# Numerical Modeling of Sampling Airborne Radioactive Particles Methods from the Stacks of Nuclear Facilities in Compliance with ISO 2889

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**Abstract:** The International Standard ISO 2889 focuses on monitoring the activity concentrations and activity releases of radioactive substances in air in stacks of nuclear facilities and sets the performance criteria and recommendations required for obtaining valid measurements. The goal of achieving an unbiased, representative sample is best accomplished where samples are extracted from a location where the radioactive materials of interest are well mixed within the free stream. The criteria those guarantee the homogeneity of the air stream at the sampling locations are the following:

- absence of angular or cyclonic flow (the mean flow angle between the flow axis and stack axis should not exceed 20°);
- symmetry of air velocity profile (the Coefficient Of Variation should be less than 20% on the centre two-thirds of the area of the stack);
- symmetry of gas concentration and particle profile, injected on the base of chimney (measured with the same principle of velocity profile).

In circumstances where the well mixed criteria are not achieved, a multi-nozzle probe (instead of a single nozzle probe) can be required to get a representative sample.

During off-normal conditions, the performance of the sampling system can be affected by the modification of several parameters (temperature, flow rate in stacks, type of airborne particles). In any case, acceptance criteria described in the International Standard for normal conditions still apply for off-normal conditions and an evaluation of the opportunity to use a special or separate air sampling system is needed.

The main objective of this study is to verify the compliance of an ongoing nuclear facilities stack design with the ISO 2889 requirements, during normal and off-normal conditions. In particular, with the numerical simulations, they have been identified well-mixed sample locations along the chimney and the compliance with the International Standard requirements as result of stack flow rate and airborne particle aerodynamic diameter modifications.

The 3D simulations have been performed with Comsol Multiphysics 4.4 (Heat Transfer and Particle Tracing Module). The stationary simulations are based on the following segregated steps: Fluid flow study (single-phase incompressible turbulent k-eps-wall function model), Transport of diluted species study and Particle tracing study (Lagrangian approach).

The results presented in this study confirm the capability of Comsol as multiphysics simulation tool. The development of this work has allowed us to obtain useful indications for the nuclear facilities stack design, reducing the field testing costs.

**Keywords:** CFD, sampling, nuclear stack, particle tracing.

## 1. Introduction

The International Standard ISO 2889 [1] focuses on monitoring the activity concentrations and activity releases of radioactive substances in air in stacks of nuclear facilities and sets the performance criteria and recommendations required for obtaining valid measurements. The recommendations are aimed at sampling that is conducted for worker and environmental protection, regulatory compliance and system control. A representative sample is best extracted from a location where the radioactive materials of interest are well mixed within the free stream. In circumstances where the well mixed criteria are not achieved, a multi-nozzle probe (instead of a single nozzle probe) can be required to get a representative sample [2]. The main objective of this study is to verify the compliance of an ongoing nuclear facilities stack design with the ISO 2889 requirements, during normal and off-normal conditions. The off-normal conditions are represented by a reduction of mass flow that evolves inside the chimney (e.g. fire scenario) and modifications on the particle size released by the facilities (accident or High-Efficiency-Particulate-Air filtration disruption) [3]. The 3D simulations have been performed with Comsol Multiphysics 4.4 (Heat Transfer and Particle Tracing Module). The stationary simulations are based on the following segregated steps: Fluid flow study (single-phase incompressible turbulent k-eps-wall function model), Transport of diluted species study and Particle tracing study (Lagrangian approach).

## 2. ISO 2889 requirements

The criteria those guarantee the homogeneity of the air stream at the sampling location are the following [1]:

a) absence of angular or cyclonic flow (the mean flow angle between the flow axis and stack axis should not exceed 20°);
b) symmetry of air velocity profile (the Coefficient Of Variation should be less than 20% on the centre two-thirds of the stack area);
c) symmetry of gas concentration and particle profile, injected on the base of chimney (measured with the same principle of velocity profile). At no measurement point the concentration of the tracer gas should differ by more than 30% from the mean value for all of the points.

The COV is expressed by the following formula:

$$COV = \frac{\sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2}}{\frac{1}{n}\sum_{i=1}^{n} x_i} \qquad (1)$$

where $n$ is the number of data points and $x_i$ is the value of the generic variable (velocity, tracer concentration) at the $i$th location on a sampling grid. The gaseous tracer should be introduced at five or more locations across the cross-section of the air stream (as far upstream as possible of the sampling probe, yet downstream of filter). For a round duct, the introduction should be at the centre and near the wall (within 20% of the diameter from the wall). The aerosol particle tracer may be introduced at only one location, located at the centre of the duct [4]-[5].

## 3. Numerical model

In this section are presented the geometrical and mechanical features of the preliminary stack design, the governing equations of the numerical modeling and their boundary conditions. It is also described the simplified approach to take into account the interaction between the particle and the stack surfaces.

### 3.1 Geometrical and mechanical stack's design

The next Figure 1 shows the chimney and the feeder duct. The stack is about 24 m high and 1,32 m inner diameter. The flow range is 22.000 $m^3/h$ (fire scenario) to 40.000 $m^3/h$ (nominal design). The test sampling stations are placed in the stack at distances of 3-5-7-9 diameters from the end of cone section.

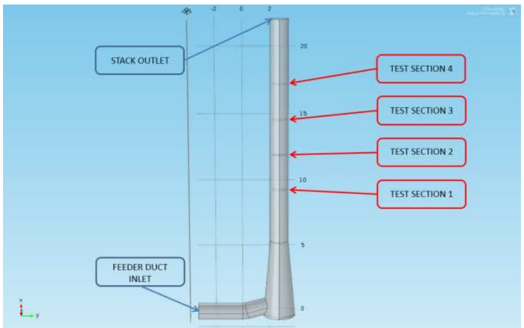


**Figure 1**. Geometry of the stack and test sampling sections positioning

### 3.2 Governing equations

The governing equations used during the study are represented by partial differential equations derived by imposing the balance of mass (2), momentum (3) and concentration of species (4) within an infinitesimal element of volume. The last equation (5) represents the Newton's second law applied to each particle. The governing equations, for incompressible case are reported in tensor form:

$$\nabla \cdot \boldsymbol{u} = 0 \qquad (2)$$

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = \nabla \cdot [-p\boldsymbol{I} + \boldsymbol{\tau}] \qquad (3)$$

$$\frac{\partial c}{\partial t} + \boldsymbol{u} \cdot \nabla c = \nabla \cdot (D\nabla c) \qquad (4)$$

$$\frac{d}{dt}(m_p\boldsymbol{v}) = \left(\frac{1}{\tau_p}\right) m_p(\boldsymbol{u}-\boldsymbol{v}) + m_p\boldsymbol{g}\frac{(\rho_p-\rho)}{\rho_p} \qquad (5)$$

where $\boldsymbol{u}$ is the velocity vector, $c$ the gas concentration and $\boldsymbol{v}$ the particle velocity vector. For the other terms, please refer to Comsol Multiphysics Reference Manual.

### 3.3 Boundary conditions

For the first simulation step (fluid flow study), the following boundary conditions are applied: atmospheric pressure on the stack outlet section (suppress back flow option), logarithmic wall function on the walls, velocity inlet condition (normal flow velocity) on the entrance of the feeder duct (see Figure 1). For the second simulation step (transport of diluted species), the next boundary conditions are imposed: no flux for all surfaces except for injection location (see Figure 2) where inflow condition is used and the stack outlet section where outflow condition is applied. The last simulation step concerns the particle tracing study. The particles are released from the entrance section of the feeder duct at initial time (t=0), with uniform distribution along the section, and initial velocity equal to the air local velocity field. The hypothesis of uniform particle distribution at inlet boundary, instead of modeling injection spray zone, is used for saving computational time. The stack walls are treated by means of general reflection wall conditions: according with Li&Ahmadi [6] approach the collision of a particle and a wall is conveniently characterized in terms of particle-surface interaction energy. Particles striking the surface with a velocity greater than a critical value are assumed to bounce, while those with a lesser velocity deposited. The critical velocity is defined by [7]:

$$v_{p,crit} = \sqrt{\frac{2E_0}{m_p}\left(\frac{1-r^2}{r^2}\right)} \qquad (6)$$

where $m_p$ is the mass of particle, $r$ is the restitution coefficient (assumed equal to one for elastic collision) and $E_0$ is the potential energy of surface. The reflection condition implemented in Comsol is based on the comparison between the critical velocity and the approaching particle normal velocity to the wall. The stack outlet section is modelled by means of freeze option. For each test section analyzed, during the particle tracing simulation, is used the stick surface condition in order to calculate the COV (the particle which trajectory meets the section analyzed sticks on it); this approach is suitable for the next reasons: 1) the process is assumed deterministic (the Brownian forces for particle with aerodynamic diameter greater than 1 micron vanish); 2) the velocity field is assumed stationary; 3) the particle distribution at inlet boundary is supposed uniform and time invariant. Each test section is divided into 16 sampling area (see Figure 3) to count the number of particles those sticks on it and to calculate the COV by means of a spreadsheet. For more details about the numerical technique refer to § 4.4.

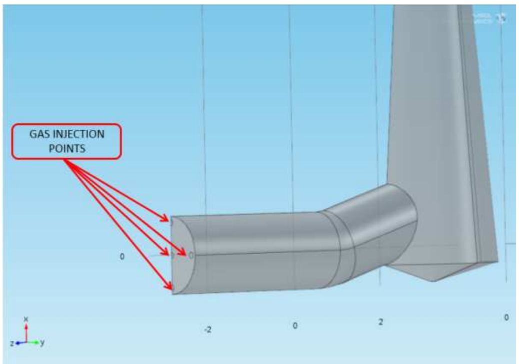


**Figure 2**. Boundary conditions detail for second step simulation

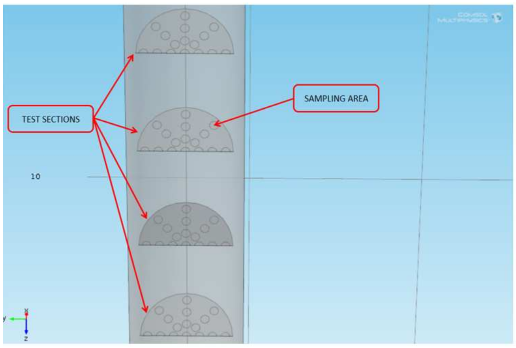


**Figure 3**. Boundary conditions detail for third step simulation

## 4. Use of COMSOL Multiphysics

The simulations are performed with Comsol Multiphysics 4.4 – Heat Transfer and Particle

Tracing Modules and are based on the following steps: 1) stationary fluid flow study (single phase incompressible turbulent k-eps closure model); 2) stationary transport of diluted species study (using the air velocity filed obtained in the previous study); 3) time dependent particle transport study (using the air velocity field obtained in the first study). During the first step are verified the requirements a) and b) of ISO 2889, with the second and the third step the last point c). The transport of diluted species theory assumes that all species present are dilute; that is, their concentration is small compared to a solvent (case of study). Due to the dilution, mixture properties such as density and viscosity can be assumed to correspond to those of the solvent. The particle transport simulation is based on the “sparse flow” approach where the continuous phase affects the motion of the particles but not vice versa (one–way coupling).

**4.1 Computational domain and meshes**

The geometrical dimensions of the chimney and its feeder duct are reproduced in 1:1 scale (see Figure 1). It is also considered the symmetry of the flow in order to speed up the simulation. The flow study mesh consist of a tetrahedral network of 1.250.000 elements with average element quality 0.5634 (minimum quality 0.014). A finer mesh is used near the wall in order to guarantee sufficient small values of wall lift-off: as shown in Figure 4 it is larger than 11.06 only at some locations into stack cone section. The mesh used for the particle tracing study is the same of the flow study while for simulation b) a finer mesh is used to avoid the introduction of inconsistent stabilization. The meshes proved to be dense enough to yield sufficiently accurate results and for a reasonably short simulation time (7 hours for the flow simulation, 2 hours for chemical study and 60 hours for 10 micron aerodynamic diameter particle study on a workstation Intel Xeon CPU @2,40 GHz, 64 GB RAM).

**4.2 Solver set-up for fluid flow study**

The stationary fluid flow study is used to obtain the velocity field inside the stack. The physics selected is single phase turbulent flow k-eps formulation as closure model (wall function). As described in § 3.2 the flow is considered incompressible. The direct, MUMPS, segregated solver configuration is used during the simulation. The solution is considered to be converged when the residual values fell below less than $10^{-3}$.

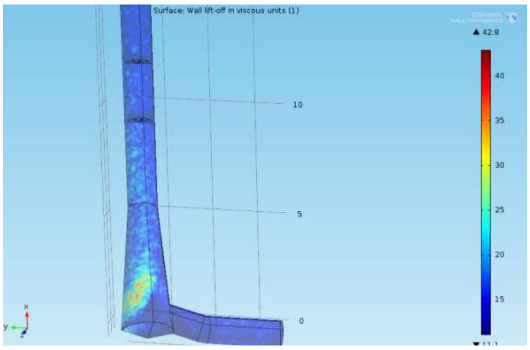


**Figure 4**. Wall lift-off in viscous unit for nominal flow

**4.3 Solver set-up for transport of dilute species study**

The stationary transport of diluted species study is used to obtain the gas concentration profile along the test sections due to gas injection at the inlet section of the feeder duct. The diffusivity coefficient is assumed equal to $7\cdot10^{-5}$ $m^2/s$. The study uses the velocity field obtained in the previous step. The physics selected is the transport of diluted species with convection term. The direct, MUMPS, segregated solver configuration is used during the simulation. The solution is considered to be converged when the residual values fell below less than $10^{-3}$.

**4.4 Solver set-up for particle transport study**

The time dependent particle transport study is used to obtain the aerosol concentration profile along the test sections due to injection at the inlet section of the feeder duct. The Transient Newtonian formulation is employed with Schiller-Naumann drag law implementation. As described in § 3.2 the forces considered are drag and gravity. They are performed 24 different computational studies that represent the combinations of two flow regime, three aerodynamic diameter and four test sections. The transient simulations are extended for a simulation time long enough to allow the adhesion of particles to the stick surfaces or to reach the outlet section. The direct, MUMPS, fully-coupled solver configuration is used during the simulation. The solution is considered to be converged when the residual values fell below less than $10^{-5}$.

## 5. Results

With reference to Figure 5 the multislice plot shows the velocity magnitude close to test sections for the case of nominal flow rate. The gas concentration field is shown in Figure 6 for the case of nominal flow rate. Lastly, the particle trajectories for the case of nominal flow rate and 10 micron aerodynamic diameter are shown in Figure 7.

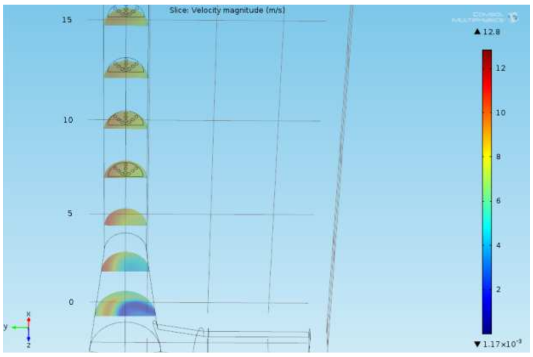


**Figure 5**. Multislice plot of velocity magnitude field (nominal flow rate)

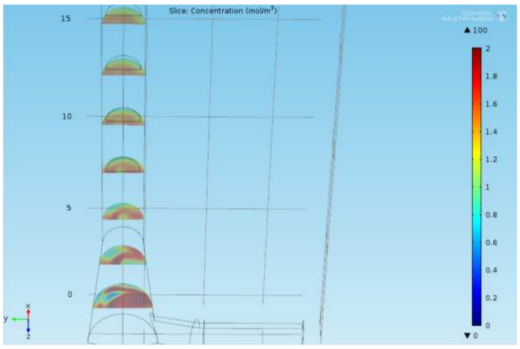


**Figure 6**. Multislice plot of gas concentration field (nominal flow rate)

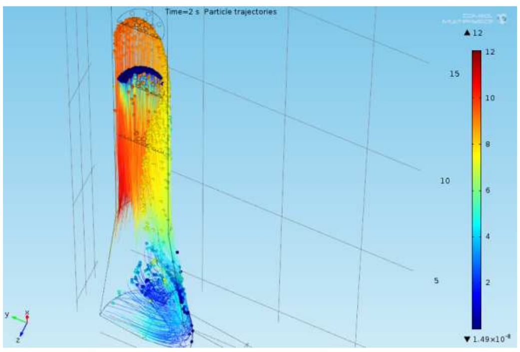


**Figure 7**. Particle trajectories at time t=2s for 10 micron aerodynamic diameter and nominal flow rate

The results in terms of cyclonic flow magnitude are shown in Figure 8. The succeeding figures show the coefficients of variation (COVs) at various downstream locations of the stack for different flow rate and particle aerodynamic diameter.

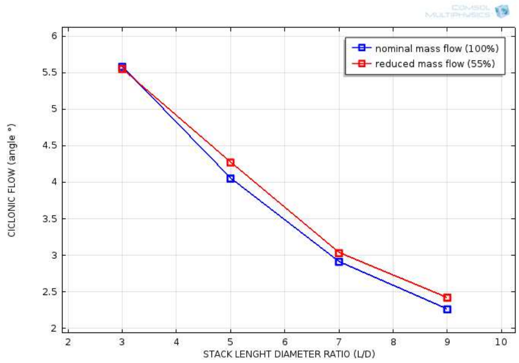


**Figure 8**. Cyclonic flow magnitude for different flow rate

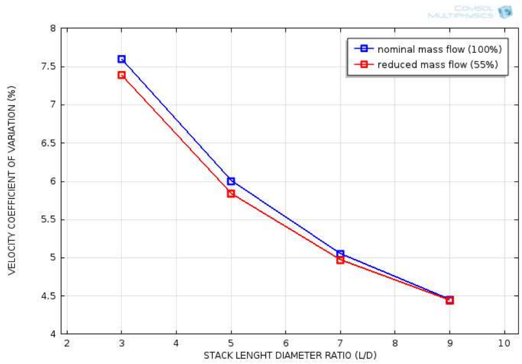


**Figure 9**. Velocity COV for different flow rate

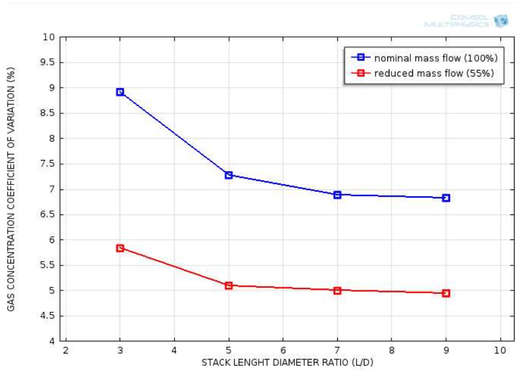


**Figure 10**. Gas concentration COV for different flow rate

The cyclonic flow, velocity and gas concentration COVs are calculated with derived values operator tool of Comsol. In particular, the COVs are expressed in terms of surface integral operator. The aerosol concentration along the test sections are calculated by means of a spreadsheet after the determination of the number of particles that sticks on the sampling areas.

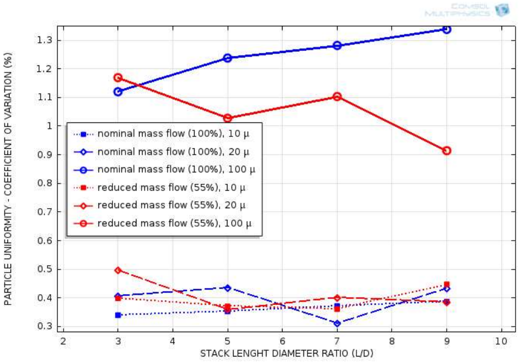


**Figure 11**. Particle COV for different flow rate and aerodynamic diameter

The velocity COV, for the nominal mass flow, decreases downstream of the elbow, from a value of 7,60% (L/D=3) to 4,45% (L/D=9). The velocity COV, for the reduced mass flow, has a similar behavior. The tracer gas concentration COV, for nominal mass flow, slightly decreased from 8,92% (L/D=3) to 6,3% (L/D=9). The tracer gas concentration COV, for the reduced mass flow, has a better behavior starting from 5,84% (L/D=3) for reducing at 4,95% (L/D=9). For each test section and flow simulated, at no measurement point the concentration of the tracer gas should differ by more than 30% from the mean value for all of the points.

The aerosol concentration profiles for all combination of flow rates and particle aerodynamic diameters are shown in Figure 11. The negative influence of inertial effects for particles greater or equal to 10 micron aerodynamic diameter is clearly shown: whereas the requirements a) and b) of ISO 2889 are widely satisfied for both flow rates studied, the point c) isn't fulfilled for any cases. The average COV values for 10 micron aerodynamic diameter are 36,3% for nominal mass flow and 39,4% for reduced mass flow. The average COV values for other cases are greater. It is important to underline that due to inertial effects and the bouncing of particles when they strike the walls, the aerosol COV does not decrease along the stack downstream of the elbow but oscillates from a maximum to a minimum value. The average particle COVs for 100 micron aerodynamic diameter are greater than 100% making particularly difficult the sampling process. It has to be considered that although the particle size most likely to directly penetrate HEPA filter media is approximately 0,1 – 0,3 micron diameter, it is erroneous to assume that the sampling system can be designed only for sub-micrometre particles. Larger size particles can be transmitted through HEPA filter banks due to small openings in HEPA frames, gasket seals and filter-media defects, especially those that develop after extended period of use.

The following Table 1 shows the percent of particles injected at t=0 along the feeder duct inlet section that stick on chimney boundaries and the percent of particles that pass through the test section 4. The "other" percent is represented by the particles that exit from the outlet section of the stack without cross the test section n.4.

**Table 1** Percent of particles that stick on the boundaries and pass through test section n.4

| Case study | Stick particles | Sampling particles | Other |
|---|---|---|---|
| 100% flow, 10 µ | 4,2% | 63.9% | 31,9% |
| 100% flow, 20 µ | 4,9% | 62,1% | 33,0% |
| 100% flow, 100 µ | 32,5% | 31,8% | 35,7% |
| 55% flow, 10 µ | 4,5% | 63,4% | 32,1% |
| 55% flow, 20 µ | 5,3% | 62,6% | 32,1% |
| 55% flow, 100 µ | 44,2% | 31,9% | 23,9% |

The effect of gravitational settling and inertial-impaction removal is evidently shown in Table 1. The percent of particle that exit from the outlet section of the stack without cross the test section n.4 is roughly constant for the case studied. Even if the interaction between the particles and the walls is quite simple and isn't considered the secondary emissions the Table 1 can give some indications about the particle deposition on the wall.

## 6. Conclusions

In this study the capabilities of Comsol Multiphysics for solving three-dimensional fluid flow problem is shown. The numerical model is used to determine whether the test stack sampling sections, for a preliminary stack design, meet the requirements of ISO 2889 under nominal and reduced exhaust flow conditions and particle aerodynamic diameter modifications. All the ISO requirements are met except for aerosol well-mixed distribution test. Future study will be performed in order to evaluate the impact of feeder duct angle modifications.

## 7. References

[1]. ISO 2889, Sampling airborne radioactive materials from the stacks and ducts of nuclear facilities, second edition 2010;

[2]. C. Rodgers, Single Point Aerosol Sampling: Evaluation of Mixing and Probe Performance in a Nuclear Stack, *23$^{rd}$ DOE/NRC Nuclear Air Cleaning and Treatment Conference*, July 24-28 1994;

[3]. J. Glissmeyer, Stack Sampler Calibration, *25$^{rd}$ DOE/NRC Nuclear Air Cleaning and Treatment Conference*;

[4]. MY Ballinger, Sampling Point Compliance Tests for 325 Building at Set-Back Flow Conditions, *DOE PNNL-20397*, May 2011;

[5]. T. Han , Evaluation of Mixing Elements in a L-Shaped Configuration for Application to Single-Point Aerosol Sampling in Ducts, *HVAC & Research*, Feb 2011;

[6]. M. Sippola, Particle deposition from turbulent flow: review of published research and its applicability to ventilation ducts in commercial buildings", *Lawrence Berkeley National Laboratory*, Gen 2012;

[7]. Amy Li, Dispersion and Deposition of Spherical Particles from Point Sources in a Turbulent Channel Flow, *Aerosol Science and Technology*, Jun 2007.