Pacific Northwest NATIONAL LABORATORY

PNNL-36017

Qualification of Mixing Criteria by Computational Fluid Dynamics Modeling for the 325 Building Stack Revision

May 2024

SR Suffield
JM Barnett
SE Gourley

U.S. DEPARTMENT OF ENERGY

Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830

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Summary

Additional ventilation capacity has been designed for the 325 Building filtered exhaust stack system. The four (4) existing main facility exhaust fans are past the end of their useful life. The fans are being replaced to provide additional exhaust capacity for future growth and to provide a more robust system. Stack operations will involve running various fan combinations at any given time. The air monitoring system of the existing stack previously was found to comply with the American National Standards Institute/Health Physics Society (ANSI/HPS) N13.1-1999 standard. Full-scale, three-dimensional computational fluid dynamics (CFD) modeling was used to evaluate the modified four-fan system for compliance with the ANSI/HPS N13.1-2021 standard, which essentially is equivalent in mixing requirements to the ANSI/HPS N13.1-1999 standard (and ANSI/HPS N13.1-2011). The four mixing criteria evaluated are 1) flow angle, 2) velocity, 3) gas tracer, and 4) particle tracer.

In addition to the evaluating the modified four-fan system a temporary single fan stack configuration was also evaluated with CFD modeling. The temporary stack is planned to be used while the four-fan system is being modified.

Modeling of the modified four-fan design and temporary ductwork showed that flow angles, velocity uniformity, gas tracer, and particle tracer were acceptable.

Acronyms and Abbreviations

acfm	actual cubic feet per minute
3-D	three-dimensional
ANSI	American National Standards Institute
cfm	cubic feet per minute
HPS	Health Physics Society
HVAC	heating, ventilation, and air conditioning
CFD	computational fluid dynamics
COV	coefficient of variation
PNNL	Pacific Northwest National Laboratory
scfm	standard cubic feet per minute

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1.0 Introduction

The 325 Building at Pacific Northwest National Laboratory (PNNL) houses radiological capabilities. Permit conditions require that air discharged from the building filtered exhaust stack system must be monitored for radionuclides. The air monitoring system must comply with applicable federal regulations, which subsequently require a sampling probe in the exhaust stream to conform to the uniformity criteria of the American National Standards Institute/Health Physics Society (ANSI/HPS) N13.1-1999 (and ANSI/HPS N13.1-2011) standard (HPS 1999, and HPS 2011). The criteria include the average angle between the flow and duct axis, the uniformity of flow velocity, the uniformity of tracer gas, and the uniformity of tracer particles. Uniformity is expressed by the coefficient of variation (COV), which is defined as the standard deviation divided by the mean, reported as a percentage. For a sampling location to be acceptable, the average flow angle must be less than 20° from the duct axis (aligned with the sample probe) to prevent cyclonic flow, and COV values for velocity, tracer gas concentration, and tracer particle concentration must be less than 20%. An additional criterion is that at no point in the sampling plane will the maximum concentration of tracer gas exceed the mean by more than 30%.

An option in the ANSI/HPS N13.1-2021 standard allows adoption of results from a previously performed full test series for a stack system of similar configuration as the basis of compliance with the standard (HPS 2021). Compliance then is confirmed by partial testing performed on the actual stack system. This approach was used to qualify the location of the sampling and monitoring equipment. Initially, a scale model of the exhaust system was construction and tested; the scale model results were compared to the actual velocity uniformity of the as-built stack and found to meet the mixing requirements (Ballinger et al. 2004, Smith et al. 2010, and Ballinger et al. 2011).

The 325 Building exhaust stack system will be updated with additional ventilation capacity. The updated system will incorporate four (4) direct drive exhaust fans with an exhaust capacity of 60,000 CFM each. In the new ANSI/HPS N13.1-2021, computational fluid dynamics (CFD) modeling is discussed as an option for optimizing and upgrading an existing system and indicates the same requirements for qualifying the sample extraction system must be met (i.e., those methods similar to either a similar exhaust system or a scale model system [HPS 2021]). The final 325-Building-stack modeled the updated design and effectively acts as a similar stack design.

2.0 Modeling Methodology

The purpose of modeling the 325 Building stack system is to simulate the stack flow, including distributions of gas and particle tracers, to assist in determining if the modified system will satisfy the ANSI/HPS N13.1-2021 standard. To provide accurate predictions of flow angle, velocity, tracer gas, and tracer particle distributions (at the sampling location) requires an accurate prediction of the turbulent air flow with transport and mixing of the tracer species within it. The geometry and flow field of the exhaust stack system is complex and highly three-dimensional (3-D). Therefore, a representative boundary-fitted, 3-D flow model also was required. The commercially available CFD flow simulation code, STAR–CCM+ (Siemens 2021) was selected for creation of the 3-D model domain and the flow simulations.

PNNL has extensive experience in modeling stack designs for compliance. Past CFD modeling has been shown to be useful both in the design process and as an effective predictor of flow angles and velocity and tracer COVs. Peer-reviewed publications authored by PNNL staff include papers that addressed the following relevant topics:

- Modeling of the 325 Building exhaust stack system to evaluate relocation of the sampling point (Barnett et. al 2005, Recknagle et. al 2009),
- Modeling and testing to assess the 3410 Building exhaust stack sampling probe location (Yu et. al 2014),
- Modeling of a modified building stack for sampling compliance (Barnett et. al 2016), and
- Modeling of filtered building effluent stack sampling points for qualification criteria (Barnett et. al 2020).

The present modeling for the 325 Building stack was performed using the same modeling methodology applied in our previous work.

2.1 Flow Model

The stack sampling methodology assumes isothermal conditions exist within the stack; therefore, that assumption was adopted in the flow model. For isothermal flow solutions, STAR-CCM+ solves the Navier-Stokes conservation of mass and momentum equations, which for steady-state compressible and incompressible fluid flows are:

$$\frac{\partial}{\partial x_j}\left(\rho u_j\right)=0 \quad (1)$$

$$\frac{\partial}{\partial x_j}\left(\rho u_j u_i-\tau_{ij}\right)=-\frac{\partial p}{\partial x_i} \quad (2)$$

where the term u_i and u_j represent absolute fluid velocity components in coordinate directions x_i (i = 1, 2, 3) and x_j (j=1,2,3), ρ is the density, p is the pressure, and τ_{ij} is the fluid stress tensor, which for turbulent flows is represented by:

$$\tau_{ij}=2\mu\sigma_{ij}-\frac{2}{3}\mu\frac{\partial u_k}{\partial x_k}\delta_{ij}-\bar{\rho}\overline{u_i' u_j'} \quad (3)$$

where μ is the dynamic viscosity, σ_{ij} is the rate of strain tensor, δ_{ij} is the Kronecker delta, u_i' and u_j' are fluctuations about the average velocity, and the overbar indicates the averaging of the fluctuations. The right-most term in Equation 3 represents the additional Reynolds stresses due to turbulent motion. These stresses are linked to the mean velocity via the turbulence model being used. In the simulations for this work, the generation and dissipation of turbulence is accounted for using a standard κ-ε turbulence model, which is a widely tested and validated two-equation closure model for the Reynolds average Navier-Stokes equations, as described in the STAR-CMM+ User Guide (Siemens 2021). In past work by Recknagle et al. (2009), a turbulence model comparison found the Reynolds average Navier-Stokes κ-ε model to be the most suitable for simulating duct flow, a finding corroborated by Jensen (2007). To capture strong secondary flows, which are frequently seen in heating, ventilation, and air conditioning (HVAC) systems, non-linear terms were added to the stress-strain relationship for the κ-ε model by selecting a cubic constitutive relationship. This modified the Boussinesq approximation with cubic terms (Siemens 2021).

These equations (Eqs. 1, 2, and 3) are independent of units. That is, the user can select the units for length, density, and velocity and make any necessary conversions to ensure consistent units.

2.2 Gas Tracer Model

For the tracer gas simulations, the model assumes each species k of a gas mixture, with local mass fraction Y_k is governed by a species conservation equation of the form:

$$\frac{\partial}{\partial x_j}\left(\rho u_j Y_k + F_{k,j}\right) = S_k \tag{4}$$

where $F_{k,j}$ is the gas diffusional flux component and S_k is the gas species source term, which is non-zero at the injection location.

2.3 Particle Tracer Model

A Lagrangian dispersed two-phase flow model is used for the particle transport simulations. The Lagrangian methodology considers the interactions of mass, momentum, and energy between the continuum and dispersed phase. In general, motion of the dispersed phase is influenced by that of the continuous phase and vice versa. The strength of the phase interactions depends on concentration, size, and density of the dispersed particle. For the present work, particle concentrations are small, as is the nominal particle size. Thus, momentum transfer from particles to air is negligibly small. In the model, the momentum equation for a particle, given by Newton's second law, is:

$$m_d \frac{du_d}{dt} = F_{dr} + F_p + F_b \tag{5}$$

where m_d and u_d are the mass and velocity of the dispersed particle phase, F_{dr} is the drag force, F_p the pressure force, and F_b is body forces, including effect of the gravity and angular velocity vectors. Surface vapor pressure and mass transfer between phases are not considered here. The problem is considered isothermal and does not involve electrically charged flow; therefore, thermophoresis and electrostatic effects are not included. Because of the low concentration of the particles, separation and coalescence models were not considered.

2.4 Model Geometry and Computational Mesh

Design drawings or computer aided design software drawings of the stack system of interest were used to create 3-D geometry models of the system. The model geometry for the updated four-fan, 325 Building system design is shown in Figure 1. Air flow upstream and through the fans is not included in the model domain but is accounted for as turbulence added at each fan duct. Thus, the model domain includes the ductwork from just downstream of the fans and damper to the stack exit. The flow from each fan is split and enters the exhaust plenum at two inlets. It was assumed that the flow from each fan was split by and 1/3rd and 2/3rd flowrate. The tracer injection locations are at the fan inlets to the exhaust plenum and assumed a 1/3rd and 2/3rd split. The sampling point is located at the 80-foot level above grade, which is approximately 8 ft below the top of the stack.

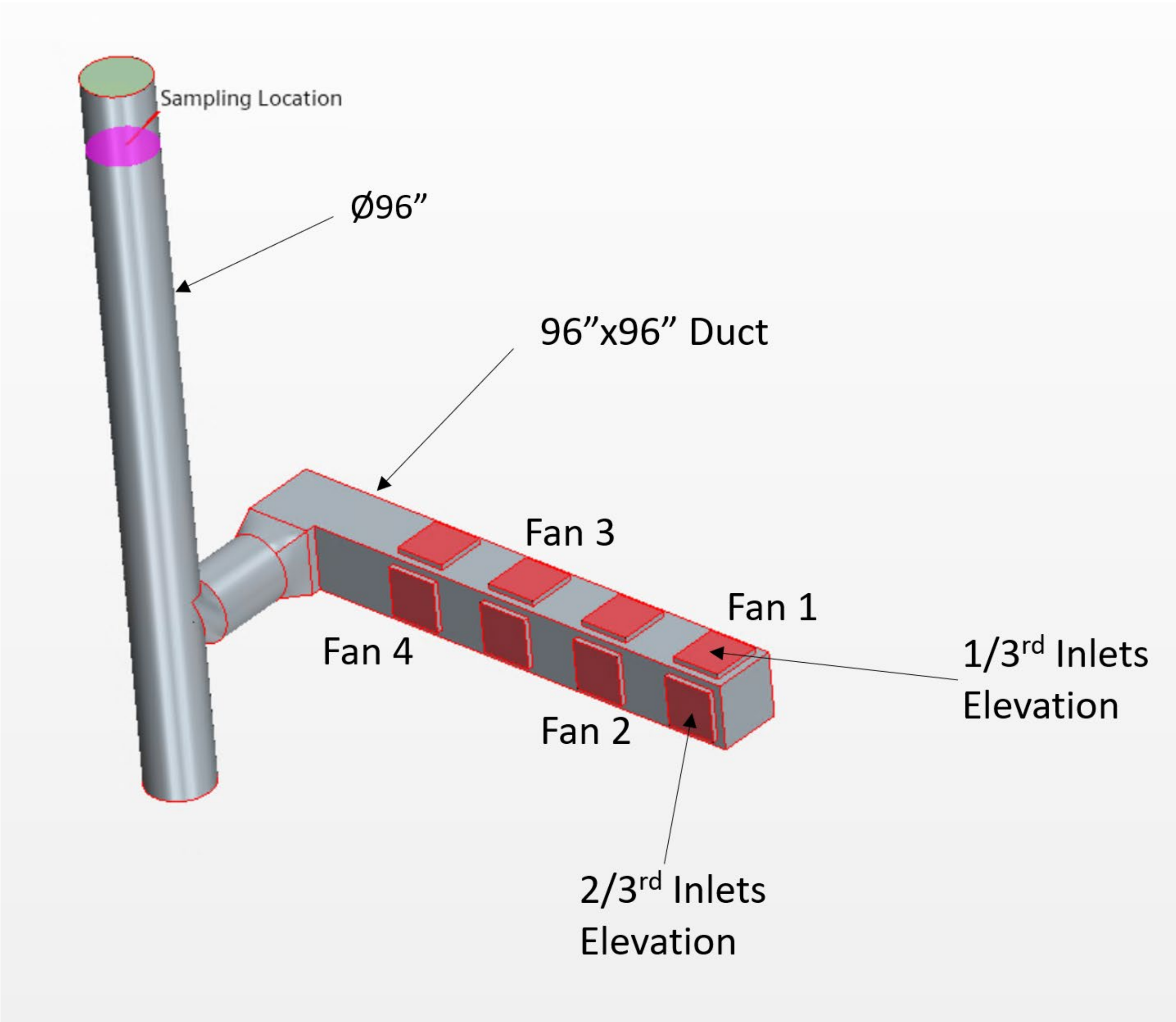


Figure 1. Model Geometry for the Updated 325 Building Stack System Design

A mesh sensitivity study was performed to ensure that the mesh was sufficiently resolved for the CFD model. The mesh sensitivity runs assumed only the fan closest to the sampling location was running at a total flowrate of 19,500 cfm. Three different resolutions of mesh were generated. An estimate of discretization error can be obtained by determining the Grid Convergence Index (GCI). This parameter is calculated following the approach outlined by Oberkampf and Roy (2010). The GCI is given by:

$$GCI = \frac{F_s}{r^p - 1} \frac{|f_2 - f_1|}{f_1} \tag{6}$$

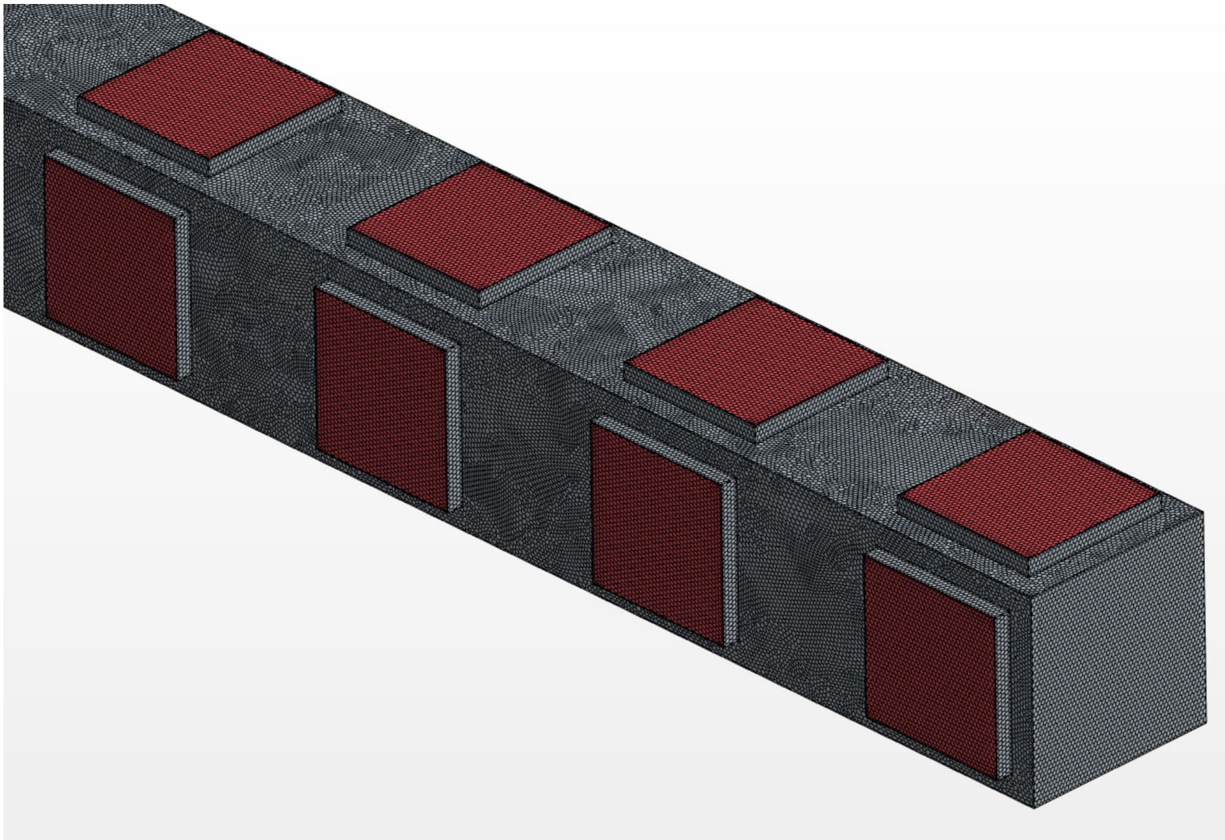
where F_s is the factor of safety (equal to 1.25 for this calculation), r is the grid refinement factor, p is the order (which is 2 for these cases), and f_i is the solution for the cases, with f_1 designating the fine mesh solution and f_2 the solution for the coarse mesh. The grid refinement ratio can be computed as:

$$effective\ r = \left(\frac{N_1}{N_2}\right)^{1/D} \tag{7}$$

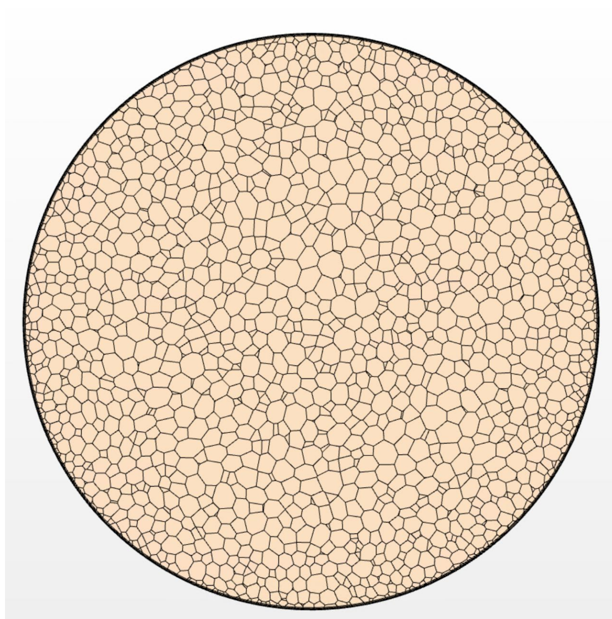
where N_1 and N_2 are the total cell count for the fine and course meshes, respectively, and D is the dimensionality of the system. Applying this for the cell counts of the different mesh resolutions and resulting gas tracer COV in the CFD model shown in Table 1 yields the two estimates of GCI as shown in Table 1. Note that the GCI is not a bounding error estimate, rather an indication of the relative error. The relative error for the coarse mesh was around 21% and the refined mesh was around 0.2%. The refined mesh is used going forward for the CFD model. Figure 2a provides a view of the mesh near Fan inlets. The typical resolution throughout the volume mesh is represented in Figure 2b which shows a cross-sectional plot of the mesh at the sampling location.

Table 1. GCI – CFD Model

Model	# Cells	Gas Tracer [%COV]	GCI	Relative Error [%]
Coarse	371,691	19.62	1.115	21.88
Refined	1,818,624	4.84	0.075	0.22
Very Refined	8,452,633	4.47	-	-



(a)



(b)

Figure 2. Detail of Computational Mesh at the (a) Near Fan Inlets, and (b) Cross-Section of the Volume Mesh at the Sampling Location

2.5 Boundary Conditions

A pressure boundary with 1 atmosphere absolute pressure was used at the stack exit. Duct walls were modeled as smooth surfaces with zero slip flow boundary conditions. The particle boundary condition at the walls was established so particles with trajectories that impact the duct walls would stick to the surface. Mass inflow boundaries were established at the duct inlets with turbulence intensity and length scale settings to account for upstream turbulence. The turbulent intensity specifies the quantity or intensity of the turbulence, and the length scale specifies the eddy size that represents the rate by which turbulence vanishes. Turbulent intensity can often be estimated from empirical correlations based on Reynolds number, but the turbulence length scale can be harder to estimate. The flow at the inlets of the model was assumed to be fully developed flow and to determine the fully developed velocity profile a simple model was constructed to replicate the 74” by 74” square inlets. Figure 3 shows the overall mesh for the simple model. The simple model allows a uniform velocity profile to be specified at the inlet and by applying a “fully developed interface” at the outlet the model calculates the resulting fully developed flow profile at the outlet. The resulting flow profile and turbulence parameters (i.e. turbulence intensity and turbulent viscosity ratio) can be extracted from the simple model and applied to the larger duct model. Figure 4 shows the resulting velocity profile for an inlet flowrate of 19,500 cfm. Table 2 provides the resulting turbulence parameters for all flowrates considered for the updated four-fan system. These turbulence parameters were applied at the inlet boundaries for each fan along with the calculated velocity profile. As a result, the Reynolds number is substantially greater than the required 10,000 (HPS 2021).

Figure 3. Mesh for Simple Inlet Model

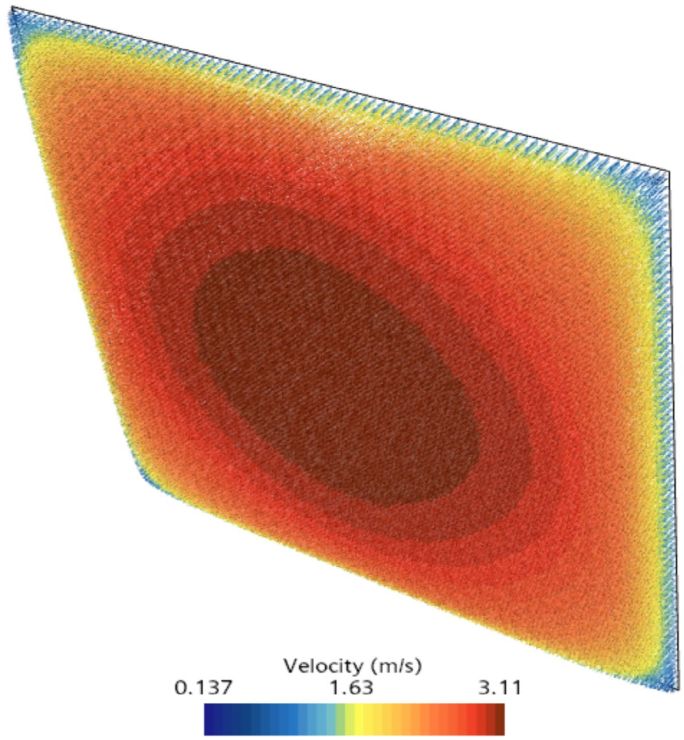


Figure 4. Resulting Velocity Profile for an Inlet Flowrate of 19,500 cfm

Table 2. Turbulence Inlet Parameters Calculated with Simple Inlet Model

Total Flow Rate [cfm]	Total Flow Rate per Fan [cfm]	2/3 Inlet [cfm]	1/3 Inlet [cfm]	2/3 Inlet		1/3 Inlet	
				Turbulence Intensity	Turbulent Viscosity Ratio	Turbulence Intensity	Turbulent Viscosity Ratio
15000	15000	10000	5000	0.051	158	0.055	77
100000	50000	33333	16667	0.038	417	0.043	231
150000	50000	33333	16667	0.038	417	0.043	231
180000	60000	40000	20000	0.037	494	0.041	271
234000	58500	39000	19500	0.037	482	0.042	265

3.0 Stack Modeling Results

In this section, we discuss results from CFD simulations of the updated four-fan exhaust system. The simulations were undertaken to examine the mixing performance of the system when operating at design conditions. The simulation cases include one, two, three, and four-fan operations. Operation of the modified exhaust system involved running in several different modes. All expected flow conditions must be examined to determine if any will fail to meet the ANSI/HPS N13.1-2011 standard. The airflow conditions for each fan are described as follows:

- *Minimum Airflow per Fan*: The minimum flow rate per fan is 15,000 cfm.
- *Maximum Airflow per Fan*: The (bounding) maximum flow rate per fan is 58,500 cfm.

The minimum and maximum airflow conditions per fan results in a minimum airflow of 19,500 cfm for a single fan in operation at the minimum airflow rate per fan and a maximum airflow of 234,000 cfm for all four-fans in operation at the maximum airflow per fan.

Simulation results for the updated four-fan system predict that in all cases, the flow angle, velocity uniformity, and tracer distributions criteria are met at the sampling location meeting the standard mixing criteria. Results are shown in Table 3. Figure 5 shows the resultant particle and tracer gas distribution at the sampling location for the 234,000-cfm case running all fans with the injection point at Fan 4. The plots show well mixed tracer distributions.

Table 3. Summary of CFD Modeling Results for the Updated 325 Building Duct with Four Fans

Total Flow Rate [CFM]	Fans in Operation	Tracer/ Aerosol Injection Position	Velocity Uniformity [% COV]	Flow Angle [% COV]	Gas Tracer Uniformity [% COV]	Gas Tracer % Deviation from Mean	Particle Tracer Uniformity [% COV]
15,000	1	Fan 1	5.3	6.0	5.2	13.3	1.0
15,000	4	Fan 4	7.1	5.0	1.6	4.8	4.5
100,000	1,4	Fan 1	3.6	6.3	6.2	13.9	9.8
100,000	1,4	Fan 4	3.6	6.3	9.3	19.6	1.8
150,000	1,2,4	Fan 1	3.0	6.0	5.1	12.3	13.8
150,000	1,3,4	Fan 4	1.9	6.7	8.4	19.1	14.3
180,000	1,2,4	Fan 4	3.6	6.3	5.6	11.3	18.5
180,000	1,3,4	Fan 1	3.0	6.1	11.0	28.9	6.8
180,000	2,3,4	Fan 3	3.2	6.1	5.5	17.7	3.9
180,000	1,2,3	Fan 3	2.7	5.7	7.6	16.2	2.8
234,000	1,2,3,4	Fan 1	3.4	6.2	5.3	12.7	1.4
234,000	1,2,3,4	Fan 4	3.6	6.3	10.7	25.5	1.6

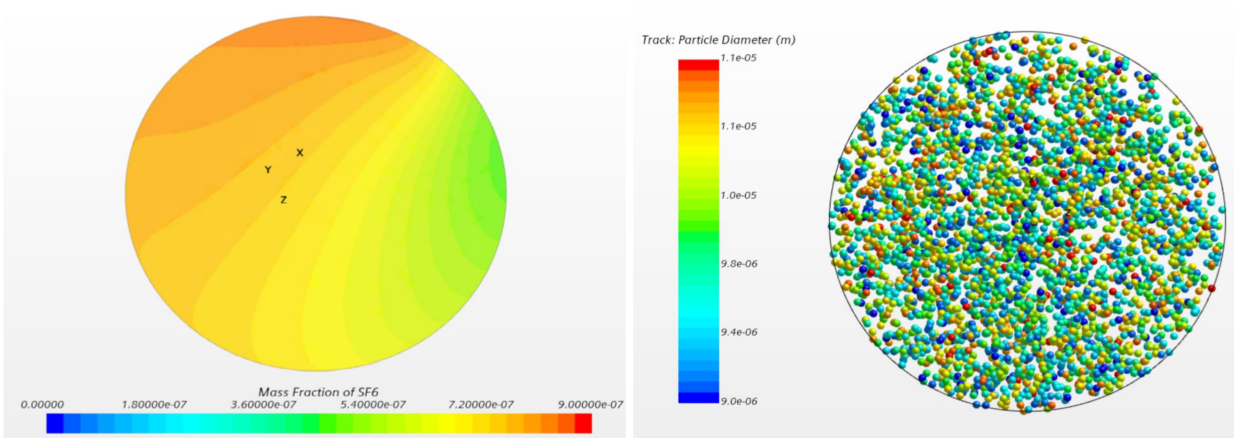


Figure 5. Tracer gas distributions at the sampling location for the 234,000-cfm case operating Fans 1, 2, 3, and 4 with the injection point at Fan 4.

4.0 Temporary Stack Modeling

A temporary single fan stack configuration was also evaluated with CFD modeling. The temporary system is planned to be used while the four-fan system is updated. The geometry for the temporary single fan stack is shown in Figure 6. The single fan duct attaches to the main exhaust duct through a hatch access near the bottom of the exhaust stack. The sampling location is at the same location as the four-fan system (~8 ft below the top of the stack).

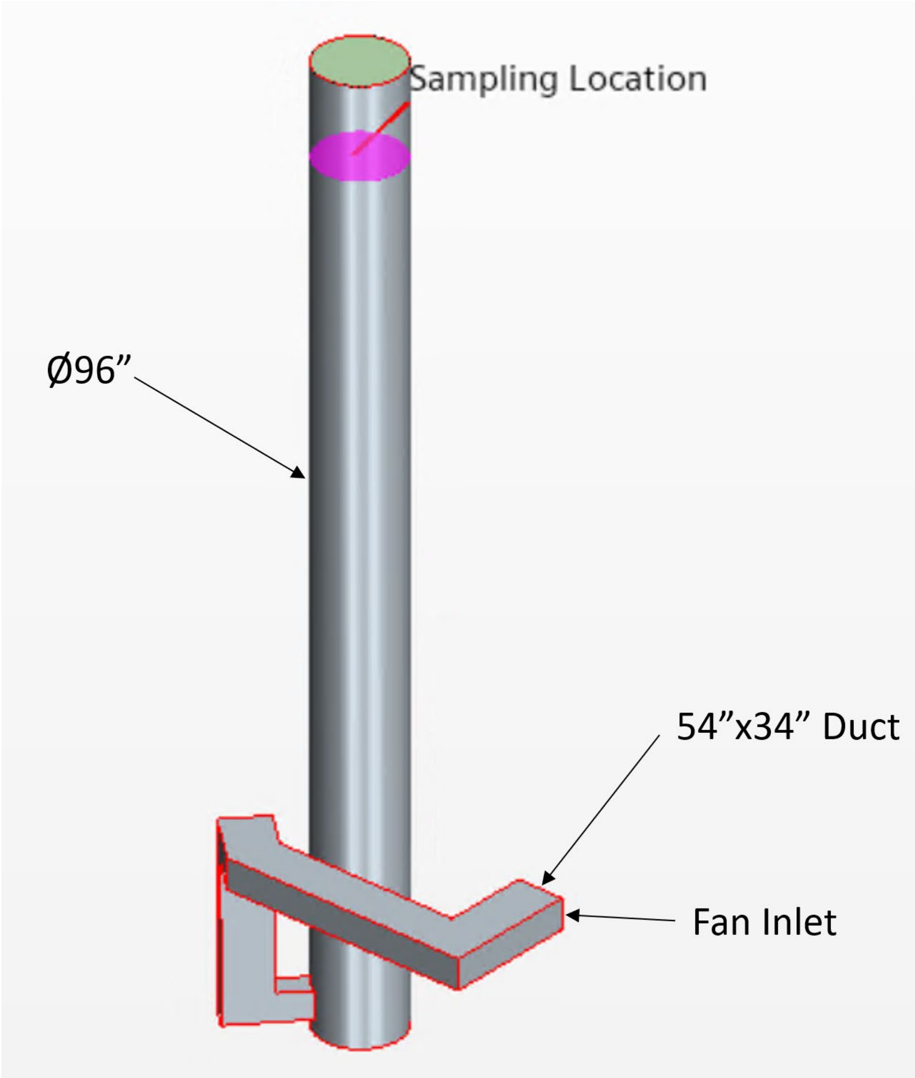


Figure 6. Temporary Duct System CAD Geometry.

The CFD model of the temporary single fan stack used the same modeling approach and methodology as described for the updated four-fan model. A single case was run with the temporary stack model assuming a total airflow of 30,000 cfm with the injection point at the fan inlet of the model. The results for the temporary single fan stack model are shown in Table 4. Results show the flow angle, velocity uniformity, and tracer distributions criteria all meet the standard mixing criteria at the sampling location.

Table 4. Summary of CFD Modeling Results for the Temporary 325 Building Duct with a Single Fan

Airflow per Fan [cfm]	Total Airflow [cfm]	Velocity Uniformity	Flow Angle	Gas Tracer Uniformity		Particle Tracer Uniformity
		% COV	% COV	% COV	% Deviation from Mean	%COV
30000	30000	8.23	16.43	0.176	0.297	8.91

5.0 Conclusions

Based on CFD modeling of the 325 Building filtered exhaust stack system, the following conclusions are drawn:

- Modeling results of the updated four-fan duct and a single fan temporary duct operating at all expected flow conditions predict that flow angle, velocity uniformity, and tracer concentration criteria established by the ANSI/HPS N13.1-2021 standard will be met.
- The process of CFD modeling meets the intent of optimizing and upgrading a new or existing system as described in Section 6.9 of ANSI/HPS N13.1-2021. Specifically, the CFD modeling of the re-designed exhaust system shows that the mixing criteria will be met.

6.0 References

Ballinger MY, JA Glissmeyer, JM Barnett, KP Recknagle, and ST Yokuda. 2011. *Sampling Point Compliance Tests for 325 Building at Set-Back Flow Conditions*. PNNL-20397, Pacific Northwest National Laboratory, Richland, Washington.

Ballinger MY, JM Barnett, JA Glissmeyer, and DL Edwards. 2004. *Evaluation of Sampling Locations for Two Radionuclide Air-Sampling Systems Based on the Requirements of ANSI/HPS N13.1-1999*. Health Physics 86(4):406-415.

Barnett JM, MY Ballinger, KP Recknagle, and ST Yokuda. 2005. *Computational Modeling of a Stack Sampling Location for Radioactive Air Emissions*. Health Physics 89(1):S39-S40.

Barnett, JM, X-Y Yu, KP Recknagle, and JA Glissmeyer. 2016. *Modeling and Qualification of a Modified Emission Unit for Radioactive Air Emissions Stack Modeling Compliance*. Health Physics 111(5):432-441. DOI: 10.1097/HP.0000000000000557

Barnett, JM, X-Y Yu, SR Suffield, KP Recknagle. 2020. *Modeling Filtered Building Effluent Stack Sampling Points for Qualification Criteria*. Progress in Nuclear Energy 124:103338. DOI: 10.1016/j.pnucene.2020.103338

Health Physics Society (HPS). 1999. *Sampling and Monitoring Releases of Airborne Radioactive Substances From the Stacks and Ducts of Nuclear Facilities*. ANSI/HPS N13.1-1999, Health Physics Society, McLean, Virginia.

Health Physics Society (HPS). 2011. *Sampling and Monitoring Releases of Airborne Radioactive Substances From the Stacks and Ducts of Nuclear Facilities*. ANSI/HPS N13.1-2011, Health Physics Society, McLean, Virginia.

Health Physics Society (HPS). 2021. *Sampling and Monitoring Releases of Airborne Radioactive Substances from the Stacks and Ducts of Nuclear Facilities*. ANSI/HPS N13.1-2021, Health Physics Society, Herndon, Virginia.

Oberkampf WL and CJ Roy. 2010. *Verification and Validation in Scientific Computing*. Cambridge University Press, New York.

Recknagle KP, ST Yokuda, MY Ballinger, and JM Barnett. 2009. *Scaled Tests and Modeling of Effluent Stack Sampling Location Mixing*. Health Physics 96(2):164-174.

Siemens PLM Software. 2022. STAR-CCM+17.06 (computer software). Siemens PLM Software, Plano, Texas.

Smith BM, MY Ballinger, JA Glissmeyer, and JM Barnett. 2010. *Sampling Point Compliance Tests for 325 Building at Full Flow Condition*. PNNL-19998, Pacific Northwest National Laboratory, Richland, Washington.

Yu X-Y, KP Recknagle, JA Glissmeyer, and JM Barnett. 2014. *Integrating Modeling and Physical Testing for Assessing Filtered Exhaust Stack Sampling Probe Location*. Health Physics 107(1):S30.

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