Experimental Evaluation of a Markov Multi-Zone Model of Particulate Contaminant Transport

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ABSTRACT

The performance of a Markov chain model of the three-dimensional transport of particulates in indoor environments is evaluated against experimentally-measured supermicrometer particle deposition. Previously, the model was found to replicate the predictions of relatively simple particle transport and fate models; and this work represents the next step in model evaluation. The experiments modeled were: 1) the release of poly-dispersed particles inside a building lobby, and 2) the release of mono-dispersed fluorescein-tagged particles inside an experimental chamber under natural and forced mixing. The Markov model was able to reproduce the spatial patterns of particle deposition in both experiments, though the model predictions were sensitive to the parameterization of the particle release mechanism in the second experiment. Overall, the results indicate that the Markov model is a plausible tool for modeling the fate and transport of super micrometer particles.

KEYWORDS

exposure model, model evaluation, particle dispersion, particle transport

INTRODUCTION

The transport and fate of supermicrometer particles, those with aerodynamic diameters ≥ 1 μm in indoor environments are important to public health. For example, particles containing infectious agents emitted from the respiratory tract vary in size by several orders of magnitude, and contribute to the transmission of numerous infectious diseases (Nicas et al., 2005). While there are many models available and appropriate to predicting the transport of particles in indoor environments, the authors have focused on the application of a Markov chain. Previously, the authors developed theory to support the application of a Markov chain to predict the three-dimensional transport and of airborne gaseous and particulate contaminants (Nicas, 2000, 2001, 2010; Jones, 2008), and applied this Markov model to the transport of *Mycobacterium tuberculosis* in aircraft (Jones et al., 2009). The evaluation of the Markov model performance, however, is incomplete.

The evaluation of a mathematical model is a multi-step process that includes: 1) development and verification of a theoretical basis for the mathematical construct, 2) benchmarking model predictions against related models, 3) evaluation of the model predictions with experimental data obtained in relatively simple contexts, and 4) evaluation of the model predictions with real-world data reflecting real-world problems. In the accompanying paper (Jones and Nicas, submitted), the Markov model predictions were benchmarked against traditional models of elutriation, stirred settling and turbulent eddy diffusion. In addition, Chen et al. (2013) showed that a different Markov model of particle transport utilizing CFD-estimated advection and turbulence was able to reproduce CFD-estimated of particle transport. Herein, the Markov model predictions are evaluated against experimental data obtained in relatively simple contexts.

The performance of mathematical models with respect to supermicrometer particle transport and fate have rarely been published in the peer-reviewed literature. This may be due to the scarcity of appropriate data, or to unsatisfactory model performance. Most experiments measuring particle transport and fate, not particle loss rates from air, use particles with aerodynamic diameters ≤ 3 μm (Murakami et al., 1992; Lu and Howarth, 1996; Miller and Nazaroff, 2001; Richmond-Bryant et al., 2006a, 2006b; Zhang and Chen, 2007). Larger particles, however, are also relevant to public health, but only two experiments were identified that involved particles with $d_a \geq 10$ μm (Sajo et al., 2002; Jones and Nicas, 2009).

Herein we evaluate the performance of the Markov model with respect to the experimental results of Sajo et al (2002) and Jones and Nicas (2009). Sajo et al (2002) simulated the accidental release of radioactive materials by releasing poly-dispersed cobaltosic oxide ($^{59}Co_3O_4$) dust in the empty, unoccupied lobby of a university building. Jones and Nicas (2009) released mono-dispersed fluorescein-labeled particles into a room-scale chamber under natural and forced mixing conditions. These studies have been selected because they feature: particles with appreciable rates of gravitational settling, descriptions and/or data about airflow, extensive monitoring of particle deposition on the room floor, and simple experimental conditions. For details of the

Markov model, the reader is referred to Jones and Nicas (submitted): Here we present only the features of model implementation for the two experiments.

METHODS

Sajo Experiment & Model

The environment studied by Sajo et al (2002) was the two-story lobby of a university building, which contained no furniture or human activity. The geometry was rectangular (400 cm $\times$ 660 cm $\times$ 1040 cm high, 275 m^3), with a second-floor mezzanine that protruded 1 m into the lobby air space. The reader is referred to Sajo et al. (2002) for a graphical depiction of the lobby. The environment was modeled using zones with length aspect Δx = 50 cm (see Supplementary Materials S1.2 for justification), such that the interior dimensions of the room were represented by 8 $\times$ 13 $\times$ 21 zones for a 400 cm $\times$ 650 cm $\times$ 1050 cm high modeled room. Adding two zones along each dimension to represent room surfaces, yields a total of 3,450 zones of which 1,258 represent room air, 104 represent room floor, 1,054 represent the walls and ceiling, and 108 represent area of air exfiltration (two hallway entrances and an open stairwell). These zone counts include “corners” where particles cannot be transported, but exist owing to programming ease in the definition of the one-step transition probability matrix.

The experiments were conducted with the mechanical ventilation system turned off (Sajo et al., 2002). Air speeds were measured with a neutrally buoyant balloon to be low, less than 0.25 cm s^{-1}. The airflow was predominantly horizontal, parallel to the 660 cm wall, but the flow changed direction 180° at height 250 cm. Advective airflow depicted by Sajo et al (2002) was resolved to 45° angles in the Markov model. In the central portion of the room, the advective flow was represented as 0.2 cm s^{-1} in the direction of increasing y, for z < 250 cm, and 0.25 m s^{-1} in the direction of decreasing y for z > 250 cm. Turbulent diffusion was not measured, and was assumed to be homogeneous, stationary and isotropic with magnitude D_T = 6.67 cm^2 s^{-1}, based on the characteristic mixing time for a quiescent space (Nicas, 2001).

In each experiment, 10 g of $^{59}Co_3O_4$ dust (ρ_p = 5.5 g cm^3) was propelled vertically from a 10 cm long, 5 cm diameter cylindrical cup by pressurized inert gas (Sajo et al., 2002). The release duration was 2 s. The release point was 2.0 m above the floor, at (x = 0, y = 0, z = 200 cm). The release rapidly formed an ellipsoidal-shaped puff (elongated horizontally): Assuming a Gaussian distribution Sajo et al (2002) estimated 68% of the discharged mass was within a lateral dimension of 200 cm and a vertical dimension of 150 cm. Given a center of mass at (x = 0, y = 0, z = 275 cm), the observed dimensions are achieved with standard deviations of the dispersion equal to σ_x = 64 cm, σ_y = 64 cm and σ_z = 48 cm. Thus, approximately 100% of the puff mass is contained within a conceptual box of size 400 cm × 400 cm × 350 cm, corresponding of 448 zones of the Markov model. The fraction of particles (and mass) at intervals from the emission location, f_x, f_y, and f_z are defined in Table S1 (see supplementary materials). For any given particle size, the fraction of particles in a zone is the product $f(x,y,z) = f_x \times f_y \times f_z$. Particles were assumed to have no initial velocity.

The supplier of the cobaltosic oxide estimated the particle size distribution could be represented as lognormal($\overline{d_p} = 1.1$ μm, GSD = 2). The particle size distribution was not verified by the investigators, and particle agglomeration was observed (Sajo, personal communication). The Hatch-Choate equations give a count median diameter of 0.865 μm, and mass median diameter of 3.36 μm (Hinds, 1999). The particle size distribution was represented in two ways (Table 1). In Simulation I, the particle size distribution was divided into ten bins each containing approximately 1 g. For each bin, a representative particle aerodynamic diameter was selected that provided the bin-average terminal settling velocity, $d_{a,w}$. To account for particle agglomeration, in Simulation II, the mass in Simulation I bins 1-4 was distributed amongst bins 5-10 in proportion to the particle surface area in each bin. The particle count was held constant and the particle diameters were re-calculated to account for the increased mass, then the $d_{a,w}$ were calculated. The terminal settling velocities were calculated using the $d_{a,w}$ specified in Table 1.

After release, particles were allowed to deposit for 90 minutes. Neutron activation was used to measure $^{59}Co_3O_4$ deposition on 12.9 cm^2 foils (36 foils on the floor in two experiments, and 56 foils on the floor in two experiments). To make the Sajo et al (2002) results comparable to Markov model predictions, for each experiment, the logarithm of measured deposited mass for each 12.9 cm^2 area of the floor was interpolated using the inverse distance weighted method. The interpolated values were returned to the arithmetic scale, and aggregated to estimate the mass deposited in 50 cm × 50 cm squares, the length aspect of the Markov model zones (Figure 1(a)). The sum total of interpolated mass that deposited on the room floor was 8.53 g, 9.52 g, 11.6 g, and 11.8 g (mean 10.3 g), indicating that all of the released material deposited. The greatest variability between experiments, indicated by the standard deviation in interpolated values, was observed in the positive x direction from the emission location, $0 < x < 100$ cm and $-50 < y < 50$ cm (data not shown). The shallow gradient in the deposition under the mezzanine ($x > 100$ cm) for $y > 0$ cm is unexpected, but may be due to unmeasured local velocity towards an open stairway in the corner ($y = 350$ cm, $100 \leq x \leq 200$ cm).

The Markov model used a time step of $\Delta t = 0.5$ s (see Supplementary Materials S1.2 for justification). For each particle size bin, for each model zone the advective air flow, turbulent diffusion coefficient and terminal settling velocity were transformed into first-order rate constants in accordance with the methods described by Jones and Nicas (submitted) and compiled to create a one-step transition probability matrix, **P**, of size 3,450 × 3,450. For each particle size bin, the model was simulated for 90 minutes, or 10,800 time steps.

The simulation output was the probability that a particle "released" into one of the $i = \{em_1, em_2, \ldots, em_{448}\}$ emission zones at time t = 0 s is in a zone $j = \{fl_1, fl_2, \ldots, fl_{104}\}$ representing the floor after 90 minutes, or 10,800 time steps. This probability is the entry in the *i*th row and *j*th column of the 10,800-step transition probability matrix $\mathbf{P}^{(10,800)}$, denoted $P^{(10,800)}(i,j)$ and calculated by multiplying the one-step transition probability matrix **P** by itself 10,800 times. Note, **P** and $\mathbf{P}^{(10,800)}$ are determined for each of the $k = \{1, 2, \ldots, 10\}$ particle size bins. Thus, the mass of particles predicted to deposit in zone *j*, M_j (g) is

$$M_j = \sum_{k=1}^{10} \sum_{i=1}^{448} E_k \times f_i \times P_k^{(10,800)}(i,j) \quad (1)$$

where E_k (g) is the mass emitted in particle size bin *k* (Table 1), f_i is the fraction of the mass emitted in emission zone *i* ($f_{(}$x,y,z)), $P_k(i,j)$ is the (*i*,*j*) entry in the one-step transition probability matrix for particle size bin *k*.

Jones and Nicas Experiment & Model

The environment studied by Jones and Nicas (2009) was a room-scale chamber, 236 cm × 292 cm × 239 cm high. The environment was modeled using zones with length aspect Δx = 30 cm. This size corresponds with the grid layout for particle deposition measurement in the experiments, but also meets the model assumptions (see Section S2.1 of the Supplementary Material). The interior of the chamber was represented by 7 × 9 × 8 zones for a modeled room 210 cm × 270 cm × 240 cm high. Adding two zones along each dimension to represent room surfaces yields a total of 990 zones, of which 504 represent room air, 63 represent room floor, and 423 represent the walls and ceiling. The grid representing the floor of the chamber is shown in Table 2.

The experiments were conducted with natural and forced mixing (Jones and Nicas, 2009). For the natural mixing condition, advection was too low to measure and was not included in the Markov model. Homogeneous isotropic turbulent diffusion was included with $D_T = 5.5$ cm^2 s^{-1}, based on the mixing time of carbon monoxide (see Section S3 of the Supplementary Material). For the forced mixing condition, three-axis ultrasonic anemometers measured advection and fluctuating velocity. Inhomogeneous istropic turbulence was included in the Markov model using the measured turbulence intensity, defined as (Yost and Spear, 1992):

$$K = \frac{\sqrt{\sigma_u^2 + \sigma_v^2 + \sigma_w^2}}{\overline{U_s}} \qquad (2)$$

where (σ_u, σ_v, σ_w) are the fluctuating velocities, and $\overline{U_s}$ is the mean air speed. Alternatively homogeneous isotropic turbulence was included with D_T = 2,050 $cm^2\ s^{-1}$, based on the mixing time of carbon monoxide. The zone length aspect, Δx = 30 cm is longer than the integral length scale of the chamber turbulence measured under forced mixing conditions (Λ in 1-9 cm), so the velocity vectors can be assumed uncorrelated between the model zones.

In each experiment, fluorescein aerosol (d_a ~ 3 μm and d_a ~ 14 μm) was emitted into the chamber via carrier gas flowing at 50 L min^{-1} out of a 3.175 cm (1.25 inch) inner diameter tube, oriented 25° from vertical, at grid location 7C and height 63 cm above the floor. The release occurred for 20 min. The fluorescein formulae and verification of the particle diameter are described by Nicas and Jones (2009). The particle terminal settling velocity was calculated for d_a = 3 μm and d_a = 14 μm (Hinds, 1999).

The release was modeled as a point source and as a jet. In the point source approach, particles emitted in time step Δt were assumed instantaneously well-mixed within the single model zone corresponding to the release location. Particles were assumed to have no initial velocity, and that the emission stream did not influence the advection or turbulence.

In the jet approach, particles emitted in time step Δt were instantaneously well-mixed and uniformly distributed between three model zones aligned diagonally in the y-z plane of the "projectile" motion. During the release period, the advective velocity in the three emission zones were equated with those measured in-line with the carrier air jet. Though the velocity of the carrier jet decreased rapidly from the exit point, the centerline velocity of two-phase jets decays more slowly than single-phase jets due to the increased momentum of the particles. Modarress et al (1984) found that the mean centerline velocity of the gas-phase in the two-phase jet was 30% higher than that of the one-phase jet; and the particle velocity was 1.5 times that of the one-phase jet. The velocity of a two-phase jet increases with mass load, and though the mass load used by Modarress et al (1984) was larger than in the Jones and Nicas (2009) experiments, a velocity increase of 1.5 times was assumed. This method required that particle transport be described using two one-step transition probability matrices: One matrix represented the transport during the release, and the other matrix represented the transport after the release stopped.

After the 20 min release, particles were allowed to deposit for 70 min giving a total experiment duration and simulation time of 90 min. Measured and modeled fluorescein concentrations were normalized to the mean value in each experiment.

The Markov model used a time-step of $\Delta t = 0.05$ s. The simulation was analogous to that for the Sajo experiments. Total simulation was 90 min, accounting for 20 min of emission and 70 min of deposition. Because particles are emitted in multiple time steps

(24,000 time steps), the number of time-steps between the emission of a particle and the end of the simulation varies from 108,000 (for particles emitted in the first time step, time 0 min) to 84,000 (for particles emitted in the 24,000th time step, time 19.95 min). Let N = 108,000 time steps of the 90 min simulation and *m* = {1,2, …, 24,000} be the time step of particle emission. The cumulative mass deposited in the *j*th zone, M_j (g), for the point source emission of particles in zone *i* = em_1 is calculated

$$M_j = \sum_{m=1}^{24,000} E \times P^{(N-m)}(i,j) \quad (3)$$

where E is the mass of particles (either d_a = 3 μm or d_a = 14 μm) emitted in each time step in the emission zone.

And, the cumulative mass deposited in the *j*th zone, M_j (g), for the jet source emission of particles in zone *i* = {em_1, em_2, em_3} is calculated

$$M_j = \sum_{m=1}^{24,000} \sum_{i=1}^{3} E \times P^{(N-m)}(i,j) \quad (4)$$

where E_i is the mass of particles emitted in each time step in each of the *i* emission zones.

Model Evaluation

Statistical summaries of model performance include (US EPA, 1991): mean bias, mean error, normalized mean bias, and normalized mean error. Correlation analyses use Spearman's rank correlation coefficient, ρ_s. The magnitude of variability is summarized by the coefficient of variation (CV), which is the relative standard deviation.

RESULTS

Sajo Experiment & Model

Simulation I predicted that 8.20 g of the 10 g released deposited on the room floor within 90 minutes of release. At 90 minutes, 1.1 g remained airborne (99% of this mass was associated with particle bins 1 to 4), 0.34 g had deposited on the mezzanine floor, and 0.34 g had left the lobby via exfiltration. Simulation II predicted that 9.7 g of the 10 g released deposited on the room floor within 90 minutes of release. At 90 minutes, 2.5×10^{-7} g remained airborne, 0.18 g had been deposited on the mezzanine floor, and 0.005 g had left the lobby via exfiltration.

The contours of the relative predicted mass deposition at 90 minutes subsequent to the release are indicated in Figures 1(b) and 1(c) for Simulations I and II, respectively. For reference, the release point is at the origin of the coordinate system (0,0). For Simulation I, more mass moved in the negative x-direction than in the positive x-direction, contrary to the observation of Sajo (comparing Figures 1(a) and 1(b)). For Simulation II, the dispersion is symmetric, more symmetric than was observed by Sajo (comparing Figures 1(a) and 1(c)). In Simulation II, more mass was predicted to deposit under the release point than in Simulation I, which makes sense given the larger mass among larger particles (Table 1).

Model performance statistics are summarized in Table 3. The negative mean bias is expected for Simulation I because only 82% of the released mass was predicted to deposit, while all mass was estimated to deposit in the interpolation. The magnitude of the mean bias is smaller in Simulation II. Other statistics indicate that Simulation II provides modest improvement relative to Simulation I. The Spearmans correlation between predicted and mean measured deposited mass increases from ρ_s = 0.4165 (p-value < 0.001) in Simulation I to ρ_s = 0.6625 (p-value < 0.001) in Simulation II. The spatial arrangement of model residuals is depicted in Figure S1 (Supplementary Material). Overall, the predicted deposited mass was within a factor of 2 for 35% and 43% of grid points in Simulations I and II, respectively; and within a factor of 3 for 59% and 61% of points, respectively.

Jones Experiments & Model

The summary statistics of the Markov model performance are summarized in Table 3, while percentage of emitted mass predicted by the Markov model to deposit, and spatial variation of those predictions are summarized in Table 4. Deposition patterns are depicted for natural mixing conditions in Figures 2 and 3 for the 3 μm and 14 μm particles, respectively, including representative experimental results (Figures 2(a) and 3(a)). For forced mixing conditions, only deposition patterns predicted for the jet source are shown in Figures 4 and 5 for the 3 μm and 14 μm particles, respectively, owing to similarity with the point source model predictions. Representative experimental results are shown in Figures 4(a) and 5(a).

Natural Mixing Conditions. For d_a = 3 μm (Figure 2), the modeled deposition had a small peak at the emission point (grid 7C), that was not observed in the experiments. However, the modeled deposition exhibited a positive gradient with increasing row number that was also observed in the experiments. This gradient suggests that advective flow, probably driven by convection, may have been present in the chamber, though it was too low to be measured.

For d_a = 14 μm (Figure 3), the increased deposition in the North-West quadrant of the room was not apparent, or was dwarfed, in the modeled deposition: The model predicted high deposition near the emission source, though the peak was broadened for the jet emission relative to the point emission source model.

The turbulence parameter used in these simulations, D_T = 5.5 cm^2 s^{-1}, was based on a global assessment of mixing time. Advection and local gradients in turbulence, however, may have facilitated dispersion of the particles during experiments; and these features were not included in the Markov model.

Statistical measures of performance (Table 3) do not indicate substantial bias, though Markov model prediction errors were larger for the larger particle size. The increased error is not surprising given the qualitative results in Figure 3.

Forced Mixing Conditions. The parameterization of turbulence had more impact on the model predictions than particle size, under forced mixing conditions. When turbulence was parameterized by D_T the predicted deposition was uniform for both 3 μm and 14 μm particles (Figures 4(b) and 5(b)). In contrast, when turbulence was parameterized by K, the predicted deposition had peaks in the South-East corner of the room (grid point 9G) and in front of the mixing fan (grid point 3D) for both particle sizes (Figures 4(c) and

5(c)). The spatial variability predicted by the Markov model with K may be expected because of the spatial variability in K, which was determined from anemometry data. However, the variability may also be driven by advection (measured by anemometry), because Markov model simulations with decreasing values of D_T predict deposition patterns that are increasingly similar to those observed with K.

The percentage of released mass that is predicted to deposit on the floor is similar for both the point and jet source emission (Table 4). Statistical measures of performance (Table 3) have small mean bias, but normalized mean bias is negative for the 14 μm particles. Measures of error are larger for Markov models parameterized by K than by D_T, which is consistent with the qualitative observations in Figures 4 and 5

DISCUSSION

The objective of this study was to evaluate the performance of the Markov model relative to observed particle transport and fate in two simple experiments (Sajo et al., 2002; Nicas and Jones, 2009). Evaluation of contaminant transport models of particles with $d_a \geq 3$ μm has been limited in the peer-reviewed literature, due to the scarcity of appropriate experimental data, and possibly, relatively poor model performance. In this study, the Markov model performance was found to be modest, but we judge appropriate for further evaluation and application. In particular, the results suggest the importance of careful characterization of particle emission, and quantitation of advection and turbulence are important for good model performance. At this time, quantitative advection and turbulence data are relatively limited, and this is one application that motivates further study of these parameters in indoor environments.

For example, in the natural mixing condition of Jones and Nicas (2009), the deposition patterns and influence of source emission type on the deposition patterns suggests that the experimental particle release mechanism was not well captured in the Markov model (Figures 2 and 3). Rather than explore a range of emission models to find an option that improved model performance, we elected to retain simple emission models (point source and jet source) that reflected our best understanding of the physical emission process.

In the forced mixing condition of Jones and Nicas (2009), the deposition patterns are similar for both particle sizes, though the experimental observations are differentiated by the relative magnitude of deposition near the mixing fans (grid point 2D) (Figures 4 and 5). Though the similarity of predictions for the two particle sizes suggest that the turbulence parameterization with D_T and K are strongly determinant of the deposition pattern, the difference diminishes with smaller values of D_T and approaches the deposition pattern predicted with K (data not shown). This suggests that advection is the driving force behind the deposition pattern observed with K. In the forced mixing condition, K was significantly negatively correlated with mean airspeed (ρ_s = -0.658, p-value < 0.001), such that areas of high airspeed have low turbulence intensity. Large values of D_T can mask spatial variation in advection.

CONCLUSION

Previous work indicates that the Markov model replicates predictions of relatively simple particle transport and fate models (Jones and Nicas, submitted), and there is theoretical support for the representation of advection-diffusion processes in a Markov chain (Jones, 2008; Nicas, 2010; Jones and Nicas, submitted). This study reflects an important step in the evaluation of mathematical models, in that the Markov model was evaluated against experimental data collected in controlled, but realistic, settings. The results show that the Markov model is a plausible tool for the modeling the fate and transport of supermicromter particles in more realistic settings. This work is a rare example of experimental evaluation of mathematical models predicting super micrometer particle transport. Experimental evaluation of models predicting supermicrometer particle transport is significant for persuading others that mathematical models can be informative and accurate.

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FIGURE CAPTIONS

Figure 1. Results of the Sajo et al. (2002) experiment and model. (a) Mean interpolated mass (mg) per 50 cm × 50 cm squares on the lobby floor at 90 minutes. Relative mass deposition predicted by (b) Simulation I and (c) Simulation II 90 minutes after the release. The release point is above the origin of the coordinate system (x = 0 cm, y = 0 cm).

Figure 2. Relative cumulative deposition of particles with d_a = 3 μm under natural mixing conditions after 90 min, including 20 min release above grid location 7C. (a) Measured relative deposition from experimental trial 1 of Jones and Nicas (2009). Markov model used (b) point source emission above grid location 7C, or (c) jet emission in three zones above grid locations 5C, 6C and 7C, with homogeneous isotropic turbulence D_T = 5.5 cm^2 s^{-1}.

Figure 3. Relative cumulative deposition of particles with d_a = 14 μm under natural mixing conditions after 90 min, including 20 min release above grid location 7C. (a) Measured relative deposition from experimental trial 5 of Jones and Nicas (2009). Markov model used (b) point source emission above grid location 7C, or (c) jet emission in three zones above grid locations 5C, 6C and 7C, and homogeneous isotropic turbulence D_T = 5.5 cm^2 s^{-1}.

Figure 4. Relative cumulative deposition of particles with d_a = 3 μm under forced mixing conditions after 90 min, including 20 min release above grid location 7C. (a) Measured relative deposition from experimental trial 8 of Jones and Nicas (2009). Markov model used jet emission in three zones, above grid locations 5C, 6C and 7C, and homogeneous isotropic turbulence (b) D_T = 2,050 cm^2 s^{-1} or (c) measured turbulence intensity, K.

Figure 5. Relative cumulative deposition of particles with d_a = 14 μm under forced mixing conditions after 90 min, including 20 min release above grid location 7C. (a) Measured relative deposition from experimental trial 12 of Jones and Nicas (2009). Markov model uses a jet emission in three zones, above grid locations 5C, 6C and 7C, and (b) homogeneous isotropic turbulence D_T = 2,050 cm^2 s^{-1} or (c) measured turbulence intensity, K.

Particle Bin	Nominal Range d_a (μm)	Simulation I		Simulation II	
		$d_{a,w}$ (μm)	Mass (g)	$d_{a,w}$ (μm)	Mass (g)
1	0.024-3.53	2.71	1.02	-	-
2	>3.53-4.79	4.19	1.02	-	-
3	>4.79-5.97	4.39	1.02	-	-
4	>5.97-7.20	6.58	1.02	-	-
5	>7.20-8.58	7.89	1.02	11.6	2.10
6	>8.58-10.2	9.39	1.02	13.2	192
7	>10.2-12.4	11.3	1.02	15.3	1.78
8	>12.4-15.4	13.8	1.02	18.0	1.64
9	>15.4-20.9	17.8	1.02	22.3	1.50
10	>20.9-35.2	26.3	0.81	31.1	1.07

Table 1. Distribution of particle sizes used in the simulations of the release experiments conducted by Sajo and colleagues. Note that $d_{a,w}$ is a terminal settling velocity weighted diameter used to represent each bin, and that in Simulation II the particle mass in bins 1-4 has been redistributed to bins 5-10 in proportion to the surface area in bins 5-10. The particles were assumed to be spherical.

North

West						
1A	1B	1C	**1D**	1E	1F	1G
2A	2B	2C	2D	2E	2F	2G
3A	3B	3C	3D	3E	3F	3G
4A	4B	4C	4D	4E	4F	4G
5A	5B	5C	5D	5E	5F	5G
6A	6B	6C	6D	6E	6F	6G
7A	7B	**7C**	7D	7E	7F	7G
8A	8B	8C	8D	8E	8F	8G
9A	9B	9C	9D	9E	9F	9G

Table 2. Floor grid layout for the Jones and Nicas (2009) experiments. Each grid location represents a 30 cm × 30 cm area. Mixing fans located at 1D. Particle release at 7C.

	Sajo Experiment		Jones Experiment					
			Natural Mixing		Forced Mixing			
Statistic	**Sim I**	**Sim II**	**3 μm-D_T**	**14μm-D_T**	**3μm-D_T**	**3μm-K**	**14μm-D_T**	**14μm-K**
MB	-20.4	-5.57	-1.0×10^{-14}	-2.4×10^{-15}	-1.9×10^{-14}	-2.0×10^{-15}	8.2×10^{-15}	-1.5×10^{-14}
ME	66.4	61.1	17.0	68.4	4.30	29.9	6.54	23.8
NMB	29.9	-8.41	-1.67	1.54	0.07	1.25	-1.04	-5.86
NME	1.13	0.78	0.80	7.36	0.75	4.74	0.20	0.38

Table 3. Statistical summary of Markov model performance, including the mean bias (MB), mean error (ME), normalized mean bias (NMB) and normalized mean error (NME). For the Jones experiment, results for the jet source emission are presented, and compared to experimental trials 4, 6 8 and 12 and statistics were calculated using results normalized to the mean value.

Mixing Type	Source Type	Particle d_a (μm)	D_T		K	
			%Mass	CV	%Mass	CV
Natural	Point	3	55	47	-	-
		14	100	240	-	-
Natural	Jet	3	50	27	-	-
		14	63	150	-	-
Forced	Point	3	29	7.1	5.8	51
		14	100	7.2	87	52
Forced	Jet	3	29	7.1	5.3	52
		14	100	7.0	86	50

Table 4. Markov model predicted cumulative percent mass deposition (% mass) and spatial variability, measured by the coefficient of variation (CV%), for the experimental conditions of Jones and Nicas (2009).