Comparison and Performance Evaluation of CFD based Numerical Model and Gaussian based Models for Urban Air Quality Prediction

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Abstract

This paper presents the comparison and performance of the numerical and Gaussian based air quality models for simple and complex terrain. For simple terrain case, monitored Sulfur Hexa Fluoride (SF_6) and meteorological data at Lillestrom, Norway and Kincaid, USA have been considered to study the model prediction performance; whereas, for complex terrain case, oxides of nitrogen (NO_x) and particulate matter (PM_{10}) with meteorological data at Hindhead, UK have been used to study the performance of the two models. In general, Gaussian based air quality model estimates pollutant concentration using analytical and probabilistic concepts; while numerical model solves the differential equations governing mass momentum and energy transfer by numerical techniques.

Statistical analysis has been carried out to evaluate the model performance by comparing measured and predicted SF_6 concentrations. Finally, a sectorwise concentration distribution of NO_x and PM_{10} has also been estimated to study the interrelationship between source emission and meteorological conditions for complex terrain features.

Key words: Air quality prediction, numerical model, Gaussian model, statistical analysis, pollutant concentration, urban air quality.

Introduction

Mathematical models are used in all aspects of air quality planning where prediction is a major component, from episode forecasting to long term planning. In general, Gaussian and Numerical models are widely used for the simulation of urban air quality. The Gaussian models calculate the pollutant concentrations from emission inventory and meteorological variables according to the solutions of various equations that represent the relevant physical processes (Ku et al.,1987a). In other words, differential equation is developed by relating the rate of change of pollutant concentration to average wind and turbulent diffusion which, in turn, is derived from mass conservation principle (Nagendra and Khare, 2002).

Numerical air quality models are based on numerical solution of partial differential equations representing atmospheric dispersion phenomena. Computational Fluid Dynamics (CFD) based numerical models use tools in a finite volume based approach to solve the partial differential equations governing mass, momentum, and energy transfer.

The purpose of this paper is to compare the prediction performance of Gaussian (Industrial Source Complex Short-Term, version 3) and numerical based (PANAIR) air quality models for simple and complex terrain features. The model performance evaluation is accomplished through the comparison of model predictions with the actual observations. Statistical indicator-mean square error (MSE) has been used to evaluate model performance (Willmott, 1982).

MODEL DESCRIPTION

Industrial Source Complex Short-Term model , Version-3 (ISCST3) is Gaussian based air quality model developed by US Environmental Protection Agency (USEPA). This model provides options to model emissions from a wide range of sources that might be present at a typical industrial source complex. The model is applicable to four types of emission sources namely point, area, volume and open pit. The model accepts hourly meteorological data records to define the conditions for plume rise, transport, diffusion and deposition. The detailed methodology of development of ISCST3 model is available elsewhere (EPA, 1995).

Fluidyn-PANAIR is a 3-dimensional high precision environmental modelling software package, which simulates dispersion of pollutants emitted into the atmosphere under different scenario. PANAIR uses computational fluid dynamics tools in a finite volume based approach to solve the three-dimensional, time dependent equations describing the laws of conservation for mass, momentum, energy, turbulence parameters and species (pollutants), subjected to the given set of boundary conditions. It consists of turbulence models such as k-diffusion, k-ε and k-L models and also includes component models for representing radiation effect, chemical reactions, gravity effect, and surface roughness.This model computes a mass consistent wind field over the domain using an interpolation technique based on Lagrangian multipliers. Turbulence models in **PANAIR** are based on the surface heat flux from the ground into the atmosphere. The sensible heat flux resulting from the energy balance between insolation, the anthropogenic heat flux and the heat flux absorbed or released from ground is a criteria for atmospheric stability (Pasquill Stability Class). In addition, the Navier-Stokes (NS) equations in three-dimensional space are applied to a curvilinear grid taking into account the undulations in the terrain and its obstacles (Transoft, 2003).

DATA

Tracer (SF6) experiments were conducted at two towns namely Lillestrom, Norway and Kincaid, USA to study the dispersion characteristics. These data have been used for the present air quality simulation under simple terrain cases. Lillestrom city is located 110 m above mean sea level at 59.89^{o} N latitude and 11.02^{o} E longitudes. Table 1 shows the details of tracer study at Lillestrom (Olesen, 1998).

The Electric Power Research Institute (EPRI), USA, performed the Kincaid tracer experiment. The tracer dispersion study was conducted at the Kincaid power plant, situated in Illinois, USA (39.59^{o} N latitude, 89.49^{o} W longitude). The area is surrounded by flat farmland with some lakes. The terrain is at an elevation of approximately 180m above mean sea level. Table 2 provides the tracer study details at Kincaid (Olesen, 1998).

For complex terrain case, emissions from trafic tunnel of length 1.9 KM connecting between London and Portmouth near Hindhead, U.K have been used. The tunnel is part of A3 trunk road at Hindhead and is the last remaining single carriageway section of the A3 trunk road. The southern portal is located in Tyndall’s Wood, approximately 250 m from the residentail area of Hindhead city. The northern portal is positioned in the Boundless Corpse, approximately 500 m from the residentail area. The emissions from the southern portal has been considered for the complex terrain dispersion study. Table 3 gives the details of model input parameters for Hindhead.

Table 1. Tracer experimentation details and modelling parameters for Lillestrom, Norway.

Sl. No.	Particulars	Data	
		Set- 1	Set- 2
1.	**Terrain Data**		
	Longitude	11.051 ^{0}E	11.051 ^{0}E
	Latitude	59.889 ^{0}N	59.889 ^{0}N
	Roughness length (m)	0.50	0.50
	Computation Domain (m^3)	1000 x 400 x 150	1000 x 400 x 150
	Monitor Point Height (m)	3.0	3.0
2.	**Source Data**		
	Type of source	Point	Point
	Exit velocity (m/sec)	6.50	6.50
	Chemical Species	SF6	SF6
	Height of source (m)	36.0	36.0
	Mass flux (Kg/sec)	0.000102	0.000102
	Temperature (^{o}C)	87.0	87.0
	Composition (Mole Fraction)	1.00	1.00
3.	**Weather Data**		
	Wind speed (m/sec)	2.10	1.70
	Anemometer height (m)	10.0	10.0
	Ambient temperature (^{o}C)	-25.65	-25.65
	Ambient Pressure (mbars)	1000.00	1000.00
	Relative humidity (%)	45.00	45.00
	Cloud cover (Scale of 10)	0	0
	Wind profile		
	- *Power Law* (Exp)	0.0995	0.0985
	Temperature profile		
	- Two Step		
	- Lapse Rate (^{o}C/m)	-3.7e-005	-1.46e-005
	- Mixing Height (m)	900	900
	- Inversion Lapse Rate (^{o}C/m)	0.0065	0.0065
4.	**Simulation Option**		
	Mesh size chosen	46 x 19 x 11	46 x 19 x 11
	Grid fineness parameter	7	7
	Date	10/01/1987	10/01/1987
	Time (Hrs.)	9.30 – 9.45	9.45 – 10.00
	Time zone	1	1
	Fluid type	Incompressible	Incompressible
	Temperature model	Solve	Solve
	Wind model	Solve	Solve
	Buoyancy model	No Gravity	No Gravity
	Wall type	Log Law1	Log Law1
	Turbulence model	K-Diff	K-Diff

Table 2. Tracer experimentation details and modelling parameters for Kincaid, USA.

Sl no.	Particulars	Data	
		Set - 1	Set – 2
1.	**Terrain Data**		
	Longitude	89.49 ^{0}W	89.49 ^{0}W
	Latitude	39.59 ^{0}N	39.59 ^{0}N
	Roughness length (m)	0.1	0.1
	Computation Domain (m^3)	32500 x 22900 x 400	24,000 x 6000 x 500
	Monitor Point Height (m)	3.0	3.0
2.	**Source Data**		
	Type of source	Point	Point
	Exit velocity (m/sec)	29.2	11.0
	Chemical Species	SF6	SF6
	Height of source (m)	187.0	187.0
	Mass flux (Kg/sec)	0.0112	0.0102
	Temperature (^{o}C)	159.00	123.85
	Composition	1.0	1.0
3.	**Weather Data**		
	Wind speed (m/sec)	2.10	2.80
	Anemometer height (m)	10.0	10.0
	Ambient temperature (^{o}C)	12.20	22.05
	Ambient Pressure (mbars)	995.00	993.40
	Relative humidity (%)	35.0	38.0
	Cloud cover (Scale of 10)	2.0	1.0
	Wind profile	Log Law	Power Law (Exp = 0.635)
	Temperature profile	Log Law	*Two Step:*
		---	Lapse Rate (^{o}C/m) = 0.01333
		---	Mixing Height (m) = 226.0
		---	Inv Lapse Rate (^{o}C/m) = -0.01
4.	**Simulation Option**		
	Mesh size chosen	23 x 16 x 9	79 x 20 x 13
	Grid fineness parameter	4	8
	Date	25/04/1980	13/07/1980
	Time (Hrs.)	12.00 –13.00	9.00 –10.00
	Time zone	-6	-6
	Fluid type	Incompressible	Incompressible
	Temperature model	Solve	Solve
	Wind model	Solve	Solve
	Buoyancy model	No Gravity	No Gravity
	Wall type	Log Law1	Log Law1
	Turbulence model	K-eps	K-eps

Table 3. Model input parameters for Hindhead, UK

Sl no.	Particulars	Data		
		Sector - 1	Sector – 2	Sector – 3
1.	**Terrain Data**			
	Longitude	0.18 ^{0}W	0.18 ^{0}W	0.18 ^{0}W
	Latitude	51.15 ^{0}N	51.15 ^{0}N	51.15 ^{0}N
	Roughness length (m)	0.01	0.01	0.01
	Computation Domain (m^3)	870 x 1000 x 170	870 x 1000 x 170	870 x 1000 x 170
	Monitor Point Height (m)	1.5	1.5	1.5
2.	**Source Data**			
	Type of source	Point	Point	Point
	Exit velocity (m/sec)	0.001	0.001	0.001
	Chemical Species	NOx and PM10	NOx and PM10	NOx and PM10
	Height of source (m)	3.0	3.0	3.0
	Mass flux (Kg/sec)	4.102 E-04	4.102 E-04	4.102 E-04
	Temperature (^{o}C)	15	15	15
	Composition, mass fraction			
	NOx	0.9758	0.9758	0.9758
	PM10	0.0241	0.0241	0.0241
3.	**Weather Data**			
	Wind speed (m/sec)	1.39	3.03	2.34
	Wind direction (degree)	105	225	345
	Anemometer height (m)	10.0	10.0	10.0
	Ambient temperature (^{o}C)	15	15	15
	Ambient Pressure (mbars)	1013.0	1013.0	1013.0
	Relative humidity (%)	90	90	90
	Cloud cover (Scale of 10)	3.0	3.0	3.0
	Wind profile	Log Law	Log Law	Log Law
	Temperature profile	Log Law	Log Law	Log Law
4.	**Simulation Options**			
	Mesh size chosen	60 x 62 x 11	60 x 62 x 11	60 x 62 x 11
	Time zone	0.0	0.0	0.0
	Fluid type	Incompressible	Incompressible	Incompressible
	Temperature model	Freeze	Freeze	Freeze
	Wind model	Solve	Solve	Solve
	Buoyancy model	No Gravity	No Gravity	No Gravity
	Wall type	Log Law1	Log Law1	Log Law1
	Turbulence model	K-eps	K-eps	K-eps

RESULTS AND DISCUSSION

(a) Model performance for simple terrain cases:

Table 4 and 5 lists the performance statistics of the PANAIR and ISCST3 model prediction on the Lillestrom tracer data set 1 and 2 respectively. For PANAIR, the mean of the predicted SF6 concentration (4.9 μg/m^3) is found to be matching with the observed mean (5.34 μg/m^3) values for data set 1; while for ISCST3, the difference between the observed and predicted mean value is quite high (Table 4). The MSE value for PANAIR and ISCST3 model are 0.38 and 20.71 μg/m^3 respectively. Similar observations have also been found for data set 2 at Lillestrom (Table 5). This explains that PANAIR predictions are more accurate than ISCST3 model predictions.

Table 4. Comparison for models prediction for data set at Lillestrom.

Receptor location	Distance from the source (m)	SF6 concentration in (μg/m^3)		
		Observation	Prediction	
			PANAIR	ISCST3
M1	160	7.6	6.9	0.003
M2	490	4.8	4.9	2.71
M3	810	3.7	2.9	3.47

Table 5. Comparison for models prediction for data set 2 at Lillestrom.

Receptor location	Distance from the source (m)	SF6 concentration in (μg/m^3)		
		Observation	Prediction	
			PANAIR	ISCST3
M1	140	8.3	8.1	0.174
M2	440	5.2	5.3	5.49
M3	820	3.4	3.6	2.99

Table 6 and 7 provide the performance statistics of the PANAIR and ISCST3 model prediction on the Kincaid tracer data set 1 and 2 respectively. For PANAIR, the mean of the predicted SF6 concentration (5.7 μg/m^3) is found to be matching with the observed mean (5.6 μg/m^3) values for data set 1; while for ISCST3, the difference between the observed and predicted mean value is quite high (Table 6). The MSE value for PANAIR and ISCST3 model are 0.023 and 22.09 μg/m^3 respectively. Similar observations have been found for data set 2 at Lillestrom (Table 7). From the results it is evident that, for simple terrain cases i.e. for Lillestrom and Kincaid, PANAIR is found to be more accurate in predicting the air pollutant concentration.

Table 6. Comparison for models prediction for data set 1 at Kincaid.

Receptor location	Distance from the source (m)	SF6 concentration in ($\mu g/m^3$)		
		Observation	Prediction	
			PANAIR	ISCST3
M1	5000	1.316	1.145	0.156
M2	7000	0.999	0.833	0.513
M3	10000	0.710	0.605	1.08

Table 7. Comparison for models prediction for data set 2 at Kincaid.

Receptor location	Distance from the source (m)	SF6 concentration in ($\mu g/m^3$)		
		Observation	Prediction	
			PANAIR	ISCST3
M1	5000	1.346	1.24	0.1
M2	7000	1.397	1.407	0.359
M3	10000	1.395	1.475	0.751

(b) Model performance for complex terrain cases:

Table 8 describes the sectorwise performance statistics of the PANAIR and ISCST3 model prediction for complex terrain case (Hindhead). PANAIR predicted the NOx concentration of 320 $\mu g/m^3$ at the receptor located at a distance of 125 m from the source for the wind direction of 345^0 N. While for ISCST3, the predicted concentration of NO_x at the same receptor, was found to be 156.5 $\mu g/m^3$. The high concentration predicted by PANAIR is due to the wind flow from the elevated terrain towards the valley, thus passing over the valley without causing much mixing of pollutants. This complex relationship has been accurately explained by PANAIR when compared to ISCST3. Figure 1 shows the NO_x and PM_{10} concentration contours for the 105^0 N wind direction. Figure 2 describes the windfield established by PANAIR over the undulated terrain.

Table 8. Sector wise comparison of NO_x and PM_{10} predictions at Hindhead, UK.

Sl. No	Wind direction (degree)	Wind speed (m/s)	Receptor distance (m)	NOx in $\mu g/m^3$		PM10 in $\mu g/m^3$	
				PANAIR	ISCST3	PANAIR	ISCST3
M1	105	1.39	105	240.0	337.4	5.9	9.9
M2	225	3.03	60	134.0	291.0	3.3	8.5
M3	345	2.34	125	320.0	156.5	7.9	4.6

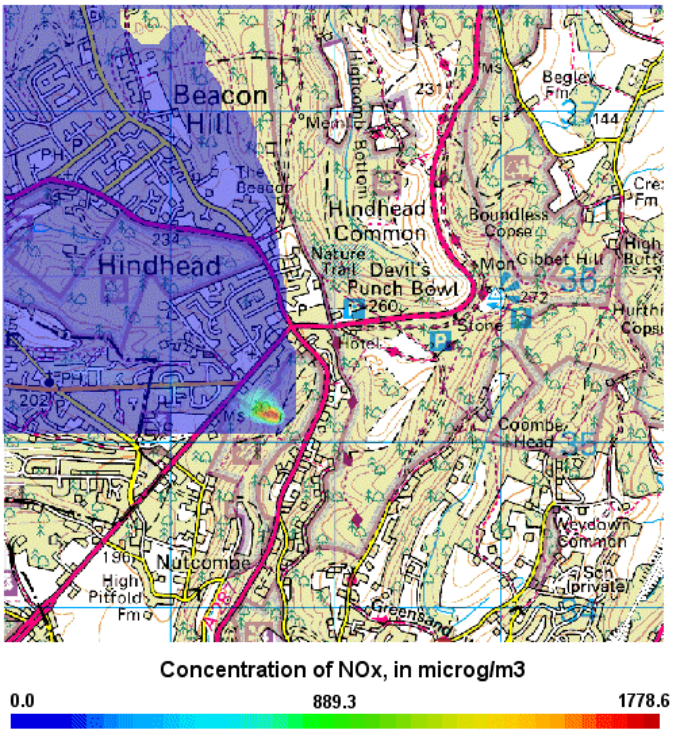

Figure 1a: Concentration contours for NOx, in μg/m3.
(Wind speed, 1.39 m/s, Direction 105^{0}N)

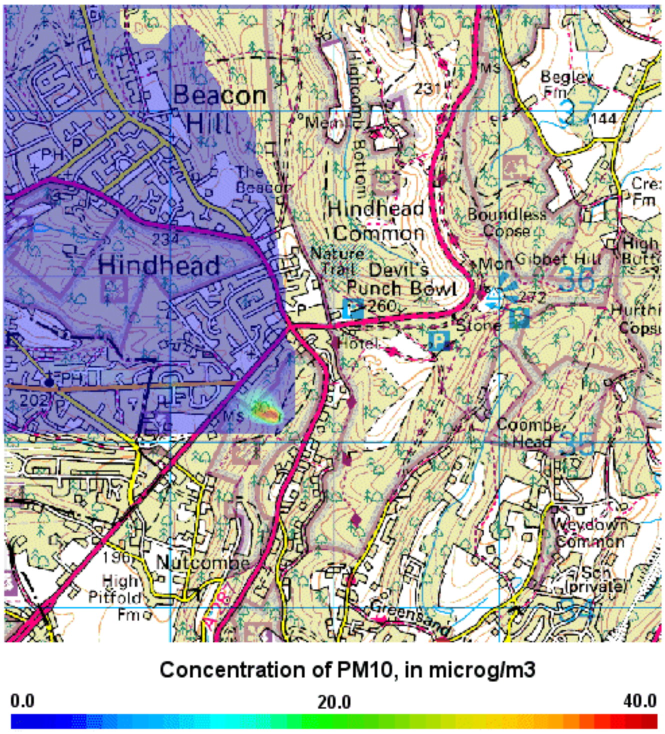

Figure 1b: Concentration contours for PM_{10}, in μg/m3.
(Wind speed, 1.39 m/s, Direction 105^{0}N)

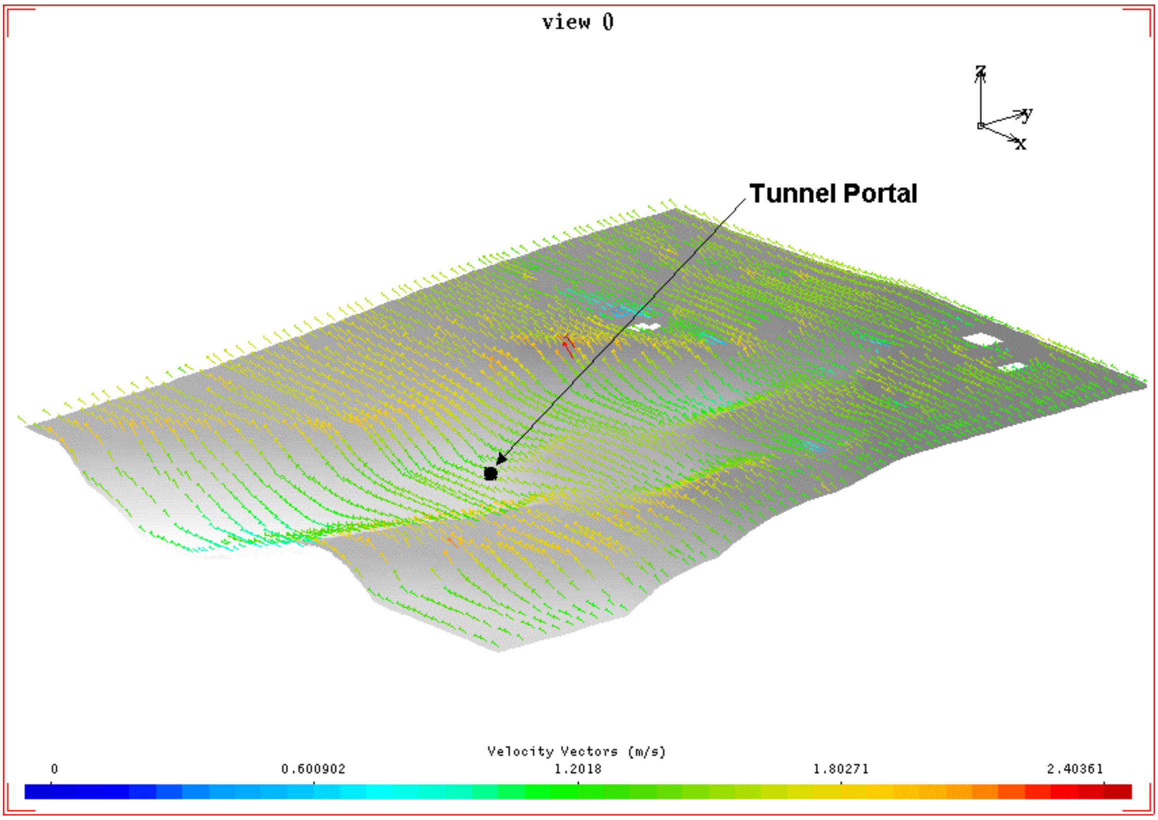

Figure 2: Wind field over the domain for the direction of 105^0 *at* wind speed 1.39 m/s

CONCLUSIONS

Gaussian (ISCST3) and numerical (PANAIR) based air quality models have been evaluated for both simple and complex terrain cases. Statistical indicator mean square error has been used to evaluate model performance. For simple terrain cases (Lillestrom, Norway and Kincaid, USA) PANAIR predictions are found to be in accordance with the filed measurements. Similarly, for complex terrain case (Hindhead, UK) PANAIR accurately considers the terrain features and meteorological conditions when compared to ISCST3 model. The overall study suggests that for urban air quality, CFD based numerical model predictions are more reliable than the Gaussian models. Further, CFD models are more effective in simulating the dispersion of pollutants for complex terrains.

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