CFD Simulation of Short-Range Plume Dispersion from a Point Release in an Urban like Environment

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Abstract

An accurate simulation of the short-range plume dispersion of a hazardous pollutant in a geometrically complex urban region is a prerequisite in emergency preparedness and to assist regulators for developing effective policies. This study critically examines the real predictive capability of a three-dimensional Computational Fluid Dynamics (CFD) model, Fluidyn-PANACHE, to apply it in emergency contexts of an accidental or deliberate airborne release in urban regions. The model is evaluated with the Mock Urban Setting Test (MUST) field experiment of a continuous point source release in an idealized urban geometry of a regular array of shipping containers in various atmospheric stability varying from neutral to stable, and very stable conditions. The simulations are performed using three combinations (*cases 1, 2, & 3*) of inflow boundary conditions for wind and turbulence profiles. A detailed analysis with statistical measures shows that the performance of the Fluidyn-PANACHE against MUST experiment with all the

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three *cases* of the inflow boundary conditions is well achieved within the acceptable standards for air quality applications. The model with three *cases* 1, 2, & 3 predicts respectively 52.8%, 59.9%, and 67.9% of the total concentrations within a factor of two and shows an overall under-prediction. The sampling line maximum concentrations are better simulated by the CFD model with *case*-3 (95% within a factor of two) in comparison to other *cases* 1 & 2. A comparative statistical analysis is also performed with other evaluation studies in the literature for the averaged and sampling line maximum concentrations. The present evaluation of the Fluidyn-PANACHE strengthen the evidence that it is capable of dealing properly with the dispersion phenomena in geometrically complex urban environments.

Keywords: CFD modeling, Fluidyn-PANACHE, Short-range dispersion, MUST field experiment, Urban dispersion.

1. Introduction

An accurate simulation of the short-range plume dispersion in urban regions is of great importance for the informative studies of the adverse effects of a hazardous pollutant exposure on human health and environment, emergency preparedness, and developing effective policies. It is difficult to simulate the short-range plume dispersion of a hazardous pollutant with certainty due to the complex interaction between atmospheric flow and flow around buildings and other obstacles in an urban area (Tominaga and Stathopoulos, 2013). In urban regions, the intricacy of simulations increases due to the composite dynamics of flow field and pollutants perturbed by the buildings and obstacles.

12 Over the years, the Computational Fluid Dynamics (CFD) simulation of
13 wind flow in geometrically complex environments has led a remarkable im-
14 provement to the modelling of pollutant's dispersion within built-up urban
15 regions (Hanna et al., 2004; Milliez and Carissimo, 2007; Donnelly et al., 2009;
16 Pontiggia et al., 2010; Efthimiou et al., 2011, 2015; Gromke and Blocken,
17 2015, etc.). The CFD models have potential to provide the precise and real-
18 istic simulations of wind flow and dispersion around and within the buildings
19 and other complex structures in urban regions. These models have an ad-
20 vantage over the simple Gaussian and other analytical/numerical dispersion
21 models due to their ability to efficiently capture the effects of complex ur-
22 ban geometries on dispersion process. However, these CFD models need to
23 be set up, tested, and evaluated correctly to obtain the reliable results for
24 emergency preparedness (Antonioni et al., 2012).

25 One of the prerequisite of a CFD model simulation in the Atmospheric
26 Boundary Layer (ABL) is the realistic inflow boundary conditions at the
27 boundary located upstream of the simulation domain. In a CFD simulation,
28 the atmospheric dispersion process in the ABL depends on the vertical pro-
29 files of wind and turbulent kinetic energy, from which the fluctuating veloc-
30 ity components are derived to predict the turbulent dispersion (Gorlé et al.,
31 2009). Appropriate wind and turbulence profiles for these inflow boundary
32 conditions are considered as important input variables to a CFD model that
33 also provide actual weather state of the natural environment and should be
34 identical to the measurement conditions. For a given atmospheric stability
35 class, the fully developed vertical profiles of wind and turbulence along with
36 appropriate ground boundary conditions (Blocken et al., 2007) have been

37 used in CFD models for the flow-field and dispersion simulations (Hanna
 38 et al., 2004; Milliez and Carissimo, 2007; Pontiggia et al., 2010; Efthimiou
 39 et al., 2015, etc.). However, most of the wind profiles are either based on
 40 log-law or derived using the Monin-Obukhov similarity theory, which are ap-
 41 plicable only to the atmospheric surface layer. Some recent investigations
 42 for the vertical wind profiles in various atmospheric stability conditions that
 43 are applicable in entire atmospheric boundary layer (ABL) (Gryning et al.,
 44 2007; Pena et al., 2009) allow to analyze the effects of these extended profiles
 45 on the dispersion process. These extended profiles have been successfully
 46 applied in the analytical models for dispersion process in the homogeneous
 47 terrains (Kumar and Sharan, 2009, 2012b). However, the applicability of
 48 these extended wind profiles for the turbulent dispersion process in complex
 49 urban geometries is required to analyse with a CFD model.

50 The evaluation of a CFD model against representative experimental ob-
 51 servations is necessary to critically examine its real predictive capability to
 52 apply in emergency contexts of an accidental or deliberate airborne release
 53 in urban regions. A comprehensive observational set of meteorological, tur-
 54 bulence, and concentrations from Mock Urban setting Test (MUST) field
 55 experiment (Biltoft, 2001; Yee and Biltoft, 2004) provides an unique dataset
 56 for evaluation of the dispersion models in an idealized urban-like complex
 57 geometry. The MUST experiment was a short-range ($\approx 200 \text{ m} \times 200 \text{ m}$)
 58 field campaign of a point source release in an idealized urban geometry of a
 59 regular array of shipping containers in different atmospheric stability condi-
 60 tions. This dataset has been extensively used for evaluating the CFD models
 61 in complex environment (Hanna et al., 2004; Milliez and Carissimo, 2007;

62 Donnelly et al., 2009; Antonioni et al., 2012, etc.). Therefore, a CFD model
63 Fluidyn-PANACHE is evaluated with the observations from the MUST field
64 observations.

65 In this study, three-dimensional numerical simulations are performed for
66 the short-range plume dispersion using a CFD model Fluidyn-PANACHE.
67 The simulated results are evaluated with the observations in an urban-like en-
68 vironment of MUST field experiment. The high-resolution CFD simulations
69 are performed using three combinations (*cases* 1, 2, & 3) of inflow boundary
70 conditions of wind and turbulence profiles. The remainder of this paper is or-
71 ganized as follows. A brief description of the MUST field experiment and the
72 meteorological and turbulence observations used in this study are described in
73 Section 2. Section 3 briefly presents about a CFD model Fluidyn-PANACHE
74 and the mesh structures in the defined simulation domains. The boundary
75 conditions, particularly the wind and turbulence profiles at inlet of the do-
76 main are discussed in Section 4. The details of numerical simulation and
77 statistical evaluation methods are mentioned in Section 5. The discussions
78 of the simulated results and a comparative performance analysis are give in
79 Section 7. Some concluding remarks are summarized in Section 8.

80 **2. Description of Mock Urban Setting Test (MUST) field experi-** 81 **ment**

82 Mock Urban Setting Test (MUST) field experiment (Biltoft, 2001) is one
83 of the standard and extensively utilized experimental dataset for formula-
84 tion and evaluation of the atmospheric dispersion models in an urban like
85 environment. The dataset includes a comprehensive set of meteorological,

86 turbulence, and tracer concentration observations in an idealized urban ge-
 87 ometry. MUST dataset is very useful to study the flow fields, turbulence,
 88 dispersion and other parameters in an idealized urban settings that can
 89 be view as being most consistent with a small industrial facility (Yee and
 90 Biltoft, 2004; Milliez and Carissimo, 2007; Donnelly et al., 2009, etc.). The
 91 detailed descriptions of MUST set-up, geometry, positions of containers (ob-
 92 stacles), meteorological towers, sources, receptors, tracer releases summary
 93 are given in Biltoft (2001). The experiment was conducted mostly in night
 94 or in the early morning hours during neutral and stable atmospheric condi-
 95 tions at the U.S. Army Dugway Proving Ground (DPG) Horizontal Grid test
 96 site ($40^{\circ}12.606'N$, $-113^{\circ}10.635'W$) from 6^{th} to 27^{th} September, 2001 (Biltoft,
 97 2001). Most of the trials in this experiment were conducted with prevailing
 98 south-easterly winds. The terrain of the experimental test site was primarily
 99 flat with an averaged surface roughness length (z_0) of 0.045 ± 0.0005 m (Yee
 100 and Biltoft, 2004). The MUST experiment represents an urban roughness
 101 geometry by placing 120 shipping containers (each 12.2 m $\times$ 2.42 m $\times$ 2.54
 102 m) in a large array of building-like obstacles (Figure 1). These containers
 103 were placed in a regular formation of 10 rows and 12 columns forming an
 104 idealized urban geometry of an approximately 200 m $\times$ 200 m array (Figure
 105 1).

106 In this study, 20 trials from a total 68 releases are selected to simulate the
 107 flow field and forward atmospheric dispersion of a tracer in an urban-like envi-
 108 ronment (Table 1). These selected trials are similar with the trials utilized in
 109 earlier studies (Yee and Biltoft, 2004; Milliez and Carissimo, 2007; Donnelly
 110 et al., 2009, etc.), so that a comparative analysis of the simulated dispersion

111 results can be performed with other investigations. The meteorological and
 112 source parameters for each trial are taken from Biltoft (2001) and Yee and
 113 Biltoft (2004) and given in Table 1. In all selected trials, Propylene (C_3H_6)
 114 tracer gas was continuously released from a point source into the atmosphere
 115 for approximately 15 min and measured at 48 receptors (both horizontal and
 116 vertical cross-sections of the dispersing plume) located downwind from the
 117 source. The location and height of tracer source were altered mostly in each
 118 trial. The tracer was released without buoyancy at one of the five vertical
 119 heights 0.15, 1.3, 1.8, 2.6, and 5.2 m above the ground surface. The concen-
 120 tration measurements were recorded at a height of 1.6 m (at 40 receptor) on
 121 four horizontal sampling lines. The concentrations were also measured at 8
 122 receptors in vertical direction on a single point in the domain at a height of 1,
 123 2, 4, 6, 8, 10, 12, and 16 m above the ground surface. These four horizontal
 124 sampling lines or arcs were approximately 25, 60, 95, and 195 m downwind
 125 from the release locations. Digital photo-ionization (dPID) detectors were
 126 used to measure the C_3H_6 concentrations at a frequency response of 50 Hz
 127 and with a detection limit of about 0.04 parts per million by volume (ppmv).
 128 As an input for model simulation, the mean wind speed and direction are
 129 taken at 4 m height above the ground surface from upstream South tower
 130 (Yee and Biltoft, 2004). The observations of the surface friction velocity (u_*),
 131 Obukhov length (L), and turbulent kinetic energy (k) are taken at 4 m level
 132 from a 32-m tower (tower T) in centre of the domain.

133 Following Yee and Biltoft (2004), 200 s quasi-steady periods within each
 134 15 min plume dispersion experiment were extracted from the selected trial to
 135 remove the non-stationary from the data. The concentration measurements

136 during these extracted 200 s quasi-steady periods were used to evaluate the
137 simulated dispersion results in each trial. Measurements from three hor-
138 izontal two-dimensional (2-D) sonic anemometer/thermometers at a 16 m
139 telescoping pneumatic mast (located 30.5 m upwind of the midpoint of front
140 obstacle array) were used to generate the inflow boundary conditions.

141 **3. CFD model and mesh structure**

142 *3.1. Description of the model Fluidyn-PANACHE*

143 In this study, a three-dimensional (3-D) Computational Fluid Dynam-
144 ics (CFD) diagnostic model Fluidyn-PANACHE (version 4.0.7.52) (Mazzoldi
145 et al., 2008; Fluidyn-PANACHE, 2010) is utilized to compute the flow field
146 and dispersion of pollutants in the MUST geometry. Fluidyn-PANACHE
147 is dedicated to the 3-D simulation of accidental dispersion from industrial
148 sites and simulates the atmospheric processes related to the pollution and
149 hazards in complex geometric environments. Fluidyn-PANACHE solves the
150 Reynolds Averaged Navier-Stokes (RANS) fluid dynamics equations of air
151 motion along with the equations describing conservation of species concen-
152 tration, mass, and energy for a mixture of ideal gases using 3-D finite-volume
153 techniques. It solves the Reynolds averaged forms of these equations for tur-
154 bulent flow. Fluidyn-PANACHE uses modified standard $k - \varepsilon$ turbulence
155 model to resolve the turbulence structure within the domain. It includes a
156 built-in automatic 3-D mesh generator that generates a computational finite-
157 volume mesh around obstacles and body-fitting the complex terrain undula-
158 tions. The mesh can be considered as structured or unstructured in simula-
159 tions by the CFD model Fluidyn-PANACHE. Clustering of mesh points in

certain regions is also possible with nested domains. Dispersion of gaseous pollutants is modelled by solving the standard Eulerian advection-diffusion equation governing the transport and diffusion of C_3H_6 concentrations in MUST field experiment.

3.2. Simulation domain and grid resolution

A study domain for the high-resolution numerical simulations of MUST field experiment comprises the outer and inner (nested) domains. Since the overall width and length of the obstacles array in MUST experiment were 193 m and 171 m respectively (Yee and Bilotft, 2004), the inner domain is defined a size of 250 m $\times$ 225 m. To ensure a smoothly varying wind flow over the boundary of defined inner domain that contains the main experimental geometry of MUST obstacles array, outer domain boundary is kept away from obstacles. Accordingly, the size of the outer computational domain is considered 800 m $\times$ 800 m (approximately four times of the inner domain consisting the obstacles arrays). The extension of outer domain far from the experimental site is essential to reduce the effect of the boundary conditions on the simulations. The maximum heights of the inner and outer domains are taken as 100 m and 200 m respectively.

The mesh in this study is selected to be 3-D unstructured for both outer and nested domains. A finer mesh is generated in the nested domain and grids are adjusted to the containers. The mesh is further refined near the source and monitor points. The computational domain consists of total 2849276 grid cells in the embedded mesh. The outer and inner domains are discretized respectively in 61 and 56 vertical levels. The first vertical level is corresponding to the ground surface. The minimum vertical grid spacing in both domains

185 is 0.25 m at close to the ground surface and the maximum are 10 m and 20
186 m at top of the inner and outer computational domains, respectively. The
187 lowest 40 vertical levels in both domains are set to a uniform 0.25 m grid
188 spacing that comprising the lowest 10 m (approximately four times of the
189 obstacles height 2.54 m) of the vertical domains. Above the 10 m level, the
190 vertical grid spacing are set to uniform 2 m (5 vertical levels between 10 m
191 - 20 m), 5 m (4 levels between 20 m - 40 m), 10 m (6 levels between 40 m -
192 100 m), and, 20 m (5 levels between 100 m - 200 m for outer domain only).
193 A grid sensitivity analysis with other mesh resolutions is also performed to
194 adapt the defined horizontal and vertical mesh for the numerical simulation.

195 **4. Boundary conditions**

196 Boundary conditions characterize the profiles of model variables at outer
197 computational domain boundaries and directly influence the simulated flow-
198 field and thus, dispersion of the air pollutants. Boundary conditions at the
199 outer domain boundary, ground, and on obstacles are required to solve the
200 governing equations. The top boundary is considered as an outflow bound-
201 ary. The lateral boundaries of the domain are treated as inflow and outflow
202 boundaries depending on the direction of the wind with respect to the domain
203 boundary. Several profiles are available in the literature for inflow boundary
204 conditions for wind and turbulence variables. Following boundary conditions
205 are specified in this study.

206 *4.1. Bottom boundary condition and wall functions*

207 The Fluidyn-PANACHE uses wall functions to compute the drag forces
208 on solid walls existing in computational domain in the turbulent boundary

209 layer. The bottom boundary condition is defined as a no-slip condition where
 210 velocity components are set to zero at the ground surface and standard wall
 211 functions are used for other variables (Hanjalic, 2005). The wall functions
 212 result from the solution of the Navier-Stokes equations for a turbulent bound-
 213 ary layer in equilibrium. The logarithmic law of the wall for momentum is
 214 given by:

$$u^+ = \begin{cases} \frac{1}{\kappa} \ln(Ey^+), & \text{for } y^+ > 11.63 \\ y^+, & \text{for } y^+ < 11.63 \end{cases} \quad (1)$$

215 where $\kappa (= 0.41)$ is the von Karman constant, $u^+ = U_p/u_*$ is the non-
 216 dimensional velocity, in which U_p is the fluid velocity parallel and relative to
 217 wall, $y^+ = \rho u_* y / \mu$ is non-dimensional wall to cell-centre distance, in which y
 218 is the cell-centre to wall distance and μ is the dynamic viscosity of fluid, and
 219 E is a function of wall roughness. The effective viscosity (μ_e) at the wall is
 220 computed by $\mu_e = \mu \max(y^+/u^+, 1)$.

221 For equilibrium ABL modelling, Blocken et al. (2007) discussed the prob-
 222 lems of generating a horizontally homogeneous ABL profile over an uniformly
 223 rough terrain in the upstream and the downstream (or at least the upstream)
 224 regions of the computational domain. This problem is resolved by following a
 225 relationship between the equivalent sand-grain roughness height of the ABL
 226 (K_s) and aerodynamic roughness length (z_0) by $K_s = Ez_0/C_s$ (Blocken et al.,
 227 2007), where $E = 9.793$, and C_s is a constant required in the wall function.
 228 The value of C_s is set to 3.55 so that a common requirement for the selection
 229 of the height of wall adjacent cell centroid ($z_p = 0.125$ m) greater than K_s
 230 (i.e. $z_p > K_s$) is satisfied. This condition is also required to ensure a reason-
 231 able vertical grid resolution (0.25 m for the lowest 10 m) close to the ground

232 surface (Blocken et al., 2007).

233 4.2. Inflow boundary condition

234 The velocity, temperature, turbulence variables, and species concentra-
235 tions are needed to be specified at inlet of the domain. Pressure was extrap-
236 olated from inside the domain. Specifications of the wind and turbulence
237 variables are explained in the following sections.

238 4.2.1. Wind profile

239 The vertical wind profile is an important factor in defining the structure
240 of the ABL. Generally, the log-law profile in neutral stability condition and
241 the profiles based on the Monin-Obukhov (MO) similarity theory in stable
242 and unstable atmospheric conditions have been used to parametrize the in-
243 flow boundary condition (Hanna et al., 2004; Milliez and Carissimo, 2007;
244 Donnelly et al., 2009; Efthimiou et al., 2015, etc.). However, these profiles
245 are valid only in the surface layer and may not be able to characterize the
246 entire ABL and thus, can affect the flow field and dispersion. To overcome
247 this limitation of the profiles, Gryning et al. (2007) extended the surface layer
248 wind profiles and proposed new parametrizations that are valid in the entire
249 ABL. In this study, these extended profiles for velocity are utilized to specify
250 the inflow condition as follows:

251 (a) *Gryning et al. (2007) profile*

252 By defining three different length scales for surface, middle, and upper
253 layers of the ABL, Gryning et al. (2007) extended the surface layer wind
254 speed profiles in various atmospheric stability conditions that can be ap-
255 plicable in the entire ABL. In stable atmospheric conditions during MUST

256 filed experiment, following wind profile from Gryning et al. (2007) is used to
 257 parametrize the inflow boundary condition:

$$U(z) = \frac{u_*}{\kappa} \left[\ln \left(\frac{z}{z_0} \right) + \frac{bz}{L} \left(1 - \frac{z}{2h} \right) + \frac{z}{L_{MBL}} - \frac{z}{h} \left(\frac{h}{2L} \right) \right] \quad (2)$$

258 where z is the height above the ground surface, h is the ABL height, $b(= 4.7)$
 259 is an empirical constant in the stability function (Businger et al., 1971; Dyer,
 260 1974), and a length scale L_{MBL} in middle layer of the ABL is given by:

$$L_{MBL} = \frac{h}{2} \left[\left\{ \left(\ln \left(\frac{u}{fz_0} \right) - B(\mu_f) \right)^2 + A^2(\mu_f) \right\}^2 - \ln \left(\frac{h}{z_0} \right) - \frac{bh}{2L} \right]^{-1} \quad (3)$$

261 where f is the Coriolis parameter and, $A(\mu_f)$ and $B(\mu_f)$ are the resistance law
 262 functions in the geostrophic drag law (Stull, 1988). $A(\mu_f)$ and $B(\mu_f)$ depend
 263 on a dimensionless stability parameter $\mu_f = u_*/fL$. Arya (1975) empirically
 264 determined resistance law functions $A(\mu_f)$ and $B(\mu_f)$ from observations in
 265 stable boundary layer. These empirical functions are used in Eq. (3) to
 266 parametrize L_{MBL} in the wind profile (Eq. (2)).

267 *(b) Mixing length profile by Pena et al. (2009)*

268 Pena et al. (2009) proposed a mixing length parametrization of the wind
 269 speed profiles in different atmospheric stability conditions that extend the
 270 validity of the wind profiles much higher than the surface layer. For stable
 271 atmospheric conditions, following wind profile is utilized to analyse the effect
 272 of different inflow conditions on the pollutant dispersion in a complex urban
 273 environment (Pena et al., 2009):

$$U(z) = \frac{u_*}{\kappa} \left[\ln \left(\frac{z}{z_0} \right) + \frac{bz}{L} \left(1 - \frac{z}{2h} \right) + \frac{\kappa z}{\lambda} \left(1 - \frac{z}{2h} \right) - \frac{z}{h} \right] \quad (4)$$

274 where $\lambda = 0.00027G/f$, in which G is the geostrophic wind magnitude. This
 275 wind profile includes the effect of the ABL height. An evaluation by Pena
 276 et al. (2009) showed that it has good agreement with the measurements,
 277 correcting the underestimation of the traditional surface layer wind profile.

278 4.2.2. Turbulence profile

279 Appropriate vertical profiles of the turbulent kinetic energy (k) and the
 280 turbulence dissipation rate (ϵ) are required to accurately specify the bound-
 281 ary conditions in the $k - \epsilon$ turbulence model. The simulations of each trial
 282 in MUST field experiment are performed by applying two turbulence profiles
 283 of k and ϵ . These profiles of k and ϵ are described as follows:

284 (a) Prognostic turbulence profile

285 The turbulence profiles in the ABL are computed as a prognostic profiles
 286 for k and ϵ that are consistent with the vertical profiles of velocity and
 287 temperature (Ye, 1998). These prognostic profiles are derived from a one-
 288 dimensional (1-D) transport equation for k and ϵ . The transport equations
 289 for k and ϵ are simplified with the assumptions: (i) constant density (ρ)
 290 (ii) steady flow (iii) neglecting convection, and (iv) neglecting horizontal
 291 gradients of all quantities. With these approximations, one obtains:

$$\frac{\partial}{\partial z} \left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial z} + P_k + P_b - \rho\epsilon = 0 \quad (5)$$

$$\frac{\partial}{\partial z} \left(\mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial z} + \frac{\epsilon}{k} [C_{\epsilon 1}(P_k + C_{\epsilon 3}P_b) - C_{\epsilon 2}\rho\epsilon] = 0 \quad (6)$$

293 where σ_k is the turbulent kinetic energy Prandtl number, σ_ϵ is the turbu-
 294 lent dissipation Prandtl number and, $C_{\epsilon 1}$, $C_{\epsilon 2}$ and $C_{\epsilon 3}$ are empirical con-
 295 stants. The shear stress-related production of turbulent kinetic energy (P_k),

296 buoyancy-related production of turbulent kinetic energy (P_b), and the tur-
 297 bulent eddy viscosity (μ_t) in Eqs. (5) & (6) are given by

$$P_k = \mu_t \left(\frac{\partial U}{\partial z} \right)^2, \quad P_b = \beta \frac{\mu_t}{Pr_t} g \frac{\partial \theta}{\partial z}, \quad \text{and} \quad \mu_t = \rho C_\mu \frac{k^2}{\epsilon} \quad (7)$$

298 where β is the coefficient of thermal expansion, g is the gravitational ac-
 299 celeration, Pr_t is the turbulent Prandtl number for energy, and θ is the
 300 temperature. The constants of the $k - \epsilon$ turbulence model (Eqs. (5)-(7)) are
 301 given in Table 2. $C_{\epsilon 3}$ does not play a role as buoyancy production in neutral
 302 stability conditions and therefore, it sets to zero. $C_{\epsilon 3}$ is set to -0.4 in sta-
 303 ble condition (Peters and Baumert, 2007). For the selected vertical profiles
 304 for velocity and temperature, Eqs. (5) & (6) are solved using a conjugate
 305 gradient method.

306 (b) *Equilibrium ABL model*

307 Using an approximate analytical approach, Yang et al. (2009) derived a
 308 set of inflow turbulence boundary conditions for the standard $k - \epsilon$ turbulence
 309 model to simulate an equilibrium ABL. A solution of the k -equation of the
 310 standard $k - \epsilon$ turbulence model with assumption of equilibrium between
 311 turbulence dissipation and production, and logarithmic mean wind profile
 312 gives the following relations of k and ϵ for the inflow boundary conditions
 313 (Yang et al., 2009)

$$k(z) = \frac{u_*^2}{\sqrt{C_\mu}} \sqrt{C_1 \ln \left(\frac{z + z_0}{z_0} \right) + C_2} \quad (8)$$

$$\epsilon(z) = \frac{u_*^3}{\kappa(z + z_0)} \sqrt{C_1 \ln \left(\frac{z + z_0}{z_0} \right) + C_2} \quad (9)$$

315 where C_1 and C_2 are constants that need to be determined using the observa-
 316 tions of turbulent kinetic energy (k). The constants C_1 and C_2 are estimated
 317 by fitting the turbulent kinetic energy relation (Eq. (8)) to the measured
 318 vertical profile of k at a 16 m telescoping pneumatic mast located 30.5 m up-
 319 wind of the midpoint of the front of obstacle array. Turbulent kinetic energy
 320 at this pneumatic mast was obtained with the measurements from three hor-
 321 izontal two-dimensional (2-D) sonic anemometers at the 4, 8, and 16 m levels
 322 (Biltoft, 2001). Since C_1 and C_2 in these equations are estimated by fitting
 323 the observed values of k , the approximated analytical profiles (Eqs. (8)&(9))
 324 follow the actual representation of k in each trial of the MUST experiment.

325 **5. Numerical simulations and statistical methods for evaluation**

326 A fully implicit NT-unsteady CFD solver in Fluidyn-PANACHE is used
 327 for wind-field computations that can handle the nested domains and both
 328 structured and unstructured meshes. The NT solver is a pressure-based fully
 329 implicit segregated method on unstructured meshes that solves all governing
 330 equations separately and uses an iterative procedure for both steady state and
 331 transient cases. A modified standard $k - \epsilon$ 3-D prognostic turbulence model
 332 is used to resolve the turbulence structure within the domain. It solves the
 333 transport equations for turbulent kinetic energy (k) and its dissipation rate
 334 (ϵ) for the constants given in Table 2. The SIMPLEC (SIMPLE-Consistent)
 335 algorithm of Doormaal-Raithby (Van Doormaal and Raithby, 1984) was used
 336 to couple the pressure and momentum equations. Since the released tracer
 337 gas C_3H_6 in MUST field experiment is heavier than the air, the buoyancy
 338 model is used to model the body force term in the Navier-Stokes equations.

339 The buoyancy model is suitable for the dispersion of heavy gases where den-
 340 sity difference in the vertical direction drives the body force. Residuals were
 341 used to check the convergence of the solution during simulation. For an ideal
 342 CFD simulation, the scaled residuals for all variables were considered to be
 343 equal or less than $O(10^{-4})$. The model Fluidyn-PANACHE took ≈ 6 hours
 344 to complete each CFD simulation on 20 processors (Intel(R) Xeon(R) CPU
 345 E5-2695 v2 @ 2.40GHz) on a cluster CentOS release 6.5.

346 Fluidyn-PANACHE is not capable of incorporating atmospheric stratifi-
 347 cation through surface cooling or heating and whatever stability effects are
 348 included are through the inflow boundary condition (via advection). Fluidyn-
 349 PANACHE includes the ABL model that serves as the interface between
 350 the meteorological observations and the boundary conditions required by
 351 the CFD solver. Fluidyn-PANACHE meteorological pre-processor uses the
 352 meteorological observations (Table 1) for each trial of MUST field experi-
 353 ment along with the date/time to generate the micro-meteorological param-
 354 eters that characterize the structure of the ABL. These computed micro-
 355 meteorological parameters, along with the terrain undulations and obstacles,
 356 determine the three-dimensional wind field for each trial. The estimated val-
 357 ues of coefficients C_1 and C_2 in Eqs. (8)&(9) vary in each trial for inflow
 358 boundary conditions. The averaged values of these coefficients for all trials
 359 are estimated as $C_1 = -0.15$ and $C_2 = 1.33$. It was observed that the be-
 360 haviour of k profile in Eqs. (5)-(7) is the opposite of Eqs. (8)&(9) and is
 361 contrary to the observations near the surface in most of the MUST trials.
 362 However, the magnitude of the ϵ profile obtained from (5)-(7) is greater than
 363 that obtained from Eqs. (8)&(9) in most of the trials.

364 In comparison to the observations, it was observed that the wind speeds
 365 obtained from Eq. (2) are better than Eq. (4) for most of the MUST trials
 366 considered for simulation. The vertical temperature profile directly deter-
 367 mines the buoyancy contribution to the turbulence and thus, it has significant
 368 bearing on the dispersion patterns both in vertical and horizontal directions.
 369 A logarithmic temperature profile, based on the MO-similarity theory for
 370 atmospheric surface layer, is used to describe its vertical variation in neu-
 371 tral and stable conditions in the MUST field experiment. The ABL height
 372 (h) in the vertical wind profiles at inlet in Eqs. (2)-(4) was computed us-
 373 ing $h = 0.3u_*/f$ (Tennekes, 1973) in neutral stability, and $h = 0.4\sqrt{u_*L/f}$
 374 (Zilitinkevich, 1972) in stable atmospheric conditions.

375 Three combinations of the inflow boundary conditions for wind and tur-
 376 bulence profiles (section 4) are considered for the simulations. These combi-
 377 nations are defined as (i) *case 1*: wind profile of Pena et al. (2009) (section
 378 4.2.1), and prognostic turbulence profile (section 4.2.2); (ii) *case 2*: wind pro-
 379 file of Pena et al. (2009) (section 4.2.1), and turbulence profile of Yang et al.
 380 (2009) (section 4.2.2); and (iii) *case 3*: Gryning et al. (2007) wind profile
 381 (section 4.2.1), and turbulence profile of Yang et al. (2009) (section 4.2.2).
 382 It was noted that the wind profile proposed by Gryning et al. (2007) (Eq.
 383 (2)) is not applicable in the trials (trial no. 4, 5, & 6 in Table 1) of very
 384 stable atmospheric conditions. The intermittent turbulence in very stable
 385 conditions produces strongly nonstationary events during which the valid-
 386 ity of turbulent transport and storage measurements is uncertain (Kumar
 387 and Sharan, 2012a). A wind profile based the similarity function, proposed
 388 by Beljaars and Holtslag (1991), was used to parametrize the vertical wind

389 profiles in these three trials.

390 6. Performance evaluation methods

391 The performance of the Fluidyn-PANACHE against MUST experiment
392 is evaluated both qualitatively (unpaired analysis) and quantitatively using
393 the standard statistical measures (Chang and Hanna, 2004), such as, Nor-
394 malized Mean Square Error (NMSE), Fractional Bias (FB), Geometric Mean
395 bias (MG), Geometric Variance (VG), Correlation coefficient (COR), Factor
396 of Two (FAC2), and Index of Agreement (IA). These statistical measures
397 characterize the agreement between the model predictions and observations.
398 The NMSE emphasizes the scattering in a sample and FB indicates an over-
399 all under- or over-prediction from the observations. A prefect model would
400 have NMSE and $FB = 0$; and COR, FAC2, MG, VG, and $IA = 1$ (Chang
401 and Hanna, 2004). However, for an *acceptable* model performance, Chang
402 and Hanna (2004) provided the following bounds of the statistical measures:

403 $NMSE < 4$, $-0.3 < FB < 0.3$, $FAC2 > 0.5$, $VG < 1.6$, $0.7 < MG < 1.3$.

404 For a point to point evaluation of the model with observations, Chang
405 and Hanna (2004) suggested to replace the concentration values, which are
406 below detection limit of the samplers, by the detection threshold. However,
407 some other methods were also used to deal with these below detection limit
408 concentrations (Milliez and Carissimo, 2007; Donnelly et al., 2009). The
409 sampling calibration range of the detectors used in MUST experiment was
410 0.04-1000 ppmv (Biltoft, 2001). By following Donnelly et al. (2009), if both
411 concentrations values in a pair of simulated and observed concentrations
412 are lower than the detection limit, both are set to zero and removed from

the dataset. If one of the concentration value in a pair is greater than the detection limit and other is lower than it, the lower concentration value is set to the detection limit.

7. Results and Discussion

For each trial of the MUST field experiment (Table 1), the 3-D wind flow and the plume dispersion of a tracer C_3H_6 released from a point source are simulated by Fluidyn-PANACHE. The simulated concentrations at all receptors are evaluated and analysed for the selected 20 trials (Table 1). All 20 trials are classified in neutral, stable and very stable classes by using the Obukhov length (L). Based on this, two trials are in neutral conditions ($L \geq 2500$), 11 trials in slightly stable to near-neutral conditions ($130 \leq L \leq 330$), and seven trials are in very stable to stable atmospheric conditions ($4.8 \leq L \leq 91$).

Figure 2 shows the horizontal cross-section of concentration field (Kg/m^3) for two representative trials (a) 2671852 with an inflow wind direction of -49° and (b) 2672213 with an inflow wind direction of 30° . The contour plots in both trials show the influence of the elongated buildings on plume deflection. In trial 2672213, the source is just behind a building and the concentration contour in Figure 2(b1) exhibits that pollutant is first reflected back by the building fronted on the source, and traveled with the flow between the array of buildings and then divert with a deflection from mean wind direction near to the source. These contours show the ability of CFD model to capture the effects of urban geometry on plume dispersion. The vertical profiles of the concentration on a location of the 32-m tower near the centre of the

437 obstacle array is also shown in Figure 2. The vertical profiles of the observed
 438 concentrations at heights of 1, 2, 4, 6, 8, 10, 12, and 16 m on the 32-m tower
 439 is also shown in this figure. It shows that, the simulated concentrations in
 440 vertical direction is satisfactory with the observations. These contours are
 441 plotted for *case-1* of boundary conditions; however, the characteristics of the
 442 concentration field are comparable for others *cases 2 & 3*.

443 As shown by Milliez and Carissimo (2007) using a CFD model Code_Saturne,
 444 the shifting of the plume centerline from mean wind direction, especially close
 445 to the source, is also sensitive to the source location. Figure 3 shows a com-
 446 parison of the iso-surface of concentration ($C = 4.0 \times 10^{-5} Kg/m^3$) for two
 447 representative trials (a) 2640138 and (b) 2672303, with same upstream wind
 448 direction (17°), but different source locations. The source was located be-
 449 hind a building in trial 2640138; whereas, it was placed on a cross-road in
 450 trial 2672303. Similar features of the plumes as illustrated by Code_Saturne
 451 (Milliez and Carissimo, 2007) are found with the present simulations in both
 452 trials (Figure 3). For a source behind a building, Figure 3(a) shows that
 453 the pollutant is first travelled into the eastwest oriented streets of the array.
 454 However, the tracer is first channelled into the northsouth oriented streets
 455 for a source located in a cross-road in trial 2672303 (Figure 3(b)).

456 The statistical performance measures are computed and analyzed for the
 457 simulated results with all three combinations (*cases 1, 2, & 3*) of inflow
 458 boundary conditions. Figure 4(a) shows a scatter diagram between the pre-
 459 dicted and observed concentrations for all 20 MUST trials. The scatter plot
 460 in this figure is shown for all the three *cases* of inflow boundary conditions. It
 461 shows that a good agreement is found between the observed and simulated

concentrations by the CFD model. For an unpaired analysis, a quantile-quantile ($Q - Q$) plot (Figure 4(b)) is also drawn by arranging both, the observed and predicted concentrations, in increasing order of their magnitudes. The $Q - Q$ plot shows that the predicted concentrations are close to a one-to-one line. The statistical performance measures for the simulated concentrations with all three *cases* of inflow boundary conditions are given in Table 3.

As visible in the scatter plot (Figure 4(a)), the false negative and false positive values are important in evaluation of a dispersion model for emergency response applications (Donnelly et al., 2009). The false negative values are that concentrations when a simulated concentration is below detection limit that sets to the detection limit and the corresponding observations have a visible tracer concentration greater than the threshold limit. These false negative predictions remain a cause of concern in emergency applications (Donnelly et al., 2009). However, the magnitude of the false negative values are very small (mostly less than ≈ 1 ppmv; however, only two points are greater than 1 ppmv and < 8 ppmv). Donnelly et al. (2009) also observed a similar pattern for these false negative concentrations.

7.1. Comparative analysis with respect to different inflow boundary conditions

In order to analyse the effect of different inflow boundary conditions on plume dispersion in MUST experiment, three distinct simulations for each trial are performed for three *cases* (section 5) of the inflow boundary conditions. The simulated concentrations from Fluidyn-PANACHE for all three *cases* of inflow boundary conditions are analysed and inter-compared.

487 *7.1.1. Overall performance*

488 To compare an overall performance of Fluidyn-PANACHE for all the
489 three *cases* of different inflow boundary conditions, the simulated concen-
490 trations from all 20 trials are exhibited in form of the scatter (Figure 4(a)),
491 $Q - Q$ (Figure 4(b)) plots, along with the statistical performance measures
492 (Table 3). In the scatter plot (Figure 4(a)), it is observed that the simulated
493 concentrations have good agreement with the observations for all the three
494 *cases* of inflow boundary conditions. The simulated higher concentrations,
495 at the receptors near to the source, are close to one-to-one line; however,
496 comparably more scatter is observed for lower concentrations at far from the
497 source. This trend of the predicted concentrations is more visible in $Q - Q$
498 plot (Figure 4(b)) that shows a comparison of simulated and observed con-
499 centration distributions. As the statistical measures NMSE characterizes the
500 scattering in a sample, it is observed that the *case-3* has relatively smaller
501 scatter (NMSE = 0.67) in comparison to *case-1* (NMSE = 1.66) and *case-*
502 *2* (NMSE = 1.51). However, the NMSE values for all the three *cases* are
503 smaller than its acceptable bound (NMSE < 4) (Chang and Hanna, 2004).
504 The correlation coefficients (COR) for all three *cases* 1, 2, & 3 are 0.89, 0.89,
505 and 0.92, respectively (Table 3) and it shows a good one-to-one correspon-
506 dence between the simulated and observed concentrations.

507 An overall under-prediction of the simulated concentrations is observed
508 for all the three *cases* (Figures 4(a) & (b)) and it is also re-affirmed by
509 the positive values of FB in all *cases* (Table 3). The magnitudes of the
510 FB for each *cases* in Table 3 show that the *case-3* has relatively smaller
511 under-prediction (FB = 0.10) than the *case-1* (FB = 0.42) and *case-2* (FB

512 = 0.37). It also shows that the *case-1* and *case-2* have comparable under-
513 predictions with the observations (Figures 4(a) & (b), Table 3). The FB
514 value (= 0.10) for *case-3* is relatively small, implying this *case-3* of the inflow
515 boundary conditions is performing good with the observations. The degree of
516 under-prediction in each *case* is also visible with the ratio of predicted ($\overline{C_p}$)
517 and observed ($\overline{C_o}$) concentrations, where the over-bars indicate the average
518 over all measurements. It shows a comparable under-prediction for *case-1*
519 ($\overline{C_p}/\overline{C_o} = 0.65$) and *case-2* ($\overline{C_p}/\overline{C_o} = 0.69$), and a slight under-prediction
520 for *case-3* ($\overline{C_p}/\overline{C_o} = 0.90$). The MG values, which shows more significant
521 under-prediction than the FB and also systematic errors (Chang and Hanna,
522 2004), are 1.77, 1.62, and 1.35 for *cases* 1, 2, & 3, respectively (Table 3).
523 It also shows that the MG value for *case-3* is approximately close to its
524 acceptable bound (MG < 1.3) and thus, it exhibits comparatively smaller
525 under-predictions.

526 The three *cases* 1, 2, & 3 are predicting respectively 52.8%, 59.9%, and
527 67.9% of total concentrations within a factor of two (FAC2) (Table 3). All
528 the *cases* are predicting more number of concentration points within a FAC2
529 than its acceptable bound (FAC2 > 50%) (Chang and Hanna, 2004). It also
530 shows that the simulated FAC2 points (67.9%) with *case-3* are relatively
531 greater than the *cases* 1 & 2. The value of IA is maximum and close to its
532 ideal value for *case-3* (IA = 0.96) and comparable for *cases* 1 and 2 (IA =
533 0.90 and 0.91, respectively) (Table 3).

534 7.1.2. Performance at each horizontal line

535 To investigate the near source plume dispersion and for quantifying the
536 quality of simulations in each *cases*, the statistical performance measures

are analysed with respect to the downwind distance from the source. Accordingly, all performance measures are calculated for each horizontal line separately for all the three *cases*. The computed statistical indices at each horizontal line are given in Table 3 and the performance measures with downwind distance from the source are shown in Figure 5. As evident from the trends in NMSE (Figure 5(a), Table 3), the maximum scatter for *case-1*, *case-2*, and *case-3* is respectively observed at line 1 (NMSE = 1.36), line 2 (NMSE = 1.32), and line 4 (NMSE = 0.62). The variation of FB at each horizontal line shows that the extent of under-prediction for all the three *cases* increases with increasing downwind distance from the source. First three lines have almost invariant one-to-one correlation between the observed and simulated concentrations for each *cases* and minimum correlation is observed at line 4 for all *cases*. The *case-3* predicts 72.7%, 73.0%, 65.2%, and 50.9% points within a FAC2 for lines 1, 2, 3, and 4, respectively and it shows that the *case-3* simulates more points within FAC2 at each line in comparison to the *cases* 1 & 2 (Table 3). The Figure 5(a),(b)(e),&(f) shows that the *case-3* has smaller NMSE, FB, MG, and VG at each horizontal lines in comparison to other *cases* 1 & 2. Also the FAC2 and COR at each horizontal lines are also greater for *case-3* than *cases* 1 & 2 (Figures 5(c) & (d)). In each *case*, IA is maximum at line 1 and minimum at line 4 and comparable at lines 2 & 3 (Table 3).

7.1.3. Performance at all horizontal, and all vertical receptors

The performance measures for each *case* are calculated for the datasets from all receptors at four horizontal lines altogether and, also separately for the data from eight receptors in vertical direction at a single point in the

562 MUST array (Table 3). An overall under-prediction is observed for all hori-
563 zontal receptors and 50.8%, 58.4%, and 66.8% points are simulated within a
564 FAC2 (Table 3) by the three *cases*, respectively. The *case-3* gives minimum
565 under-predictions ($FB = 0.07$) at all horizontal lines in comparison to *case-1*
566 ($FB = 0.41$), and *case-2* ($FB = 0.36$) (Table 3). The statistical measures
567 for the concentrations at the vertical receptors show that the vertical extent
568 of plume dispersion simulated by Fluidyn-PANACHE is in good agreement
569 with the observations for all three *cases*. For vertical profile of the concen-
570 trations, the three *cases* 1, 2, & 3 simulate 60.1%, 65.3%, and 71.7% points,
571 respectively, within a FAC2 (Table 3).

572 7.1.4. Performance analysis with respect to atmospheric stability

573 The statistical indices in each *case* are calculated with the sets of sim-
574 ulated and observed concentrations from trials categorized in (i) neutral (2
575 trials), (ii) near-neutral to stable (11 trials), and (iii) stable to very stable
576 (7 trials) atmospheric conditions (Table 4). The values of FB in Table 4
577 show that the overall under-prediction is minimum ($FB = 0.29, 0.23, \& 0.07$
578 for *cases* 1, 2, & 3, respectively) in near-neutral to stable conditions. The
579 maximum under-prediction is observed in stable to very stable conditions
580 for *case-1* ($FB = 0.49$) and *case-2* ($FB = 0.46$), and in neutral conditions
581 for *case-3* ($FB = 0.23$). The three *cases* 1, 2, & 3 respectively simulates (i)
582 45.5%, 63.6%, and 66.7% points within a FAC2 in neutral conditions, (ii)
583 57.2%, 64.1%, and 71.5% points in near-neutral to stable conditions, and
584 (iii) 47.6%, 51.6%, and 62.0% points in stable to very-stable conditions (Ta-
585 ble 4). The performance measures in Table 4 show that the performance of
586 *case-3* excels in comparison to other two *cases* 1 & 2 in all stability conditions

587 varying from neutral to very stable conditions.

588 7.1.5. Performance of sampling line maximum (SL-Max) concentrations

589 Simulations of the sampling line maximum (SL-Max) concentrations has
590 an utmost importance for accurately quantifying the maximum concentra-
591 tions in the most affected regions. Figures 6 (a) & (b) show the scatter and
592 $Q - Q$ plots of the SL-Max concentrations simulated by Fluidyn-PANACHE
593 for *cases* 1, 2, & 3 of the inflow boundary conditions. It shows that the per-
594 formance of the Fluidyn-PANACHE is well in agreement for SL-Max concen-
595 trations in all the three *cases*. Most of the simulated SL-Max concentrations
596 are close to one-to-one line (Figures 6 (a) & (b)) and have good correlations
597 with the SL-Max observed concentrations. The statistical measures for sim-
598 ulated SL-Max concentrations are given in Table 5 for each *case* of inflow
599 boundary conditions. The simulated SL-Max concentrations for *case-3* shows
600 the best performance of Fluidyn-PANACHE in comparison to the other *cases*
601 1 & 2 (Figures 6 (a) & (b), Table 5). The model with *case-3* predicts 95% of
602 SL-Max concentrations within FAC2; whereas, the values of FAC2 for *cases*
603 1 & 2 are 77.5% & 85.0%, respectively. The performance of the Fluidyn-
604 PANACHE against MUST measurements is obtained within the bounds of
605 all statistical measures (Chang and Hanna, 2004) in each *case*.

606 Based on the above statistical analysis, we can conclude that the CFD
607 model with *case-3* of inflow boundary conditions gives relatively better agree-
608 ment with the observations in comparison to the *cases* 1 & 2 (Tables 3, 4,
609 & 5 and Figures 4, 5, & 6). The *case-3* exhibited a better agreement with
610 the observed concentrations at all horizontal and vertical receptors in vari-
611 ous stability conditions. SL-Max concentrations are also better simulated by

612 *case-3* in comparison to *cases* 1 & 2 of the inflow boundary conditions.

613 7.2. Comparison with other evaluation studies

614 7.2.1. Comparison with Milliez and Carissimo (2007)

615 A comprehensive evaluation study of all 20 trials (Table 1) of the MUST
616 field experiment was performed by Milliez and Carissimo (2007) using a 3-
617 D CFD model Code_Saturne. In their evaluation, Milliez and Carissimo
618 (2007) used a threshold of detection limit ($= 0.04$ ppmv) for both simulated
619 and observed averaged concentrations. Thus, a similar statistical evaluation
620 method is used here for the comparison purpose. The Code_Saturne showed
621 a slightly over-prediction ($FB = -0.063$) with the observations for all 20 trials;
622 however, the present simulations for each *case* of inflow boundary conditions
623 exhibit an overall under-prediction ($FB = 0.42, 0.37, \& 0.10$ for *cases* 1, 2,
624 & 3, respectively). Present simulations predicts respectively 67.0%, 71.9%,
625 & 77.5% of the concentrations within a FAC2 for *cases* 1, 2, & 3, which
626 are more than the Code_Saturne's (Milliez and Carissimo, 2007) simulated
627 67.1% points within a FAC2. Code_Saturne predicts 92.5% of the SL-Max
628 concentrations within a FAC2 which is smaller than the points predicted with
629 *case-3* ($FAC2 = 95.0\%$) and greater than the FAC2 values for *case-1* ($FAC2$
630 $= 77.5\%$) and *case-2* ($FAC2 = 85.0\%$).

631 7.2.2. Comparison with Donnelly et al. (2009)

632 In another study, Donnelly et al. (2009) performed an evaluation of the
633 MUST field experiment with the simulation results from a numerical model
634 WinMISKAM, a 3-dimensional non-hydrostatic flow model and an Eulerian
635 dispersion model. However, only 19 trials (excluding trial no. 2682353 in

636 Table 1) were simulated by Donnelly et al. (2009). In order to compare
637 the evaluation results from the present study, the statistical performance
638 measures for each *cases* are computed for these 19 trials only. The values of
639 NMSE for the present simulated concentrations at all horizontal receptors for
640 the *cases* 1, 2, & 3 are 1.77, 1.62, & 0.69, respectively; which are smaller than
641 the NMSE (= 3.36) reported by Donnelly et al. (2009). The WinMISKAM
642 model predicts 46% of points within a FAC2; whereas, the present model
643 simulates 51.1%, 58.0%, & 66.3% of concentrations within a FAC2 for the
644 inflow boundary conditions in *cases* 1, 2, & 3, respectively.

645 The statistical measures for SL-Max concentrations for all 19 MUST tri-
646 als are also compared to the WinMISKAM simulations. The WinMISKAM
647 is simulating 83% of points within a FAC2 for all SL-Max concentrations;
648 which is slightly higher than the present simulations with *case*-1 (FAC2 =
649 77.6%), comparable to the *case*-2 (FAC2 = 84.2%), and, relatively smaller
650 than the *case*-3 (FAC2 = 94.7%). The NMSE values for SL-Max concen-
651 trations simulated by the Fluidyn-PANACHE with *cases* 1, 2, & 3 are 0.69,
652 0.65, & 0.26, respectively; which are also smaller than the simulations by
653 WinMISKAM (NMSE = 1.12).

654 7.2.3. Comparison with a Gaussian model in Winiarek (2014)

655 In order to evaluate the usefulness of the CFD over a simple regulatory
656 model under non-flat terrain cases, it is obvious to examine the performance
657 of a simple Gaussian model compared to the CFD model for the MUST
658 urban experiment. Recently, Winiarek (2014) used a Gaussian model with
659 appropriate dispersion parameters to simulate its performance in urban con-
660 ditions in MUST field experiment. However, only 14 trials were simulated by

Winiarek (2014). In order to compare the dispersion results from the present CFD study with Gaussian model (Winiarek, 2014), the statistical performance measures for each *cases* are computed for identical 14 trials only and given in Table 6.

The NMSE values are respectively 0.70, 0.65, & 0.68 with *cases* 1, 2, & 3 for the present CFD model simulated concentrations for 14 trials at all receptors; which are smaller than the NMSE ($= 4.24$) reported by a Gaussian model in Winiarek (2014). The Gaussian model predicts 45% of points within a FAC2; whereas, the CFD model simulates 68.0%, 74.3%, & 78.7% of concentrations within a FAC2 for *cases* 1, 2, & 3, respectively. Gaussian model gives an over-prediction ($FB = -0.33$); whereas, an overall under-prediction ($FB = 0.36, 0.25, \& 0.07$ for *cases* 1, 2, & 3, respectively) is observed in present CFD simulations. Even the one-to-one correlation ($COR = 0.59$) between the Gaussian model predicted and observed concentrations is smaller than the COR values 0.95, 0.94, & 0.95 with *cases* 1, 2, & 3, respectively. The (MG, VG) values for Gaussian model were respectively (0.72, 40.41) (Winiarek, 2014). However, (MG, VG) for *case* 1, 2, & 3 are (1.50, 1.93), (1.39, 1.83) and (1.26, 1.73), respectively (Table 6). The acceptable statistical performance measures shows an overall usefulness of CFD models over a simple regulatory Gaussian model under non-flat terrain cases.

8. Conclusions

The present study performed a 3-D CFD simulation of the short-range plume dispersion in an urban like environment of the MUST field experiment. A CFD model Fluidyn-PANACHE is used and evaluated for a tracer disper-

685 sion in various atmospheric stability varying from neutral to stable, and very
686 stable conditions in MUST experiment. The simulations are performed with
687 three *cases* comprising the three combinations of inflow boundary conditions
688 of wind and turbulence profiles at the inlet of computational domain. These
689 inflow boundary conditions comprises the two vertical profiles of wind speed
690 that are applicable in the entire atmospheric boundary layer. Two vertical
691 turbulence profiles are modelled by the numerical, and approximate analytical
692 solutions of the standard one-dimensional $k - \epsilon$ prognostic equations.

693 The statistical evaluation methods are used to analyze the performance
694 of the simulated concentrations in all three *cases* of the inflow boundary
695 conditions. A detailed comparative analysis for three *cases* is performed (i)
696 overall 20 trials, (ii) at each horizontal line, (iii) separately at all horizontal,
697 and all vertical receptors, (iv) with respect to the atmospheric stability, and
698 (v) for the sampling line maximum concentrations. A comprehensive statistical
699 analysis shows that the performance of the Fluidyn-PANACHE against
700 MUST field experiment with all three *cases* is well within the acceptable
701 bounds of statistical measures for air quality applications. The CFD model
702 with three *cases* 1, 2, & 3 of the inflow boundary conditions predicts respectively
703 52.8%, 59.9%, and 67.9% of the total concentrations within a factor of
704 two. The positive fractional bias in all the simulated results show that the
705 model gives an overall under-prediction of the observed concentrations.

706 From a comprehensive comparative analysis, it was observed that the
707 inflow boundary conditions in *case-3*, that comprises the Gryning et al. (2007)
708 wind profile and the turbulence profiles of Yang et al. (2009) empirically
709 fitted with observations, give relatively better agreement with the observed

710 concentration in comparison to the *cases* 1 & 2. The analysis shows that
711 the performance of the CFD model with the *case-3* excels at all horizontal
712 and vertical receptors in various stability conditions and it has an overall
713 smaller scatter (normalized mean square error = 0.67) and under-prediction
714 (fractional bias = 0.10). The sampling line maximum concentrations are
715 also better simulated by *case-3* (95% within a factor of two) in comparison
716 to other *cases* 1 & 2.

717 A comparative statistical analysis of the Fluidyn-PANACHE simulations
718 is performed with other evaluation studies in the literature for the sampling
719 line maximum and overall simulated concentrations. A slightly better perfor-
720 mance was observed for the present simulations. The acceptable statistical
721 performance measures shows an overall usefulness of CFD models over a
722 simple regulatory Gaussian model under non-flat terrain cases. The study
723 shows that a parametrization of inflow boundary conditions with a realistic
724 wind profile that is applicable in entire atmospheric boundary layer yields
725 an overall good performance of a CFD model. The evaluation results show
726 that the CFD model Fluidyn-PANACHE can be used for emergency response
727 planning and management.

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Table 1: The selected 20 trials of the MUST field experiments with source, meteorological, and turbulence parameters (Biltoft, 2001; Yee and Biltoft, 2004). H_s , t_s , and Q_s are respectively the height, duration, and rate of the tracer release. S_{04} and α_{04} are the wind speed and direction respectively at a 4 m level of mast S. The Obukhov length (L), friction velocity (u_*), and turbulent kinetic energy (k) are measured at 4 m level of tower T.

Trial	Trial Name	Q_s	t_s	H_s	S_{04}	α_{04}	u_*	L	k
No.	(JJJhhmm)	(l/min)	(min)	(m)	(m/s)	(deg)	(m/s)	(m)	(m^2s^{-2})
1	2640138	175	21	0.15	2.35	17	0.26	91	0.359
2	2640246	200	15	0.15	2.01	30	0.25	62	0.306
3	2671852	200	22	0.15	3.06	-49	0.32	330	0.436
4	2671934	200	15	1.8	1.63	-48	0.08	5.8	0.148
5	2672033	200	15	1.8	2.69	-26	0.17	4.8	0.251
6	2672101	200	14	0.15	1.89	-10	0.16	7.7	0.218
7	2672150	200	16	0.15	2.30	36	0.35	150	0.409
8	2672213	200	15	1.8	2.68	30	0.35	150	0.428
9	2672235	200	15	2.6	2.32	36	0.26	48	0.387
10	2672303	200	19	1.8	2.56	17	0.25	74	0.367
11	2681829	225	15	1.8	7.93	-41	1.10	28000	1.46
12	2681849	225	16	0.15	7.26	-50	0.76	2500	0.877
13	2682256	225	15	0.15	5.02	-42	0.66	240	0.877
14	2682320	225	15	2.6	4.55	-39	0.50	170	0.718
15	2682353	225	15	5.2	4.49	-47	0.44	120	0.727
16	2692054	225	22	1.3	3.34	39	0.36	170	0.362
17	2692131	225	17	1.3	4.00	39	0.42	220	0.582
18	2692157	225	15	2.6	2.98	43	0.39	130	0.505
19	2692223	225	15 ₄₂	1.3	2.63	26	0.35	120	0.484
20	2692250	225	17	1.3	3.38	36	0.37	130	0.537

Table 2: $k - \epsilon$ turbulence model constants.

$C_{\epsilon 1}$	$C_{\epsilon 2}$	$C_{\epsilon 3}$	C_{μ}	σ_k	σ_{ϵ}
1.44	1.92	-0.4	0.09	1.0	1.3

Table 3: Statistical performance measures of the concentrations for all 20 simulated trials of the MUST field experiment. The *cases* 1, 2, and 3 are defined in section 5 and m is the sample size. FAC2 is given in percentage (%).

<i>cases</i>		m	NMSE	FB	COR	FAC2	MG	VG	IA
<i>case 1</i>	All	672	1.66	0.42	0.89	52.8	1.77	3.07	0.90
	Line 1	168	1.36	0.35	0.88	60.7	1.87	3.70	0.90
	Line 2	137	1.23	0.48	0.89	53.3	1.87	2.19	0.86
	Line 3	111	1.06	0.52	0.86	43.2	2.02	3.71	0.84
	Line 4	108	1.34	0.50	0.77	39.8	1.52	4.81	0.78
	horizontal	524	1.80	0.41	0.89	50.8	1.82	3.41	0.90
	vertical	148	0.92	0.46	0.94	60.1	1.58	2.12	0.88
<i>case 2</i>	All	673	1.51	0.37	0.89	59.9	1.62	2.69	0.91
	Line 1	171	1.20	0.29	0.89	67.2	1.57	3.12	0.91
	Line 2	137	1.32	0.46	0.89	62.0	1.67	1.83	0.84
	Line 3	112	0.96	0.48	0.88	55.4	1.84	3.18	0.84
	Line 4	106	1.25	0.46	0.76	42.4	1.49	4.92	0.78
	horizontal	526	1.63	0.36	0.89	58.4	1.63	2.99	0.91
	vertical	147	0.85	0.42	0.93	65.3	1.57	1.86	0.88
<i>case 3</i>	All	672	0.67	0.10	0.92	67.9	1.35	2.44	0.96
	Line 1	172	0.52	-0.03	0.93	72.7	1.16	2.73	0.96
	Line 2	137	0.56	0.20	0.91	73.0	1.38	1.62	0.93
	Line 3	112	0.36	0.24	0.92	65.2	1.56	2.87	0.94
	Line 4	106	0.62	0.21	0.82	50.9	1.28	4.85	0.89
	horizontal	527	0.70	0.07	0.93	66.8	1.32	2.70	0.96
	vertical	145	0.48	0.24	0.91	71.7	1.46	1.69	0.93

Table 4: Statistical performance measures of the concentrations for trials categorized in (i) neutral, (ii) near-neutral to stable, and (iii) stable to very stable atmospheric conditions. The *cases* 1, 2, and 3 are defined in section 5 and the stability classification is described in section 7. Here m is the sample size and FAC2 is given in percentage (%).

<i>cases</i>	stability class	m	NMSE	FB	COR	FAC2	MG	VG	IA
<i>case 1</i>	neutral	66	0.41	0.47	0.91	45.5	2.07	2.28	0.89
	near-neutral to stable	381	0.47	0.29	0.95	57.2	1.76	2.48	0.96
	stable to very stable	225	1.35	0.49	0.89	47.6	1.69	4.80	0.88
<i>case 2</i>	neutral	66	0.24	0.26	0.91	63.6	1.74	1.98	0.93
	near-neutral to stable	382	0.46	0.23	0.94	64.1	1.62	2.34	0.96
	stable to very stable	225	1.24	0.46	0.89	51.6	1.59	3.74	0.88
<i>case 3</i>	neutral	66	0.23	0.23	0.91	66.7	1.69	1.94	0.93
	near-neutral to stable	382	0.51	0.07	0.95	71.5	1.40	2.10	0.96
	stable to very stable	224	0.46	0.11	0.92	62.0	1.18	3.37	0.95

Table 5: Statistical performance measures of the ground-level sampling line maximum (SL-Max) concentrations for all 20 simulated trials of the MUST field experiment. The *cases* 1, 2, and 3 are defined in section 5 and m is the sample size. FAC2 is given in percentage (%).

<i>cases</i>	m	NMSE	FB	COR	FAC2	MG	VG	IA
<i>case 1</i>	80	0.70	0.31	0.92	77.5	1.58	1.36	0.93
<i>case 2</i>	80	0.65	0.27	0.91	85.0	1.44	1.25	0.93
<i>case 3</i>	80	0.26	0.02	0.95	95.0	1.20	1.12	0.97

Table 6: Comparison of the statistical performance measures for the identical 14 trials of the MUST field experiment with Gaussian model results in Winiarek (2014). FAC2 is given in percentage (%).

<i>cases</i>	NMSE	FB	COR	FAC2	MG	VG
<i>case 1</i>	0.70	0.36	0.95	68.0	1.50	1.93
<i>case 2</i>	0.65	0.25	0.94	74.3	1.39	1.83
<i>case 3</i>	0.68	0.07	0.95	78.7	1.26	1.73
<i>Gaussian</i>	4.24	-0.33	0.59	45.0	0.72	40.41

Figure 1: Layout of the MUST array showing 120 containers. The black circles denote the position of receptors. The stars denote source locations - only one was operational at a given time.

Figure 2: Horizontal cross-section of concentration field (Kg/m^3) for two trials (a) 2671852 and (b) 2672213 at a vertical height $z = 1.6m$ for *case-1*. Second column represents the vertical profiles of the concentration for all for *cases* on the 32-m tower near the centre of the obstacle array, along with observations (Obs) at heights of 1, 2, 4, 6, 8, 10, 12, and 16 m.

Figure 3: Comparison of the iso-surface of concentration ($C = 4.0 \times 10^{-5} \text{ Kg/m}^3$) for two trials (a) 2640138 and (b) 2672303 with same upstream wind direction but different source locations for *case-1*.

Figure 4: (a) Scatter and (b) quantile-quantile ($Q - Q$) plots between the predicted and observed concentrations for all 20 trials of the MUST field experiment. The middle solid line is one-to-one line between observed and simulated concentrations whereas the dotted lines correspond to factor of two.

Figure 5: The statistical performance measures (a) NMSE, (b) FB, (c), COR, (d) FAC2, (e) MG, and (e) VG with increasing downwind distances from the source (at each horizontal lines) and at vertical receptors for all 20 trials of the MUST field experiment.

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