terms of total momentum flux F_{ij} :

$$\rho \frac{\partial u_i}{\partial t} + \frac{\partial F_{ij}}{\partial x_j} = f_{e,i},$$

$$F_{ij} = \rho u_i u_j + p \delta_{ij} - \tau_{ij}, \quad \text{Eq. 2-4}$$

The generalized form of the momentum equation is then given by:

$$\frac{\rho}{J} \frac{\partial u_i}{\partial t} + \frac{\partial}{\partial \xi} \left(\frac{1}{J} \frac{\partial \xi}{\partial x_j} F_{ij} \right) + \frac{\partial}{\partial \eta} \left(\frac{1}{J} \frac{\partial \eta}{\partial x_j} F_{ij} \right) + \frac{\partial}{\partial \zeta} \left(\frac{1}{J} \frac{\partial \zeta}{\partial x_j} F_{ij} \right) = \frac{f_{e,i}}{J},$$

Eq. 2-5

While the CFD model is able to utilize curvilinear coordinates, the present simulations are performed on a stretched Cartesian grid, and thus, the forthcoming development will be presented using Cartesian notation for simplicity.

2.2.2 Large-Eddy Simulation

The solution of the incompressible Navier-Stokes equations was approached as a large-eddy simulation (LES), in which the motion of large “resolvable” turbulent eddies is solved, while the effects of smaller eddies are modeled. The resolvability of eddies depends on the local spatial mesh resolution. The justification for the modeling of smaller-eddy effects lies in the assumption that small-scale turbulent motion is mostly isotropic and universal. In contrast, the larger eddies contain most of the turbulent kinetic energy and dictate the anisotropic fluid motion.

In a LES, a filtered set of the Navier-Stokes equations is solved, which contains a sub-grid scale (SGS) stress term. This formulation is summarized in [27] and is obtained by decomposing flow properties into resolved (filtered) and unresolved scales:

$$q_i = \bar{q}_i + q'_i. \quad \text{Eq. 2-6}$$

Here, $\bar{q}_i$ represents a resolvable quantity, and q'_i represents a sub-grid scale quantity.

The filtered flow variables are defined by the convolution integral, as follows:

$$\bar{q}_i(x_1, x_2, x_3) = \iiint_{\mathbb{V}} \left[\prod_{j=1}^3 G_j(x_j, x'_j) \right] q_i(x'_1, x'_2, x'_3) dx'_1 dx'_2 dx'_3, \quad \text{Eq. 2-7}$$

shown here in tensor notation, where G is a filter function, which must satisfy

$$\iiint_{\mathbb{V}} \left[\prod_{j=1}^3 G_j(x_j, x'_j) \right] dx'_1 dx'_2 dx'_3 = 1 \quad \text{Eq. 2-8}$$

in order to return the correct values where q_i is constant. The resulting form of the incompressible Navier-Stokes equations contains separate terms for filtered and unfiltered quantities, as follows:

$$\frac{\partial \bar{u}_j}{\partial x_j} = 0$$

$$\frac{\partial \rho \bar{u}_i}{\partial t} + \frac{\partial \left(\rho \bar{u}_i \bar{u}_j + \delta_{ij} \bar{p} - \mu \frac{\partial \bar{u}_i}{\partial x_j} + \tau_{SGS,ij} \right)}{\partial x_j} = f_{e,i},$$

$$\text{where } \tau_{SGS,ij} = \rho \left(\overline{u_i u_j} - \bar{u}_i \bar{u}_j \right) + \left(\overline{u'_i u'_j} - \bar{u}'_i \bar{u}'_j \right) + \overline{u'_i u'_j}. \quad \text{Eq. 2-9}$$

Here, $\tau_{SGS,ij}$ is the SGS stress tensor. The three terms shown on the right-hand side are known as (from left to right) the Leonard stress, cross-term stress, and Reynolds stress. The cross-term stress and Reynolds stress cannot be directly calculated, and thus, must be modeled to achieve closure of the solution. It is possible to compute the Leonard stress directly, but its magnitude is small enough and its solution complicated enough that it is generally not considered to be a worthwhile endeavor. Therefore, all three terms are typically included in the sub-grid scale model.

Several options exist for the modeling of sub-grid scale effects. Among the simplest and most widely used is that proposed by Smagorinsky [26].

$$\begin{aligned}\tau_{SGS,ij} &= 2\mu_T S_{ij} \\ S_{ij} &= \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \\ \mu_T &= \rho (C_s \Delta)^2 \sqrt{2 S_{ij} S_{ij}}\end{aligned}\tag{Eq. 2-10}$$

Here, μ_T is the eddy viscosity, S_{ij} is the strain rate tensor, $\Delta = (\Delta x \Delta y \Delta z)^{1/3}$ is the local filter width, and C_s is the Smagorinsky constant. The latter is not considered to be universal and must be chosen according to the particular application (in this case, a value of 0.1 is used). Henceforth, the bar notation for resolved-scale quantities will be omitted, and it can be assumed that all quantities referenced with respect to the numerical solution are filtered quantities.

2.2.3 Time Integration

In the absence of compressibility, the continuity equation does not contain a time derivative. This creates a dilemma when seeking a time-dependent hydrodynamics solution. One way to address this issue is to extract an alternative formulation of the continuity equation from known fluid property relations that contains an artificial time derivative. From the equation of state, $\frac{\mathcal{P}}{a^2} = \rho$, a relationship between the time-derivative of pressure and that of density, which appears in the compressible form of the continuity equation, can be derived. Thus, it can be asserted, $\frac{1}{\beta^2} \frac{\partial p}{\partial t} \approx \frac{\partial \rho}{\partial t}$, where β is a velocity scale. Chorin's artificial compressibility method [4] utilizes this relationship as a means of obtaining a steady-state solution of the continuity equation:

$$\frac{1}{\beta^2} \frac{\partial p}{\partial t} + \frac{\partial u_i}{\partial x_i} = 0. \quad \text{Eq. 2-11}$$

Here, β controls the propagation of physical information. Selecting a value of β that is of the order of magnitude of the local flow velocity will produce a pseudo-compressible solution that can easily be advanced in time. However, to obtain a time-accurate solution that satisfies a divergence-free velocity constraint, β would have to be of the same order as the sound speed, which approaches infinity in an incompressible flow. This dichotomy is reconciled by implementing an implicit dual time-stepping technique that ensures a divergence-free velocity field at each physical time step without having to use a very large β . This procedure involves constructing an approximate solution based on an

incomplete LU factorization, and repeating over multiple “pseudo-time steps” until a time-accurate divergence-free solution is achieved at time level $n+1$.

While the present system of equations is to be discretized in both space and time, it is useful to treat the spatial and temporal discretizations separately by employing what is referred to as the method of lines [17]. In such an approach, the spatial derivatives are treated as steady terms in the time-advancement of the solution in each cell, and flow properties in each cell are treated as functions of time. Thus, the momentum equation reduces to the ordinary differential equation (ODE):

$$\rho \frac{du_i}{dt} + \frac{\partial \left(\rho u_i u_j + \delta_{ij} p - \mu \frac{\partial u_i}{\partial x_j} + \tau_{SGS,ij} \right)}{\partial x_j} - f_{e,i} = 0,$$

$$\text{or } \rho \frac{du_i}{dt} + R_{m,i} = 0, \quad \text{Eq. 2-12}$$

where $R_{m,i}$ represents the residual of the steady terms in the momentum equation. In a similar manner, the pseudo-time problem for the momentum equation can be expressed as follows:

$$\rho \frac{du_i}{d\tau} + \rho \frac{du_i}{dt} + R_{m,i} = \rho \frac{du_i}{d\tau} + R_{m,i}^* = 0, \quad \text{Eq. 2-13}$$

where τ is the pseudo-time variable, and $R_{m,i}^*$ is the residual of the “pseudo-steady” terms, referred to as such because the solution at each physical time level is approached as a steady-state solution to the pseudo-time problem. Since the continuity equation does not contain a time derivative, its steady and pseudo-steady residuals are the same:

$$R_c^* = R_c = \frac{\partial u_j}{\partial x_j}. \quad \text{Eq. 2-14}$$

In the dual time-stepping procedure, the pseudo-steady residual is driven toward zero, iteratively, in order to converge a time-accurate solution at the next physical time step. Thus, a divergence-free time-dependent solution can be achieved if the pressure is advanced in pseudo-time, leaving

$$\frac{1}{\beta^2} \frac{dp}{d\tau} + R_c^* = 0 \quad \text{Eq. 2-15}$$

as the pseudo-time problem for the continuity equation. The system of ODEs can now easily be reduced to the compact notation:

$$\frac{d\vec{V}}{d\tau} + \vec{R}^*(\vec{V}) = 0 \quad \text{Eq. 2-16}$$

where $\vec{V} = [p, u, v, w]^T$ is the dependent primitive variable vector for which a solution is sought. In the context of the representation shown here, implementation of the artificial

compressibility approach can be viewed as a preconditioning of the pseudo-time derivative, as follows:

$$\bar{\bar{P}}^{-1} \frac{d\bar{V}}{d\tau} + \bar{R}^*(\bar{V}) = 0, \text{ where } \bar{\bar{P}}^{-1} = \begin{bmatrix} \frac{1}{\beta^2} & & & \\ \frac{u}{\beta^2} & \rho & & \\ \frac{v}{\beta^2} & & \rho & \\ \frac{w}{\beta^2} & & & \rho \end{bmatrix} \quad \text{Eq. 2-17}$$

for the case of the primitive variable formulation. This preconditioner is intended to be applicable in low-speed convection-dominated flows, in which the maximum achievable time steps are otherwise restricted by large acoustic wave speeds. Generally, a good choice for β is the global maximum convection speed, but more complicated dependencies have been proposed. The main point is not to allow β to become small relative to the convection speed, as this can cause large numerical error; and not to allow it to become too high, as this creates stiffness.

The basic idea behind an implicit approach is to approximate the residual at a future time (or pseudo-time) level; e.g., $\bar{\bar{P}}^{-1} \frac{d\bar{V}}{d\tau} + \bar{R}^*(\bar{V}^{n+1,l+1}) = 0$, where l represents a pseudo-time level between n and $n+1$. In semi-discrete form, a fully implicit dual time-stepping scheme for this equation is given by:

$$\bar{\bar{P}}^{-1} \frac{\bar{V}^{n+1,l+1} - \bar{V}^{n+1,l}}{\Delta\tau} + \frac{3\bar{V}^{n+1,l} - 4\bar{V}^n + \bar{V}^{n-1}}{2\Delta t} + \bar{R}(\bar{V}^{n+1,l+1}) = 0. \quad \text{Eq. 2-18}$$

Here, two and three-level backward difference formulas are used for the pseudo-time and time-derivative discretizations, respectively. In the present notation, $n+1, l=0$ is equivalent to the n th physical time level, and $n+1, l=l_{\max}$ represents the actual $n+1$ th level. Generally, the pseudo-time problem can be converged in a prescribed number of sub-iterations, dependent upon the chosen iterative method. Steady data at the $l+1$ sub-level is given by a Taylor series expansion:

$$\bar{R}(\bar{V}^{n+1,l+1}) = \bar{R}(\bar{V}^{n+1,l}) + \frac{\partial \bar{R}}{\partial \bar{V}} (\Delta \bar{V}^{n+1,l+1}) + O(\Delta \bar{V}^{n+1,l+1})^2, \quad \text{Eq. 2-19}$$

where $\Delta \bar{V}^{n+1,l+1} \equiv \bar{V}^{n+1,l+1} - \bar{V}^{n+1,l}$. Substituting this into Eq. 2-18 and neglecting higher-order terms gives:

$$\bar{P}^{-1} \frac{\Delta \bar{V}^{n+1,l+1}}{\Delta \tau} + \frac{3\bar{V}^{n+1,l} - 4\bar{V}^n + \bar{V}^{n-1}}{2\Delta t} + \bar{R}(\bar{V}^{n+1,l}) + \frac{\partial \bar{R}}{\partial \bar{V}} (\Delta \bar{V}^{n+1,l+1}) = 0. \quad \text{Eq. 2-20}$$

Rearranging, the equation can be put into the form of a standard linear system:

$$\left[\frac{1}{\Delta \tau} \bar{P}^{-1} + \frac{\partial \bar{R}}{\partial \bar{V}} \right] \Delta \bar{V}^{n+1,l+1} = -\frac{3\bar{V}^{n+1,l} - 4\bar{V}^n + \bar{V}^{n-1}}{2\Delta t} - \bar{R}(\bar{V}^{n+1,l}), \quad \text{Eq. 2-21}$$

for which a solution of the correction vector, $\Delta \tilde{V}^{n+1,l+1}$, is sought. A multitude of linear iterative methods may be applied to solve this system. For brevity, the above system will be represented by the standard convention $A\bar{x} = \bar{b}$ in the forthcoming discussion of its solution.

While a direct solution of the linear system is possible, by LU factorization for example, such an approach has drawbacks for ODE solutions. Linear systems resulting from the discretization of differential equations are sparse, but the factors of A (L and U) generally are not, which leads to large storage requirements. An alternative approach involves using iterative methods. These methods tend to be robust and require little storage, but they can be hampered by slow convergence. A compromise can be achieved by implementing a preconditioned iterative method based on an approximate factorization of A . Since the convergence rate is dependent upon the spectrum of A , improving the spectrum location by applying a preconditioner will improve convergence [28]. (Note that the preconditioner discussed here is not the same as the artificial compressibility preconditioner described above.)

In the present case, the preconditioner is constructed by performing an “incomplete” LU (ILU) decomposition of A . This partial decomposition $\tilde{L}\tilde{U}$ is intended to approximate A reasonably well (i.e., $(\tilde{L}\tilde{U})^{-1}A$ is close to I), but at less computational expense. Several options exist for the definition of $\tilde{L}$ and $\tilde{U}$, but they are generally dictated by sparsity requirements and other numerical and computational criteria. In this case, a block-ILU(0) decomposition is employed in which the sparsity patterns of $\tilde{L}$ and $\tilde{U}$ are forced to be the same as the L -part and U -part of A , respectively, thus limiting storage cost. On the other hand, a more accurate factorization (better convergence) can

be achieved by allowing some “fill-in” with additional nonzero entries. Generally, $\tilde{L}$ and $\tilde{U}$ are constructed without pivoting, thereby keeping the time to compute them down. [28]

2.2.4 Spatial Discretization

A finite volume approach is used to solve the present system. The idea behind such an approach is to break the system into a finite number of computational cells in which an average solution of $\tilde{U}$ is sought in each cell. This solution is based on the integral form of the system, given by

$$\frac{d}{dt} \int_{\forall} \tilde{U} d\forall + \oint_{\partial\forall} \overline{\overline{F}} \cdot d\vec{S} = \int_{\forall} \tilde{Q} d\forall$$

$$\overline{\overline{F}} = \begin{bmatrix} (\tilde{F}_i - \tilde{F}_v)^T \\ (\tilde{G}_i - \tilde{G}_v)^T \\ (\tilde{H}_i - \tilde{H}_v)^T \end{bmatrix}, \quad \text{Eq. 2-22}$$

where $\forall$ is the cell volume. $\tilde{F}$, $\tilde{G}$, and $\tilde{H}$ represent fluxes in the x , y , and z -direction, and i and v indicate inviscid and viscous contributions. Finite volume methods solve the above integral by constructing numerical flux functions that approximate the exact physical fluxes at cell interfaces based on cell-average data.

The spatial discretization of inviscid terms is performed using a low-diffusion flux splitting scheme (LDFSS) by Edwards [10]. This upwind splitting method is a derivative of Van Leer’s flux-vector splitting scheme, but it is capable of exactly capturing stationary contact discontinuities and captures moving ones as well as most

other widely used methods. As with most Van Leer family schemes, LDFSS is simple, robust, and monotonicity-preserving. The construction of the numerical flux at each interface involves a separate splitting of convective and pressure fluxes. As an example, the x -direction numerical flux is constructed as follows:

$$\begin{aligned}\bar{F}_{i+\frac{1}{2}} &= \bar{F}_{C,i+\frac{1}{2}} + \bar{F}_{P,i+\frac{1}{2}}, \\ \bar{F}_{C,i+\frac{1}{2}} &= \tilde{a}_{i+\frac{1}{2}} \rho \left\{ C_E^+ \begin{bmatrix} 1 \\ u \\ v \\ w \end{bmatrix}_L + C_E^- \begin{bmatrix} 1 \\ u \\ v \\ w \end{bmatrix}_R \right\}, \\ \bar{F}_{P,i+\frac{1}{2}} &= \left\{ \frac{1}{2} (p_L + p_R) + \rho \tilde{a}_{i+\frac{1}{2}}^2 (D^+ + D^- - 1) + \frac{1}{2} (D^+ - D^-) (p_L - p_R) \right\} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix},\end{aligned}$$

Eq. 2-23

where $i + \frac{1}{2}$ indicates the interface between cells (i, j, k) and $(i + 1, j, k)$; the superscripts $+$ and $-$ indicate positive and negative splitting, respectively; and the subscripts L and R indicate states to the immediate left and right of the interface, respectively. In the above form, intended for low-speed incompressible flows, $\tilde{a}_{i+\frac{1}{2}}$ is the “effective sound speed” evaluated at the cell interface:

$$\tilde{a}_{i+\frac{1}{2}} = \frac{\sqrt{(1 + \tilde{M}_{i+\frac{1}{2}}^2)^2 u_{i+\frac{1}{2}}^2 + 4\beta_{i+\frac{1}{2}}^2}}{1 + \tilde{M}_{i+\frac{1}{2}}^2},$$

$$\text{where } \tilde{M}^2 = \frac{\beta^2}{a^2} \text{ and } \beta^2 = \min[a^2, \max(u^2, u_{ref}^2)]. \quad \text{Eq. 2-24}$$

Here, u_{ref} represents a reference velocity, usually taken as the maximum expected in the flow. Using β in the definition ensures that the interface sound speed scales with the maximum convection speed and that it does not approach infinity near the incompressible limit. Instead, $\tilde{a}_{i+\frac{1}{2}} \rightarrow \sqrt{u_{i+\frac{1}{2}}^2 + 4\beta_{i+\frac{1}{2}}^2}$ as $a_{i+\frac{1}{2}} \rightarrow \infty$. The Mach number splitting $C_E^\pm$ is given by:

$$C_E^\pm = C_{VL}^\pm \mp M_{\frac{1}{2}}^\pm, \quad \text{Eq. 2-25}$$

where $C_{VL}^\pm$ is the subsonic splitting developed by Van Leer,

$$\begin{aligned} C_{VL}^+ &= \frac{(M_L + 1)^2}{4} \\ C_{VL}^- &= -\frac{(M_R - 1)^2}{4} \end{aligned} \quad \text{Eq. 2-26}$$

The split interface Mach number is defined as:

$$\begin{aligned} M_{\frac{1}{2}}^+ &= M_{\frac{1}{2}} \left[1 - \frac{p_L - p_R}{2\rho\beta_{i+\frac{1}{2}}^2} \right] \\ M_{\frac{1}{2}}^- &= M_{\frac{1}{2}} \left[1 + \frac{p_L - p_R}{2\rho\beta_{i+\frac{1}{2}}^2} \right], \end{aligned}$$

$$\text{where } M_{\frac{1}{2}} = \frac{1}{2} [C_{VL}^+ - \alpha_L^+ M_L - C_{VL}^- + \alpha_R^- M_R]. \quad \text{Eq. 2-27}$$

$\alpha_{L,R}^\pm$ is a function that ensures the correct behavior at stagnation points:

$$\alpha_{L,R}^\pm = \frac{1}{2} [1 \pm \text{sgn}(M_{L,R})]. \quad \text{Eq. 2-28}$$

In the subsonic pressure flux splitting, $D^\pm$ is defined as:

$$D^+ = \frac{1}{2} (1 + M_L), \quad D^- = \frac{1}{2} (1 - M_R). \quad \text{Eq. 2-29}$$

In the above developments, the left and right-state Mach numbers are based on an effective sound speed averaged at the interface:

$$M_{L,R} = \frac{u_{L,R}}{\tilde{a}_{i+\frac{1}{2}}}. \quad \text{Eq. 2-30}$$

Having defined the LDFSS as a basis for the discretization, spatial accuracy is enhanced by the use of the weighted essentially non-oscillatory (WENO) variable extrapolation method. By constructing high-order (3rd/5th) polynomial approximations to flow properties at cell interfaces based on their cell-averaged values in adjacent and nearby cells, a more accurate numerical flux construction can be achieved. In order to obtain an “essentially non-oscillatory” behavior near discontinuities, different sets

(stencils) of nearby cells are used to reconstruct pointwise data, and the resulting approximations are evaluated for smoothness.

When constructing the numerical flux at a particular interface, one seeks approximations of the states on either side of the interface, i.e., at the corresponding boundaries of the two adjacent cells. In each of these cells, the WENO scheme approximates flow properties at the interface. The following describes the WENO method utilized in the present model, as applied to a single cell i at boundary point $x_{i+\frac{1}{2}}$. The general procedure is carried out in a one-dimensional fashion in each of the three dimensions. This method is presented in a more detailed and comprehensive fashion in [25].

First, all stencils of dimension d that contain cell C_i are identified. In each one of these stencils, a polynomial approximation to the exact boundary data $\phi(x_{i+\frac{1}{2}})$ is sought, which must have the same cell average as the solution $\bar{\phi}_j$ in each cell of the stencil (where the overbar denotes a cell-average quantity). Here, $\phi(x)$ represents the exact pointwise solution. The candidate stencils can be distinguished by the number of cells l to the left of cell i that they contain – the “left-shift”. Thus, the stencils can be defined:

$$S_l(i) \equiv \{C_{i-l}, \dots, C_{i-l+d-1}\}. \quad \text{Eq. 2-31}$$

Defining the primitive function,

$$\tilde{\phi}(x) \equiv \int_{x_{i-l-\frac{1}{2}}}^x \phi(\psi) d\psi, \quad \text{Eq. 2-32}$$

$\check{\phi}(x_{i+\frac{1}{2}})$ can be expressed as a linear combination of cell averages $\bar{\phi}_i$, as follows:

$$\check{\phi}(x_{i+\frac{1}{2}}) = \sum_{j=i-l}^i \int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} \phi(\psi) d\psi = \sum_{j=i-l}^i \bar{\phi}_j \Delta x_j. \quad \text{Eq. 2-33}$$

If a polynomial $\check{P}(x)$ of degree $\leq d$ interpolates $\check{\phi}(x)$ at the boundary points $\{x_{i-l-\frac{1}{2}}, \dots, x_{i+d-1-\frac{1}{2}}\}$, with its derivative is given by

$$P(x) \equiv \check{P}'(x), \quad \text{Eq. 2-34}$$

then it can be shown that

$$\frac{1}{\Delta x_j} \int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} P(\psi) d\psi = \bar{\phi}_j \quad \text{for } j = i-l, \dots, i+d-1-l. \quad \text{Eq. 2-35}$$

Therefore, given the cell averages $\bar{\phi}_j$ within the stencil $S_l(i)$, the boundary data can be reconstructed by:

$$P_{l,i+\frac{1}{2}} = \sum_{j=0}^{d-1} \gamma_j \bar{\phi}_{i-l+j}, \quad \text{where } P_{l,i+\frac{1}{2}} = \phi(x_{i+\frac{1}{2}}) + O(\Delta x^d). \quad \text{Eq. 2-36}$$

The linear weights γ_{lj} depend on mesh properties within stencil l , but not on the solution

$\phi(x)$ or its cell averages:

$$\gamma_{lj} = \left(\frac{\sum_{m=0}^d \prod_{q=0}^d (x_{i+\frac{1}{2}} - x_{i-l+q-\frac{1}{2}})}{\sum_{n=j+1}^d \frac{\prod_{m=0}^d (x_{i-l+n-\frac{1}{2}} - x_{i-l+m-\frac{1}{2}})}{m \neq n, q \neq n, m}} \right) \Delta x_{i-l+j} . \quad \text{Eq. 2-37}$$

By computing a weighted sum of the d polynomial approximations $P_{l,i+\frac{1}{2}}$, a new approximation of order at least d and as much as $2d-1$ (where data is smooth in all stencils l) can be achieved:

$$P_{i+\frac{1}{2}} = \sum_{l=0}^{d-1} \hat{w}_l P_{l,i+\frac{1}{2}} . \quad \text{Eq. 2-38}$$

The weights $\hat{w}_l$ are required to be ≥ 0 and normalized, such that $\sum_{l=0}^{d-1} \hat{w}_l = 1$. In the event that $\phi(x)$ is smooth in all candidate stencils, there are known coefficients $\hat{w}_l = \alpha_l$ that yield an approximation $P_{i+\frac{1}{2}}$ of order $2d-1$ (e.g., for $d = 3$: $\alpha_0 = \frac{3}{10}$, $\alpha_1 = \frac{3}{5}$, $\alpha_2 = \frac{1}{10}$). On the other hand, in a stencil l where a discontinuity occurs, it is desired that $\hat{w}_l \approx 0$, such that an essentially non-oscillatory behavior is maintained. This criteria gives rise to the following method for determining suitable weights:

$$\hat{w}_l = \frac{w_l}{\sum_{s=0}^{d-1} w_s}, \quad l = 0, \dots, d-1$$

$$w_l = \frac{\alpha_l}{(\varepsilon + \beta_l)^2}$$
Eq. 2-39

Here, ε is a small positive number ($\sim 10^{-12}$) that prevents a divide-by-zero, and β_l is a “smoothness indicator” defined on S_l as:

$$\beta_l = \sum_{m=1}^{d-1} \int_{x_{i-1/2}}^{x_{i+1/2}} \Delta x^{2m-1} \left(\frac{\partial^m P_l(x)}{\partial x^m} \right)^2 dx.$$
Eq. 2-40

For the case of $d = 3$, this definition returns:

$$\begin{aligned} \beta_0 &= \frac{13}{12} [\bar{\phi}_j - 2\bar{\phi}_{j+1} + \bar{\phi}_{j+2}]^2 + \nu [3\bar{\phi}_j - 4\bar{\phi}_{j+1} + \bar{\phi}_{j+2}]^2 \\ \beta_1 &= \frac{13}{12} [\bar{\phi}_{j-1} - 2\bar{\phi}_j + \bar{\phi}_{j+1}]^2 + \nu [\bar{\phi}_{j-1} - \bar{\phi}_{j+1}]^2 \\ \beta_2 &= \frac{13}{12} [\bar{\phi}_{j-2} - 2\bar{\phi}_{j-1} + \bar{\phi}_j]^2 + \nu [\bar{\phi}_{j-2} - 4\bar{\phi}_{j-1} + 3\bar{\phi}_j]^2 \end{aligned}$$
Eq. 2-41

The second term on the right adds a small amount of numerical dissipation. In the present LES, ν is taken as 2.5E-3.

Since viscosity is considered to be a diffusive effect, a central-difference discretization is used to compute the viscous fluxes at cell interfaces, which are then subtracted from the inviscid flux to obtain the total numerical flux.

2.2.5 Human Body Representation

The first step in the human-body simulation is to generate surface data defining the shape of the body. This data can be generated in a number of ways, but for the present simulations, a computer-aided design (CAD) software package was used to create the geometry, and grid-generation software was utilized in the creation of the surface mesh. The body was developed as separate components, each representing a different body part, in the SolidWorks CAD package. The components were then combined into an assembly, and the geometries were exported in an IGES format, a universal CAD file format that is compatible with most grid generation packages. The assembled mannequin was 6 feet (1.83 m) in height with proportionally sized body parts.



Figure 2-1: CAD depiction of human-body geometry

The surface mesh generation was performed using the Gridgen software package (Pointwise, Inc.). Unstructured triangulations were created on the surface of each

component, with a maximum edge length less than 6 mm. The surface data was then exported in an STL file format, which provides the vertices of each planar surface element, along with its outward unit normal vector. The STL data for each body component was compiled into a single surface data file, containing surface nodes (representing the center of a surface element) with their corresponding outward unit normal vectors.

It is important that the surface mesh be very fine, relative to the domain grid. In other words, the maximum length of surface element edge should be much less than the minimum dimension of any nearby computational cell. The reason for this will become apparent later in this section.

Once the surfaces are generated, it is necessary to define the immersed components as a function of space. That is, it must be determined which computational cells are inside of the body and which are outside of the body. To do this, a signed distance function (SDF) is first defined at the center of each cell, which gives the distance from the cell center to the nearest surface node, with a sign determined from the dot product of the distance vector and the outward normal vector. This is done at each cell for every immersed component:

$$\Phi_s(x_{k,i}, t) = \text{sgn}((x_{k,i} - x_{s,l(k),i}) \cdot n_{s,l(k),i}) |x_{k,i} - x_{s,l(k),i}|. \quad \text{Eq. 2-42}$$

An efficient “approximate nearest neighbor” searching technique by Arya et al. [1] is employed to determine the closest surface node. To further reduce computing time, all cell centers outside of a “bounding box” surrounding each immersed component s are

assigned large positive values. A global SDF is then defined as the minimum signed distance at each cell, thereby specifying whether a cell center is inside any part of the human body or completely outside:

$$\Phi(x_{k,i}, t) = \min_s (\Phi_s(x_{k,i}, t)). \quad \text{Eq. 2-43}$$

Thus, the zero iso-surface of the global SDF represents the surface of the human body in computational space.

The motion of the human body is governed by rate laws, which are prescribed at each surface node. In these simulations, only rigid-body translation and rotation are allowed. However, with additional precautions, deforming geometries can be simulated. At each time step, the SDF is updated in accordance with the new location and orientation of the immersed components. From here on, SDF will refer to the global definition, as the component-based definition is no longer of use once a global definition is acquired.

2.2.6 Hydrodynamics/Immersed Boundary Coupling

In order to couple the solution of the hydrodynamics with the motion of the immersed components, an immersed boundary method based on that proposed by Fadlun et al. [11] is used. The main point of immersed boundary methods, originally developed by Peskin [21], is that the velocity of the fluid at the surface of an immersed body must be equal to the velocity of the surface, itself. In this model, the dual time-stepping approach used to ensure a divergence-free velocity field also facilitates the adjustment of

the velocity field to the immersed-body motion. Thus, when coupled with the immersed-body motion, the pseudo-steady residuals of the continuity and momentum equations become:

$$\begin{aligned}
R_c^{*n+1,l} &= (1 - H(\Phi^{n+1}))R_c^{n+1,l} + H(\Phi^{n+1}) \left[\frac{p^{n+1,l} - p_f^{n+1,l}}{\beta^2 \Delta t} \right], \\
R_{m,i}^{*n+1,l} &= (1 - H(\Phi^{n+1})) \left[\frac{\rho(3u_i^{n+1,l} - 4u_i^n + u_i^{n-1})}{2\Delta t} + R_{m,i}^{n+1,l} \right] \\
&\quad + H(\Phi^{n+1}) \left[\frac{\rho(u_i^{n+1,l} - u_{f,i}^{n+1,l})}{\Delta t} \right].
\end{aligned} \tag{Eq. 2-44}$$

Notice that particulate phase information is not included in this formulation. The particulate phase is assumed dilute, and thus, particulate properties do not affect the solution of the hydrodynamics phase. $H(\Phi)$ represents a sharp Heaviside function, which is zero or unity. At all interior cells and cells that are “immediate neighbors” of interior cells, $H(\Phi)$ is set to unity. In this case, immediate neighbors are defined as any of the 26 surrounding cells of an interior cell (i.e., any cell sharing at least one corner boundary with the interior cell), but other definitions can be applied as well. At all cells that are not interior cells or immediate neighbors of interior cells, $H(\Phi)$ is set to zero. When $H(\Phi)=0$, the Navier-Stokes mass and momentum equations are solved, and when $H(\Phi)=1$, a forcing function is applied to the solution of fluid properties. Thus, we can classify all cells based on their SDF and Heaviside function. From here on, “field points”

will refer to cells where $\Phi > 0$ and $H(\Phi)=0$; “band points” will refer to cells where $\Phi > 0$ and $H(\Phi)=1$; and “interior points” will mean cells where $\Phi < 0$.

$u_{f,i}$ and p_f are the values of velocity and pressure to which the forcing function will relax over the $l_{\max}$ sub-iterations at points where the forcing function is applied. At interior points, $u_{f,i}$ is set to the velocity of the nearest surface point, and p_f is fixed at the freestream pressure. At band points, these values are determined by interpolation methods based on the SDF. Simultaneously, the solution at field points will adjust to the conditions imposed at the band points.

Band point interpolations are performed based on the approximate normal distance between the band point and the nearest surface. A velocity distribution function based on the normal coordinate n is defined as follows:

$$u_{f,i}(n) = u_{T,i}(n) + u_{N,i}(n) + u_{s,i}. \quad \text{Eq. 2-45}$$

Thus, the velocity enforced in each band cell can be viewed as the sum of the velocity of the nearest surface node, $u_{s,i}$, and a relative velocity, decomposed into normal and tangential components, $u_{N,i}$ and $u_{T,i}$, respectively. Since it is unlikely that a nearby field point would lie exactly on the normal coordinate, an interpolation point outside of the band must be defined, at which fluid properties are determined based on the nearby field points. The solution at the band point is then a function of its location along the normal coordinate between the interpolation point and surface point. By defining the relative

velocity function appropriately, the proper boundary layer profile can be achieved near the immersed surface. With this goal, the relative velocity components are defined:

$$u_{T,i}(n) = \left\{ u_{T,i}(d_I) + \left(1 - \frac{n}{d_I}\right) \left[k u_{T,i}(d_I) - d_I \frac{du_{T,i}}{dn} \Big|_{n=d_I} \right] \right\} \left(\frac{n}{d_I} \right)^k,$$

$$u_{T,i}(d_I) = (u_i(d_I) - u_{s,i}) - \hat{n}_i (u_j(d_I) - u_{s,j}) \cdot \hat{n}_j,$$

$$u_{N,i}(n) = \left\{ u_{N,i}(d_I) + \frac{1}{2} \left(1 - \left(\frac{n}{d_I} \right)^2 \right) \left[u_{N,i}(d_I) - d_I \frac{du_{N,i}}{dn} \Big|_{d_I} \right] \right\} \left(\frac{n}{d_I} \right),$$

$$u_{N,i}(d_I) = \hat{n}_i (u_j(d_I) - u_{s,j}) \cdot \hat{n}_j, \quad \text{Eq. 2-46}$$

where d_I is the location of the interpolation point along the normal coordinate, and $\hat{n}_i$ is the outward surface normal vector at a surface point $x_{s,i}$. Evaluating the above algorithm at $n = \Phi(x_{b,i}, t)$ returns the forcing velocity at band point $x_{b,i}$.

In this form, the tangential component is a power-law function of the normal coordinate, and the normal component is a cubic function. The exponent k is a power-law variable, which should be set according to the desired velocity profile. For an attached turbulent flow of suitably high Reynolds number ($\text{Re} > 100000$), values around 1/7 or 1/9 produce an approximation to the expected logarithmic profile. For low Reynolds numbers ($\text{Re} < 1000$), a linear profile ($k = 1$) is more applicable.

The forcing pressure at band points is computed assuming a second-degree polynomial distribution:

$$p_f(n) - p_\infty = A + Bn + Cn^2. \quad \text{Eq. 2-47}$$

For such a distribution, boundary conditions at the surface of the immersed body require that

$$\begin{aligned} (p_f(n) - p_\infty)|_{n=0} &= p_w - p_\infty = A \\ \left. \frac{d(p_f(n) - p_\infty)}{dn} \right|_{n=0} &= B \end{aligned} \quad , \quad \text{Eq. 2-48}$$

where the subscript w denotes a “wall” quantity. The quantity B depends only on the acceleration of the immersed body and will be zero when the body is stationary or moving at constant velocity. Given a value of B , the values of p_w and C can be determined by substituting the above boundary conditions into the polynomial function and its first derivative, and evaluating at the interpolation point:

$$\begin{aligned} p_f(d_I) - p_\infty &= (p_w - p_\infty) + Bd_I + Cd_I^2 \\ \left. \frac{d(p_f(n) - p_\infty)}{dn} \right|_{n=d_I} &= B + 2Cd_I \end{aligned} \quad . \quad \text{Eq. 2-49}$$

The final form of the forcing pressure is then:

$$p_f(n) = p_f(d_I) + Bn - \frac{1}{2} \left(\left. \frac{dp}{dn} \right|_{n=d_I} - B \right) \left(1 - \left(\frac{n}{d_I} \right)^2 \right) d_I. \quad \text{Eq. 2-50}$$

Reconstruction of an interpolation point located along the normal coordinate requires identifying all of the points close to the band point in question from which information is to be taken. Weighted summations can then be performed to set the location and flow properties at the interpolation point.

To define a set of points to be used in the interpolation, all nearest-neighbor field points of the band point in question are identified. If none exist, all nearest-neighbor band points are used, instead. Once these points are selected, each one is weighted according to its distance from the band point and the projection of that distance along the normal coordinate:

$$w_l = \frac{1}{\sqrt{(|\vec{x}_l - \vec{x}_b|)^2 - ((\vec{x}_l - \vec{x}_b) \cdot \hat{n})^2} + \varepsilon} \quad \text{if } (\vec{x}_l - \vec{x}_b) \cdot \hat{n} > 0,$$

Eq. 2-51

$$w_l = 0 \quad \text{otherwise.}$$

Here, l indicates a point used in the interpolation, and b denotes the band point in question. By this formula, points lying close to the band point and close to the normal axis receive a large weight. The quantity ε is a very small positive number ($\sim 10^{-12}$), the inverse of which w_l will be set to if l lies exactly on the normal axis. The weights are normalized by dividing each by the summation over the entire set:

$$\hat{w}_l = \frac{w_l}{\sum_m w_m}.$$

Eq. 2-52

The location of the interpolation point along the normal coordinate is then defined as the weighted sum of the projection of the distance vectors along the normal axis:

$$d_I = \sum_l \hat{w}_l (\bar{x}_l - \bar{x}_b) \cdot \bar{n} . \quad \text{Eq. 2-53}$$

The weights are also used to reconstruct flow properties at the interpolation point,

$$q(d_I) = \sum_m q_m \hat{w}_m , \quad \text{Eq. 2-54}$$

as well as gradients,

$$\left. \frac{dq}{dn} \right|_{n=d_I} = \nabla q(n) \big|_{n=d_I} \cdot \bar{n} , \quad \text{where} \quad \nabla q(n) \big|_{n=d_I} = \sum_m \hat{w}_m \nabla q_m . \quad \text{Eq. 2-55}$$

The methodology presented here for interpolating data at band points is applicable not only on Cartesian meshes, but on generalized meshes (including unstructured meshes), as well.

2.2.7 Governing Equations of Particulate Transport

The governing equations of particulate motion can be formulated in an Eulerian manner as mass and momentum conservation laws, as follows:

$$\begin{aligned}
\frac{\partial M_k}{\partial t} + \frac{\partial (M_k (u_{k,j} - v_{k,j}))}{\partial x_j} &= Q_{c,k} \\
M_k \frac{\partial u_{k,i}}{\partial t} + M_k u_{k,j} \frac{\partial u_{k,i}}{\partial x_j} &= Q_{m,k,i}
\end{aligned}
\tag{Eq. 2-56}$$

In this form, k denotes a discrete “size class” composed particles of diameter d_k , M_k represents the mass concentration, $u_{k,i}$ is a mass-average particle velocity, and $v_{k,i}$ is a diffusive velocity that accounts for the effects of Brownian motion and small-scale turbulence. The mass concentration can be defined as $M_k = \rho_k \forall_k N_k$, where ρ_k is the intrinsic density of particle class k , $\forall_k$ is the volume of a single particle in class k , and N_k is the local number concentration of particles in class k . $Q_{c,k}$ is a mass source term that can include effects such as nucleation, condensation, and deposition. $Q_{m,k,i}$ is a momentum source term that includes all external forces acting upon the particles; such as hydrodynamic drag and buoyancy.

2.2.8 Particle Size Distribution

As each field k has a characteristic size of particulate, a discrete population density function (PDF) must be initialized, specifying how much mass of each size class is present. A PDF expresses the frequency (or probability) of occurrences of particles as a function of some property; in this case, size. In most applications, particle distribution is observed to be a log-normal function of diameter; i.e. the frequency of observations of a particular size of particle is a normal function of the log of its diameter. [14]

The frequency is typically expressed in terms of number or mass of particles. By gathering experimental statistics, an approximate PDF can be generated. In the case of a mass PDF, a mass mean diameter (MMD) and geometric standard deviation (GSD) are adequate to approximate the log-normal distribution, as follows:

$$f_m(\log(d_p)) = \frac{1}{(\sqrt{2\pi})\log(\sigma_g)} \exp\left[\frac{-(\log(d_p) - \log(\bar{d}))^2}{2(\log(\sigma_g))^2}\right], \quad \text{Eq. 2-57}$$

where $f_m(\log(d_p))$ is the normalized mass frequency of particles of diameter d_p , $\bar{d}$ is the MMD, and σ_g is the GSD. Since the distribution is a normal function of the log of particle diameter, it satisfies the constraint

$$\int_0^\infty f_m(\log(d_p)) d(\log(d_p)) = 1. \quad \text{Eq. 2-58}$$

Thus, a mass fraction for a range of particle diameters can be obtained by integrating $f_m(\log(d_p))$ over that range, as follows:

$$\frac{\Delta m(d_p)_{d_1}^{d_2}}{M} = \int_{\log(d_1)}^{\log(d_2)} f_m(\log(d_p)) d(\log(d_p)). \quad \text{Eq. 2-59}$$

This distribution can then be discretized by calculating sectional averages of the diameters, thus dividing the PDF into a finite number of “size bins”, each with its own frequency and mass fraction. A mean diameter, $\bar{d}_k$, of size bin k is calculated by:

$$\log(\bar{d}_k) = \int_{\log(d_k)}^{\log(d_{k+1})} f_m(\log(d_p)) \log(d_p) d(\log(d_p)), \quad \text{Eq. 2-60}$$

where d_k and d_{k+1} are the small and large limits of size bin k , respectively. The experimental particle data collected in the present experiments were partitioned into two size bins, $0.5\mu m \leq d_p < 5.0\mu m$ and $d_p \geq 5.0\mu m$. In keeping with these experimental limits (i.e., $d_1 = 0.5\mu m$, $d_2 = 5.0\mu m$, and $d_3 \rightarrow \infty$), two discrete size bins were used to approximate the size distribution, given by:

$$\begin{aligned} \bar{d}_1 &= 2.7\mu m, \quad \frac{\Delta m(\bar{d}_1)}{M} = 0.275 \\ \bar{d}_2 &= 7.7\mu m, \quad \frac{\Delta m(\bar{d}_2)}{M} = 0.725 \end{aligned}.$$

While the particle distribution can vary in space, its spatial dependence can be difficult to determine by experimental means. In the present experiment, particle data was averaged throughout the room, and an average MMD and GSD were calculated. Thus, the mass fractions specified above are initialized at all points. More on the specification of initial conditions is presented later in this section.

2.2.9 Numerical Solution of Particle Fields

A similar implicit sub-iteration approach to that in the hydrodynamics solution is taken to adjust the particulate motion to the position and motion of the immersed body, though in a two-level time-advancement form. The solution at each sub-level is obtained by the same implicit technique, using a TVD upwind scheme to perform the spatial discretization. However, the Heaviside function described previously is modified for particle mass conservation. The previous form, when implemented, led to significant mass loss as a result of particle mass flux across the immersed body surface. The modified form of the mass equation seeks to prevent any transport through the surface by setting the mass flux between interior and band cells to zero and solving the continuity equation in the band cells. An additional measure is taken by the inclusion of a mass source term to ensure conservation when the immersed body is moving.

$$\begin{aligned}
 R_{c,k}^{*n+1,l} &= (1 - \bar{H}(\Phi^{n+1})) \left[\frac{M_k^{n+1,l} - M_k^n}{\Delta t} + \frac{\partial(M_k(u_{k,j} - v_{k,j}))^{n+1,l}}{\partial x_j} - Q_{c,k}^{n+1,l} \right] \\
 &\quad + \bar{H}(\Phi^{n+1}) \frac{M_k^{n+1,l} - M_{f,k}^{n+1,l}}{\Delta t} \\
 R_{m,k,i}^{*n+1,l} &= (1 - H(\Phi^{n+1})) \left[M_k^{n+1,l} \frac{u_{k,i}^{n+1,l} - u_{k,i}^n}{\Delta t} + M_k^{n+1,l} u_{k,j}^{n+1,l} \frac{\partial(u_{k,i})^{n+1,l}}{\partial x_j} - Q_{m,k,i}^{n+1,l} \right] \\
 &\quad + H(\Phi^{n+1}) M_k^{n+1,l} \frac{u_{k,i}^{n+1,l} - u_{f,k,i}^{n+1,l}}{\Delta t} = 0
 \end{aligned}$$

Eq. 2-61

The modified Heaviside function $\bar{H}(\Phi)$ is set to zero for all points outside of the immersed body ($\Phi > 0$) and unity for all interior points ($\Phi < 0$). Thus, the particle mass

conservation equation is solved in band cells. $M_{f,k}$ is the forcing value of mass concentration, set to zero at interior points. $Q_{m,k,i}$ and $Q_{c,k}$ are momentum and mass source terms, respectively. The diffusive velocity is given by:

$$v_{k,j} = \left(\frac{\mu + \mu_T}{M_k \rho_k Sc} \right) \frac{\partial M_k}{\partial x_j}, \quad \text{Eq. 2-62}$$

where Sc is the Schmidt number, which is proportional to the ratio of kinematic viscosity to molecular diffusivity.

The momentum source term, $Q_{m,k,i}$, accounts for various forces to which particles may be subjected. These include net buoyancy, hydrodynamic drag, lift due to shear, and contact forces such as van der Waals and electrostatic forces.

Net buoyancy is the sum of the buoyant force of the air, resulting from displacement by particles, and the force of gravity on the particles. This quantity (as force per volume) can be calculated as:

$$Q_{m,k,i} \Big|_{\text{buoyancy}} = g_i (\rho_k - \rho), \quad \text{Eq. 2-63}$$

where g_i is the gravitational acceleration, and ρ is the local fluid density. Net buoyancy determines the settling rate of particulate in the absence of drag and lift forces.

The hydrodynamic drag force is a function of the velocity of the fluid relative to that of the particulate, as well as particulate size and fluid properties. For low Reynolds numbers (small particles with $Re_k \ll 1$) the Stokes drag assumption can be applied:

$$Q_{m,k,i}|_{drag} = C_h M_k (u_i - u_{k,i}). \quad \text{Eq. 2-64}$$

The hydrodynamic drag coefficient is computed based on fluid and particle properties by:

$$C_h = \frac{3}{4} \frac{\tilde{C}_D \rho \alpha_g^{-2.65}}{\rho_k \bar{d}_k},$$

$$\tilde{C}_D = \begin{cases} \frac{24}{\left(\frac{Re_k}{|u_i - u_{k,i}|}\right) (1 + 0.15 Re_k^{0.687})}, & Re_k < 1000, \\ 0.44 |u_i - u_{k,i}|, & \text{otherwise,} \end{cases}$$

$$Re_k = \frac{\alpha_g \rho \bar{d}_k}{\mu} |u_i - u_{k,i}|, \quad \text{Eq. 2-65}$$

where α_g is the volume fraction of gas (very near 1).

Lift due to shear, also known as Saffman lift force [24], is determined as follows:

$$Q_{m,k,i}|_{lift} = L d_{ij} (u_j - u_{k,j}),$$

$$L = \frac{5.188 \mu^{\frac{1}{2}} \rho^{\frac{1}{2}}}{\rho_k \bar{d}_k (d_{ml} d_{lm})^{\frac{1}{4}}}, \quad \text{Eq. 2-66}$$

where d_{ij} is the deformation tensor. Notice that the Saffman lift is zero in the absence of velocity gradients. This effect is most significant with small sub-micron particles.

When particulate and carpet fibers are in contact, a variety of attractive and repulsive forces combine. Most significant among these are van der Waals and electrical double layer forces. [13] The net effect of such forces is an attractive force that scales with the inverse of the square of the particle diameter. More on the modeling of contact forces will be discussed later in this section.

While the aforementioned modifications to the mass conservation solution provides good results for a stationary body, they do not account for the displacement of particulate by a moving body. The source term is introduced to achieve the correct response when the body moves into cells initially containing particles. That is, the source term ensures that particles are “pushed” into neighboring cells, rather than being “lost” as the body displaces them. Thus, $Q_{c,k}$ represents particle mass (per volume) that is pushed into a cell by the movement of the body during one time step. The procedure for computing the source term is as follows:

1. At each interior cell m that shares an interface with at least one band cell at the $n+1$ time level, compute the net outward volume flow rate from m to each such band cell neighbor l . This can be approximated as a function of the velocity of the nearest surface node, its outward normal vector, and the area of each interface.

$$q_{m,l} = \max(0, u_{s,i}|_{\sim m} \cdot n_{s,i}|_{\sim m}) A_{m,l} \quad \text{Eq. 2-68}$$

Here, the interface in question is identified by the interior cell m and band cell l that share it, q is the outward volume flow rate, s denotes values at a surface point, and $\sim m$ means “nearest to m ”.

2. Normalize the volume flow rates by the sum over all cell m interfaces shared with band cells to obtain a mass transfer fraction Y .

$$Y_{m,l} = \frac{q_{m,l}}{\sum_j q_{m,j}}, \sum_j q_{m,j} > 0$$

$$Y_{m,l} = 0 \quad \text{otherwise}$$
Eq. 2-69

3. At each band cell l that shares at least one interface with an interior cell m at the $n+1$ time level, sum the mass transfer contributions from all such interior cells.

$$Q_{c,k,l} = \sum_m Y_{m,l} \frac{M_{k,m}^n \forall_m}{\Delta t}$$
Eq. 2-70

Here, $\forall_m$ is equal to the volume of cell m .

It is important that the immersed body not move more than one cell-length in distance during a single time step, as this would result in “new” interior cells at the $n+1$ time level that do not share interfaces with band cells. This procedure is also restricted to two-level time integration methods, such as Euler explicit or Crank-Nicholson.

2.2.10 Carpet Effects

The presence of carpet in a dwelling has important consequences for the resuspension and transport of particulate. Carpet fibers interact with the carrier fluid and directly with the particulate. The structure of a carpet is very random and complicated, and the length-scale of fibers can be several orders of magnitude smaller than the present grid resolution. Therefore, it is a goal of this study to model these interactions at a macroscopic level through volume-averaged approximations. A successful formulation requires knowledge of carpet properties, as well as fluid and particle dynamics within this type of porous medium.

Cicciarelli et al. [5] performed a detailed analysis of typical carpet structure and found a void fraction λ of about 0.9 (90% air). The individual filaments were found to have trilobal-shaped cross-sections with circumscribed diameters of about 60 μm .

As air flows through the region occupied by the carpet, drag caused by the fibers creates resistance to the flow. Since the alignment of carpet fibers tends to be random and disorganized, it is reasonable to assume that this resistance is nearly isotropic. The most common way of approximating the resistive effect of a porous medium on a fluid is by Darcy's Law:

$$-\frac{\partial p}{\partial x_i} = \mu R_{ij} u_j, \quad \text{Eq. 2-71}$$

where R_{ij} is a resistance tensor specific to the medium. For an isotropic case, only the magnitude of the resistance must be approximated. Darcy's law applies to fluid flow

with negligible inertial effects, but is not adequate to describe stronger flows, such as those induced near the moving feet and vents. For flows with noticeable inertial effects, Forchheimer's approximation,

$$-\frac{\partial p}{\partial x_i} = \mu A_{ij} u_j + \rho |u_i| B_{ij} u_j, \quad \text{Eq. 2-72}$$

can be applied, which takes into account viscous and inertial effects. Here, A_{ij} and B_{ij} are tensors that, like R_{ij} , depend on the structure of the porous medium. In order to achieve the correct response of the flow within a porous medium when solving the incompressible Navier-Stokes equations, the resistance must be accounted for in the momentum source term such that the momentum equation reduces to the above forms in their corresponding steady flow regimes. The transition between Darcy and Forchheimer flow regimes is not well understood, but models are available that interpolate the resistance in the transition regime based on an experimentally determined range of Reynolds numbers. Liu and Masliyah [19] approximate the resistive force of an isotropic porous medium on an incompressible fluid by:

$$\begin{aligned}
f_{e,i}|_{porosity} &= \mu F u_i, \\
F &= \frac{(1-\lambda)^2 \left(85.2 + \frac{0.69 \text{Re}_\lambda^3}{16^2 + \text{Re}_\lambda^2} \right)}{\lambda^{1/3} d_s^2}, \\
\text{Re}_\lambda &= \left(\frac{1 + \left(1 - \lambda^{\frac{1}{2}} \right)^{\frac{1}{2}}}{(1-\lambda)\lambda^{\frac{1}{6}}} \right) \left(\frac{d_s \rho |u_i|}{\mu} \right), \\
d_s &= 6 \frac{\nabla_s}{A_s},
\end{aligned} \tag{Eq. 2-73}$$

where F is the magnitude of shear resistance, d_s is an equivalent spherical diameter (of the carpet filament), and $\frac{\nabla_s}{A_s}$ is the volume-to-surface area ratio of the filament.

While the resistance of the carpet to fluid motion, in turn, affects particulate motion, surface-to-surface effects also become important when particles come into contact with fibers. Prominent among these are van der Waals and electric double layer forces, the net effect of which will tend to attract two surfaces together within a very small distance ($\ll 1 \mu m$). Since particles in the carpet are initially at rest, prior to commencement of human motion, it can be assumed that surface forces act on all particles contained therein. Thus, an adhering force is applied, which must be overcome by net drag and buoyant forces in order for particulate to be resuspended. Approximating such forces is very complicated, due to the complex interactions and carpet structure. However, studies have indicated a near linear relationship with the inverse of the square of particle diameter [13]:

$$Q_{m,k,i}|_{sticking} \approx \frac{A_{stick}}{d_k^2}. \quad \text{Eq. 2-74}$$

Here, $Q_{m,k,i}|_{sticking}$ is the force per volume. This quantity contributes to the momentum source term in Eq. 2-61. The coefficient A_{stick} was determined by parametric studies in which its value was varied during repetition of resuspension simulations, and resulting emission factors (mass resuspended per second per initial mass in carpet) were compared with the experimental results.

2.3 Model Implementation

2.3.1 Initial Conditions

In order to define an appropriate initial condition for the resuspension simulation, it is necessary to consider the preexisting hydrodynamic flow within the room. This flow field is driven by the ventilation system, which is already active prior to any human motion. Thus, several minutes of vent flow are simulated prior to moving the immersed body so that a quasi-steady flow can be obtained. This portion of the simulation is initialized by setting the velocity throughout the room to zero and fixing the pressure to a constant value.

Once a quasi-steady flow within the room is obtained, the particulate fields and immersed body components are initialized. The particulate mass concentration is set to a uniform value within the carpet, such that the mass per unit area of carpet is equal to that determined approximately by experiment. The airborne mass concentration is set to the

average background concentration measured prior to the experiment. The same discrete particle size distribution is initialized everywhere, as given in Sec. 2.2.8.

2.3.2 Boundary Conditions

Boundary conditions are enforced by specifying data at “ghost cells”, which can be described as computational cells adjacent to the actual solution domain in which conditions are enforced such that particular boundary conditions are achieved at the actual domain boundaries. Domain boundaries, in a finite volume system, can generally be thought of as the interfaces between computational cells inside of the solution domain and ghost cells outside of the solution domain.

The velocity at the inflow vents is set according to experimental measurements. However, as most residential vents are angled to enhance dispersion of inflow air, it is beneficial to apply perturbations to the inflow direction at the vents to simulate the breakup of the inflow jet. In this light, random perturbations are applied to the velocity vectors at inflow ghost cells in such a way that the mean normal velocity stays constant, at the measured value of 2.0 m/s. No additional particulates are introduced to the room by the inflow jet; i.e., the ventilation system is assumed to be perfectly filtered.

At outflow boundaries (doorways), a constant atmospheric pressure is fixed, and outflow velocities are extrapolated from interior cells at each time step as the solution evolves. Particles are allowed to pass through the doorways, exiting the room (and thus, exiting the computational domain), but are not allowed to enter (or re-enter).

All boundaries where vents or doorways do not exist are treated as walls. In the present case of a viscous fluid, it is appropriate to enforce “no-slip” boundary conditions

at wall boundaries. Since the walls are not permeable, no nonzero fluid velocities at a wall can be allowed. Thus, fluid velocities in the ghost cells adjacent to the wall are fixed such that all velocity components at wall interfaces are zero. For the present simulation, no surface-capturing of particles is considered. Thus, particle velocity boundary conditions are treated similarly to those of the fluid. However, if deposition of particulate matter on particular wall boundaries were allowed, accumulation could easily be monitored by tracking particulate flux “into” the walls. Note that since no-slip is enforced on the fluid, any mass flux of particulate into the wall (including the floor and ceiling) would occur as a result of particulate inertia and net buoyancy.

2.3.3 Simulation Details

In the present simulation, as in the corresponding experiment, the human body begins by standing still near the doorway to the hall for 1.5 seconds, walks forward for 1.5 seconds at a speed of 1.3 m/s, and stamps in place for 20 seconds. An alternating sinusoidal up-and-down motion is ascribed to the human’s “feet” (each comprised of a fused foot and leg) to simulate a walking motion. The bottom surfaces of the feet are allowed to sink partially into the carpet, thus displacing some of the particulate initially contained therein. The amplitude and frequency of the feet motion (given below in Table 2-1) are assigned to values that approximate typical walking and stomping motions.

In the experiment, the in-place stomping of the human subject occurred within a 1.5 ft × 1.5 ft area of carpet. However, the motion of the person within that area was somewhat random (although, the rate of stomping was relatively constant) and not known exactly. Therefore, two simulations were performed to represent two possibilities of

human motion within the stomp region. In one case, the human body stomps in place in the middle of the square with no additional movement prescribed. In the other case, the entire human body rotates in place while stomping (at 5 seconds per revolution), enabling the feet to penetrate more of the carpet area. Performing these two simulations makes it possible to analyze the relative effects of different human-body movements on particulate resuspension.

The simulation was performed on a computational domain of the same dimensions as those of the EPA test room ($13.8 \text{ ft} \times 12.5 \text{ ft} \times 8.0 \text{ ft}$) with a grid resolution of $193 \times 193 \times 145$ ($\sim 5.4 \times 10^6$ grid points). The grid was Cartesian with uniform spacing in the x and y (horizontal) directions, but was stretched in the z direction to allow better resolution of the carpet layer. The carpet was resolved (vertically) by 5 uniform cell layers (0.2 cm, each), outside of which the vertical grid spacing was stretched to a maximum cell height of 2.0 cm. The simulations were mapped to 36 Intel Xeon processors on an IBM Blade Center Linux Cluster using the MPI message passing standard. Domain decomposition techniques were used to distribute the numerical data among the processors.

Table 2-1: Simulation Parameters

room dimensions	13.8 ft × 12.5 ft × 8.0 ft
grid resolution	193 × 193 × 145
human body initial location	$x=3.0$ ft, $y=2.7$ ft
human body stomp location	$x=3.0$ ft, $y=8.1$ ft
amplitude of foot motion	2.5 in (walking); 10.0 in (stomping)
period of foot step/stomp	1.0 seconds
period of body rotation	5.0 seconds
initial carpet particle mass loading	430 $\mu\text{g}/\text{in}^2$
initial background particle mass loading	7.1 $\mu\text{g}/\text{ft}^3$
"small" particle size class diameter	2.7 μm
"large" particle size class diameter	7.7 μm
carpet thickness	1.0 cm
maximum foot penetration into carpet	0.5 cm
average vent velocity	2.0 m/s

3 Model Validation

Several validation and proof-of-concept studies have been performed in an effort to evaluate the accuracy and applicability of the CFD model. These studies include examination of steady and unsteady characteristics of flow over various stationary immersed bodies, as well as analysis of moving immersed bodies in the presence of particulate fields. Results have been obtained, for the purpose of validation, for steady and unsteady low Reynolds number flow over a two-dimensional cylinder, steady and unsteady low Reynolds number flow over a three-dimensional sphere, and steady high Reynolds number flow over a NACA-0012 airfoil. Additional results for immersed boundaries in motion (relative to the grid) have been obtained in order to evaluate mass conservation and induced flow characteristics, as compared with stationary cases.

3.1 Flow Over a Two-Dimensional Cylinder

Flow over a two-dimensional cylinder, represented as an immersed boundary, was simulated at Reynolds numbers of 20 and 40 in order to evaluate steady flow characteristics. The calculations were performed on a Cartesian mesh, with the domain extending to ± 10 m in the stream-wise direction and a resolution of 321×321 . The immersed-boundary cylinder had a diameter of 1 m and was located within a uniformly spaced 2×2 m² region of the domain with a grid resolution of 81×81 . Both first and second-order velocity interpolation techniques (the latter of which is given by Eq. 2-46) were utilized, and the quantitative results were compared with values obtained from documented experimental and computational studies.

Table 3-1 shows a comparison of the non-dimensional reattachment length (L/D), flow separation angle (θ), and drag coefficient (C_D) with some of those found in literature, as well as with a calculation performed with the current flow solver on a body-fitted grid.

Table 3-1: Reattachment length, flow separation angle, and drag coefficient of two-dimensional flow over a cylinder

	$Re=20$			$Re=40$		
	L/D	θ	C_D	L/D	θ	C_D
Tritton [29]	—	—	2.22	—	—	1.48
Coutanceau & Bouard [7]	0.73	42.3	—	1.89	52.8	—
Fornberg [12]	0.91	—	2.00	2.24	—	1.50
Dennis & Chang [8]	0.94	43.7	2.05	2.35	53.8	1.52
Calhoun [3]	0.91	45.5	2.19	2.18	54.2	1.62
Russell & Wang [23]	0.94	43.3	2.13	2.29	53.1	1.60
Ye et al. [31]	0.92	—	2.03	2.27	—	1.52
Body-fitted grid	0.92	43.8	1.98	2.21	53.6	1.49
<u>Present</u>						
First order	0.89	35.3	2.03	2.24	45.1	1.52
Second order	0.90	40.8	2.02	2.25	51.0	1.52

The drag coefficient and reattachment length results agree well with the values found in the previous studies for both the first and second-order velocity interpolations, but the first-order method significantly under-estimates the separation angle. While the second-order method also under-estimates this value, the error incurred is much more acceptable.

Figure 3-1 shows the pressure coefficient (C_p) and span-wise vorticity results along the surface of the cylinder at a Reynolds number of 40, as compared with results obtained

by Kim et al.'s immersed boundary method [16] and the present solver on a body-fitted grid.

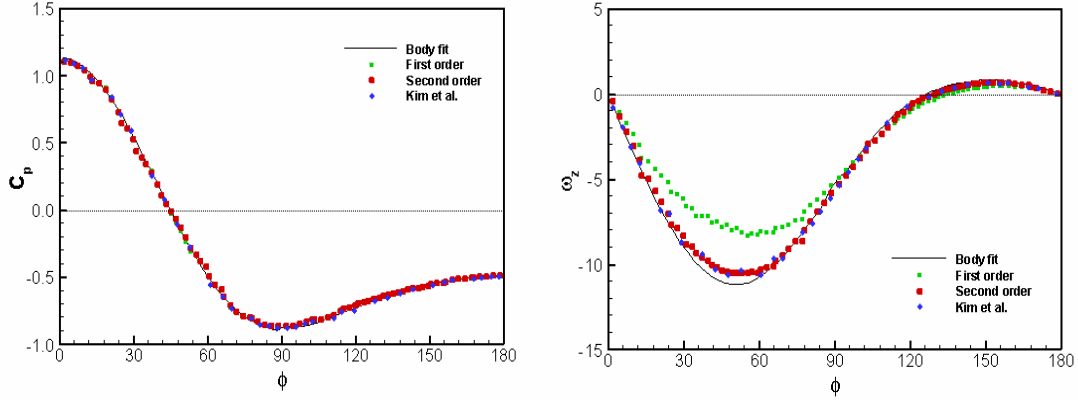


Figure 3-1: Pressure coefficient and vorticity along cylinder surface for $Re = 40$

It can be seen that both the first and second-order methods predict the surface pressure well, but only the second-order method does a good job of predicting surface vorticity.

Unsteady flow characteristics were examined for a similar case, but with Reynolds numbers of 100 and 200. Lift and drag coefficients and Strouhal number (a non-dimensional measure of vortex shedding frequency: $St = \frac{fL}{U_\infty}$) were compared with

values given in literature. Mean values and oscillations of flow variables were both obtained in order to assess temporal accuracy. Table 3-2 shows the computed results using the second-order velocity interpolation method compared with values from previous studies.

Table 3-2: Lift, drag, and vortex shedding frequency of flow over a cylinder

	$Re=100$			$Re=200$		
	C_D	C_L	St	C_D	C_L	St
Rosenfeld et al. [22]	—	—	—	1.31 ± 0.04	± 0.65	0.20
Wright et al. [30]	—	—	—	1.33 ± 0.04	± 0.68	0.196
Braza et al. [2]	1.36 ± 0.015	± 0.25	—	1.40 ± 0.05	± 0.75	—
Liu et al. [18]	1.35 ± 0.012	± 0.339	0.164	1.31 ± 0.049	± 0.69	0.192
Calhoun [3]	1.35 ± 0.014	± 0.300	0.175	1.17 ± 0.058	± 0.67	0.202
Russell & Wang [23]	1.38 ± 0.007	± 0.322	0.169	1.29 ± 0.022	± 0.50	0.195
Kim et al. [16]	1.33	± 0.32	0.165	—	—	—
Present						
Second order	1.34 ± 0.011	± 0.315	0.164	1.36 ± 0.048	± 0.64	0.191

All of the computed results agree well with values found in the literature, including both mean values and oscillations. Figure 3-2, below, clearly shows the capturing of vortex shedding behind the cylinder, using the present immersed boundary method.

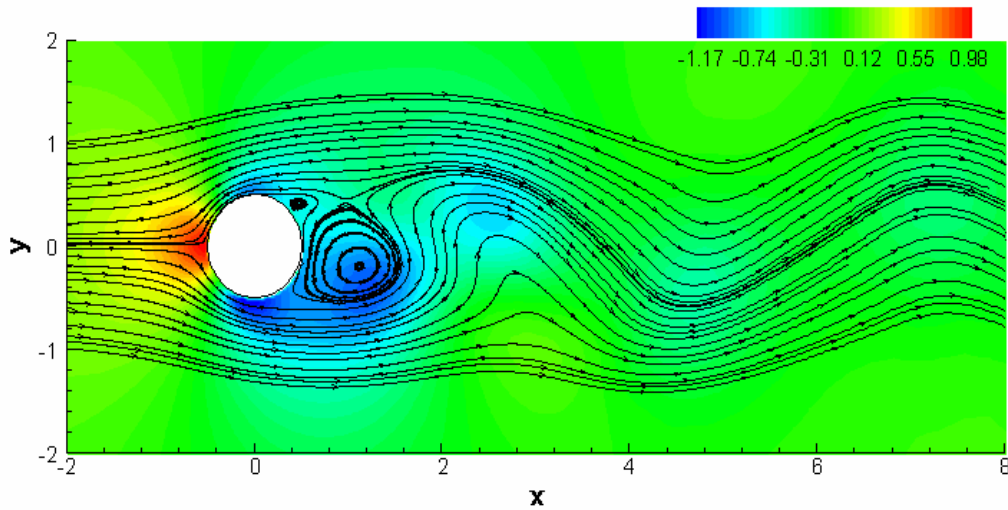


Figure 3-2: Unsteady wake induced behind cylinder with pressure coefficient contours at $Re = 100$

3.2 Flow Over a NACA 0012 Airfoil

High Reynolds number flow characteristics were examined for the case of flow over a NACA-0012 airfoil at $Re = 9$ million. These steady simulations were performed on a stretched Cartesian (non-body-fitted) grid with a resolution of 243×177 . The grid points were clustered near the leading and trailing edges, as well as near the top and bottom surfaces. Results were obtained using the first-order velocity interpolation near the airfoil surface, with varying powers k , as given in Eq. 2-46, and with an angle of attack (α) of 16 degrees. Values of k near unity allowed large flow separation on the bottom of the airfoil, more consistent with laminar flow. Lower values of k did a better job of producing the re-energizing effect seen in turbulent boundary layers, which transfers energy from the flow into the boundary layer, promoting attachment. A power of $1/9$ is intended to model a fully-developed turbulent boundary layer, and thus, results in the most flow attachment.

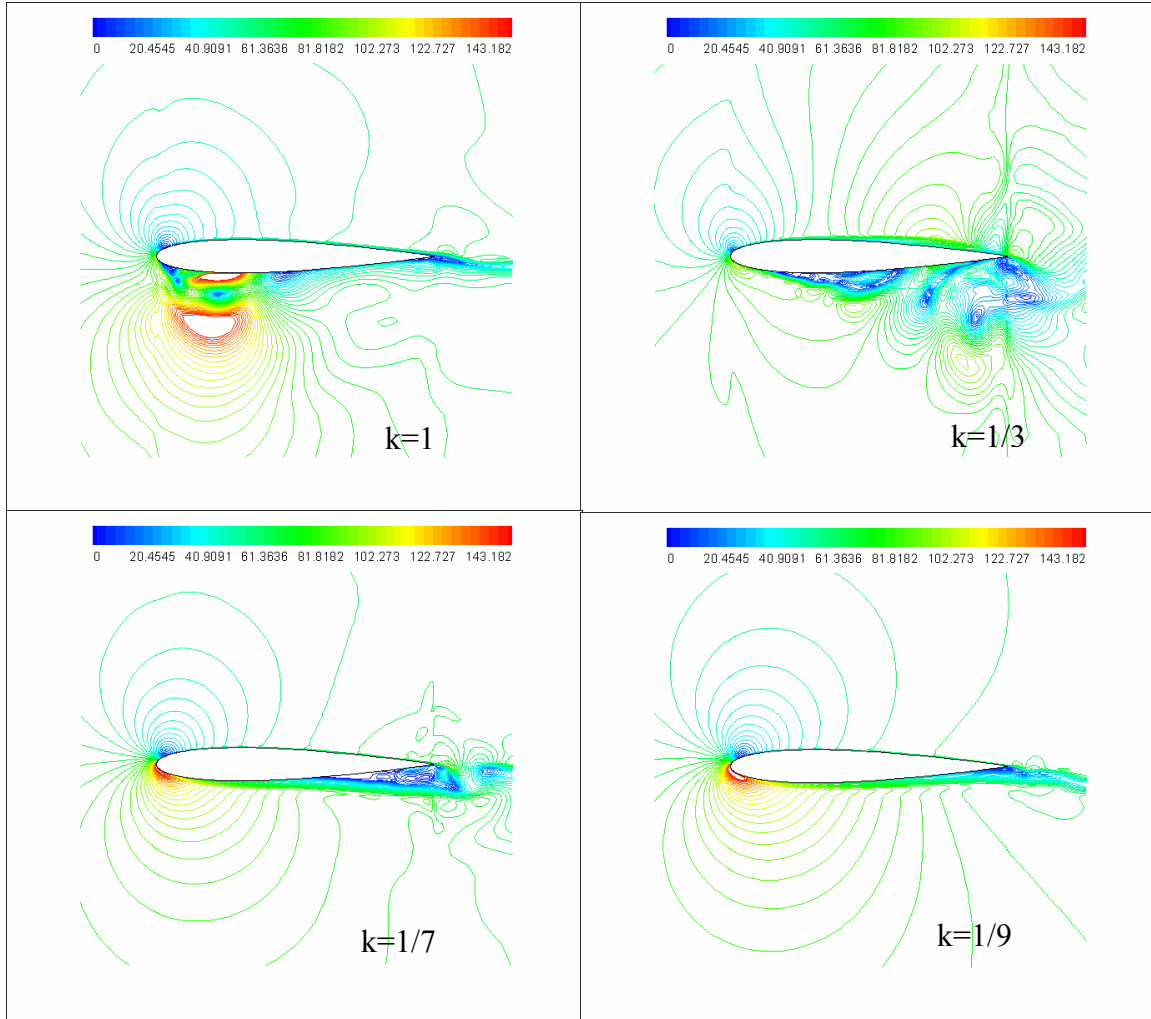


Figure 3-3: Velocity magnitude for flow over a NACA-0012

A lift curve (C_L vs. α) produced by the immersed boundary simulations, using a velocity interpolation power of $1/7$, is displayed in Figure 3-4 against those obtained experimentally and with XFOIL [9], an established computer code for predicting airfoil characteristics. Results agree very well, despite the lack of turbulence modeling or resolution of fine-scale boundary layer effects in the present simulations.

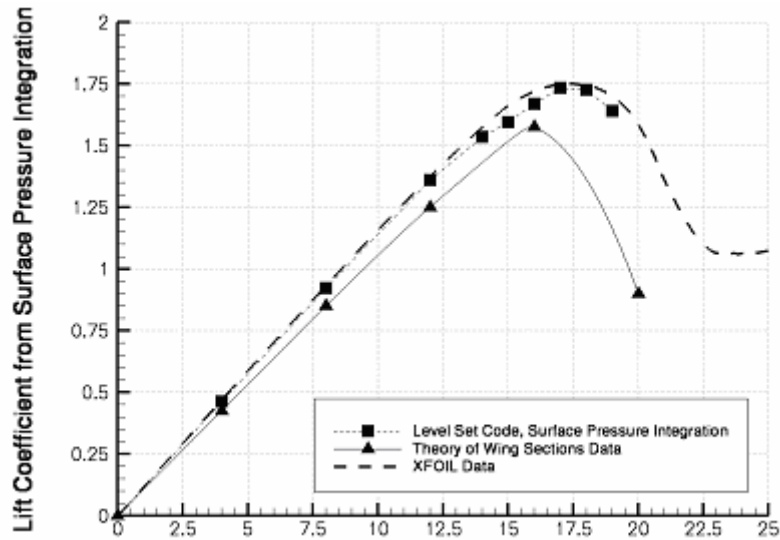


Figure 3-4: Lift curve for flow over a NACA 0012 airfoil

3.3 Flow Over a Three-Dimensional Sphere

For the validity case of flow over a three-dimensional sphere, the accuracy of the immersed boundary method was assessed over three different flow regimes – steady axisymmetric, steady asymmetric, and unsteady flow. These simulations were performed at Reynolds numbers of 100, 250, and 300, representing the three flow regimes, respectively, with a $196 \times 196 \times 196$ grid resolution. The sphere had a diameter of 1 m and was located within a $2 \times 2 \times 2$ m³ region of the domain with a grid resolution of $81 \times 81 \times 81$. Spatial accuracy was assessed in all cases, as well as temporal accuracy in the unsteady case. Drag coefficient results agree very well with the values found in literature for all three cases, and while the lift coefficient is slightly under-predicted in the Re=250 case, it is very accurate in the Re=300 case. Time-dependent characteristics are

also well predicted, as the computed Strouhal number (dimensionless frequency, $St \equiv \frac{fL}{U}$, where L and U are characteristic length and velocity values) is in line with the results given by past researchers.

Table 3-3: Drag and lift coefficients and Strouhal number for flow over a sphere

	Re					
	100	250		300		
	C_D	C_D	C_L	C_D	C_L	St
Johnson & Patel [15]	1.08	0.70	0.062	0.656	0.069	0.137
Kim et al. [16]	1.09	0.70	0.059	0.657	0.067	0.134
Constantinescu & Squires [6]	—	0.70	0.062	0.655	0.065	0.136
Present	1.09	0.70	0.052	0.658	0.068	0.134

The pressure coefficient and vorticity along the surface of the sphere closely match the curves of Kim et al. and Johnson and Patel [16], as shown in Figure 3-5, plotted as a function of azimuthal coordinate, ϕ . Furthermore, Figure 3-6 clearly shows that the immersed boundary method captures both axisymmetric and asymmetric vortex shedding behind the sphere.

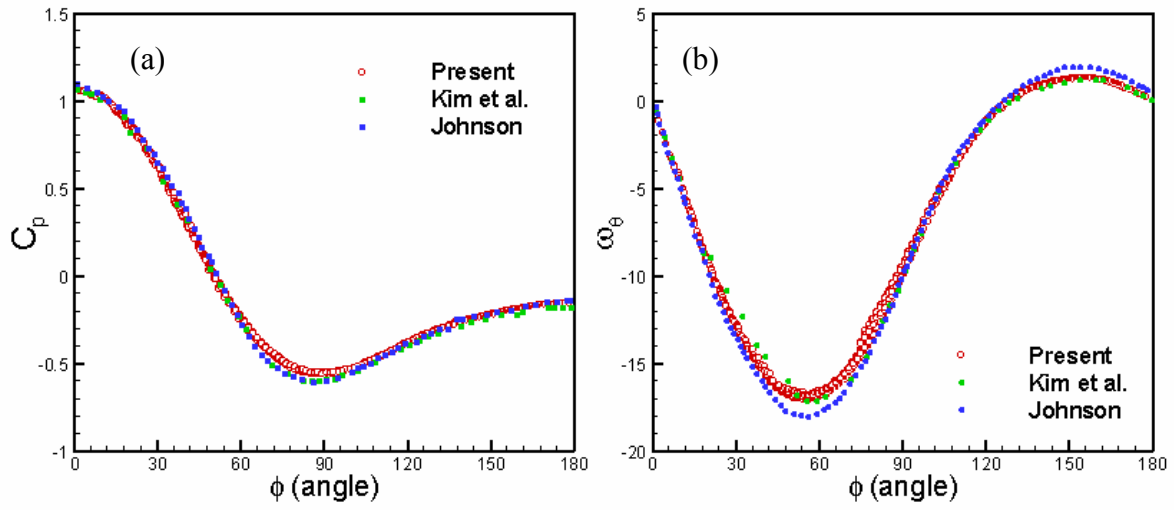


Figure 3-5: Flow variables along sphere at $Re=100$: (a) wall pressure coefficient; (b) wall azimuthal vorticity

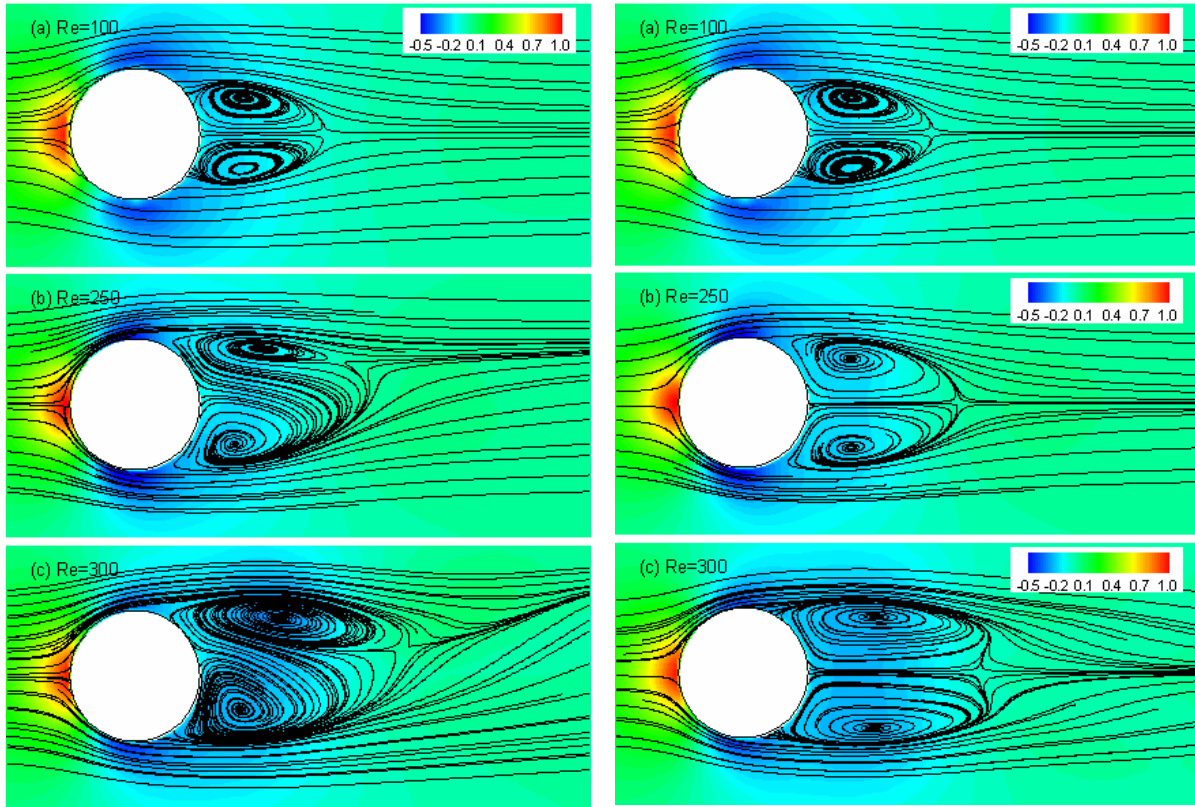


Figure 3-6: Streamlines of projected vectors for (x,y) plane (left) and (x,z) plane (right). (a) $Re=100$, (b) $Re=250$ and (c) $Re=300$

3.4 Movement of Cylinder and Cube Through Particle Field

In order to assess the ability of moving immersed boundaries to induce realistic motion of particulate fields, the movement of a simple two-dimensional cube and cylinder in a closed channel filled with particulates was simulated. The simulations were performed on a uniformly spaced 513×129 computational grid. Two initial distributions of particulate matter were imposed – one in which a “band” of particulates was located in the middle of the channel, inside of which the concentration was constant, and one of constant concentration throughout the entire channel. In the simulations, the immersed bodies were moved to the right for 8.5 seconds at a speed of 1 m/s, then back to their initial position. The initial flow and particle velocities were set to zero.

Figure 3-7 shows the mass error percentage as a function of time for the case of the cylinder moving through the channel. The results obtained using the particulate mass source term $Q_{c,k}$ (as presented in Sec. 2.2.9) are compared with those obtained with no source term implemented. The improvement in mass conservation is very significant, yielding a total mass error of only 0.003% over the duration of the simulation, compared to about 2% without the source term. Mass conservation was good for both initial particulate distributions.

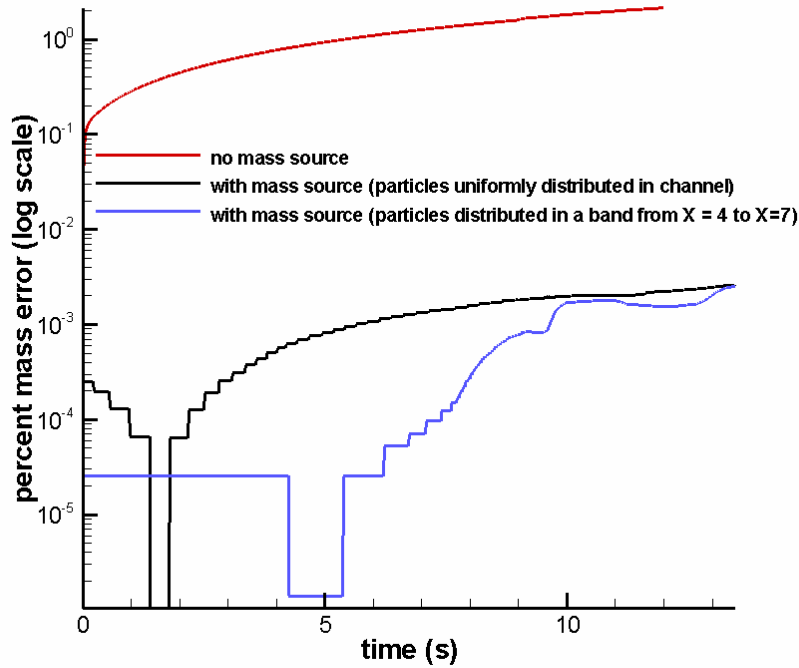


Figure 3-7: Mass error versus time for cylinder moving through a stationary particle

Figure 3-8 shows the motion of the particulate field, initially contained within a band between $x=6$ m and $x=9$ m, induced by the movement of the cube. It can be seen that particles are entrained in the vortices induced by the immersed-body motion, and dispersed as the wake breaks down into smaller, disorganized eddies.

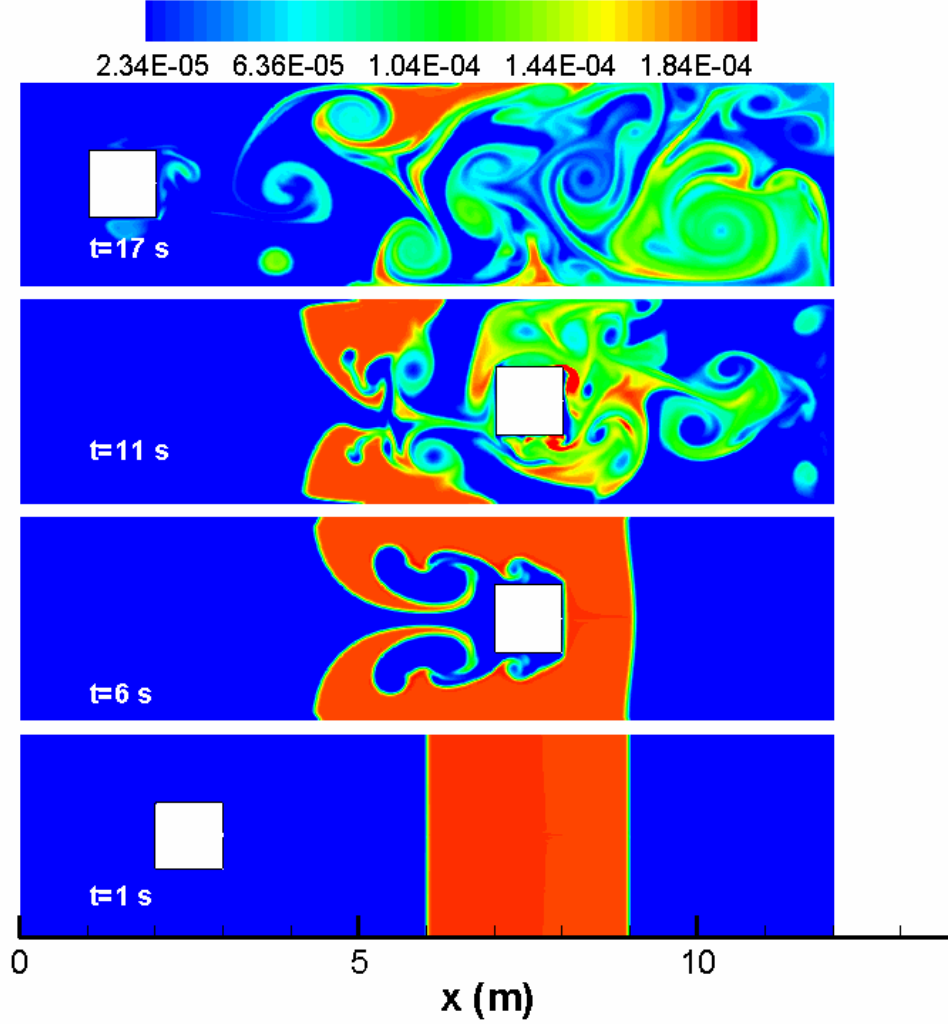


Figure 3-8: Snapshots of particle mass concentration for cube propagating through a channel

3.5 Movement of Multiple Immersed Bodies Through a Particle Field

The use of the present immersed boundary method to simulate humans walking through rooms containing particulate was examined. The results of interest in this preliminary simulation include particulate mass conservation in the presence of multiple immersed bodies in simultaneous motion, wake structure produced by the “human-body” motion as a function of k (power law variable), and the particulate motion induced. In these simulations, one or two humans move through a room (of the same size as that in

the EPA test house) and into a hallway, passing through a spherical “cloud” of 0.1 g of particulate matter, 1 m in diameter. Each human is composed of seven separate, but overlapping, immersed bodies. The “legs” of the human bodies move up and down in a sinusoidal motion to simulate walking. The computational domain is composed of approximately 8 million cells and, thus, has a similar resolution to the room-only simulations to be discussed in the next section. The immersed-body movement occurs over a 5-second period.

The maximum total mass error that occurred in these simulations was about 0.05% with two human bodies, as shown in Figure 3-9. This amount of mass is insignificant, given the number and size of immersed bodies in motion and the total amount of mass transported.

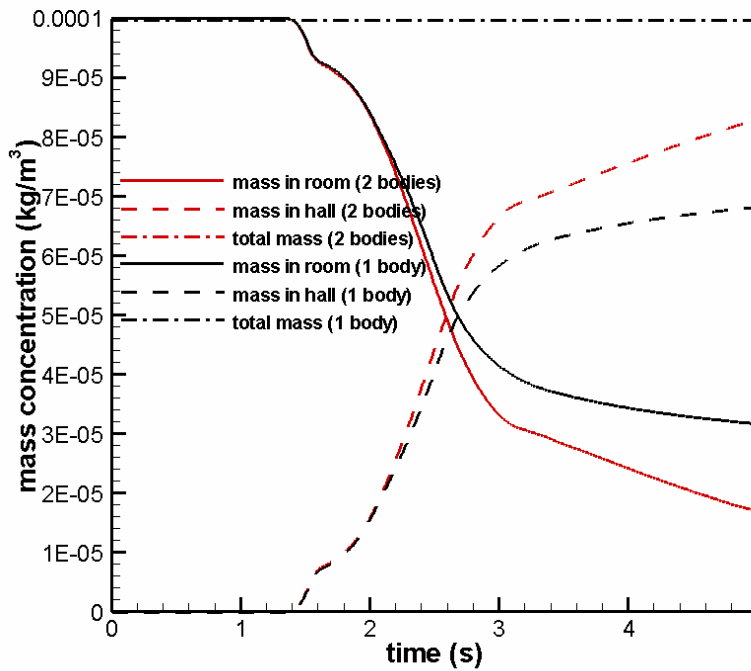


Figure 3-9: Room-to-hall mass transport due to human-induced motion

Figure 3-10 shows the wake structure behind the two humans at 2.5 and 5 seconds, as displayed by the Smagorinsky eddy viscosity contours (indicative of shear). It was found that using lower values of k allows greater flow separation along the immersed surfaces, and thus, creates broader wakes behind the moving “people”. The broader wakes promote particulate mass entrainment and are transported with the bodies, as can be seen in Figure 3-11. Both results shown here were obtained using $k=1$.

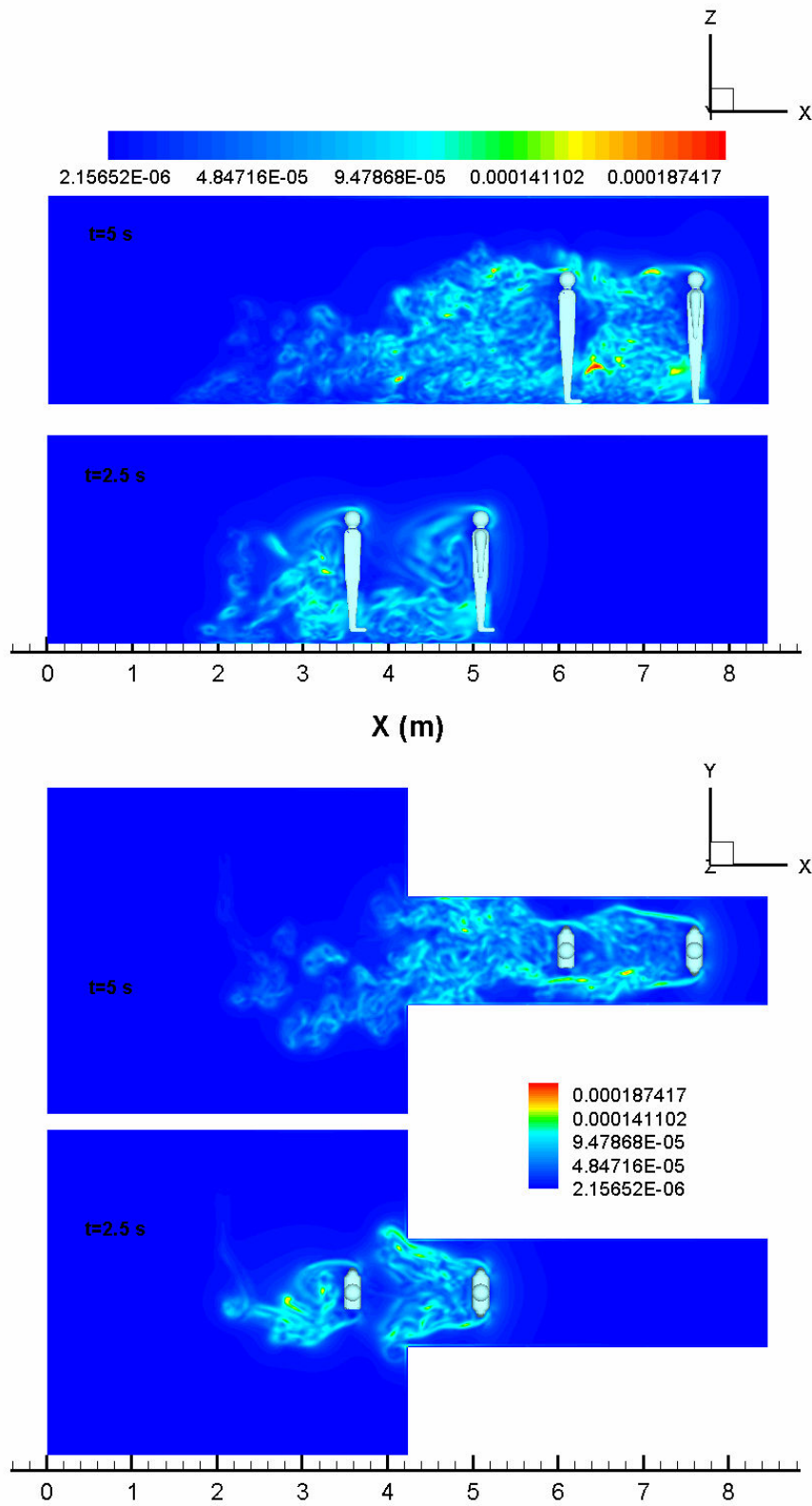


Figure 3-10: Snapshots of Smagorinsky eddy viscosity during human walking event

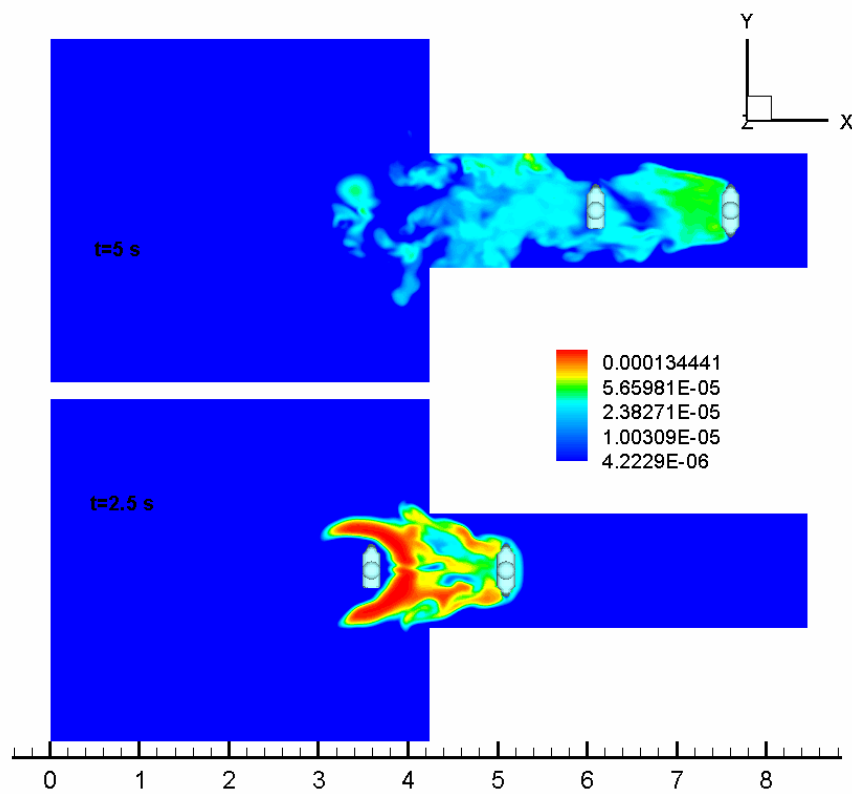
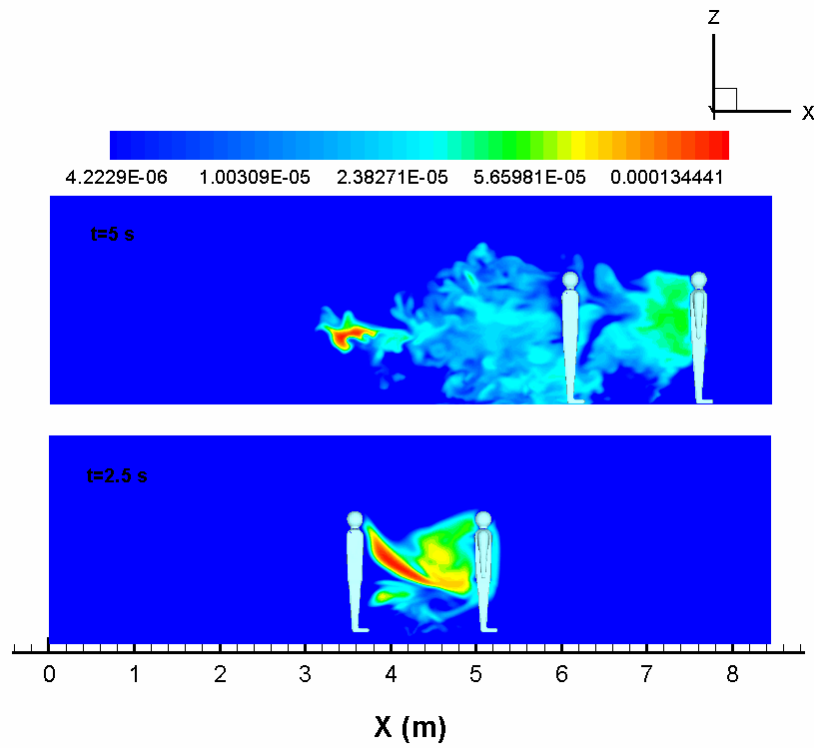


Figure 3-11: Snapshot of particle mass concentration for human walking event

4 Results and Discussion

4.1 “Feet-Only” Simulations

Prior to performing simulations with the full human body, it was necessary to determine an adequate “sticking force” to be applied to the particles entrapped in the carpet layer. Since the particle-fiber interactions occur over much smaller length scales than those resolved by the computational grid used, it was necessary to perform parametric tests using volume-averaged adhesion forces. The goal was to determine a suitable coefficient, A_{stick} , to parameterize the sticking force, $Q_{m,k,i}|_{sticking} \approx \frac{A_{stick}}{d_k^2}$. For these preliminary simulations, one or two “legs” were simulated in a small, closed $1.25 \times 1.25 \times 1.75 \text{ m}^3$ chamber with a grid of the same spatial resolution as that used for the full room (as described in Sec. 2.3.3). The initial particle sizes and concentrations in the carpet and air were the same as those given for the full-room simulations (Sec. 2.3.1). A series of stomping events were enacted over 9 and 20-second periods with A_{stick} varying from 10^3 to $10^4 \text{ N}\cdot\text{m}^2/\text{kg}$. The effect of the penetration depth of the feet into the carpet was also examined.

Table 4-1: “Feet-Only” Simulation Details

chamber dimensions	1.25×1.25×1.75 m ³
grid resolution	63×63×109
amplitude of foot motion	10 in
period of foot stomp	1.0 second
initial carpet particle mass loading	430 µg/in ²
initial background particle mass loading	7.1 µg/ft ³
"small" particle size class diameter	2.7 µm
"large" particle size class diameter	7.7 µm
carpet thickness	1.0 cm

Results of these simulations indicate that the magnitude of the sticking force has little effect on the amount of particulate resuspended out of the carpet in the vicinity of the feet, as can be seen in Figure 4-1. This is likely due to the fact that most of the mass resuspended is emitted from very close to the feet as a result of displacement by the feet and relatively high velocities generated by the stomping. That is to say, a small sticking force may be enough to adhere particulate in cells away from the immersed body disturbance, but near the feet, roughly the same amount of particulate will be dislodged, even when varying the sticking parameter significantly.

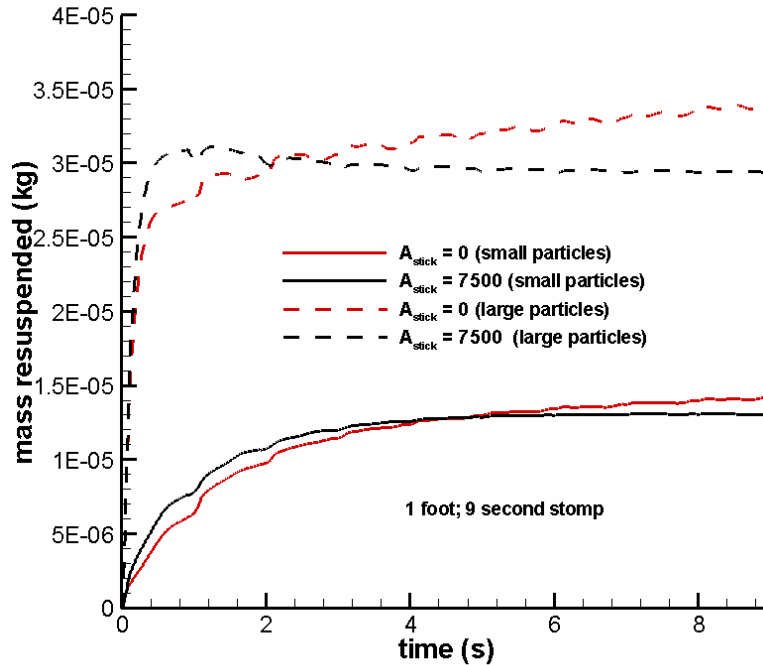


Figure 4-1: Effect of sticking force on particle mass resuspended

Figure 4-2 depicts the velocity field generated by the stamping of two feet at the moment of greatest penetration depth. It can be seen that the downward motion of the left foot (on the right in the figure) generates large lateral velocities as it approaches the floor, as well as vortices to either side of the foot. Thus, after the particles are forced downward by the foot (primarily, a result of displacement), they are propelled laterally by hydrodynamic drag effects, and some are resuspended by the circulating motion of the vortices. These high velocities impact a region within approximately 6 inches of the foot. This is the region from which a large majority of the particles are resuspended. Notice, also, that the upward motion of the right foot generates large vertical velocities, helping to elevate the particulate forced out of the carpet by the motion of the left foot.

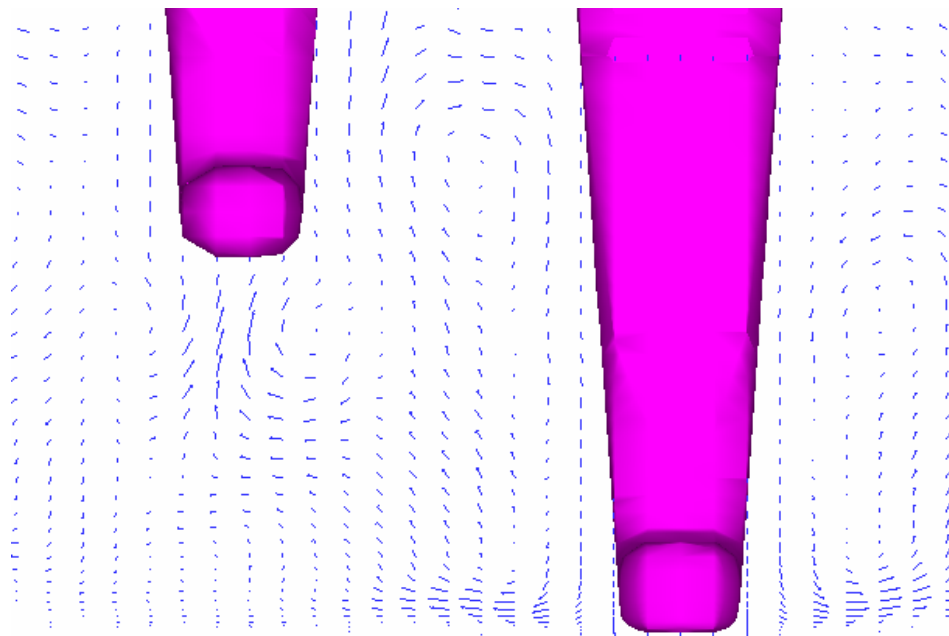


Figure 4-2: Velocity field induced by stomping “feet”

The choice of foot penetration depth has a more substantial effect on the amount of particle mass resuspended. Particles are emitted from all carpet-layer cells into which the foot penetrates. In addition, as the foot moves closer to the floor, higher lateral velocities are generated by the forcing of air out from under the foot. Figure 4-3 compares the mass resuspended by two feet when penetrating halfway into the carpet, versus when stopping at the surface of the carpet. Allowing the feet to penetrate the carpet results in approximately 35% more total mass being resuspended.

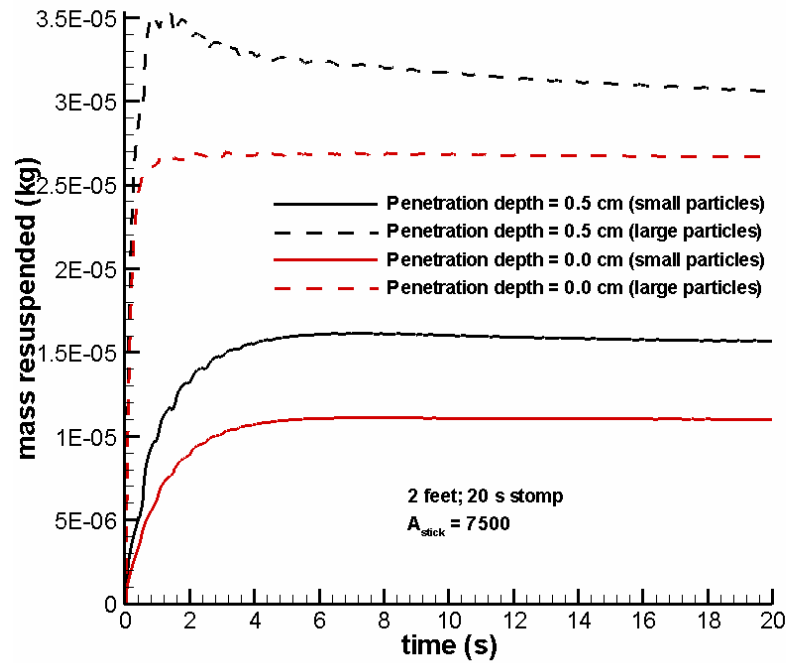


Figure 4-3: Effect of “foot” penetration depth on mass resuspended

Based on the findings of these preliminary simulations, as well as experimental observations, a sticking parameter of $7500 \text{ N}\cdot\text{m}^2/\text{kg}$ and a penetration depth of 0.5 cm were prescribed for the full human-body simulations. These parameters allowed realistic penetration of the carpet layer, while preventing particulates from being transported out of the carpet in regions of low-speed flow.

4.2 Full Human-Body Simulations

As discussed previously, the focus of this study was to predict the particle mass resuspension and transport induced by human-body motion in a vented, carpeted room. Results were obtained for two main simulations, both of which are intended to mimic the experiments performed at the EPA test house. In the first of these full-room simulations,

which will be referred to as Case 1, the “human” stands still for 1.5 seconds, walks forward for 1.5 seconds to the designated location, stamps in place for 20 seconds, and is stationary for the remainder of the simulation. In the second simulation (Case 2), the “human” performs the same sequence of motions, except that its entire body rotates while stamping in place. In both of these cases, the ventilation system (modeled here by two inflow vents) was on for the duration of the simulations.

In the EPA experiments, number concentrations were monitored by particle samplers, which were positioned at five locations throughout the room, and time-averaged over 1-minute intervals. For the purpose of comparison and validation, average concentrations within a 1 ft³ volume surrounding these sampling locations were continuously monitored during the simulations. It should be noted that, although the heights of these probe locations are known from the experiment, the *xy*-locations are approximate.

Table 4-2: Computational Probe Locations

Label	Coordinates (m)
18 source	1.37, 1.29, 0.46
18 MBR door	0.61, 0.30, 0.46
48 MBR door	0.61, 0.30, 1.22
36 bathroom door	3.30, 0.30, 0.91
18 closet	3.91, 0.61, 0.46

Additionally, the total particulate mass (of each size class) in both the air and carpet were tracked in order to determine time-dependent trends of resuspension, deposition, and transport out of the room. The simulations were run for at least 7 minutes of physical time in order to obtain predictions of the particulate concentrations throughout the room.

during the “unsteady” portion of the experiments. It was also a goal of this study to identify a “steady decay” rate of particulate concentration within the room, once a “well-mixed” state is achieved.

In a typical particle-emission event, time-dependent concentrations will exhibit three distinguishable phases of varying growth and decay trends, as described by Mage and Ott [20]. The first is the alpha phase, during which a source emits particulates and concentrations grow, especially near the source. Usually, this phase occurs over a short period of time, relative to the duration of the event, and may display a constant or periodic emission rate, a sudden release of particles, or a more unsteady emission behavior. In this case, the alpha phase involves the walking and stomping of the human body. While the up-and-down motion of the legs is periodic, and the translational and rotational motion of the body is piecewise-constant in time, the unsteady hydrodynamic flow field and complex interactions of the particles with the feet and carpet would make it quite difficult to accurately identify a theoretical time-dependent emission rate.

The second phase is the beta phase, during which the source is no longer emitting particles, but the system is not yet well-mixed. It is during this phase that particles are transferred to different regions of the system by forces such as hydrodynamic drag. Also during this phase, high deposition rates may be exhibited by large particles (those too large to become entrained in the mean flow once alpha-phase forcing has stopped), and turbulent diffusion may promote the spread of small particles. The beta phase involves the inherently unsteady, non-uniform effects that occur in the transition period between concentration growth and decay.

The final phase is known as the gamma phase, during which the system is well-mixed, and concentrations decay as a result of coagulation, deposition, transport out of the system, and other effects. It is during this phase that time-dependent concentrations are most easily predicted by theoretical means, as most effects at this stage are steady and nearly uniform. The present simulations are intended to include all of the alpha and beta phases, as well as part of the gamma phase so that a steady decay rate may be identified and used to predict conditions beyond the duration of these simulations.

Figure 4-4 shows snapshots of the first 4 seconds of the Case 1 simulation, depicting particle number concentration iso-surfaces representative of ten times the background concentrations. The lavender iso-surface represents the small particles, and the magenta represents the large. This figure clearly illustrates the resuspension of particulate as induced by the human walking. Notice, in the first two frames, that most of resuspended particles emanate from where the foot has penetrated the carpet, or very nearby. For a better understanding of why emissions are localized so near the feet, Figure 4-5 shows the velocity magnitude within the carpet at 2 seconds, when the person is walking forward. Notice that velocities are highest where the foot is penetrating the carpet and where the vents are located. Since only background concentration levels initially exist above the vents, most of the resuspended particles are emitted from where the feet step. Since high velocities also occur in the wake of the feet (behind and to the right of the red “footprint”, for instance), it is likely that many particles are emitted from the carpet where the feet pass over but do not penetrate. Elsewhere in the room, velocities within the carpet stay quite low, thus, it is unlikely that hydrodynamic forces will overcome the applied sticking force entrapping the particulates.

As the human continues to walk, particles become entrained in the person's wake, transporting them forward with the body. After the person has stopped moving forward, the particle cloud continues to advance forward, but also begins to disperse as the wake breaks down. During this initial resuspension period, both small and large particles are emitted from the carpet and are entrained in the wake as a result of the strong hydrodynamic forces induced by the human body.

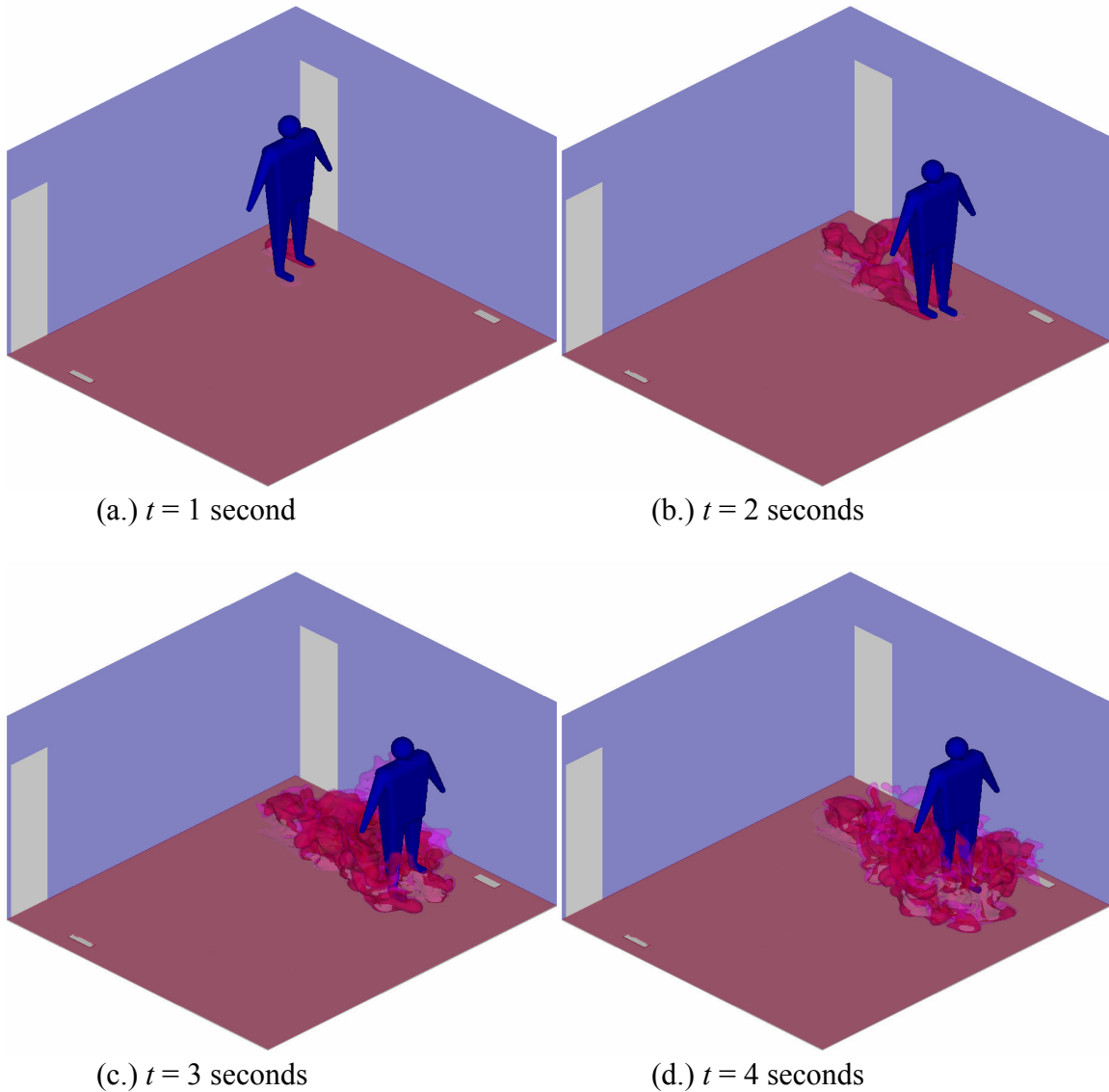


Figure 4-4: Case 1 number concentration iso-surfaces ($10 \times$ background) of small (lavender) and large (magenta) particles at $t = 1$ (a.), 2 (b.), 3 (c.), and 4 (d.) seconds

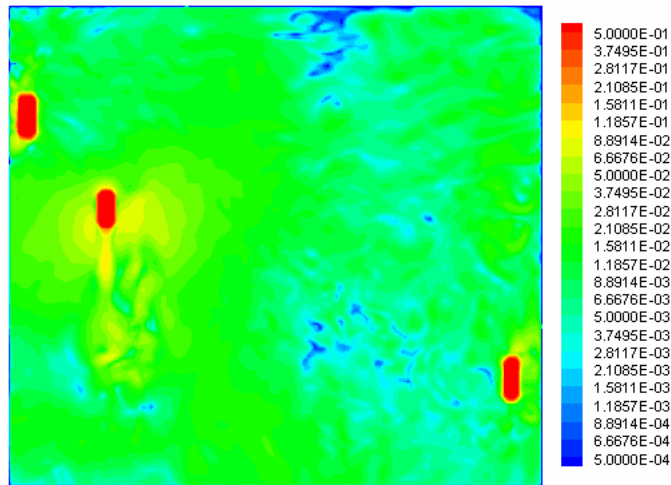


Figure 4-5: Velocity magnitude (m/s) within carpet layer at $t = 2$ seconds

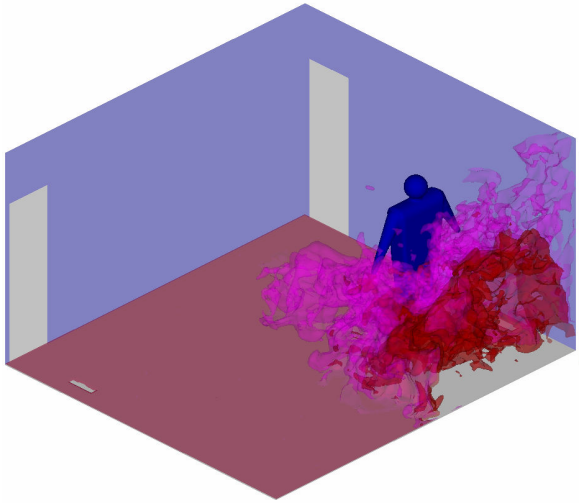
Figure 4-6 shows a sequence of snapshots at 15-second intervals over the first minute of the Case 1 simulation. It can be seen in frame (a.) that the momentum of the wake generated by the forward motion of the human caused large concentrations of particulate to gather between the human and the wall. At this stage, the person is still stomping in place, so alpha-phase forcing has not yet ceased. It can also be seen that small and large-particle motion is starting to deviate, as more small particles have spread toward the ceiling as a result of entrainment in the upward-circulating flow, particularly that caused by the vents.

At 30 seconds, after all immersed-body motion has stopped, the particulate cloud has started spreading to the opposite side of the room (to the right, with respect to the person). This is not an unexpected result, as it is consistent with the circulating flow pattern produced by the vent flow. Figure 4-7 illustrates this flow pattern, showing velocity magnitude iso-surfaces representing 0.5 m/s, several seconds after the human has stopped moving. The upward jet produced by the vent nearest the person aids in propelling the particles upward, once they have been resuspended. The circulation that

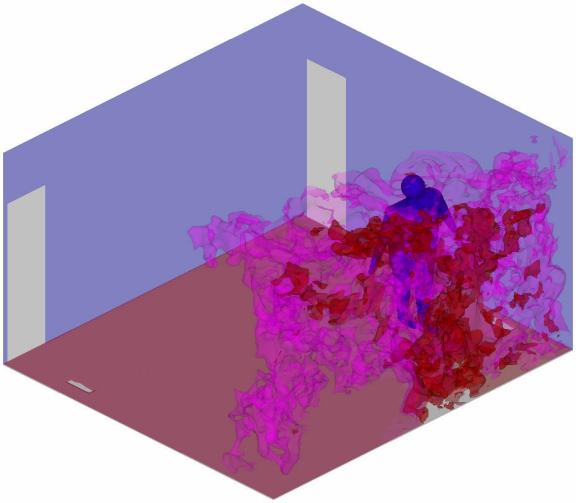
occurs as the flow encounters the ceiling then transports the particles to the person's right.

At 45 seconds (Figure 4-6c), the concentration of large airborne particles has decreased significantly as a result of settling and deposition. At this stage, the strong hydrodynamic forces produced during the alpha phase have mostly dissipated, and buoyancy effects have become more dominant over large-particle motion. The small particles, however, continue to be easily advected throughout the room. Deposition is also evident on the head and shoulders of the person, but this effect is not well accounted for in the present code, and the amount of such deposition is not monitored.

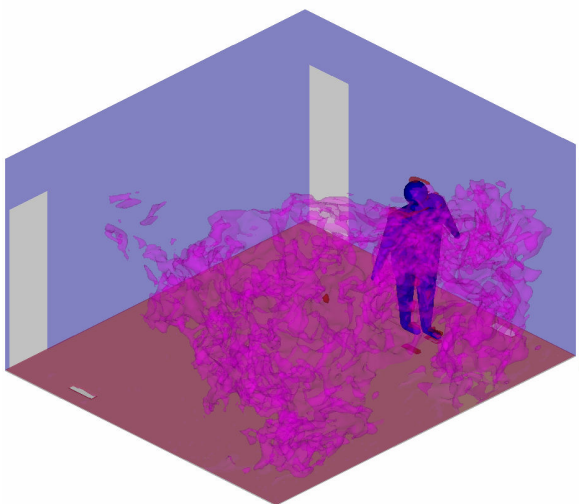
Finally, at 60 seconds (Figure 4-6c), particle concentrations in front of the person have reduced substantially. At this point, enough clean air from the vent has been introduced to dilute local concentrations and force airborne particles to other parts of the room.



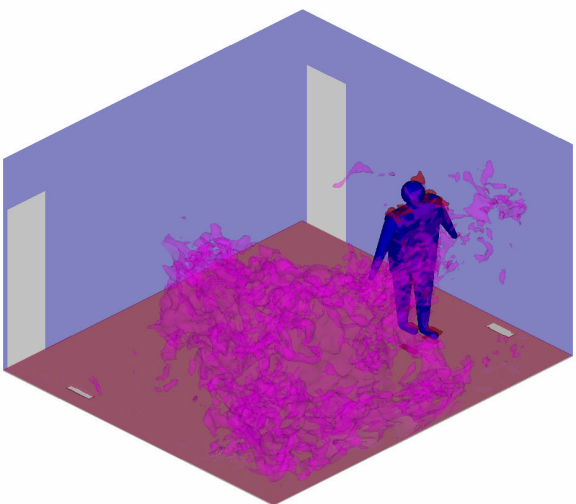
(a.) $t = 15$ seconds



(b.) $t = 30$ seconds



(c.) $t = 45$ seconds



(d.) $t = 60$ seconds

Figure 4-6: Case 1 number concentration iso-surfaces ($10\times$ background) of small (lavender) and large (magenta) particles at $t = 15$ (a.), 30 (b.), 45 (c.), and 60 (d.) seconds

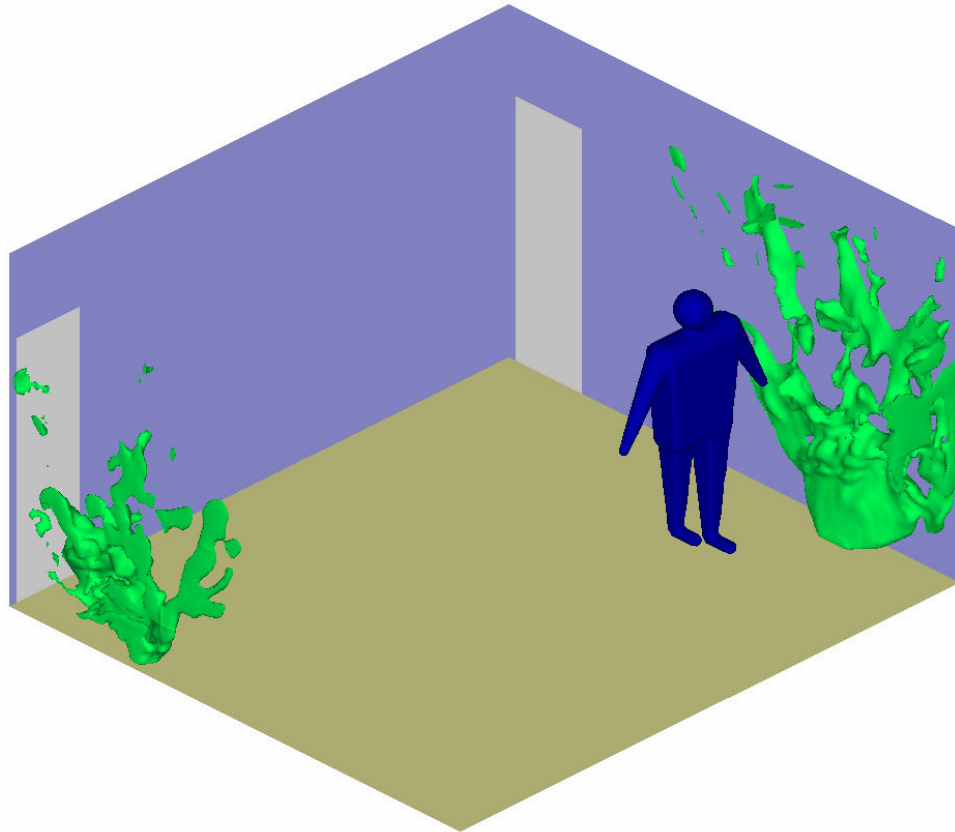


Figure 4-7: Vent velocity magnitude iso-surfaces (0.5 m/s)

Figure 4-8 shows a similar sequence of snapshots to that in Figure 4-6 over the first minute of the Case 2 simulation. Here, it can be seen that the rotating of the human while stomping results in more particles being resuspended. It is also apparent, from frames (a.) and (b.), that the flow pattern induced by the rotating body causes the particulate to spread more quickly throughout the room. At 45 and 60 seconds, significantly more fine particles remain airborne than in Case 1.

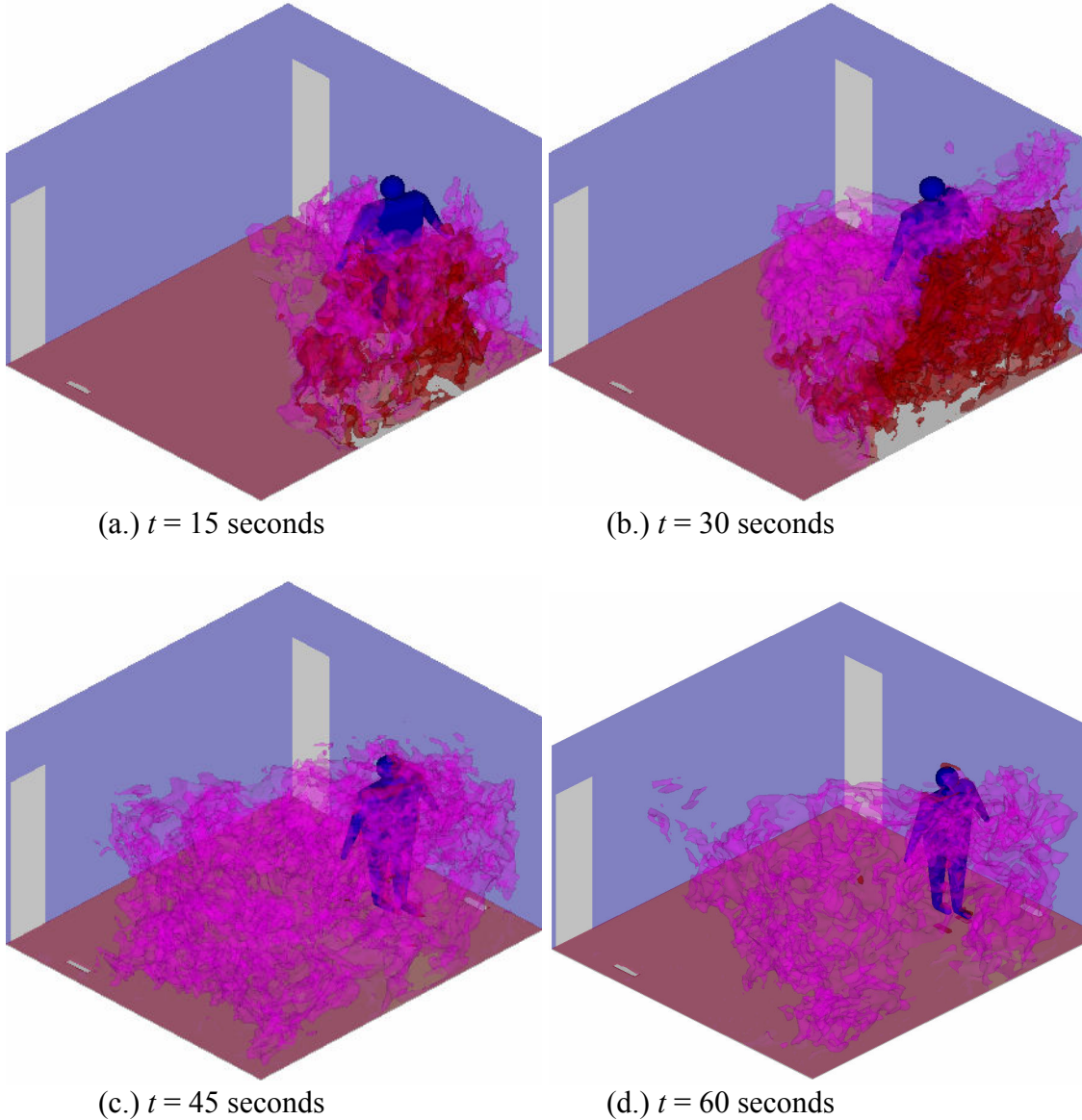


Figure 4-8: Case 2 number concentration iso-surfaces ($10 \times$ background) of small (lavender) and large (magenta) particles at $t = 15$ (a.), 30 (b.), 45 (c.), and 60 (d.) seconds

Figure 4-9 shows a comparison of small and large-particle behavior in Case 1, viewed on a plane bisecting the human, during the first minute. Contour levels here range from the background concentration ($\#/\text{ft}^3$) to 100 times that value. During the first 10 seconds, the results are somewhat similar between the small and large particles,

although it is apparent that small-particle concentrations are somewhat higher (relative to the background level). By 15 seconds, it is apparent a greater number of large particles have settled back into the carpet, while more small particles have remained airborne. It can also be seen that a significant number of small particles have been transported toward the ceiling by the vent jet (located near the bottom-right corner). Figures 4-9d and 4-9e show clearly how the circulation generated by the vent flow transports the particulate through the room. In this viewing plane, a mean counter-clockwise circulation is apparent, which transports particles upward first, then across the room (to the viewer's left), then back down, and finally toward the right. By 30 seconds, many of the large particles have re-settled, and those remaining are well entrained in the circulating flow. At 45 seconds, the small particles are approaching a well-mixed state in this part of the room, but the large particles are taking longer to respond to the mixing effects due to greater inertia and gravitational forces.

Figure 4-10 shows the same particle concentration contours for Case 2 as those shown in Figure 4-9 for Case 1. It is obvious from looking at the first few frames that initial airborne concentrations of both small and large particles are higher, indicating more overall resuspension. This result can be attributed to more area of carpet being penetrated by the feet. In addition to the higher concentration levels, the particles also appear to mix more quickly within this viewing plane than in Case 1. This is very apparent in Figure 4-10e, in which small particles appear very well-mixed, and large particles are approaching such a state.

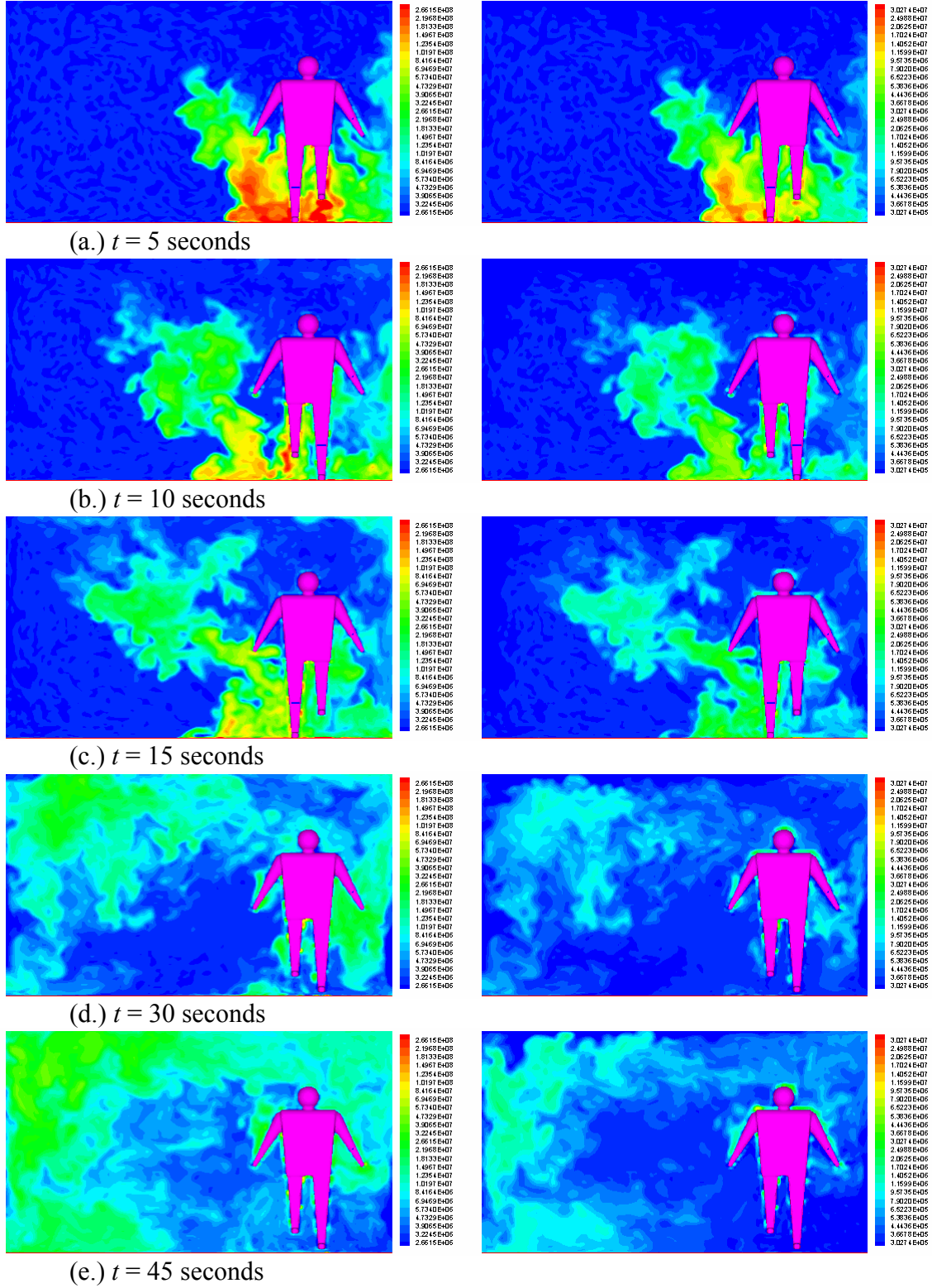


Figure 4-9: Small (left) and large (right) particle concentrations ($\#/ft^3$) at $t = 5$ (a.), 10 (b.), 15 (c.), 30 (d.), and 45 (e.) seconds for Case 1

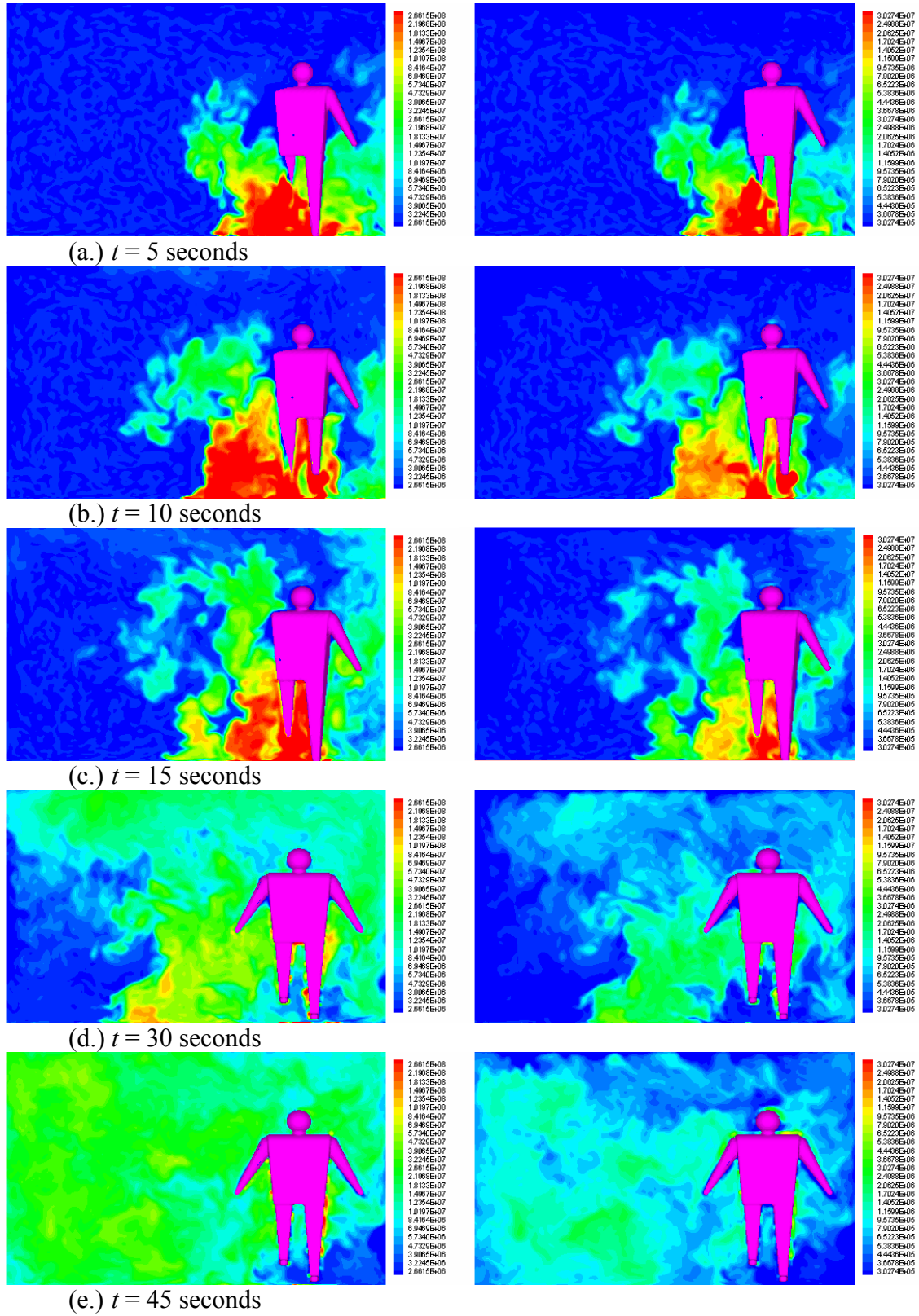


Figure 4-10: Small (left) and large (right) particle concentrations ($\#/ft^3$) at $t = 5$ (a.), 10 (b.), 15 (c.), 30 (d.), and 45 (e.) seconds for Case 2

For a better illustration of how particulate is transported through the entire room, Figure 4-11 shows the small-particle number concentrations at a height of 1.22 m (half the height of the ceiling) at 1-minute intervals. The contour levels here are the same as those in Figure 4-9 and 4-10, ranging from the background concentration to 100 times that value. At 1 minute, it can be seen that concentration gradients are still large, and a significant portion of the room has not yet been filled with a substantial number of particles. Eventually, however, the particles are transported through the room, in a mostly clockwise manner (with respect to the present viewpoint), and concentrations become much more uniform. By 3 minutes, concentration gradients have diminished enough that the room could perhaps be considered well-mixed.

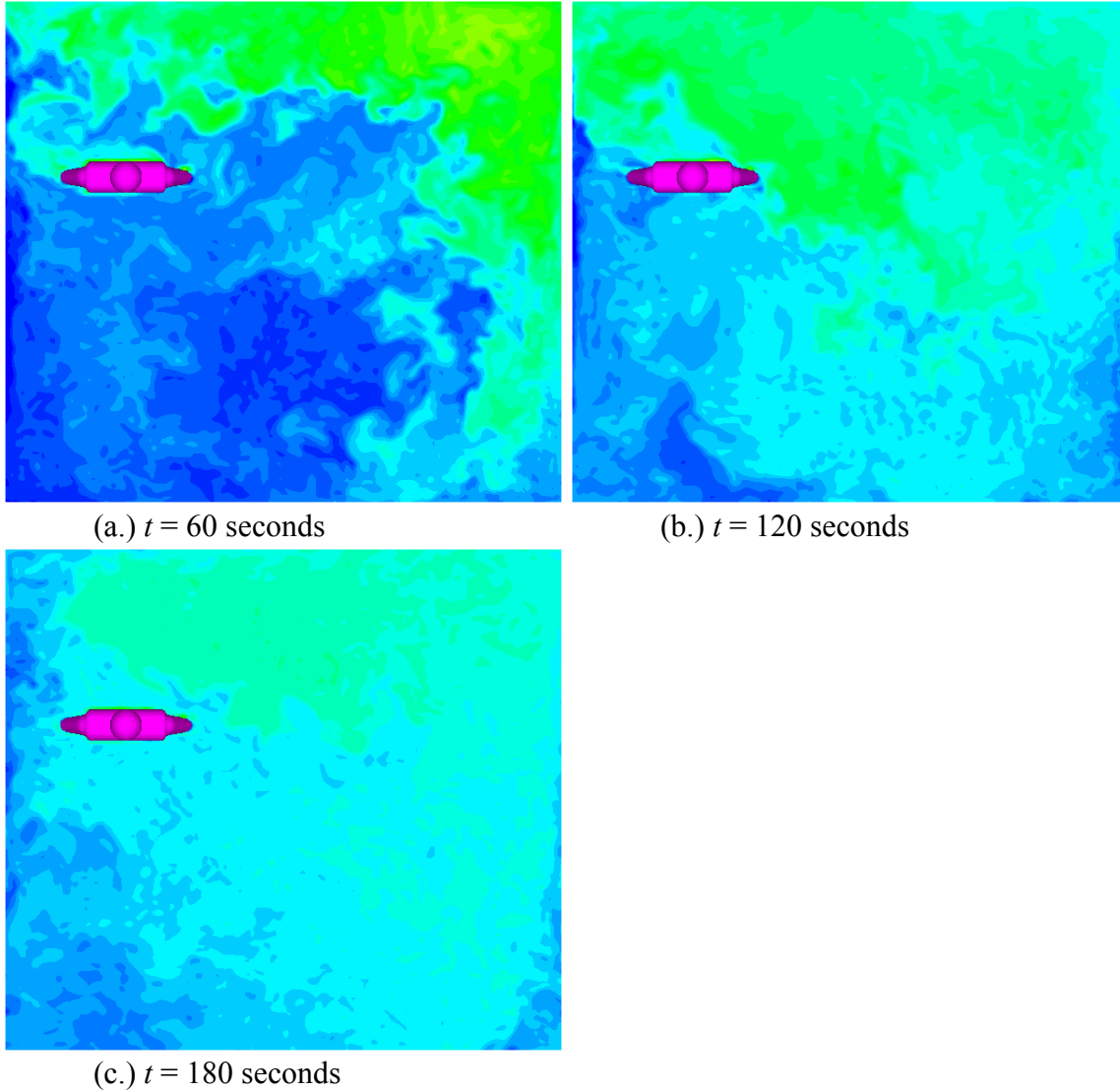


Figure 4-11: Small-particle concentrations ($\#/ft^3$) at $t = 60$ (a.), 120 (b.), and 180 (c.) seconds for Case 1

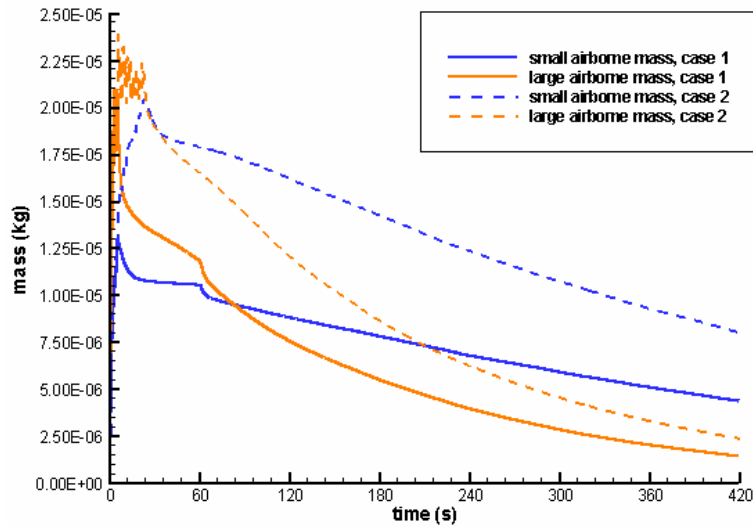
By the time the room has become well-mixed, most of the remaining airborne particulate mass is due to small particles. This can be seen in Figure 4-12, which shows the airborne particle mass due to small and large particles in the entire room over the duration of the simulation. The total mass of large particles resuspended was greater, but more small-particle mass remained airborne. The fact that more large particle mass was resuspended is not a surprising result. Since 72.5 % of the mass initially in the carpet

was due to large particles, and the large particles were exposed to a weaker sticking force than the small ones, it is obvious that more of the resuspended mass should be from the large particles. However, the greater gravitational effects, and thus, higher settling rate, causes most of the large-particle mass to settle out. By the end of the Case 1 simulation, the ratio of small-particle mass to large-particle mass that remained airborne was approximately 3.0. For Case 2, this ratio was 3.4. Since the small particles contained only 4.3 % as much mass per particle as the large particles, this discrepancy is much greater when comparing the number of airborne particles.

Notice also, in Figure 4-12, that the mass of large airborne particles oscillated during the alpha phase in Case 2 – a trend that was not exhibited in Case 1 or by the small particles in Case 2. These oscillations can be attributed to two opposing effects: one being the settling of the large particles while the person is still rotating, and the other being the resuspension of additional large particles as the person is stomping. The reason this trend does not occur in Case 1 is that, since the human is stomping in place without rotating, no new areas of carpet are being disturbed, and therefore, little additional particle mass is resuspended during the stomping. The small particles do not exhibit this trend in either case because hydrodynamic forces predominate the buoyant forces to which they are subjected.

It is also interesting to note the difference in settling trends between the two cases. In Case 1, for both sizes of particulate, a large drop in mass levels occurs around 5 seconds. This is shortly after the person has stopped moving forward and during the march-in-place portion of the simulation. This means that the immediate settling of particles not exposed to strong enough hydrodynamic forces to stay airborne

predominates the resuspension of additional particles by the stomping in place. The drop in large-particle mass at this point is, of course, greater than that of the small particles as a result of the greater settling rate. In Case 2, the most significant decrease in airborne particle mass occurs, for both particle sizes, at 23 seconds – just when the human has stopped stomping and turning. Thus, the turning while stomping causes enough additional particles to be resuspended that airborne mass levels do not drop off significantly until stomping has ceased. This is due to the feet penetrating new areas of carpet while rotating, resulting in more “fresh” mass being resuspended, as opposed to Case 1 in which the same area of carpet is disturbed continuously. It should be noted, however, that the large-particle mass in Case 2 peaks before the oscillations begin and drops off slightly during the course of the stomping and turning, indicating that the settling rate is slightly higher than the emission rate during this period.



(a.)

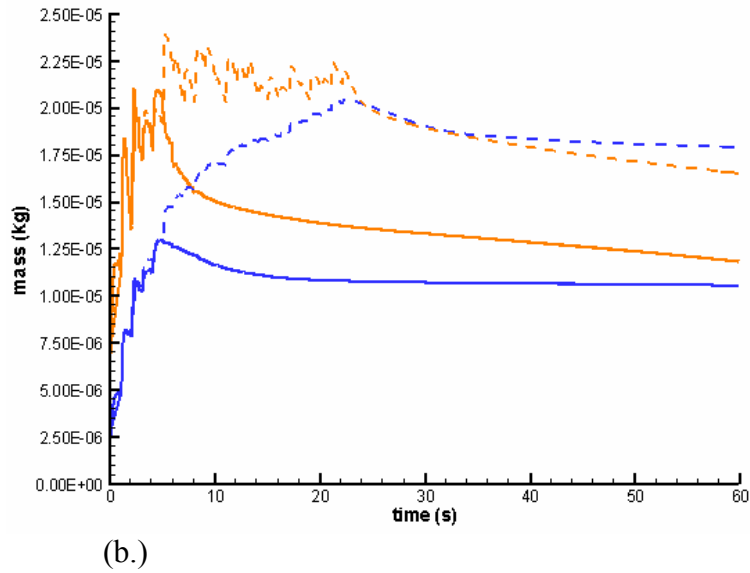
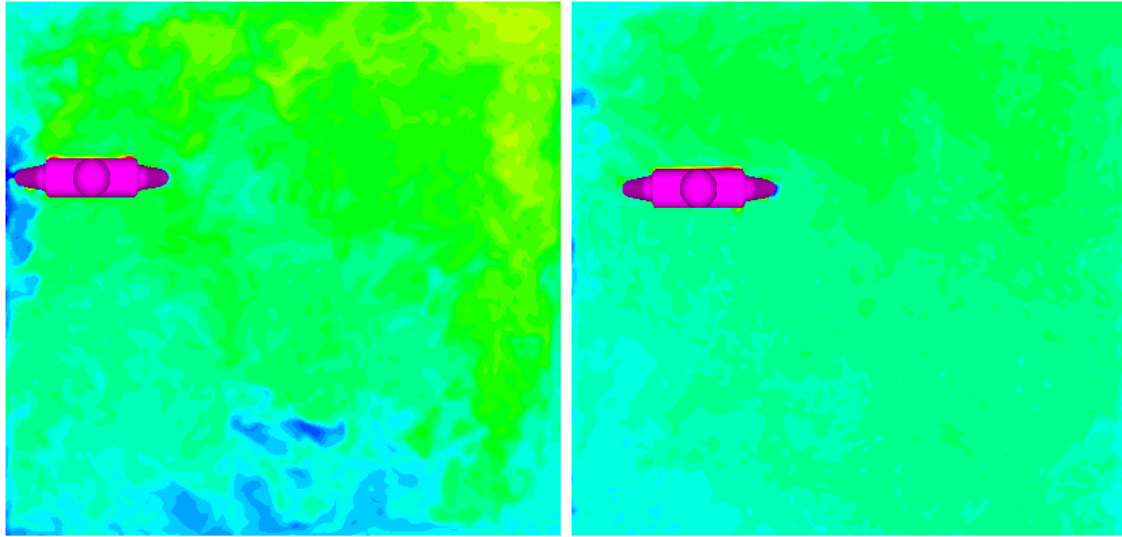


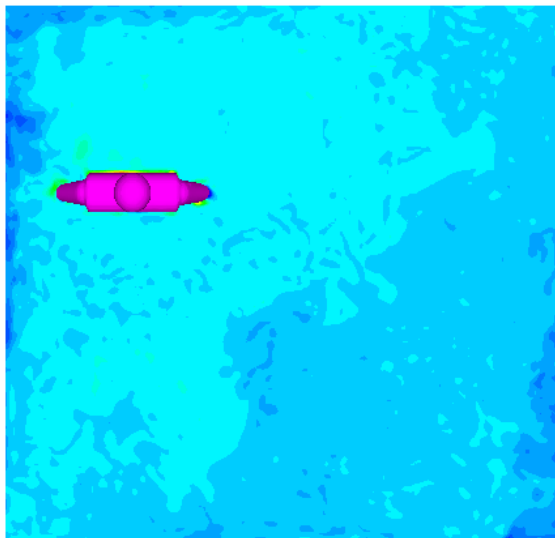
Figure 4-12: Comparison of small and large airborne particle mass in entire room over entire simulation (a.) and first minute (b.)

In Case 2, a well-mixed state is achieved in the room much earlier, as can be seen in Figure 4-13. The rotating motion of the human appears to promote mixing, in addition to allowing more particles to resuspend. In this case, the room can be considered well-mixed after only 2 minutes.



(a.) $t = 60$ seconds

(b.) $t = 120$ seconds



(c.) $t = 180$ seconds

Figure 4-13: Small-particle concentrations ($\#/ft^3$) at $t = 60$ (a.), 120 (b.), and 180 (c.) seconds for Case 2

In order to compare the results of the simulations with those of the EPA experiments, the concentrations at five probe locations throughout the room were time-averaged over 1-minute intervals. It can be seen in Figure 4-14 that, with a few exceptions, experimental number concentrations at the various probes tended to be higher

than those in the Case 1 simulation, but lower than those in Case 2. The greatest discrepancies occurred at the probe located near the source of the particulates (where the person was stomping), at a height of 18 inches. Since this location is so close to the person, it is likely to show large fluctuations in concentration. The concentrations observed are also more strongly influenced by the motion of the person.

Since neither simulation of the human body *exactly* matches the motion of the actual human subject in the experiment, it is not surprising that there would be significant discrepancies in the results near the source. However, it is unclear at this point why the experimental source probe concentration did not peak after the first minute (it instead peaks after the second and fourth minutes). This is surprising, given that all alpha-phase forcing occurs during the first minute. It may be due to localized effects that occurred during the experiment, perhaps due to the presence of the sampling apparatus, which was not modeled in the simulations. More favorable, however, is the fact that source probe concentrations in all three cases exhibit a secondary peak after the fourth minute. This peak is likely due to a re-circulation of particles back into the region, as dictated by the mean flow in the room.

Predicted concentrations at other probe locations tended to be closer to the experimental results. Notice that, in each case, concentrations toward the end of the 7 minutes were nearly uniform as a result of mixing effects. Also, concentrations in all cases exhibit a somewhat steady decay trend over the last 2 minutes. This can be seen more clearly in Figure 4-15, which shows the average of the (time-averaged) probe concentrations. This quantity has little significance when the room is not yet well-mixed, but it gives a more clear comparison of decay rates over the last few minutes.

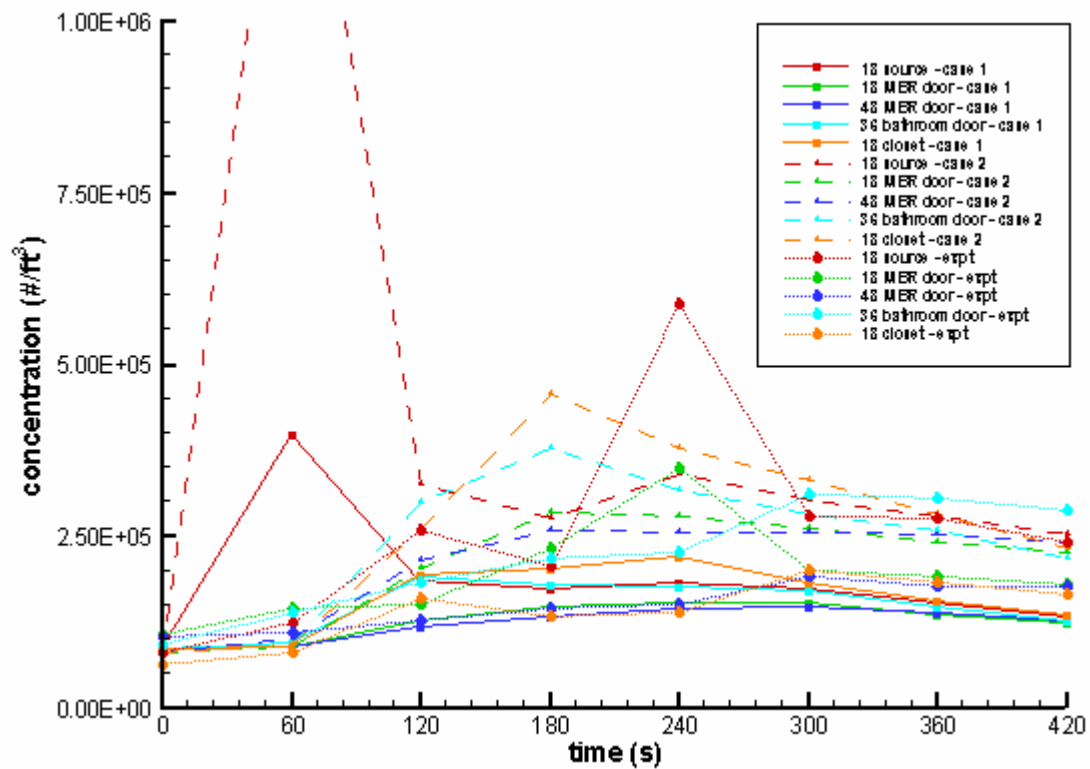


Figure 4-14: 1-minute time-averaged probe concentrations

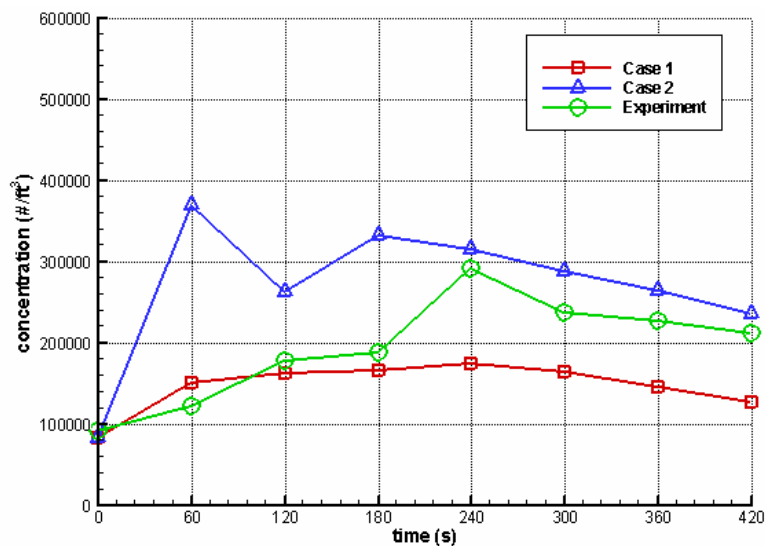


Figure 4-15: Average of probe concentrations

It is important to note that some of the error in the airborne particle concentrations seen in these simulations is due to the use of a discrete population density function.

Since the actual size distribution of particles is continuous, the simulation results may not accurately predict results that are due largely to particles of very small or large diameters. For instance, Figure 4-12 indicates that many more small particles are airborne near the end of the simulations than large particles. In the experiment, particles much smaller than 2.7 μm are present, which could account for a significant portion of the airborne particles at 7 minutes. Thus, it stands to reason that if more discrete size classes were modeled, the Case 1 simulation might more closely predict the number concentration at 7 minutes, and the Case 2 simulation might over-predict by even more.

Figure 4-16 shows the instantaneous number concentrations at the probe locations for the two simulations (shown on a log-scale). While no such data was available for the experiment, the instantaneous data better depicts the short-term temporal behavior of particle concentrations. It also illustrates how well-mixed the room is throughout the simulations. From this figure, the room appears to be fairly well-mixed, in both cases, at around 2 minutes and continues to become more uniformly mixed through the rest of the simulation.

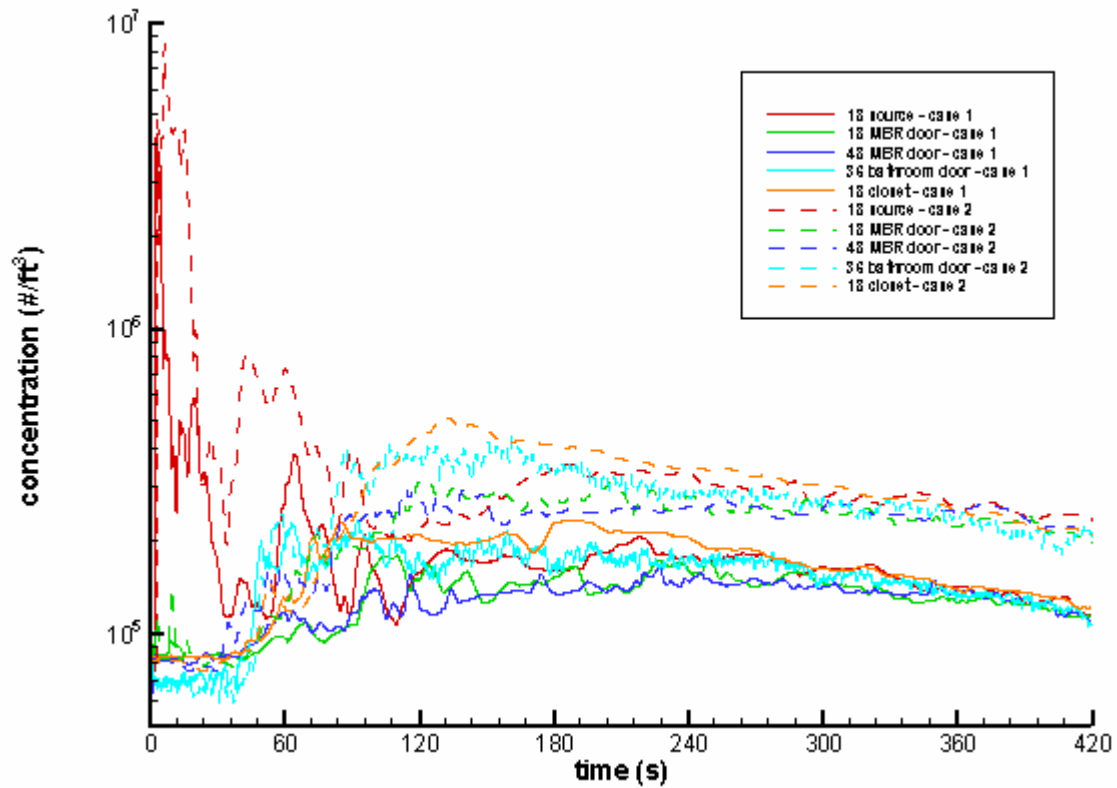


Figure 4-16: Instantaneous probe concentrations

In order to assess how accurately the probe measurements approximate the airborne particle mass present in the room, an average of the instantaneous probe concentrations was taken and converted to a mass approximation, assuming uniform mixing. This approximation is compared with the actual airborne mass present in the room in Figure 4-17. Here, it can be seen that the probe-average approximation approaches the actual mass value as the room becomes more uniformly mixed. Thus, the probe measurements should not be considered an accurate representation of conditions throughout the entire room until after about 5 minutes of mixing time.

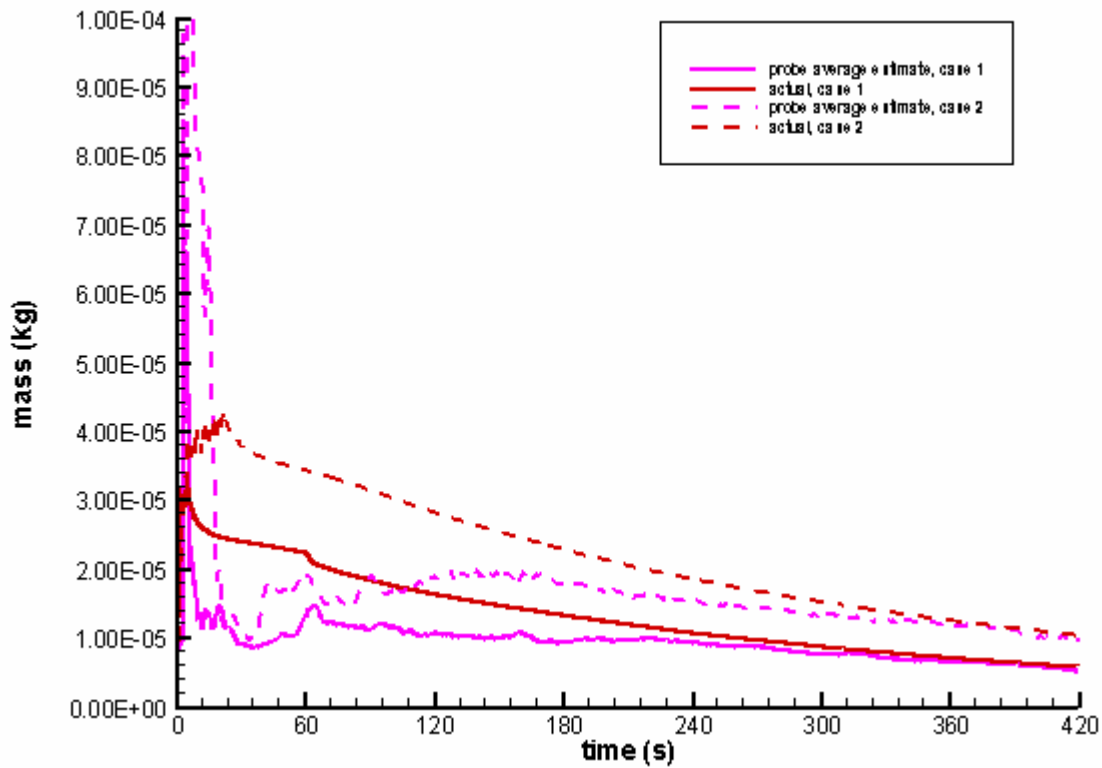


Figure 4-17: Comparison of probe-average estimate with actual mass in room

Once the room has become well-mixed, expensive computations become less necessary to predict the particulate concentrations within the room. By this point, concentrations throughout the room are more uniform, and the rate of change in airborne mass is more steady. Particle decay in this system is primarily a function of settling and transport out of the room, both of which are easy to determine, analytically.

The airborne particle mass can be predicted, as a function of time, based on the volumetric flow rate and net settling velocities. At a time when the room is well-mixed, the mass rate of change can be approximated as:

$$\frac{dm}{dt} = -\frac{q(m_1 + m_2)}{\nabla_{mix}} - \frac{w_{s,1}A_{floor}m_1}{\nabla_{mix}} - \frac{w_{s,2}A_{floor}m_2}{\nabla_{mix}} \quad \text{Eq. 4-1}$$

where q is the volumetric flow rate (which can be determined from the vent flow rate), $w_{s,k}$ is the terminal settling of size class k , A_{floor} is the area of the floor, and ∇_{mix} is the “active mixing volume” of the room. The active mixing volume is a relative measure of how well-mixed the system is, and its significance will become clear shortly. The Stokes Law form of terminal settling velocity for a particle of diameter d_k is given by:

$$w_{s,k} = \frac{\rho_p g d_k^2}{18\mu} \quad \text{Eq. 4-2}$$

where g is a the gravitational acceleration constant. Note that, in Eq. 4-1, it is assumed that the net settling rate of particles is due strictly to net buoyancy. Integrating Eq. 4-1, the mass as a function of time can be found:

$$m(t) = m(t^*) \exp(a(t^* - t)),$$

$$\text{where } a = -\left[\frac{q(m_1 + m_2) + w_{s,1}A_{floor}m_1 + w_{s,2}A_{floor}m_2}{\nabla_{mix}(m_1 + m_2)} \right], \quad \text{Eq. 4-3}$$

and t^* is a time chosen at which the room is well-mixed. Thus, the above analysis predicts an exponential decay of airborne particle mass.

The parameter $\forall_{mix}$, the active mixing volume as given by Young and Lees [32], is a relative measure of how well-mixed the system is. In a perfectly-mixed situation, $\forall_{mix}$ would be taken as the volume of the entire system (in this case, that of the room). However, in most cases, error is incurred when a perfectly-mixed system is assumed. In the present case, particles may be very well-mixed in the middle of the room, but concentrations may deviate near the vent inflow or the ceiling. Thus, a mixing volume slightly smaller than the room is assumed. Since $\forall_{mix}$ is the only free parameter in this solution, its value can be approximated by fitting the function to the mass results obtained in the simulations.

Figure 4-18 shows the airborne mass results of the simulations (for both cases) compared with theoretical mass curves. One of the theoretical curves (in each case) assumes uniform mixing, while the other is fit to the actual mass by adjusting the mixing volume parameter. In these curves, the reference mass, $m(t^*)$, was taken at $t^* = 420$ seconds, as the room is very well-mixed at this time. Thus, all of the mass curves converge at 420 seconds. This comparison shows that the airborne mass decay rate in the room is, indeed, exponential. The theoretical curve for perfect mixing does not match the actual mass curve well, as it under-estimates the particle decay rate. By adjusting the $\forall_{mix}$ parameter, however, a theoretical approximation can be obtained that very closely predicts the actual mass during the gamma phase. For Case 1, a good curve-fit was achieved using $\forall_{mix} = \frac{2}{3} \forall_{room}$, and for Case 2, $\forall_{mix} = \frac{5}{7} \forall_{room}$ produced an accurate approximation. Thus, the additional rotating of the person in Case 2 resulted in a slightly higher active mixing volume.

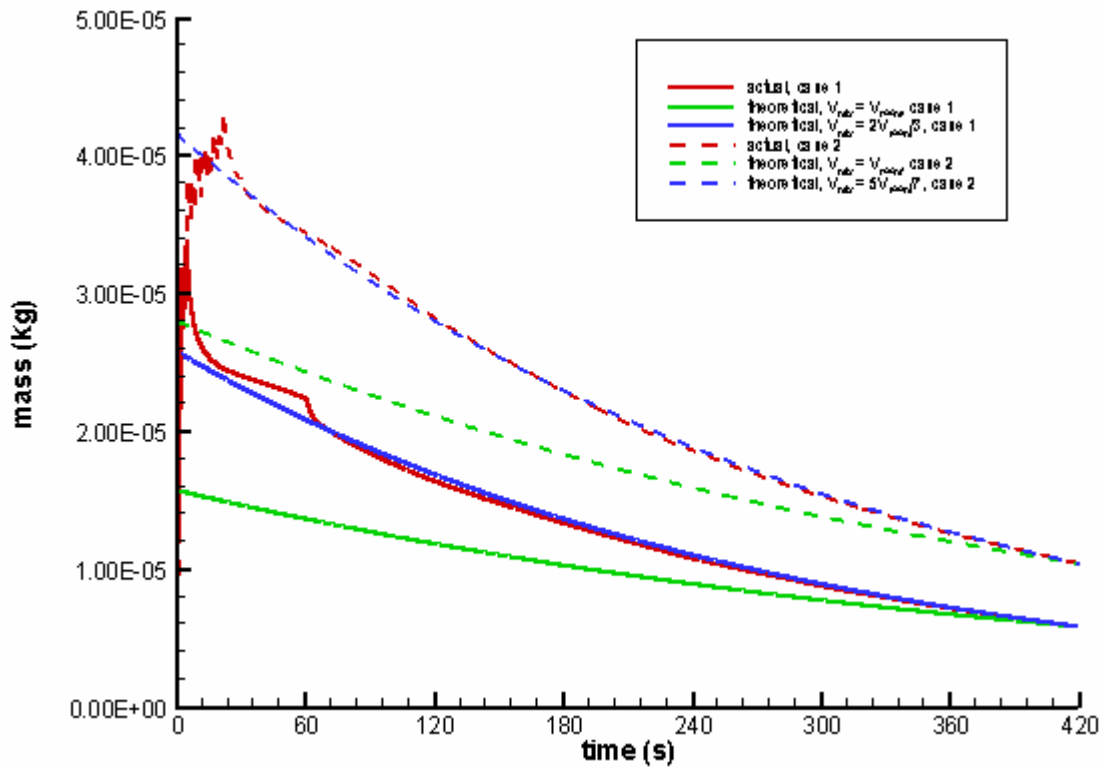


Figure 4-18: Theoretical airborne mass curve-fits

It should be noted that the mixing volume approximations assume that the volumetric flow rate is accurate. Since the flow rate was determined from an approximate vent velocity, it could be that the actual flow rate is greater than that estimated here, which would account for some of the difference between the actual and theoretical decay rates. If this is the case, the active mixing volume will be closer to the total room volume.

5 Concluding Remarks

A large-eddy simulation method for solving incompressible, particle-laden flows with embedded moving solid bodies has been developed. Spatial discretization is performed by a low-diffusion upwind difference scheme in conjunction with weighted essentially non-oscillatory variable extrapolation. Time integration is facilitated by an artificial compressibility approach with dual time-stepping. The particle motion is solved by an Eulerian approach, which requires separate solutions for each size of particle simulated. The motion of moving bodies is simulated by an immersed boundary method, which forces fluid and particle fields to respond to the moving surfaces, without requiring grid-adaptation.

Several validation and proof-of-concept simulations were performed to assess the accuracy of the immersed boundary methods. These simulations included the two-dimensional cases of steady low-Reynolds number flow over a stationary (relative to the grid) cylinder, steady high-Reynolds number flow over a stationary NACA 0012 airfoil, and movement of a cube and cylinder through a particulate-filled channel. The two stationary cases yielded results that agree closely with prior studies, despite using Cartesian non-body-fitted grids. The moving cylinder and cube simulations show realistic results with good mass conservation. Three-dimensional cases included steady (axisymmetric and asymmetric) and unsteady flow over a stationary sphere and movement of multiple immersed bodies through a chamber with a particulate source. The sphere simulation predicted both steady and unsteady flow characteristics that agree well with previous studies. The simulation of multiple three-dimensional immersed bodies yielded good mass conservation and realistic transport of particles.

The immersed boundary method was applied to the simulation of particulate resuspension and transport induced by the motion of a human body. The simulations involve a “human” walking through a room and stamping in place, causing particles to be emitted from a carpet in which they are embedded. The carpet is modeled as a porous medium, which is accounted for in both the fluid and particle governing equations. The simulations were carried out for several minutes such that theoretical decay rates of particle concentration due to settling and transport out of the room could be approximated. Time-dependent concentrations were monitored at several probe locations in order to compare the simulation results with experiments performed by the EPA and RTI.

The simulations yielded similar levels of particle concentration in the room to those of the experiment. Most of the particles resuspended originated from the carpet very near where the “feet” penetrated. Therefore, the particular motion of the feet in each case had a large influence on how much particulate mass was resuspended. Most of the mass initially resuspended was due to large particles, but many of these settled out before they could be transported very far through the room. After a few minutes, the room became well-mixed with particles, and most of the remaining airborne mass was due to small particles.

While the concentrations observed in the simulations were similar to the values observed in the experiment at most locations, some localized discrepancies did occur. Possible sources for such error include the lack of resolution of fine-scale effects within the carpet layer, the discrete particle population density function, and the lack of

modeling of the experimental apparatus as physical boundaries within the room, as well as the uncertainty of their precise location.

6 Recommendations

While the immersed boundary approach presented in this paper has yielded promising results, there are several areas in which the method can be improved, or in which further testing should be done to assess its accuracy. Upon some further research and development, many avenues exist for the use of this model in future applications.

One of the weaknesses of the present model involves the modeling of interactions that occur within the carpet between the fluid, particles, fibers, and feet. Currently, the computational model accounts for drag resistance imposed on the fluid by the carpet, adhesion forces imposed on the particles initially trapped in the carpet, and displacement of particles by the feet. However, the model does not account for the effects on the porous characteristics of the carpet due to compression by the feet. Nor does it account for direct particle-carpet interactions once the particles have been dislodged.

The likely result of compression of the carpet is a decrease in porosity. The carpet would subsequently impose greater drag on the fluid while compressed. Another effect to consider would be the recoil of the carpet once the foot is lifted. Some particles, rather than being dislodged as a result of displacement by the foot, may remain trapped in the carpet throughout compression and recoil. Once particles are initially dislodged from the carpet (adhesion forces are overcome), further interactions that are not currently modeled occur between the fibers and particles. For instance, the structure of the carpet will prevent some particles from being transported even after adhesion forces are overcome, thus, filtering out some of the airborne (dislodged) particles. This filtering effect could be implemented by introducing a particle-capture probability based on

“effective pore diameter” statistics. While the mesh resolution in the current simulations is not fine enough to directly model all of the carpet interactions discussed here, finer-scale simulations and additional experiments with greater emphasis on resuspension mechanisms could aid in developing more accurate volume-averaged approximations.

Further insight into the accuracy of the present results can easily be gained by increasing the number of particle sizes simulated. As previously discussed, the large proportion of airborne mass is due to large particles early in the simulations, and due to small particles late in the simulations. Since only two particle sizes were simulated, the results neglect the potentially significant contributions of much larger and much smaller particles. Using more size classes would provide a more accurate particle size distribution and reveal how much error is incurred by using fewer size classes.

Much more analysis of the accuracy of the computational model can be performed if new experiments designed specifically for CFD simulation are carried out. Since the experiments simulated in this study were not designed and conducted with the goal of CFD simulation, several difficulties occurred in designing an adequate simulation and comparing results. With better-coordinated experiments, the exact conditions and measurement procedures can be more easily duplicated computationally, and results can be compared with more certainty.

For example, if the motion of the human subject is more controlled (less random), it can be approximated better by the immersed-body time-dependent motion algorithm. Also, if particle concentration measurements are taken at much smaller time increments, then comparisons of time-dependent concentrations can be made during the forcing stage of the experiment/simulation, instead of relying on data averaged over 60 seconds. This

would also reduce the amount of computing time required before an initial comparison of results can be made. Further difficulties can be avoided by recording the exact location of experimental sampling apparatus and all of the physical boundaries (tables, equipment, etc.) within the room. With this information, more accurate predictions of particle concentrations can be made, as the local flow field will be correctly modeled. Also, since the steady-state decay rate of particle concentration is strongly dependent on the volumetric flow rate out of the room, great care should be used in determining this quantity (rather than just an approximate vent velocity).

Finally, in the current model, all particles that contact the moving body remain airborne. In reality, however, some of the particles that contact the person, either by deposition or impaction, will be captured. Incorporating a physically accurate surface-capturing model would improve the accuracy of this approach and provide additional useful feedback.

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