NIST Technical Note 2004

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National Institute of Standards and Technology
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Abstract

Engineered nanoparticles (ENP) are being used in many applications including consumer products. There are many different means by which ENPs may be incorporated into these products (freely-dispersed, embedded, reactive or passive) which can impact the potential for consumer exposure to ENPs. This study was motivated by the desire to better understand inhalation exposure to ENPs, and this report addresses airborne ENPs that could affect indoor air quality (IAQ). Occupant exposure to airborne nanoparticles can be characterized by indoor airflow and contaminant transport analysis models. The U.S. Consumer Product Safety Commission (CPSC) is working with the National Institute of Standards and Technology (NIST) to develop modeling tools to enable evaluation of consumer exposure to airborne ENPs in the built environment.

NIST has developed two tools, the first is an online tool that provides estimates of indoor exposure to airborne particles. This first tool, referred to as the single-size particle tool, is based on the NIST multizone modeling software, CONTAM, and demonstrates some of the capabilities that an aerosol exposure assessment tool should entail. The second tool, referred to as the size-resolved tool, includes additional physical models that account for the properties of nanoparticles that may impact their transport within the built environment including some beyond those that CONTAM is currently capable of modeling, e.g., coagulation. This report describes the development and application of these two analysis tools that could provide the basis of modeling consumer exposure to ENPs for future development.

Key Words: consumer products; engineered nanoparticle; exposure; indoor air quality; modeling; validation

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Users are warned that this software is intended for use only by persons competent in the field of particle exposure analysis and is intended only to supplement the judgement of the qualified user. The computer programs described in this report are prototype methodologies for computing particle exposure in buildings. The calculations are based upon a simplified model of the complexity of real buildings. These simplifications must be understood and considered by the user.

Certain commercial entities, equipment, or materials may be identified in this document in order to describe an experimental procedure or concept adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the entities, materials, or equipment are necessarily the best available for the purpose.

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1 Introduction

Engineered nanoparticles (ENP), those particles synthesized as having one or several dimensions in the 1 nm to 100 nm size range, are being used in a number of applications including consumer products [1]. There are many different means by which ENPs may be incorporated into these products (freely-dispersed, embedded, reactive or passive) [2], which can impact the potential for consumer exposure to ENPs. The work presented here was motivated by the desire to better understand inhalation exposure to ENPs, and this report is focused on airborne ENPs that could affect indoor air quality (IAQ). Occupant exposure to airborne nanoparticles can be characterized by indoor airflow and contaminant transport analysis software. The U.S. National Institute of Standards and Technology (NIST) has been developing CONTAM for many years [3], which is the most widely used software of this type. As such, the U.S. Consumer Product Safety Commission (CPSC) is working with NIST to develop modeling tools to enable evaluation of consumer exposure to airborne ENPs in the built environment.

Modeling of airborne particles has been performed for various reasons, including interest in atmospheric and indoor air [4, 5], and multiple methods are available to capture various transport processes involved. Models of the indoor environment can implement macro-flow or micro-flow assumptions. Typically, macro-flow models consider control volumes of air, e.g., rooms, to be characterized by uniform contaminant (e.g., particle) concentrations throughout, while micro-flow models yield detailed room air motion and potential non-uniformity of contaminant concentrations within a given space. The former is often referred to as multizone or nodal modeling and the latter as computational fluid dynamics (CFD).

While CFD can provide detailed characteristics of particle transport, it can be relatively computationally intensive/expensive to simulate on a whole building scale for which multizone modeling is more well-suited. In addition to how airflow is modeled, particle dynamics can also be modeled at varying levels of detail. Particle characteristics of interest can include: the range of particle sizes, number distribution, chemical composition, reactivity and shape of the particles. Modeling relatively large, non-reactive particles, e.g., respirable particles in the 2.5 μm ($PM_{2.5}$) to 10 μm (PM_{10}) size ranges, in concentrations encountered in non-industrial indoor environments, pose relatively minimal challenge to either the macro-flow or micro-flow analysis methods [6]. However, modeling a particle distribution that consists of a broad range of particle sizes and a large number of particles may involve inter-particle interactions, e.g., coagulation, which could significantly increase computational intensity and complexity [7]. Therefore, trade-offs are involved between computational expense, spatial and temporal resolution, and inclusion of inter-particle interaction.

It is not always clear the extent to which ENPs are contained within consumer products nor the potential for their release into the indoor air. However, there is evidence that products exist that do have the potential to release ENPs into the air [8-10]. While specific properties of ENPs may affect their transport within the built environment, modeling ENPs in indoor air is likely to require the ability to capture transport properties similar in nature to other ultrafine particles (UFPs) [6, 11, 12]. Capturing these fundamental, and well-understood, transport processes will serve as the foundation for modeling ENPs and enable the future inclusion of properties specific to ENPs should they prove relevant to their fate within the indoor environment. The fundamental transport processes and modeling thereof will be addressed within sections 2.1.1 and 2.2.1 of this report.

Two particle modeling tool development efforts were undertaken by NIST in collaboration with CPSC. Under the first effort, NIST developed an online tool to provide estimates of indoor exposure to airborne particles. This first tool was based on the NIST multizone modeling software, CONTAM [3], and provides a basis for an exposure assessment tool. The second effort involved identifying physical models that account for the properties of nanoparticles that may impact their transport within the built environment including those beyond which CONTAM is currently capable of modeling, e.g., coagulation. This report presents the results of these two efforts and the development of two particle analysis tools that could aid in modeling consumer exposure to indoor nanoparticles in the future after further development.

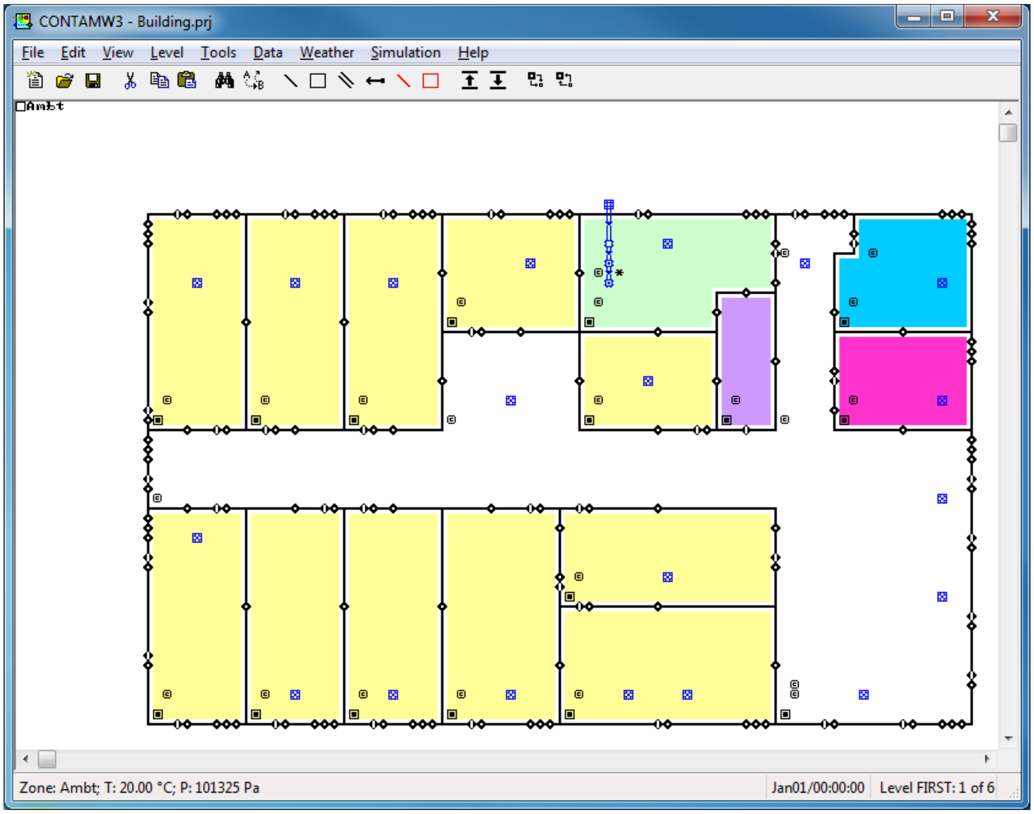
2 Tool Development

This section presents the approach to developing the two ENP modeling tools, both of which are single zone models. The first tool will be referred to as the CONTAM-based, single-size particle model and the second tool as a size-resolved particle model. These tools can be accessed from the following web page:

https://pages.nist.gov/CONTAM-apps/

2.1 CONTAM-based, Single-size Particle Tool

The single-size particle model was developed to take advantage of the existing CONTAM software. CONTAM is a multizone IAQ and ventilation analysis computer program that can be used to predict whole-building airflow and contaminant transport. CONTAM consists of two programs: ContamW – the graphical user interface shown in Figure 1, and ContamX – the solver. ContamW allows users to draw multilevel building floor plans; define zones, openings between zones including the ambient, ventilation systems, contaminant sources and sinks, and occupants that can be scheduled to move throughout building; and save the information to a project file. ContamX reads the project file, formulates a set of mass balance equations, and solves for the zone pressures and resultant interzone airflows as influenced by wind, buoyancy-induced pressures and ventilation system airflows. Once the airflows are determined, ContamX then performs contaminant mass balances to determine the time histories of contaminant concentrations and occupant exposures for up to a year long simulation for timesteps between 1 and 60 seconds.



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Level FIRST: 1 of 6

Figure 1 – ContamW Graphical User Interface

The set of user-defined inputs required to define a building in CONTAM can be significant, and the possible building configurations are limitless. Therefore, the goal of this project was to allow users to focus on a set of inputs that provides a more manageable means to evaluate particle transport properties that are relevant to investigating occupant exposure to ENPs.

2.1.1 Single-zone Mass Balance Model

The CONTAM-based tool, shown schematically in Figure 2, consists of a single zone of uniform particle concentrations. The model implements a simple air handling system (SAHS) that provides supply air to and removes return air from the zone. The supply and return airflow rates, Q_{sup} and Q_{ret} respectively, and the outdoor air fraction of the SAHS are user inputs, and the SAHS model determines the resulting zone air balance, including the system outdoor air intake Q_{oa} and envelope infiltration Q_{inf}. If the supply and return airflows are not balanced, then the zone will either be negatively or positively pressurized, thus determining the value of Q_{inf} in Equation (1).

The single-zone mass balance equations for the zone volume and interior surface areas are provided in Equations (1) and (2) respectively. Equation (1) indicates the time rate of change in mass of particles within the zone air is equal to the rate that particles are added to the zone air (from the outdoors via infiltration, from the supply airflow of the SAHS, and from surface resuspension) and removed from the zone air (via the return airflow of the SAHS and deposition to the room surfaces). Equation (2) indicates the time rate of change of particle mass on the surfaces of the zone is equal to the rate that particles are deposited on the surfaces from the air minus the rate at which they are resuspended to the air. CONTAM performs all contaminant calculations in mass-based units. However, the tool provides the ability to convert to particle number units based on the particle density and diameter.

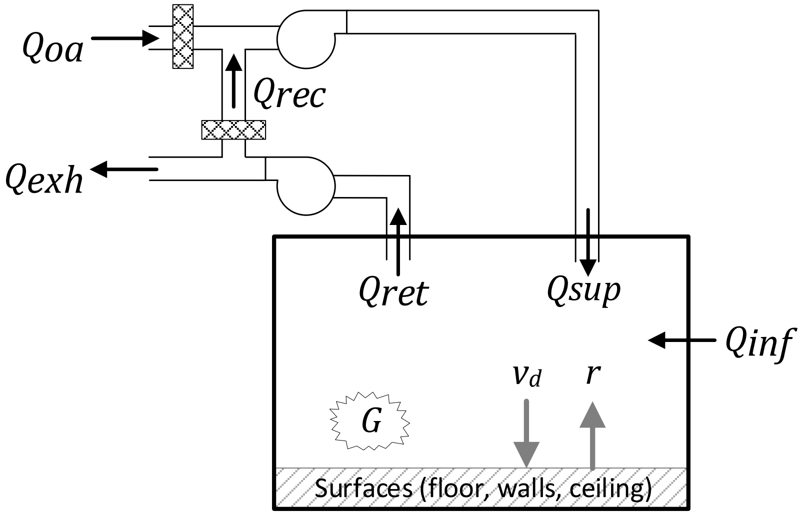


Figure 2 – Schematic of Single-zone Model

$$V\frac{dC_z}{dt} = PQ_{inf}C_{oa}(t) + Q_{sup}C_{sup}(t) + \sum_{i=1}^{N_s} r_i A_{ri} L_{si}(t) + G(t) - Q_{ret}C_z(t) - \sum_{i=1}^{N_s} v_{di} A_{si} C_z(t) \qquad (1)$$

$$A_{si}\frac{dL_{si}}{dt} = v_{di} A_{si} C_z(t) - r_i A_{ri} L_{si}(t) \qquad (2)$$

where:

C = concentration in air [kg/m^3], subscripts: **z**one, **o**utdoor **a**ir, **sup**ply and **ret**urn
Q = volumetric airflow rate [m^3/s], subscripts: **inf**iltration, **sup**ply and **ret**urn
L_{si} = surface loading for surface *i* [kg/m^2]
V = zone volume [m^3]
A_{si} = deposition surface area for surface *i* [m^2]
A_{ri} = resuspension surface area for surface *i* [m^2]
r_i = particle resuspension rate for surface *i* [1/s]
ν_{di} = particle deposition velocity for surface *i* [m/s] ($\nu_d = k_d\, V / A_s$)
N_s = number of surfaces (floor, walls and ceiling)
k_d = particle deposition rate [1/s]
G = particle generation rate [kg/s]
P = particle penetration factor [-]
t = time [s]

2.1.2 *Online Tool Development*

A single zone CONTAM model was created in ContamW and forms the basis of the online tool. The single zone CONTAM representation is shown in Figure 3. The web interface is divided into two main sections: Inputs and Results as shown in Figure 4 and Figure 5, respectively. The inputs are further subdivided into *Zone Geometry*; *Ventilation System*; *Particle Properties*, *Particle Source, Particle Deposition Velocities* and *Particle Resuspension*; *Initial Concentration* and *Surface Loadings*; and *Occupant Exposure* period. Details of each input are provided in Appendix A – Single-size Particle Tool User Guide.

Users set the desired inputs and then run a 24-hour simulation. Results are provided in the form of integrated exposure based on the occupant exposure period, average and peak concentrations for the exposure period and for the full 24-hour simulation period. Charts are also provided showing the time histories of the zone concentration, exposure concentration and surface loading. The concentration plots also show the average concentrations associated with the 24-hour period and the exposure period.

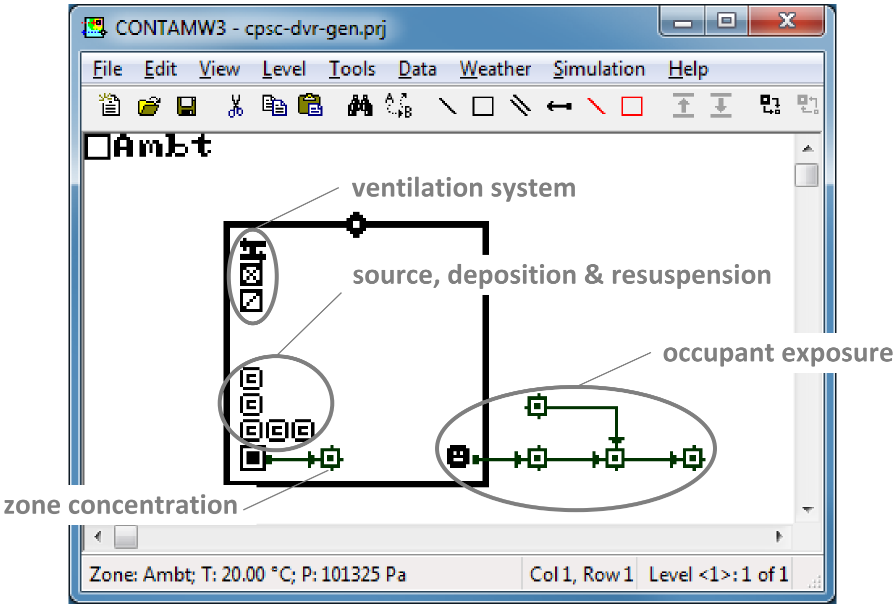
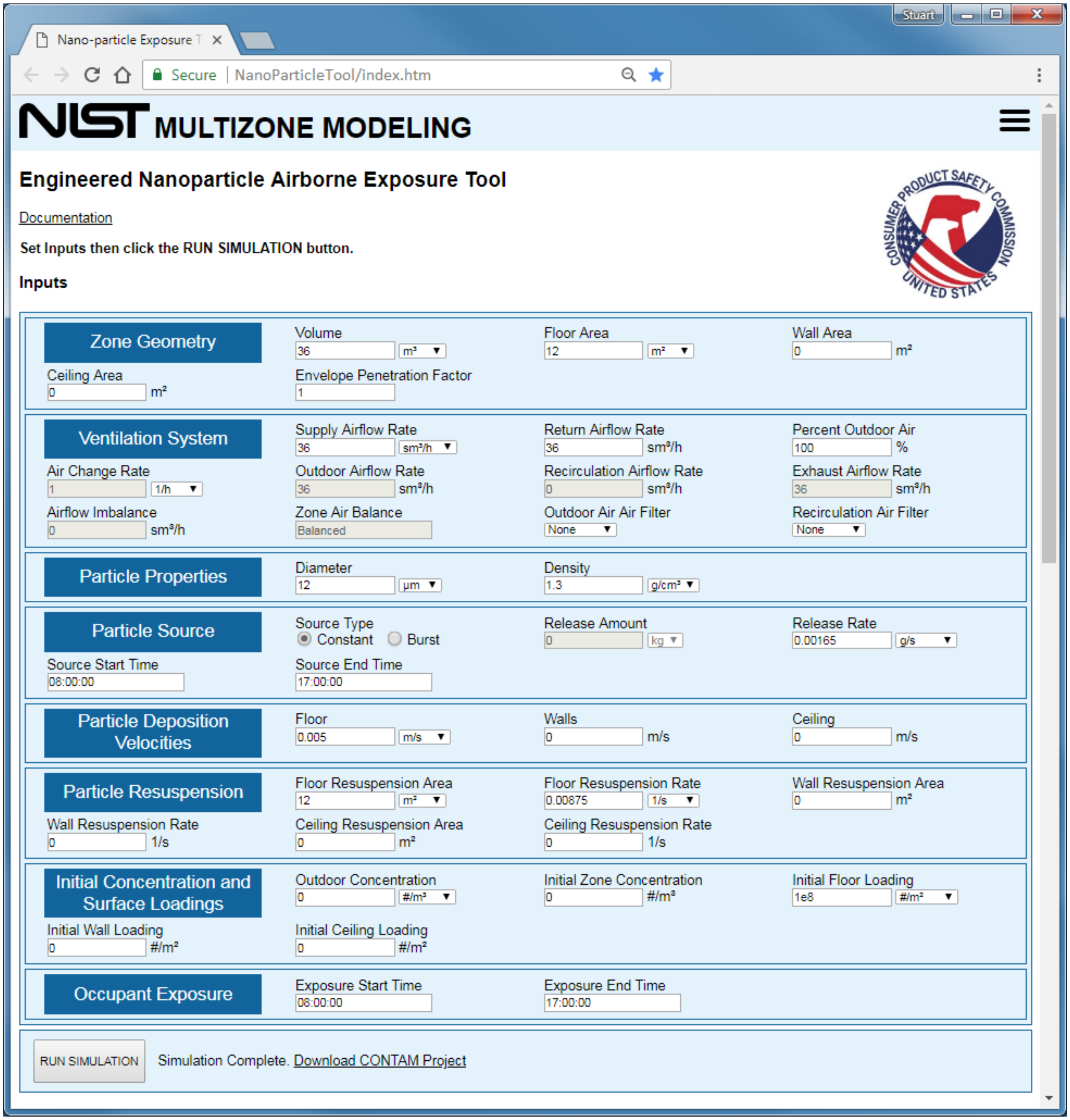


Figure 3 – Single Zone CONTAM Representation



Engineered Nanoparticle Airborne Exposure Tool

Documentation

Set Inputs then click the RUN SIMULATION button.

Inputs

Zone Geometry
Volume: 36 m³
Floor Area: 12 m²
Wall Area: 0 m²
Ceiling Area: 0 m²
Envelope Penetration Factor: 1

Ventilation System
Supply Airflow Rate: 36 sm³/h
Return Airflow Rate: 36 sm³/h
Percent Outdoor Air: 100 %
Air Change Rate: 1 1/h
Outdoor Airflow Rate: 36 sm³/h
Recirculation Airflow Rate: 0 sm³/h
Exhaust Airflow Rate: 36 sm³/h
Airflow Imbalance: 0 sm³/h
Zone Air Balance: Balanced
Outdoor Air Air Filter: None
Recirculation Air Filter: None

Particle Properties
Diameter: 12 µm
Density: 1.3 g/cm³

Particle Source
Source Type: ● Constant ○ Burst
Release Amount: 0 kg
Release Rate: 0.00165 g/s
Source Start Time: 08:00:00
Source End Time: 17:00:00

Particle Deposition Velocities
Floor: 0.005 m/s
Walls: 0 m/s
Ceiling: 0 m/s

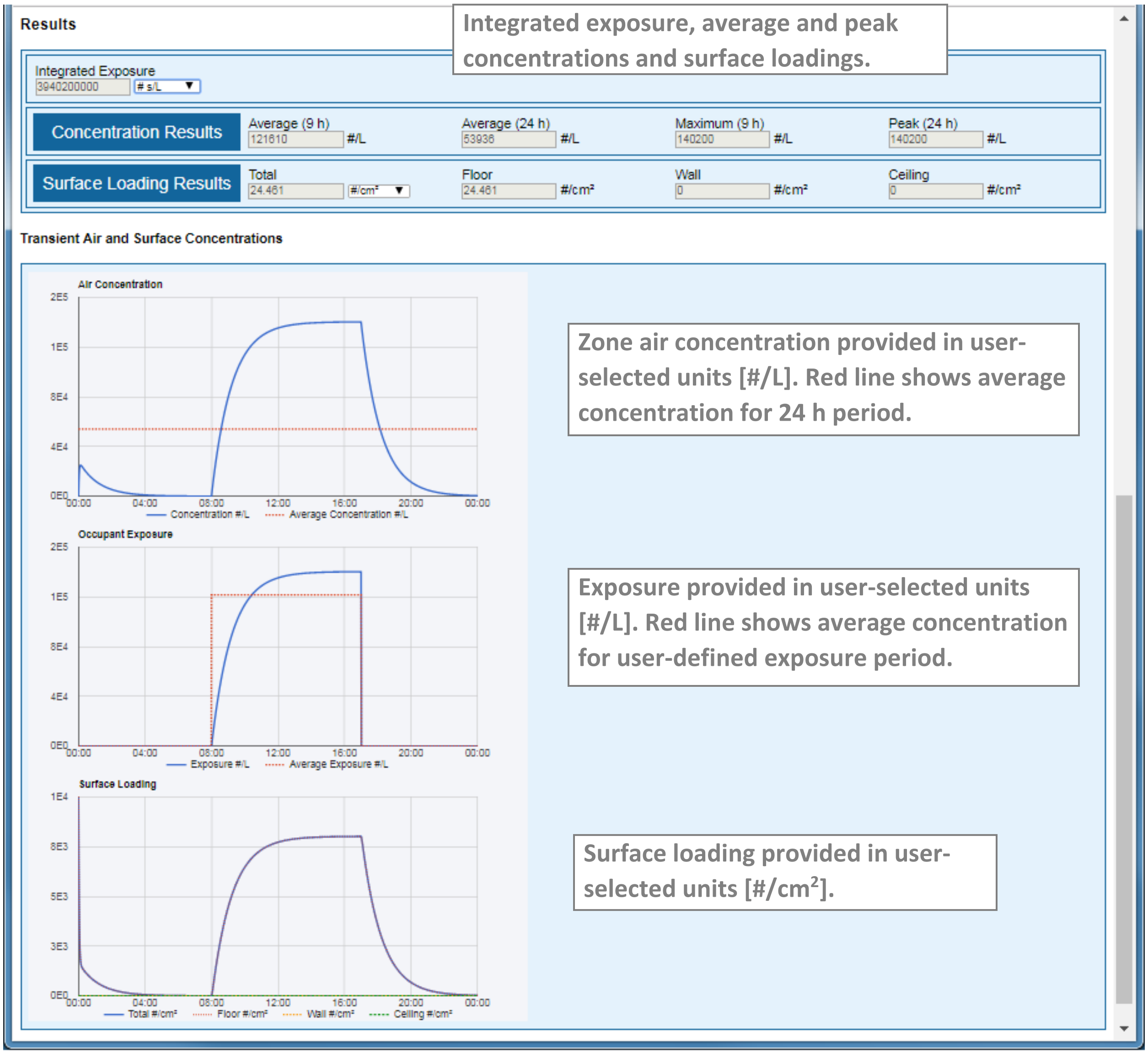
Particle Resuspension
Floor Resuspension Area: 12 m²
Floor Resuspension Rate: 0.00875 1/s
Wall Resuspension Area: 0 m²
Wall Resuspension Rate: 0 1/s
Ceiling Resuspension Area: 0 m²
Ceiling Resuspension Rate: 0 1/s

Initial Concentration and Surface Loadings
Outdoor Concentration: 0 #/m³
Initial Zone Concentration: 0 #/m³
Initial Floor Loading: 1e8 #/m²
Initial Wall Loading: 0 #/m²
Initial Ceiling Loading: 0 #/m²

Occupant Exposure
Exposure Start Time: 08:00:00
Exposure End Time: 17:00:00

RUN SIMULATION
Simulation Complete. Download CONTAM Project

Figure 4 – Web Interface of Single-size Tool (Input section)



Results

Integrated exposure, average and peak concentrations and surface loadings.

Integrated Exposure: 3940200000 # s/L

Concentration Results
Average (9 h): 121610 #/L
Average (24 h): 53936 #/L
Maximum (9 h): 140200 #/L
Peak (24 h): 140200 #/L

Surface Loading Results
Total: 24.461 #/cm²
Floor: 24.461 #/cm²
Wall: 0 #/cm²
Ceiling: 0 #/cm²

Transient Air and Surface Concentrations

Zone air concentration provided in user-selected units [#/L]. Red line shows average concentration for 24 h period.

Exposure provided in user-selected units [#/L]. Red line shows average concentration for user-defined exposure period.

Surface loading provided in user-selected units [#/cm^2].

Figure 5 – Web Interface of Single-size Tool (Results section)

2.1.3 Web-based CONTAM Solver

The CONTAM program was originally developed to run under the Windows operating system. Currently, ContamW must be run under Windows, but the solver, ContamX which is written in the C programming language, has been developed to run cross-platform under Windows, Linux and MacOS. However, for the purposes of developing this tool, ContamX was converted to run in a web-based environment.

An Open Source tool, *Emscripten* [13, 14], was used to compile ContamX to JavaScript. This process required minor modifications to the ContamX code to manage input and output. The benefit of this approach is that the single-particle model is actually running the ContamX solver, which has been well validated [15-18] and is considered by many to be the de facto tool for performing whole-building IAQ analysis.

Details of the CONTAM solver are provided in the CONTAM User Guide [3]. For the purposes of this tool, ContamX utilizes the web-based, user inputs to establish the ventilation system airflow rates and determine the air balance of the single zone. Once the airflow rates are obtained, ContamX performs a contaminant mass balance as per Equations (1) and (2) using an implicit solution method to simultaneously determine the zone and surface concentrations for each time step over the simulation period. For this tool, the time step is hard-coded to 1 minute and the simulation period to 24 hours.

2.1.4 Verification Test Case

The following inputs were used to verify the CONTAM-based tool against an analytical solution. This case is based on the experimental work of Karlsson et al. (1999) and consists of persons walking on the floor of a chamber that has been initially loaded with particles, which serves as the source for airborne particles. While this case is based on relatively large particles, it includes airborne particles and surface loading as well as removal by air change and a particle source in the form of resuspension. The basic mathematics are the same for any size particles for the model presented in Equations (1) and (2).

Zone Geometry:	Volume = 45 m^3, Floor area = 20 m^2
Ventilation System:	Air change rate = 0.5 h^{-1}, Outdoor air fraction = 100 %
Particle Properties:	
	Diameter = 12 μm, Density = 1.3 g/cm^3
	Deposition velocity = 0.005 m/s
	Resuspension rate = 0.0025 s^{-1}, Resuspension area = 0.028 m^2
	Initial surface loading = 1.0 x 10^8 particles/m^2 = 1.1762 x 10^{-4} kg$_p$/m^2

While experimental measurements are not provided directly in the reference, this simple two-zone (air and surface) model has an analytical solution. Performing an eigen analysis yields eigenvalues of -2.3644 x 10^{-3} s^{-1} and -2.056 x 10^{-7} s^{-1}, eigenvectors (1.0, -2.55008) and (1.0, 1827.5), leading to the following set of equations for the given initial conditions (no contaminants in the air and an initial surface loading) and properties provided above.

$$y_i(t) = 6.42722 \times 10^{-8}\left[\begin{pmatrix}1.0\\1827.5\end{pmatrix} e^{-2.056\times10^{-7}t} - \begin{pmatrix}1.0\\-2.55008\end{pmatrix} e^{-2.3644\times10^{-3}t}\right] \quad (3)$$

Equation (3) provides the zone concentration, $y_1(t)$, and surface loading, $y_2(t)$, in units of kg_p/kg_a (kg of particles/kg of air) and kg_p/m^2 (the units in which CONTAM calculations are performed), respectively for time, t, in seconds. Results for a 1-hour simulation yield the following:

$C_z(3600) = 6.42117 \times 10^{-8}\ kg_p/kg_a = 7.7317 \times 10^{-8}\ kg/m^3 = 6.5734 \times 10^{4}$ particles/m^3

$L_s(3600) = 1.17371 \times 10^{-4}\ kg_p/m^2 = 9.9787 \times 10^{7}$ particles/m^2

The eigen analysis was performed using Mathematica, for which plots of zone and surface concentrations are provided in Figure 6. Results of the same case simulated with the CONTAM-based nano tool are provided in Figure 7. The results shown in Figure 7 were obtained using the PRJ file downloaded from the CONTAM-based tool and modified to perform a 1-hour simulation as opposed to the default 24-hour simulation of the tool.

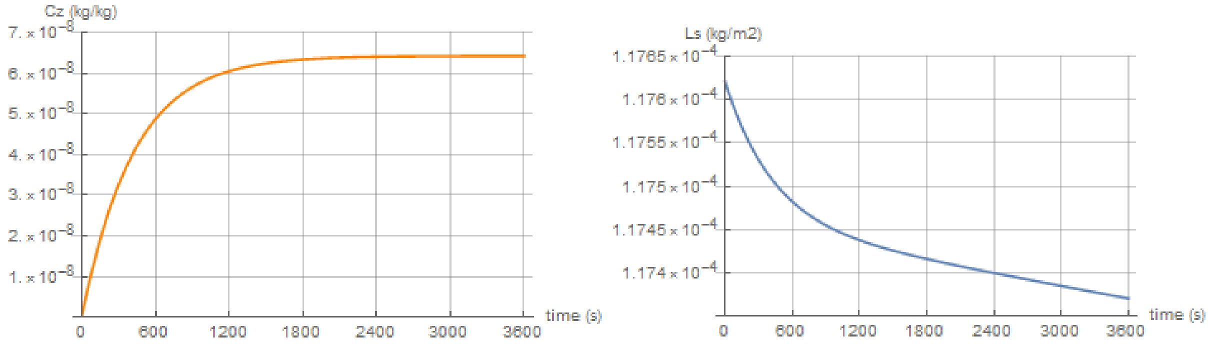


Figure 6 – Mathematica Plots of Eigen Analysis Results: Zone Air, Cz (left) and Surface, Ls (right)

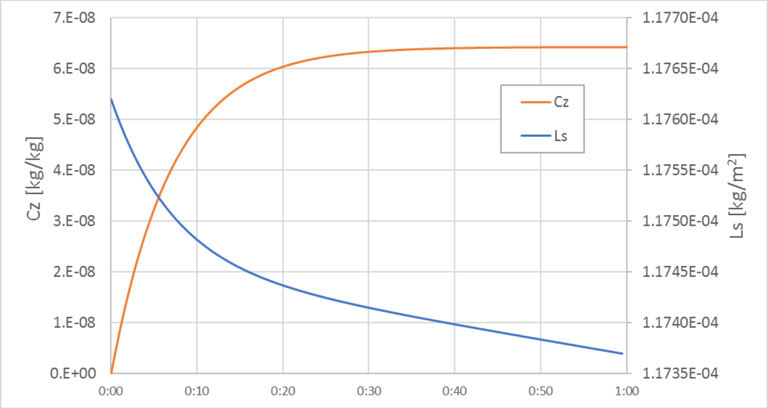


Figure 7 – CONTAM-based Tool Results of Verification Test Case

Criteria		Cz	Ls
N		361	361
r	≥ 0.9	**1.0000**	**1.0000**
m	0.75 - 1.25	**1.0039**	**1.0031**
$b/\overline{Co}$	≤ 0.25	**-0.0055**	**-0.0031**
$NMSE$	≤ 0.25	**5.22 x 10^{-6}**	**9.43 x 10^{-11}**
$\lvert FB \rvert$	≤ 0.25	**-1.57 x 10^{-3}**	**-9.49 x 10^{-6}**
$\lvert FS \rvert$	≤ 0.50	**0.0078**	**0.0063**

Table 1 – Correlation between analytical results and CONTAM-based simulations for verification test case of single-size particle tool.

Comparison between the analytical and the CONTAM-based results were made based on ASTM Standard Guide D-5157 [20], and the results are shown in Table 2. Values shown in bold in Table 2 are within the levels recommended in the ASTM guide (and provided in the left-hand column of the table). All parameters are within the guideline values for both the particle concentrations in the air and on the surface. These results confirm the validity of the calculation method for this particular case, and it is relatively simple to modify the Mathematica notebook to perform further verification as desired. While other cases were investigated, e.g., non-zero ambient concentration and constant source, they are not presented here. However, simulation of another experimental test case is presented later for purposes of comparison with the size-resolved modeling tool.

2.2 Size-resolved Particle Tool

The size-resolved particle model is being developed to capture the behavior associated with ultrafine (nano) particles that might occur concurrently in large numbers and various sizes. It has been shown that when a large number of airborne, ultrafine particles are present, then transport phenomenon, other than those captured by the existing CONTAM model, are likely to become important. In particular, coagulation of particles within the indoor environment has been shown to be significant with respect to removal rates associated with deposition and air change [12], albeit for particle emissions from cooking stoves (gas and electric) during experiments of relatively short measurement periods (approximately 20 minutes).

Size-resolved particle modeling has long been applied in the field of atmospheric and indoor air quality modeling [5, 21, 22]. However, to date there does not appear to be publicly available tools that implement these models in an easily configurable manner to address IAQ, especially with respect to consumer exposure to ENPs. The tool presented herein is an initial version developed to establish a foundation on which ENP specific properties can be incorporated as they become better understood and characterized.

2.2.1 Single-zone, Size-resolved Model

This tool implements a single zone, uniform concentration model with a user-defined, initially log-normal number distribution, and number of particles. The model incorporates the following transport mechanisms: a coagulation kernel, a size-resolved particle deposition model and a user-defined ventilation rate. This model provides the means to perform initial investigation of the relative effects of these various particle transport mechanisms on the fate of indoor particles. All particles are considered to be non-reactive species with the same density.

The mass balance model is based on the integrodifferential coagulation Equation (4) modified to include deposition and ventilation.

$$\frac{dn(v,t)}{dt} = \left[\frac{1}{2}\int_{0}^{v} \beta_{v-\bar{v},\bar{v}}\, n(v-\bar{v},t)\, n(\bar{v},t)\, d\bar{v}\right] - \left[n(v,t)\int_{0}^{\infty} \beta_{v,\bar{v}}\, n(\bar{v},t)\, d\bar{v}\right] - [(\kappa + a)\, n(\bar{v},t)] \qquad (4)$$

where:

$n(v,t)$ = number concentration of particles of volume v at time t [#/cm^3]
$\beta_{i,j}$ = coagulation rate coefficient for particles of volume i and j [cm^3/particle·s]
κ = deposition rate for particle of size $\bar{v}$ [1/s]
a = zone ventilation or air change rate [1/s]

According to Jacobson (2005), the first three terms of Equation (4) "states that the rate of change in number concentration of particles of volume v equals the rate at which particles of volume $v - \bar{v}$ coagulate with particles of volume $\bar{v}$ minus the rate at which particles of volume v are lost due to coagulation with particles of all sizes." For the purposes of this tool, the final term in brackets on the right was added to account for removal of particles by deposition and ventilation of the zone with an external, particle-free zone [11, 23]. The volume relationship between particles of volumes v, $\bar{v}$, and $v - \bar{v}$ is shown in Figure 8.

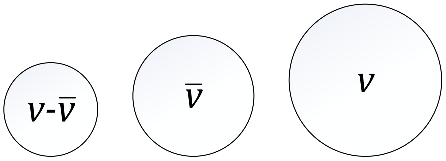


Figure 8 – Schematic of Coagulating Particle Volumes

This tool implements the semi-implicit solution method to solve Equation (4) on a volumetric basis for a volume-ratio size distribution as shown in Equation (5). This is the same as equation 15.12 provided in Jacobson (2005). The tool also utilizes a volume-ratio size distribution wherein the volume of each particle in size bin k equals that of size bin k-1 multiplied by a volume ratio, V$_{\mathrm{rat}}$, i.e., V$_{\mathrm{rat}}$ = v_k / v_{k-1}.

$$v_{k,t} = \frac{v_{k,t-\Delta t} + \Delta t \sum_{j=1}^{k}\left(\sum_{i=1}^{k-1} f_{i,j,k}\beta_{i,j}\, v_{i,t} n_{j,t-\Delta t}\right)}{1 + \Delta t \sum_{j=1}^{N_B}\sum_{i=1}^{k-1}\left(1 - f_{k,j,k}\right)\beta_{k,j}\, n_{j,t-\Delta t}} \qquad (5)$$

where:

$v_{k,t}$ = volumetric concentration of particles in bin k at time t [cm^3/cm^3] (not the same as v in Equation (4))
$f_{i,j,k}$ = bin volume fraction partitioning function (Jacobson (2005), equation 15.11)
N_B = number of particle bins
Δt = simulation time step [s]

Coagulation Kernel

Coagulation kernels refer to calculations of particle-to-particle interactions based on various particle properties. While other coagulation kernels are available, this tool implements a Brownian diffusion kernel that is based largely on particle diffusion coefficients to account for the irregular motion of particles as they are randomly and continuously impacted by the gas molecules within which they are suspended, i.e., air molecules in this case. For small particles, Brownian diffusion is the dominant coagulation process in comparison to turbulent motion which is more important for larger particles as is the case for atmospheric modeling (Jacobson (2005) section 15.6).

The Brownian diffusion kernel in this model is based on that presented in Jacobson (2005) and implements the interpolation formula of Fuchs [24] to account for particles in the transition regime. The interpolation formula reduces to Brownian diffusion formulas of the free-molecular (diffusion-dominated) and continuum (viscous force dominated) regimes. These regimes are delineated by the Knudsen number ($Kn_{a,i}$) for a given particle size within air which is also accounted for in calculating the particle diffusion coefficient as shown in the following section.

$$Kn_{a,i} = \frac{\lambda_a}{r_i} \qquad (6)$$

where:

λ_a = the mean free path of an air molecule [cm] (≈ 6.5×10^{-6} cm, 65 nm)
r_i = radius of particle, i [cm]
$Kn_{a,i} >> 10$ □ free-molecular regime (relatively small particles)
$Kn_{a,i} << 1$ □ continuum regime (relatively large particles)

Deposition Model

There have been a variety of experimental studies of particle deposition rates, including controlled chamber experiments and less controlled field experiments [25]. The mechanisms of particle deposition include advection, diffusion, thermophoresis and other external forces such as gravitational and electrostatic. Results of experimental studies are varied for reasons presented in Lai (2002); however, characteristic behaviors with respect to particle size, i.e., v-shaped deposition rate graphs, are often exhibited. These characteristics generally break down into deposition of smaller particles (< 0.1 μm) being dominated by Brownian and turbulent diffusion and large particles (> 1 μm) by gravitational settling, where for accumulation mode particles (between 0.1 μm and 1 μm) neither mechanism is dominant.

Lai and Nazaroff (2000) present a physically-based model of particle deposition onto smooth indoor surfaces that accounts for both Brownian and turbulent diffusion. The model is a function of particle size and density and incorporates enclosure geometry (rectangular or spherical) and friction velocity as inputs to the model. For purposes of this tool, only rectangular geometry is considered. Friction velocity is utilized to capture the effects of airflow intensity, i.e., the near-surface turbulent airflow. This tool enables input of friction velocity either directly or to be determined based on inputs of free stream velocity and a characteristic room dimension as detailed in Appendix B .

Equations (7) – (9) present the calculation of deposition velocities for the three surface orientations of a rectangular space, and equation (14) presents the first-order loss coefficient for deposition in a rectangular cavity. An analytical calculation for the integral, I, is presented in Lai and Nazaroff (2000) for larger particles for which Brownian diffusivity can be considered negligible, but for smaller particles I must be calculated numerically. Assuming that room air properties don't change during the simulation period, I need only be calculated once per simulation, so the tool performs the integration numerically for all particle sizes. For "typical" indoor environments, the particle turbulent eddy viscosity, ε_p, is assumed to be equal to the turbulent viscosity for which equations and associated justification are provided by equation 13 and section 2.2 respectively in Lai and Nazaroff (2000).

$$u_{dv} = \frac{u^*}{I} \tag{7}$$

$$u_{du} = \frac{u_s}{1 - exp\left(-\frac{u_s I}{u^*}\right)} \tag{8}$$

$$u_{dd} = \frac{u_s}{exp\left(-\frac{u_s I}{u^*}\right) - 1} \tag{9}$$

$$u^* = \sqrt{\frac{0.074}{2} U_\infty^2 \left(\frac{U_\infty L}{v}\right)^{-1/5}} \tag{10}$$

$$I = \int_{r^+}^{30} \left(\frac{v_{air}}{\varepsilon_p + D_p}\right) dy^+ \tag{11}$$

$$D_{p,i} = \frac{k_B T_{air}}{6\pi \, r_i \, \mu_{air}} \mathrm{G}_i \tag{12}$$

$$G_i = 1 + Kn_{a,i}\left[A' + B' e^{-C\prime/Kn_{a,i}}\right] \tag{13}$$

$$\kappa = \frac{u_{dv} A_v + u_{du} A_u + u_{dd} A_d}{V} \tag{14}$$

where:

u_{dv} = deposition velocity for vertical surfaces [cm/s]
u_{du} = deposition velocity for upward-facing horizontal surfaces [cm/s]
u_{dd} = deposition velocity for downward-facing horizontal surfaces [cm/s]
κ = first-order loss coefficient for rectangular space [1/s]
(Note: same as β in Lai and Nazaroff (2000))
$A_{v,u,d}$ = area of vertical, upward and downward surfaces, respectively [m^2]
V = Volume of rectangular space [m^3]
u^* = friction velocity [cm/s]
u_s = settling velocity [cm/s]
U_∞ = free stream velocity [cm/s]
L = characteristic room dimension [m]
v = kinematic viscosity of air [cm^2/s]
ε_p = particle turbulent (eddy) diffusivity [cm^2/s]
D_p = Brownian particle diffusivity (for each particle bin, i) [cm^2/s]
k_B = Boltzmann's constant 1.380658 x 10^{-16} [$g \cdot cm^2/s^2 \cdot K$]
T_{air} = Room air temperature [K]
r_i = particle radius (for each particle bin i) [cm]
μ_{air} = dynamic viscosity of air [g/cm·s]
G_i = Cunningham slip-flow correction (for each particle bin i) [-]
(A' = 1.257, B' = 0.42 and C' = 1.1)
r^+ = $r_i u^*/v$, where y^+ from r^+ to 30 represents the extents from the surface to the edge of the boundary layer [-]

NOTE: units are those implemented within the computer code of the tool.

The chart in Figure 9 presents the calculated deposition velocities, u_d, for three surface orientations (upward, downward and vertical facing) along with the particle settling velocity u_s. Figure 10 shows the deposition loss rate for a typical room (3 m high x 3 m x 4 m) as determined by the size-resolved tool (left) compared to values determined by Lai and Nazaroff (2000) (right).

Figure 9 and Figure 10 reveal the characteristic v-shaped plot whereby the deposition and loss rate for larger particles is independent of friction velocity, dominated by gravitational forces, and therefore aligns with the plot of settling velocity (shown in Figure 9). Smaller particles are dominated by Brownian diffusion, and therefore dependence on friction velocity is prevalent. Comparison between the two charts of Figure 10 reveals matching intercepts on the vertical axes and the minimum points of each curve confirming that the size-resolved deposition model has been properly implemented in the tool.

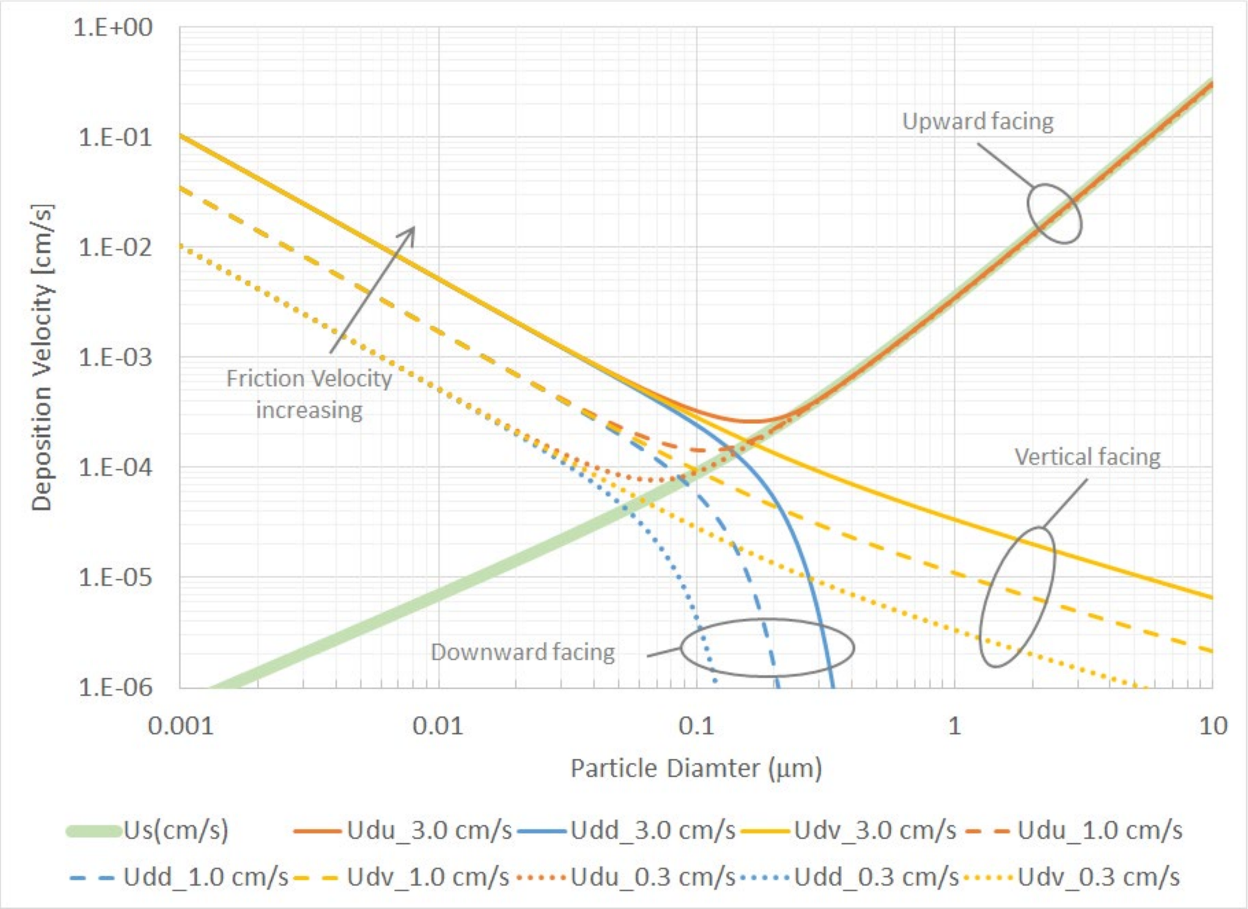


Figure 9 – Lai & Nazaroff deposition velocity model for three surface orientations and friction velocities (0.3, 1.0 and 3.0 cm/s)

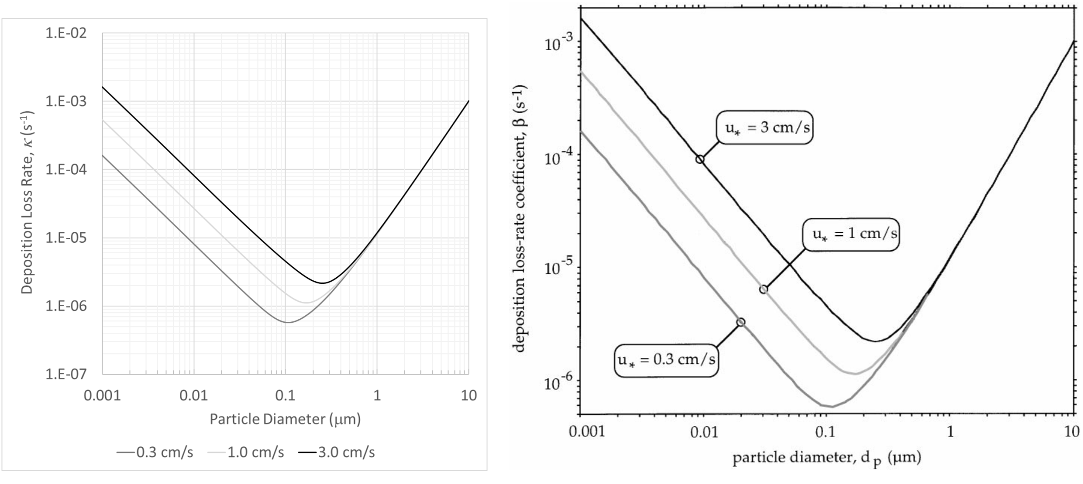


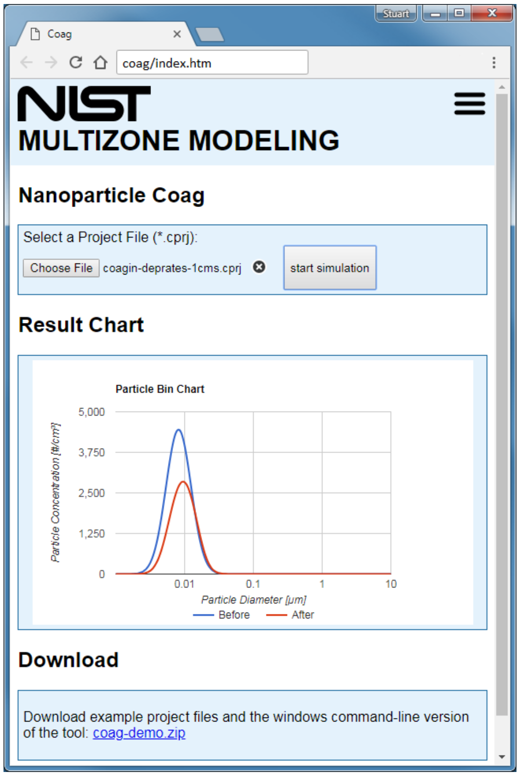
Figure 10 – Deposition loss-rate coefficient, κ, for typical room dimensions calculated using the size-resolved deposition model (left) and presented in Lai and Nazaroff 2000 (right, loss rate referred to as β).

2.2.2 Online Tool Development

FORTRAN source code, largely based on Jacobson et al. (1994), was provided to the authors by Dr. Mark Jacobson. This code was compiled for verification purposes. The code was then converted to the C programming language. The C program was then partitioned into an application programming interface (API) to produce a dynamic link library (DLL) referred to as *coagLibrary*. A client or front-end program, *coagClient*, was then developed to exercise the library module via the Windows command-line. An input file structure was created to simplify the implementation of user-defined cases and provide for future flexibility of the software. The input file is used by both the command-line client and the web-based client that will be presented in the following sections. The documentation of the input file is provided in Appendix B .

2.2.3 Web-based Solver

As was done with ContamX, *coagLibrary* was developed using Microsoft Visual C++. *Emscripten* [13, 14], was used to compile *coagLibrary* to JavaScript so that it could be run in a web browser. The initial version of the web-based, size-resolved tool has a very simple interface. The user selects an input file from the local file system and runs a simulation. Once the calculation has been completed, the initial and final particle distributions are plotted. This interface can be extended as more functionality is incorporated into the tool. For more detailed analysis, the command-line version of the program can be used to generate a results file and a log file as described in Appendix B .



Nanoparticle Coag

Select a Project File (*.cprj):

coagin-deprates-1cms.cprj

Result Chart

Download

Download example project files and the windows command-line version of the tool: coag-demo.zip

Figure 11 – Web-based Size-resolved Airborne Particle Modeling Tool

2.2.4 *Verification and Validation Test Cases*

Several test cases were developed for verification and validation purposes. For the purposes of verifying the code, comparative and analytical tests were performed. Inter-code comparisons were performed between the FORTRAN program provided to NIST and that developed for the size-resolved tool, i.e., *coagLibrary* and *coagClient*.

Figure 12 provides the results of the inter-code comparison. The initial particle distribution from both the FORTRAN and *coagClient* are shown on the left, and the final distribution on the right, revealing that the results align very well. In both plots, the FORTRAN results are represented by the dashed grey line and the *coagLibrary* version by the solid black line.

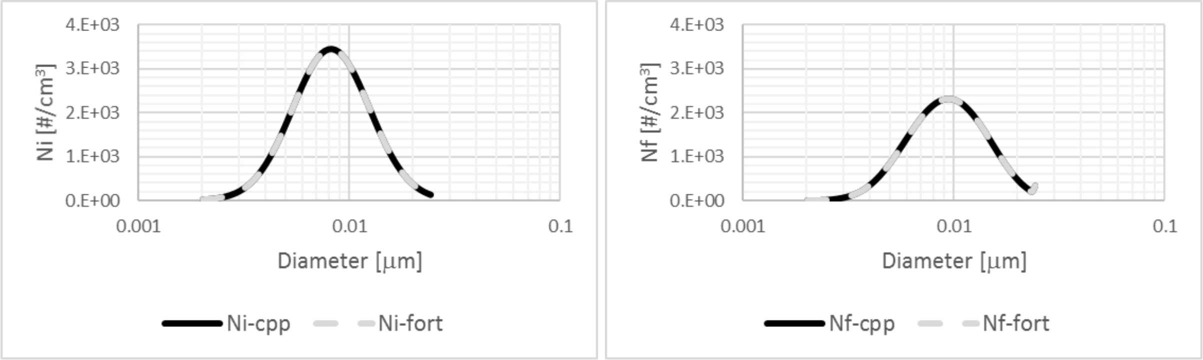


Figure 12 – Inter-code comparison test results: initial distribution (left) and final distribution (right)

There are limited analytical solutions to the coagulation equation. Smoluchowski's solution (original citation in German [27]) presented in equation (16) is one such analytical solution wherein a monomer size distribution is initially monodisperse and the coagulation kernel shown in equation (15) is constant.

$$n_{k,t} = \frac{n_{1,t-\Delta t}\left(0.5\Delta t\beta n_{1,t-\Delta t}\right)^{k-1}}{\left(1+0.5\Delta t\beta n_{1,t-\Delta t}\right)^{k-1}} \tag{15}$$

where:

$$\beta = \frac{8\ k_B T}{3\ \mu_{air}} \tag{16}$$

$n_{k,t}$ = number of particles in bin k at final time t [particles/cm^3]
$n_{0,t-\Delta t}$ = initial number of particles in bin 1 at time t-Δt [particles/cm^3]

The solution to this case is presented in Jacobson (2005). Smoluchowski's solution is implemented in *coagLibrary* as converted from the FORTRAN code. While this solution is specific to the assumed constant kernel and monodispersed initial condition, it does provide a test of the semi-implicit numerical approach implemented in the solver. Results of this test are presented in Figure 13, which shows the initial particle count all of which are in the smallest size bin and the results of three semi-implicit simulations (three different volume-ratio distributions, SI 1.2, 1.5 and 2.0) and the analytical solution. Results indicate that the

Smoluchowski and semi-implicit solution methods are performing as required and match those obtained with the FORTRAN code (not shown).

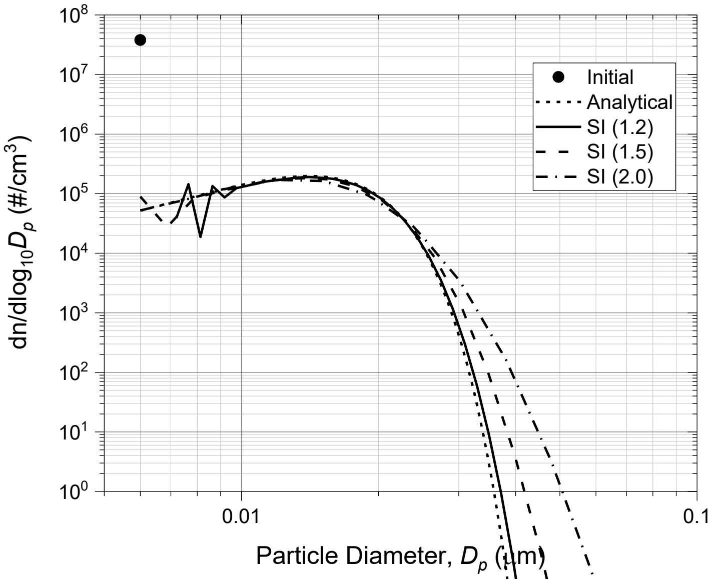


Figure 13 – Analytical solution compared with semi-implicit solutions using coagClient

Results from measurements of 3D printer emissions [28] were used to validate the performance of the size-resolved tool. The test consisted of the operation of five printers of two different types differentiated by the type of printing material used: polylactic acid (PLA) feedstock and acrylonitrile butadiene styrene (ABS) thermoplastic feedstock. Size-resolved emission rates and total loss rates were measured and reported in Stephens et al. (2013).

Measurement results for a period during which all five printers were operated and then shut off are shown in Figure 14, along with CONTAM simulation results for the several nanometer sized particles. Initial particle counts, emission rates and total removal rates for each size range were set in this tool as provided in Stephens et al. (2013). The total removal rate for each particle size was implemented by setting the ventilation rate such that the air change rate matched the total removal rate. Plots of predicted versus observed particle counts for the three simulated size ranges (11.5 nm, 36.5 nm and 64.9 nm) are provided in Figure 15 and associated correlation values, based on ASTM Standard Guide D-5157 [20], in Table 2. Values shown in bold in Table 2 are within the levels recommended in the ASTM guide (and provided in the left-hand column of the table). All parameters are within the guideline values for the two larger sized particles (36.5 nm and 64.9 nm), and the trends are all well captured by the CONTAM simulation. It is not clear why the smallest particle size is not well represented by the single-size particle model. Possible explanations include inaccuracy of the uniform concentration assumption, methods used to estimate both the emission and removal rates, and non-constant particle emission and removal rates over the period of measurements.

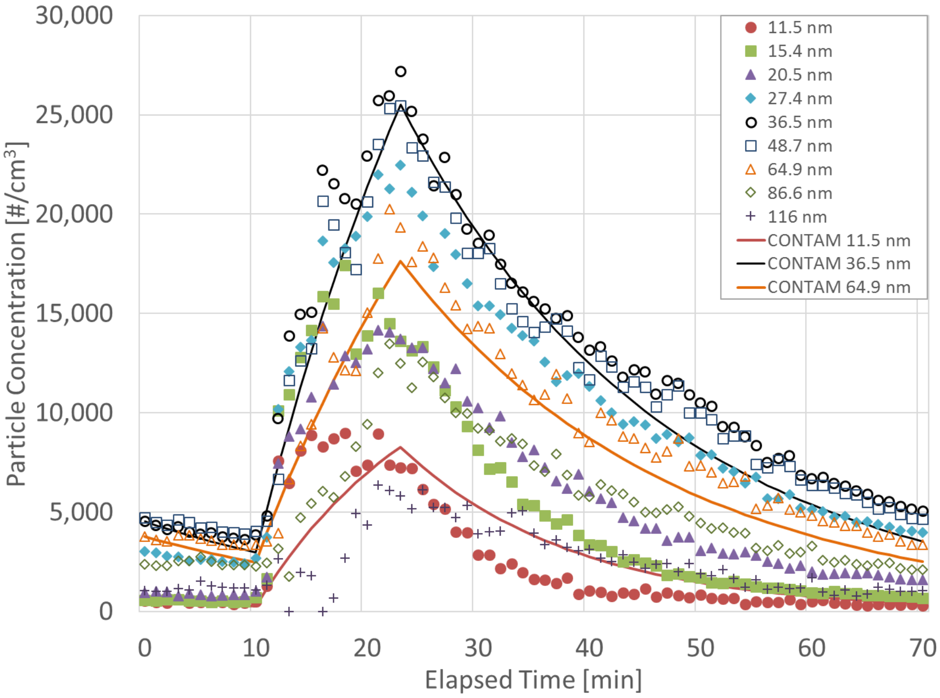


Figure 14 – CONTAM simulation of 3D printer emissions of several particle sizes vs. measurements.

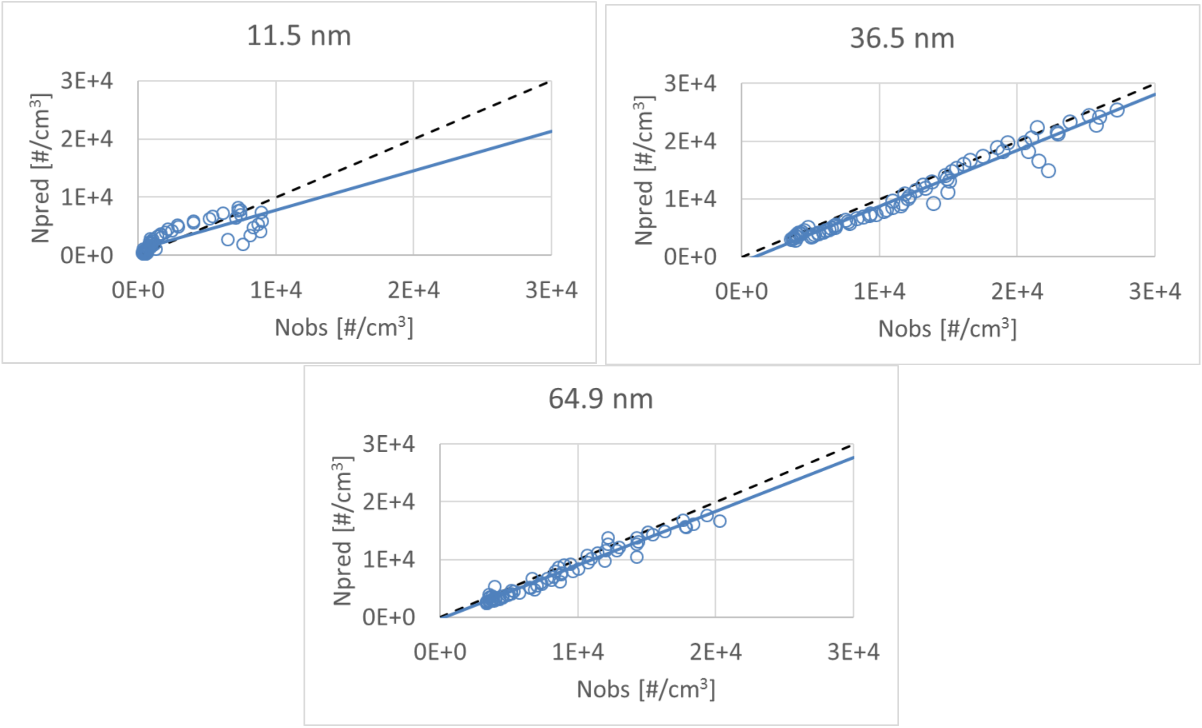


Figure 15 – Predicted vs observed particle number concentrations for CONTAM simulations of 3D printers (11.5 nm, 36.5 nm and 64.9 nm sized particles)

Criteria		11.5 nm	36.5 nm	64.9 nm
$\boldsymbol{N}$		71	71	71
$\boldsymbol{r}$	≥ 0.9	0.8156	**0.9816**	**0.9835**
$\boldsymbol{m}$	0.75 - 1.25	0.6773	**0.9649**	**0.9308**
$\boldsymbol{b/\overline{Co}}$	≤ 0.25	0.4236	**-0.0751**	**-0.0387**
$\boldsymbol{NMSE}$	≤ 0.25	0.4350	**0.0266**	**0.0251**
$\boldsymbol{\|FB\|}$	≤ 0.25	**0.0961**	**-0.1167**	**-0.1141**
$\boldsymbol{\|FS\|}$	≤ 0.50	**-0.3674**	**-0.0342**	**-0.1100**

Table 2 - Correlation between CONTAM simulations and observed particle counts for of 3D printers

To simulate this test case using the size-resolved tool, an initial particle distribution must be determined. This was done by calculating the geometric mean number diameter, μ_g, and geometric standard deviation, σ_g, based on the peak, measured number counts according to the following equations:

$$\mu_g = exp\left[\frac{\sum_{i=1}^{N_{bins}} n_i \ln d_i}{N_T}\right] \tag{17}$$

$$\sigma_g = exp\left[\frac{1}{N_T}\sum_{i=1}^{N_{bins}}\left(n_i\, ln^2 \frac{d_i}{\mu_g}\right)\right] \tag{18}$$

where:

N_T = total particle count
N_{bins} = number of particles bins
n_i = number of particles in bin i
d_i = diameter of particles bin i [cm]

The measured initial and final geometric mean and standard deviation and final simulation values are provided in Table 3 and plotted in Figure 16 (left). The closed symbols in Figure 16 correspond to the diameters of the three particle sizes simulated using CONTAM (11.5 nm, 36.5 nm and 64.9 nm) as shown in Figure 14. The measurements reveal that there is a slight increase in the geometric mean diameter indicating that removal by ventilation is not the only particle transport mechanism involved. The ventilation rate was not measured for these experiments, only the total removal rate for each particle size was determined. While the total removal rate was utilized in the CONTAM model, it is not applicable in the size-resolved model. Therefore, the air change rate used in the size-resolved model had to be estimated by trial and error. Figure 16 (right) shows the final simulated distributions comparing different simulation parameters as a result of trial and error estimation of ventilation rate. The ventilation rate was determined to be about 2.0 h^{-1}, which is reasonable for an office space in which the experiments were conducted [29]. Figure 16 (right) also shows that simulation results, assuming that both deposition and coagulation are taking place along with ventilation, are in good agreement with measurements including an increase in geometric mean number diameter. This shift can occur due to both coagulation and deposition for such small particles as can be intuited from deposition rates shown in Figure 9. (The input file associated with this test is provided as an example input file in Appendix B .)

	Measured		Simulation w/ *size-resolved tool*			
	Initial	Final	Initial	Final Vent. only 2.1 h^{-1}	Final Vent. 2.0 h^{-1} Deposition	Final Vent. 2.0 h^{-1} Deposition Coagulation
μ_g	0.03717	0.04220	0.03790	0.03790	0.03866	0.03953
σ_g	1.8265	1.6521	1.7804	1.7804	1.7729	1.7767
N_T	148,285	22,742	142,351	26,531	27,293	25,776

Table 3 – Size resolved simulation results vs Measured data

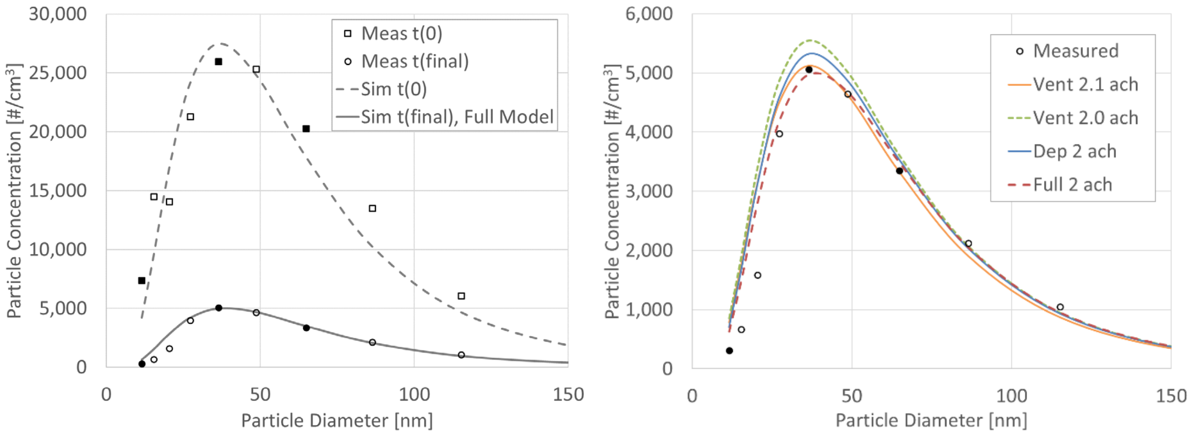


Figure 16 – Simulation of nano-particle emissions from 3D printers using the size-resolved tool. Initial and final distributions (left); comparison between final distributions for multiple sets of inputs (right).

3 Summary and Conclusions

Two tools were developed for purposes of evaluating consumer exposure to airborne ENPs: one a single-size particle model and the other a size-resolved particle model. Both tools implement a uniform concentration, single zone model. The single-size tool incorporated a web-based front-end to a JavaScript version of ContamX, the simulation engine of CONTAM. This web-based tool runs as a client-side application within a web browser. The size-resolved model was developed based largely on an atmospheric model and incorporated coagulation, deposition and ventilation. The development process, theory and assumptions were presented for both tools. Verification and validation test cases were presented, and user guides were provided for each tool along with example input values.

Future Development

While both tools can be accessed and exercised via their respective web interfaces, both tools could be further enhanced as will be outlined for each below. Enhancements could come in the form of *Transport phenomena*, *Usability*, and *Input data*. Regardless of the future modifications, the current tools provide the ability to evaluate exposures for a range of particle properties and exposure scenarios. These tools provide a foundation upon which to build as transport properties of ENPs and their relevance to consumer exposure become better understood and more data becomes available. These tools currently address the potential exposure to airborne particulates, but they do not address the dosage or uptake of such particles via human respiratory physiology. Consideration could be given as to how the results of these tools would be implemented by epidemiologists and eventually incorporated into exposure and risk assessment tools.

Single-size particle tool

The single-size tool implements a fairly simple, single zone model based on the well-validated CONTAM software. As such, much of the functionality is incorporated directly within the ContamX solver. Therefore, enhancing the *Transport phenomena* of CONTAM would require modifications to both ContamX and the Windows graphical user interface, ContamW. *Usability* improvements would mostly come in the form of modifications to the web interface, and pre-defined *Input data* being developed and made available to users.

Transport phenomena

Transport phenomena that could be incorporated within CONTAM could include those implemented by the size-resolved model. Such potential enhancements to CONTAM were identified in Axley (1995) and would involve significant modifications to CONTAM to solve the non-linear particle/contaminant calculations. These considerations could be investigated by incrementally extending the size-resolved tool to address a more simplified multi-zone approach.

The deposition model implemented in the size-resolved tool could be directly incorporated within CONTAM. While this might also improve the usability of the tool, the current command-line version of the size-resolved tool can be used to calculate these deposition rates, which could then be input by the user into the single-size tool.

Usability

Currently the single-size tool is presented as a general particle modeling tool. This is in line with the approach of the underlying CONTAM software. CONTAM provides the mathematical foundation of the model but leaves the definition of specific inputs to the user. Further, CONTAM enables the user to create custom, shareable libraries of input data. For example, one can define a particle contaminant having a given diameter, density and default background concentration, develop particle filter models, emission sources, and deposition and resuspension elements. Along these lines, usability of the size-resolved tool could be enhanced to incorporate such libraries.

The tool could be modified to enable multiple sizes to be addressed in a single simulation. This would not allow for the direct analysis of coagulation based on a size-resolved kernel, but it would still be applicable to problems with relatively “low” particle counts for which coagulation may not be a factor. However, it could allow analysis similar in nature to that presented for the validation test case wherein total removal rates are available as inputs.

The current tool provides for a single simulation to be performed and displayed. It could be modified to enable comparisons between multiple cases to evaluate differences between different exposure scenarios.

Input data

As mentioned in the previous section, libraries of input data for ENPs could be developed and provided for the tool, assuming relevant properties of ENPs exist. These libraries would be similar to the set of filters that are currently available within the tool.

Size-resolved particle tool

Development of the size-resolved tool consisted mainly of converting existing FORTRAN code to C++ and implementing it as a library of functions to be used by both a command-line and web-based client. The base functionality was verified and implemented as a simple web-based tool. While the tool allows the user to evaluate the relative impacts of coagulation, deposition and ventilation, there are still many possible enhancements that could be made to the tool.

Transport phenomena

Because the size-resolved tool was developed as a library with a readily modifiable input file, it should be easily extendable. Multiple coagulation kernels could be added, particularly those that may be relevant to nanoparticles, e.g., van der Waals (weak, fluctuating dipole interactions), viscous forces and shape-based (or fractal). While these kernels may not be specific to ENPs, if information were to emerge specific to ENPs, associated kernels could be added to the model.

The addition of source terms would provide the ability to address emissions as opposed to the current model that allows for only an initial distribution to be specified. Source terms should also be schedulable to turn on and off and to vary over time. Additionally, the ability to incorporate an outdoor particle distribution, either as a source or as a background in addition to internally-generated particles, could be added as well as envelope penetration factors. The current tool only accounts for removal by deposition and ventilation, and other removal mechanisms could be added such as filters.

The current tool only provides for direct ventilation to the zone, and does not distinguish between supply or exhaust ventilation. The tool could be modified to enable simulation of a simplified air handling system as done with the single-size tool. Such a ventilation system would provide for outdoor air intake, recirculation and filtration within the system.

Transport phenomena could be added that capture interactions between different particle types [21]. This addition could include coagulation of ENPs with background particles while tracking the composition of coagulated particles, in addition to enabling the tracking of interaction among multiple distributions based solely on the resultant particle sizes. Further, the ability to account for chemical reactions would expand the modeling capability into more general IAQ analysis which involves almost limitless combinations of inter-particle and contaminant interactions. Although the significance of such chemical interactions with respect to ENPs is currently not clear.

Input data

The current model requires the initial particle size distribution to be input as either a monomer or log-normal distribution, specified as a total initial particle count, a geometric mean number diameter and geometric standard deviation having volume-ratio based size bins. This could be modified to enable specification of different types of distributions including free-form bin and number counts or multiple size distributions or modes of particle distributions. For example, this capability would enable interaction of indoor particles with background particles. Although, accounting for the fate of particles of different types (e.g., internally and externally mixed [21]) would require modifications to the *Transport phenomena*. However, treating all particles as being of the same type may still provide insight into the fate of ENPs within the indoor air but may not fully capture the potential ramifications of occupant exposure to agglomerations of ENPs with other background particles.

Usability

Usability could be readily improved to incorporate features similar to the single-size tool. This would include modifications of the web interface to provide inputs (as opposed to directly modifying input files via text editor) and modification to the simulation code, for example, to enable calculating exposure and providing the number of particles removed by ventilation and deposition.

The tool could be modified to enable developers to extend its capabilities. For example, specific source types could be developed as in CONTAM, e.g., burst or constant, or the ability could be provided for developers to extend the library to incorporate new source terms. The source code could be made available in the public domain, or a framework could be incorporated to allow the development of modules to extend the tool. The former would likely lead to disparate, i.e., forked, code and/or require a *lead* developer to maintain a code repository and verify and incorporate modifications.

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Appendix A – Single-size Particle Tool User Guide

This appendix provides detailed information on the inputs and outputs of the *Single-size Particle Modeling Tool*. Variable names reflect those provided in Equations (1) and (2) and Figure 2.

Inputs

Building inputs are used to define the zone and ventilation system properties, particle source and removal mechanisms and the occupant exposure period.

Zone Geometry

Volume: Set the volume (V) and units.

Floor, Wall** and **Ceiling Area: Set the areas (A_{si}) and units, for those surfaces onto which deposition occurs.

Envelope Penetration Factor: Set the penetration factor (P). This will only have an effect if the outdoor concentration is greater than zero and there is an imbalance between the supply and return airflow rates that leads to infiltration.

Ventilation System

Supply Airflow** and **Return Airflow Rate: Set the supply airflow rate (Q_{sup}) and return airflow rate (Q_{ret}) of the simple air handling system.

Percent Outdoor Air: Set the fraction of outdoor air (Q_{oa}/Q_{sup}) of the simple air handling system. This must be other than 100 % in order for the zone air to be recirculated through the simple air handling system. If Q_{rec} is greater than zero, then zone air can be filtered prior to being mixed into the supply air.

Air Change Rate: Calculated from the previous inputs for informational purposes.

$$\text{Air change rate} = [Q_{oa} - \text{Min}(0.0,\ Q_{sup} - Q_{ret})]/V$$

Outdoor Airflow Rate: Calculated from the previous inputs for informational purposes. It is the amount of outdoor air brought into the zone via the simple air handling system (Q_{oa}).

Recirculation Airflow Rate: Calculated from the previous inputs for informational purposes. It is the amount of return air recirculated back into the zone via the simple air handling system (Q_{rec}).

$$Q_{rec} = \text{Min}[Q_{ret},\ Q_{sup}(1.0 - \%OA)]$$

Exhaust Airflow Rate: Calculated from the previous inputs for informational purposes. It is the amount of return air exhausted to outdoors via the simple air handling system (Q_{exh}).

$$Q_{exh} = Q_{ret} - Q_{rec}$$

Airflow Imbalance: Calculated from the previous inputs for informational purposes. It is the amount of either infiltration or exfiltration directly between the zone and outdoors (Q_{inf}). A negative flow imbalance indicates infiltration (Equation (1) uses the opposite sign convention), in which case the *Penetration* factor can remove particles from the infiltrating air.

$$Q_{inf} = Q_{sup} - Q_{ret}$$

Zone Air Balance: This will indicate the airflow imbalance leads to a *Balanced*, *Pressurized* or *Depressurized* zone depending on the ventilation system airflow rates.

Outdoor** and **Recirculation Air Filter: Select the filters from the list of Minimum Efficiency Reporting Values (MERV) to include within the outdoor and/or recirculation air streams of the simple air handling system (see Figure 2).

Particle Properties

Particle Diameter: Set the *Particle Diameter* which is used for unit conversions of particle concentrations and to establish MERV filter removal rates.

Particle Density: Set the *Particle Density* which is used for unit conversion of particle concentrations.

Particle Source

Source Type: Set the *Source Type* to be either *Constant* or *Burst* (G).

Release Amount: Set the *Release Amount* and units if using a *Burst* source. This can be set to zero if no source is desired.

Release Rate: Set the *Release Rate* and units if using a *Constant* source. This can be set to zero if no source is desired.

Source Start Time: Set the *Source Start Time* for release of a *Burst* source or the beginning of a *Constant* release.

Source End Time: Set the *Source End Time* at which to stop a *Constant* release.

Particle Deposition Velocities

Floor, Wall,** and **Ceiling: Set the *Deposition Velocity* and units for each category of surface onto which to account for particle deposition, i.e., removal of particles from zone air by deposition. You must also set the associated surface areas under Zone Geometry.

Particle Deposition Velocities

Floor, Wall,** and **Ceiling: Set the *Deposition Velocity* (v_{di}) and units for each category of surface onto which to account for particle deposition, i.e., removal of particles from zone air by deposition.

Particle Resuspension

Floor, Wall,** and **Ceiling: Set the *Resuspension Areas* (A_{ri}), *Resuspension Rates* (r_i) and units for each category of surface from which to account for particle resuspension, i.e., addition of particles to zone air by resuspension. The *Resuspension Areas* are not required to be the same as the *Areas* defined under Zone Geometry, but they should be less than or equal to those areas. For example, the surface area could simply be that of a shoe treading on the floor.

Initial Concentration and Surface Loadings

Outdoor Concentration*:* Set the *Outdoor Concentration* (C_{oa}) and units to account for particles entering the zone from the ambient via the ventilation system and/or infiltration through the building envelope.

Floor, Wall, *and* ***Ceiling***: Set the initial values for each category of surface loading (L_{si}) and units from which to account for particle resuspension. These values can be zero, or can be used to account for particle resuspension either alone or along with a source.

Occupant Exposure

Exposure Start *and* ***End Time****:* Set the time interval during which an occupant is to be located within the zone. This time interval will be used to determine the *Integrated Exposure*.

RUN SIMULATION

Click the *RUN SIMULATION* button to perform a 24-hour simulation using the currently defined Inputs. When you click the button, a notice should appear next to the button indicating “Running Simulation”. Once the simulation is complete, a “Simulation Complete” notification will be displayed along with a link that you can click to “***Download CONTAM Project***”. This will allow you to save a CONTAM project (PRJ) file to your computer. This PRJ file can be opened using ContamW for further analysis or record-keeping as desired.

Resultant Exposure

Integrated Exposure*:* This is the calculated exposure and units according to the occupant exposure period. The selected units will be reflected in all of the following results.

$$\textit{Integrated Exposure} = \int_{t_{start}}^{t_{end}} C_z(t)\, dt$$

Average and ***Peak Concentration****:* These values are for the entire 24-hour simulation period.

Average **(**Δt **h)** and ***Peak Concentration*** **(**Δt **h)***:* These values are for the entire exposure time period ($t_{end} - t_{start}$). The exposure time will be provided in the parentheses, e.g., “(8 h)”.

Transient Air and Surface Concentrations

Air Concentration*:* This chart shows the time history and the *Average Concentration* of the zone air for the entire 24-hour simulation period.

Occupant Exposure Concentration*:* This chart shows the time history and the *Average Exposure* of the occupant to the zone air for the user-defined exposure period (t_{start} to t_{end}).

Surface Loading*:* This chart shows the time history of the three surface categories (floor, walls and ceiling) for the entire 24-hour simulation period.

Appendix B – Size-resolved Particle Tool

This appendix provides documentation of the size-resolved particle modeling tool. Input files, referred to as **C**oagulation **PR**o**J**ect files (.cprj) can be utilized with the web-based front end of the tool. The input file format and an example input file are provided.

Running the web-based tool

The user clicks the "Choose File" button to select a CPRJ file from their local computer and click the "Start Simulation" button.

Running the command-line tool

The easiest way to run the command-line tool is to place the program executable (coagClient.exe) and CPRJ files in the same directory. Typing the name of the executable without any parameters will provide the following usage message:

```
Usage: coagClient [FILE] [OPTION]
Run single zone coagulation on input FILE with logging OPTION.
FILE    Name of input file having .cprj extension
OPTION 0, no logging
       1, log to stdout
       2, log to FILE.xlog
       3, log to stdout and FILE.xlog
```

CPRJ Input File Format

The input file can be used by both the web-based and command-line versions of the tool. The file is divided into sections that are terminated by a section divider string "`-999`". The first line of the file consists of a header that consists of three items, and each line after that contains a single input variable. However, comment lines can also be included which are ignored when reading the input file. Items are either read in as strings (string), integer (int) or floating-point values (float). A short form variable name is provided in the format description to simplify reference within this document. Where units are relevant, they are provided within brackets []. Refer to the Example Input File that follows this section.

The header line consists of three items:

```
COAG  // Program identifier (string)
0.4.0 // Version identifier (string)
      // Used to ensure proper file format between versions.
_list // Bitwise value defines logging (integer)
      //  0 No logging
      //  1 echo cprj file
      //  2 Log particle bins
      //  4 Log 3D volume partioning array Vijk (Jac2005, eq 15.11)
      //  8 Log initial particle distribution
      // 16 Log deposition rate calculation
      // 32 Log deposition calculation details
      // Example: 17 => echo cprj file AND deposition rate calculation
```

Ambient air properties section:

```
Tamb  // temperature [K] (float)
Pamb  // absolute pressure [Pa] (float)
-999
```

Initial particle distribution section:

```
dType // distribution type
      // 0 = log normal
      // 1 = monodispersed (use mono for Smoluchowski test)
nBins // number of particle bins (int)
rMin  // particle radius of smallest bin [cm] (float)
vRat  // volume ratio for size distribution (float)
rho   // particle density [g/cm3] (float)
gMean // geometric mean particle count diameter [µm] (float)
gStd  // geometric standard deviation [-] (float)
nTot  // initial particle number concentration [#/cm3] (float)
0     // currently not used (int)
-999
```

Simulation control section:

```
dt    // simulation time step [s] (float)
time  // simulation duration [s] (float)
dep   // deposition rate calculation method (int)
      // 0 = None
      // 1 = Lai and Nazaroff numerical & analytical
      // 2 = Lai and Nazaroff numerical only (recommended)
kern  // coagulation kernel (int)
      // 0 = None
      // 1 = Soluchowski
      // 2 = Brownian
-999
```

Zone data section:

```
Af    // floor area [m2] (float)
Aw    // wall area [m2] (float)
Vol   // volume [m3] (float)
ACR   // ventilation rate [1/h] (float)
Ufric // friction velocity [m/s] (float)
      // If Ufric <= 0.0 then f(Ufree) as per (Lai2000, eqn 20)
Ufree // free stream velocity [m/s] (float)
Lchar // characteristic length [m] (float)
      // Ufric and Lchar required for “dep” = 1 or 2
      // If Lchar <= 0.0 then Lchar = Vol^(1/3)
-999
* end project file.
```

Example Input File

This example file matches values used to simulate the 3D printer test of Stephens et al. (2013).

```
COAG 0.4.0 11
! Brent Stephens 3D printer test
!  Ventilation rate = 2.0 /h
!  Coag = yes
!  Deposition = yes
!
!--- Ambient air properties
2.93150e+02 ! Tamb(K)
1.01325e+05 ! Pamb(Pa)
-999
!--- Particle Distribution Data
0           ! type: 0=log normal, 1=monodispersed
13          ! nBins
5.77350e-07 ! rMin(cm)
2.37        ! vRat
1.0         ! rho(g/cm3)
3.70700e-02 ! gMean(um)
1.82650     ! gStd
148285.0    ! an(#/cm3)
-999
!--- Simulation Control
10.0    ! dt(s)
2880.0  ! ttime(s)
2       ! calcDepRate:
        ! 0=none, 1=LaiNazaroff(Num+Analy), 2=LN(Num only)[recommended],
2       ! coagKernel: 0=none, 1=Smoluc(test), 2=Brownian
-999
!--- Zone Data
15.0        ! Af(m2)
48.0        ! Aw(m2)
45.0        ! Vol(m3)
2.0         ! ACR(1/h)
! Ufric and Lchar required for calcDepRate = 1 or 2
2.60000e-02 ! Ufric(m/s) 0 => Ufric = f(Ufree), Lai2000 eqn 20
0.00000e+00 ! Ufree(m/s)
0.00000e+00 ! Lchar(m)   0 => Lchar = (Vol)^(1/3)
-999
* end project file.
```

Appendix C – Change Log

Revision 1 – September 30, 2020

Equation 10 was incorrect as provided in this documentation, but it is implemented correctly within the software tool. The original and corrected equations are provided below, and the corrected equation is provided within the document. The units of L within the equation are centimeters but L is provided via the input file to the program in meters.

$$u^* = \sqrt{\frac{0.074}{2} U_\infty \left(\frac{U_\infty L}{v}\right)^{1.5}} \tag{10 original}$$

$$u^* = \sqrt{\frac{0.074}{2} U_\infty^2 \left(\frac{U_\infty L}{v}\right)^{-1/5}} \tag{10 corrected}$$