MODELING AND ANALYSIS OF PLUME DISPERSION AND PARTICLE TRAJECTORIES IN SUB-URBAN ENVIRONMENT USING COUPLED METEOROLOGICAL AND DISPERSION MODELS

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by

Sabir Sardar

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Doctor of Philosophy

Department of Nuclear Engineering
Pakistan Institute of Engineering & Applied Sciences,
Niloere, Islamabad, Pakistan
February, 2014
Allah does not impose on any soul more than He has given it. Allah will provide ease after difficulty. [Qur’an, 65:7]
Declaration

I declare that all material in this thesis which is not my own work has been identified and that no material has previously been submitted and approved for the award of a degree by this or any other university.

Signature: _____________________________

Author’s Name: Sabir Sardar

It is certified that the work in this thesis is carried out and completed under my supervision.

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PIEAS, Islamabad
I dedicate this thesis to

my beloved parents, wife, daughter and sisters
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Sabir Sardar
Publications in Peer Reviewed Journals


Papers Submitted for Publication


Presentations in International Conferences


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**ABSTRACT**

Chemical or radioactive air pollutants whether emitted accidentally or by routine releases into the environment from industrial sources may be catastrophic if not monitored, assessed and controlled. Atmospheric dispersion modeling of such pollutants is an essential regulatory requirement for environmental impact assessment (EIA), safety analysis and emergency preparedness and planning (EPP). It may help in decision making regarding the emergency evacuation of population from affected areas in accidental scenario or emission reduction in specific situations when air quality is deteriorating unacceptably. Present research is directed initially on computational modeling methodology for precise atmospheric dispersion of pollutants and subsequently towards practical setups, procedures and experimentation for model validation. The proposed modeling strategy involved use of ‘coupled meteorological and dispersion models’ in Pakistan specific conditions. Thus output of a meteorological model at all nodal points of the grid under consideration can be coupled or used as precise input for dispersion model. Using this concept, advanced dispersion models such as CALPUFF and FLEXPART were coupled with appropriate meteorological models such as MM5 and WRF for realistic predictions. Sensitivity of different empirical correlations or parameterization schemes of the meteorological model was thoroughly investigated prior to coupling it with dispersion model to ensure its valid use for geographical and climatic conditions of Pakistani region. Sensitivity analysis of four parameterized schemes in MM5 model for Pakistani region indicated that Grell scheme generated better results for all parameters and resolutions for lesser precipitation intensity. A detailed study using coupled meteorological and dispersion model was performed in this research.

Modeling results in the form of ground level pollutant concentrations were verified by conducting field tracer experiments, a work that has never been carried out for any Pakistani region. In present work, experimentation was performed using two gaseous tracers, sulfur dioxide (SO$_2$) and sulfur hexafluoride (SF$_6$). The first set involved small scale dispersion experiments over a flat ground at Pakistan Institute of Engineering and Applied Sciences (PIEAS) by releasing SO$_2$ gas at a rate of 0.05 g/sec from a height of 30 ft. In the second set of experimental work, emissions from a brick kiln of 60ft height with SO$_2$ release rate of 0.3 g/s were measured at different sampling points covering larger distances up to 1640 ft. Moreover, the available data
of ground level SO$_2$ concentrations from a cluster of stacks of oil refinery and oilfield was also used for validating the results of dispersion modeling studies. In the third set of experiments, a 100 ft high experimental stack, designed, fabricated and installed as a part of this research was used to release SO$_2$ at a controlled precise rate of 0.6 g/s and air sampling was done at varied directions and distances ranging up to about 3000 ft. In the final set of experiments, SF$_6$ gas was released with a rate of about 7.0 g/s at a height of 230 ft and samples were taken at 36 sampling points simultaneously at distances ranging from 2300 ft to about 33000 ft.

Overall trends of time series plots of measured and modeled SO$_2$ concentrations using PIEAS experimental stack were found to be in reasonable agreement as reflected by correlation coefficient ‘r’ and Index of agreement ‘d’ ranging from 0.74 to 0.91 and 0.40 to 0.64 respectively. This shows that coupled model performance was satisfactory for prediction of ground level SO$_2$ concentration. The SF$_6$ test results demonstrated the cross-wind diffusion as well as down-wind dispersion very well. A slight deviation in directions of plume and sampling point locations was observed. This may be due to the difference in predicted and real wind directions. However, this indicated a limitation of the modeling strategy in reproducing instantaneous behavior of wind over a short sampling period of 10 minutes.

To incorporate the effect of atmospheric chemical reactions on predicted ground level concentrations by FLEXPART dispersion model, few new subroutines were written and suggested to be incorporated into the model. In order to trace out ‘the real time-three dimensional particle trajectory’ predicted by coupled MM5 and FLEXPART model, a three-dimensional post-processor was also developed in this research work to show the multilayered data of regional topography, geography, wind field and particles positions. The ‘coupled-model’ results and subsequent visualization of particle trajectories exhibited an irregular shaped ‘potential vulnerable area’ covered by the plume. It was quite different from expected straight line plume dispersion generally predicted by Gaussian Plume Model (GPM). This more precise visualization in an accidental scenario may help disaster management authorities in making decisions regarding emergency evacuation of population from indicated ‘potential vulnerable areas’.
<table>
<thead>
<tr>
<th>Nomenclature</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>Atmospheric pressure</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Fraction of moisture convergence to precipitation</td>
</tr>
<tr>
<td>$\alpha_d$</td>
<td>Inverse density of the dry air</td>
</tr>
<tr>
<td>AERMOD</td>
<td>American Meteorological Society/Environmental Protection Agency Regulatory Model</td>
</tr>
<tr>
<td>AGCM</td>
<td>Atmospheric General Circulation Model</td>
</tr>
<tr>
<td>ANATEX</td>
<td>Across North America Tracer Experiment</td>
</tr>
<tr>
<td>$^{41}$Ar</td>
<td>Argon-41</td>
</tr>
<tr>
<td>$\alpha_r$</td>
<td>Local rotation angle between y-axis and meridians</td>
</tr>
<tr>
<td>ASME</td>
<td>American Society of Mechanical Engineers</td>
</tr>
<tr>
<td>AUSPLUME</td>
<td>Australian Plume Model</td>
</tr>
<tr>
<td>$\chi$</td>
<td>Pollutant concentration</td>
</tr>
<tr>
<td>C</td>
<td>Discharge coefficient</td>
</tr>
<tr>
<td>$C_6F_{12}$</td>
<td>Perfluorocyclohexane</td>
</tr>
<tr>
<td>$C_7F_{14}$</td>
<td>perfluoromethylcyclohexane</td>
</tr>
<tr>
<td>$C_8F_{16}$</td>
<td>Undeca flouro (pentaflouro ethyl) cyclehexane</td>
</tr>
<tr>
<td>CADM</td>
<td>Comprehensive Acid Deposition Modeling system</td>
</tr>
<tr>
<td>CALPUFF</td>
<td>CALifornia PUFF</td>
</tr>
<tr>
<td>CAPTEX</td>
<td>Cross-Appalachian Tracer Experiment</td>
</tr>
<tr>
<td>CMAQ</td>
<td>Cumunity Multi-scale Air Quality model</td>
</tr>
<tr>
<td>CO</td>
<td>Carbon monoxide</td>
</tr>
<tr>
<td>COSPEC</td>
<td>Correlation Spectrometers</td>
</tr>
<tr>
<td>CPU</td>
<td>Central Processing Unit</td>
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<tr>
<td>d</td>
<td>Index of agreement</td>
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<tr>
<td>2D</td>
<td>Two dimensional</td>
</tr>
<tr>
<td>3D</td>
<td>Three dimensional</td>
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<tr>
<td>$d_a, d_c$</td>
<td>Distances from puff centre to receptor in along and cross wind direction</td>
</tr>
<tr>
<td>dt</td>
<td>Sampling step</td>
</tr>
<tr>
<td>$\varepsilon(t)$</td>
<td>Gaussian random number</td>
</tr>
<tr>
<td>e</td>
<td>Cosine component of coriolis term</td>
</tr>
<tr>
<td>E</td>
<td>Emission rate of pollutant</td>
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Electron Capture Detector
European Centre for Medium-Range Weather Forecast
Environmental Impact Assessment
Eulerian model for emission inventories
Environmental Protection Agency
Emergency Preparedness and Planning
European Tracer Experiment
Forcing term
Sine component of coriolis term
Central longitude
Fraction of mass of particle i
FLEXiblePARTicle
Final
Ratio of the heat capacities for dry air
Acceleration of gravity
Greenhouse Gas and Air Pollution Interactions and Synergies
Gas Chromatograph
Global Climate Models
GigaHertz
Gaussian Plume Model
Grid Analysis and Display System
Gridded Information in Binary Form
Planetary boundary layer height
Hydrogen peroxide
Hydrogen sulfide
Sulfurous acid
Sulfuric acid
Hazardous Air Pollutant Characterization and Control
Hierarchical Data Format
Plume effective height
Heavy Mechanical Complex-3
Nitric acid
High Performance Computing
HYbrid Particle And Concentration Transport
NO$_2$ ........................................................................................................ Nitrogen dioxide
NOAA........................................................................................................ National Oceanic and Atmospheric Administration
NO$_x$ .......................................................................................................... Nitrogen oxides
NWP ............................................................................................................ Numerical Weather Prediction
$\Omega_e$ ........................................................................................................ Angular rotation rate of earth
$O_3$ ............................................................................................................. Ozone
OH ............................................................................................................... Hydroxyl
p .................................................................................................................. Pressure
$\Delta p$ ......................................................................................................... Pressure difference
$p_o$ .............................................................................................................. Reference-state pressure
$p'$ ............................................................................................................... Perturbation pressure
Pak-EPA .............................................................. Pakistan Environmental Protection Agency
PANs ........................................................................................................... Peroxy Acetyl Nitrates
PBL ............................................................. Planetary boundary layer
PBS ............................................................................................................ Portable Batch System
PC ............................................................................................................... Personal Computer
PGT ........................................................................................................ Pasquill-Gifford-Turner
PIEAS .............................................................. Pakistan Institute of Engineering and Applied Sciences
$PM$ ........................................................................................................... Particulate Matter
PMD ........................................................................................................... Pakistan Meteorology Department
PMT ........................................................................................................ Photo Multiplier Tube
ppb .............................................................................................................. parts per billion
ppm .............................................................................................................. parts per million
$p_{so}$ ......................................................................................................... Surface pressure
$p_t$ ............................................................................................................... Top pressure
PVC ............................................................................................................ Polyvinyl Chloride
Q .................................................................................................................. Total exhaust flow
Q$^\circ$ .............................................................................................................. Diabetic heating rate per unit mass
$Q_m$ .......................................................................................................... Generic coupled moisture variable
$q_v$ .............................................................................................................. Specific humidity
$\rho$ ............................................................................................................ Reference state density
$r$ ............................................................................................................... Correlation coefficients
R .................................................................................................................. Amount of precipitation
$R$ .............................................................................................................. Total solar radiation
R & D ................................................................. Research and Development
RAM ......................................................................... Random Access Memory
RAMS ................................................................. Regional Atmospheric Modeling System
RAQMS .............................................................. Regional Air Quality Modeling System
RCMs ..................................................................... Regional Climate Models
\( R_d \) ........................................................................ Gas constant for dry air
RegCM ................................................................. Regional Climate Model
RH ........................................................................... Relative Humidity
\( RH_c \) ................................................................. Critical Relative Humidity
RHC ......................................................................... Reactive Hydrocarbons
\( RH_{\text{mean}} \) ....................................................... Mean Relative Humidity
\( \sigma_x, \sigma_y, \sigma_z \) .................................................. standard deviations of Gaussian distribution in
............................................................................... along, cross and vertical directions
\( s \) ........................................................................... Distance travelled by the puff
\( s_0 \) ................................................................. Value of ‘s’ at beginning of sampling step
\( S \) ........................................................................... Stability index
SCCCAMP ................ South Central Coast Cooperative Aerometric Monitoring Program
\( SF_6 \) ................................................................. Sulfur hexafluoride
\( SO_2 \) ....................................................................... Sulfur dioxide
\( SO_4 \) ........................................................................ Sulfate
SODAR ............................................................. Sonic Detection and Ranging System
\( SO_x \) ............................................................... Sulfur oxides
SP ................................................................. Sampling Point
SPM ............................................................... Suspended Particulate Matter
STEM − 1 ........................................................ Simple Thermal Environment Model
\( \theta \) ........................................................................ Potential temperature
\( t \) ........................................................................... Time
\( \Delta t \) ...................................................................... Time increment
\( T \) .......................................................................... Temperature
\( T_r \) ......................................................................... Reference state temperature
TexAQS ............................................................. Texas Air Quality Study
\( T_f \) .......................................................................... Flue gas temperature
\( T_{lv}, T_{lw} \) .................................................. Lifetime of fluctuations in v and w components of wind
TMI ................................................................. Three Mile Island
TRACT ......................................... TRAnsport of pollutants over Complex Terrain
TRMM ................................................................ Tropical Rainfall Measuring Mission
u ........................................................................... horizontal component of velocity in x-direction
u* ........................................................................... Friction velocity
UCIL .................................................................... Union Carbide India Limited
USGS ..................................................................... United States Geological Survey
UVF ....................................................................... Ultra Violet Fluorescence
V ........................................................................... Grid cell volume
v ........................................................................... Horizontal component of velocity in y-direction
\( \dot{v} \) ............................................................ Turbulent velocity component cross wind
\( \bar{v} \) ................................................................. Averaged wind speed
VFD ..................................................................... Variable Frequency Drive
VOCs ..................................................................... Volatile Organic Compounds
w ........................................................................... Turbulent velocity component vertical wind
w* ........................................................................... Convective velocity scale
WHO ..................................................................... World Health Organization
WRF ..................................................................... Weather & Research Forecasting Model
x .......................................................................... Downwind distance
\( \Delta x \) .............................................................. Grid distance along x-direction
X .......................................................................... Position vector
\(^{133}\text{Xe} \) ........................................................... Xenon-133
\( \Delta y \) .............................................................. Grid distance along y-direction
\( z_0 \) ................................................................. Surface roughness length
CHAPTER 1

Introduction

Industrialization is the most important pillar of economy, however, introduction of unwanted by-products due to industrial activities may be damaging if not monitored, assessed and controlled. Industrial activities may even become catastrophic in case of inadvertent or accidental release of toxic chemicals or radioactive pollutants into environment. Events like toxic chemicals release at Union Carbide Industries in Bhopal [Gehlawat, 2005] or radioactivity release at Fukushima and Chernobyl nuclear power plant [Baba, 2013; Cardis, 2011] are terrible examples of accidental discharge of hazardous contaminants into atmosphere.

Even if there are no accidental releases of substantial quantities of pollutants, routine releases from industries may affect general air quality due to non-compliance of regulatory limits. Atmospheric effluents emanating from specific industrial sources may be primary pollutants such as SO$_x$, NO$_x$, CO, VOCs, Particulate etc. or may further be transformed into toxic chemicals such as peroxy acetyl nitrates (PANs), ozone etc. Toxic chemicals refer to those which through their chemical action on life processes can cause health effects including temporary incapacitation, permanent harm or even death to humans or animals.

Hazardous air pollutants whether emitted accidentally or by routine releases can easily travel and affect areas far away from their points of origin. Atmospheric dispersion modeling of radioactive or toxic pollutants accidentally released from nuclear or other industrial sources is an essential regulatory requirement for environmental impact assessment (EIA) and emergency preparedness and planning (EPP). Focus of this work, therefore, is on accurate prediction of ground level concentrations and trajectories of air pollutants in case of any accidental release into atmosphere involving large doses to general public. Atmospheric dispersion computations using best available modeling tools may help in decision making regarding emergency evacuation of population from affected areas thereby shifting them to places that are surely safe according to accurate and experimentally validated predictive model.

Pakistan has been facing a tremendous increase in population, urbanization and industrial growth from the last few decades. Consequently, a significant rise has
occurred not only in the number of emission sources of various types of air pollutants, the general ambient concentrations of noxious pollutants have also increased. However, due to non-compliance as well as lack of air quality management capabilities, the country is suffering from deterioration of air quality. Various governmental organizations and international bodies have reported that air pollution has become a significant risk to the environment, quality of life, and health of the population in Pakistan [Colbeck, 2010]. Hence the situation demands immediate actions to tackle this emerging environmental issue.

There are two emission control strategies i.e. observational and predictive which are generally adopted for emission reduction in specific situations when air quality is deteriorating unacceptably. In observational control strategy, emissions are rapidly reduced when air quality sensors indicate an alarming situation of National Ambient Air Quality Standards (NAAQS) violation. Application of this approach is limited because, in many situations, emissions do not influence the sensors until hours after they have been emitted. Secondly, a large network of sensors is required to protect all areas around a source. Keeping these limitations in view, observational approach seems to be most helpful when applied with predictive approach. Predictive approach is based on the knowledge that the atmospheric conditions and frequent changes occurring in it within certain time interval can be predicted with some accuracy. In specific conditions, the pollutants causing an NAAQS violation are emitted several hours before the violation occurs. For emission reduction to be effective in this case, it is necessary to reduce emissions several hours before the predicted violation [Noel, 1995]. The above mentioned situation justifies the need to develop and suggest more accurate modeling techniques and methods for regulatory requirement and general environmental monitoring.

1.1 Dispersion Modeling, Validation and Visualization

Fate of the pollutants released in atmosphere is decided by the phenomenon of atmospheric dispersion. The process of dispersion is primarily dependent on prevailing meteorological conditions. Gases and particles in the atmosphere are transported due to the average wind speed and diffused due to wind velocity fluctuations or turbulence. Atmospheric dispersion modeling is an imperative predictive modeling technique. It is used to simulate the release of hazardous
pollutants from a wide variety of sources and the way they are transported and diffused in the atmosphere.

1.1.1 Coupling of a Dispersion Model with a Regional Climate Model (RCM)

Meteorology being a key input to a dispersion model, a dispersion model is coupled with a Regional Climate Model for performing atmospheric dispersion studies. Regional Climate Models (RCMs) are used to determine local meteorological conditions over a limited area. Local climate changes are affected greatly by local topographical features such as mountains etc. and hence due to their high spatial resolution, RCMs incorporate small-scale topographical features. Examples of some well-known RCMs are MM5 and WRF. The MM5 is the abbreviation of Mesoscale Model generation 5 whereas WRF stands for Weather & Research Forecasting Model. The input data of initial conditions, time-dependent lateral meteorological conditions and surface boundary conditions for high-resolution RCMs are derived from analyses of observations or Global Climate Models (GCMs). A GCM, sometimes also called General Circulation Model, is a mathematical model of general circulation of the planet's atmosphere based on mathematical equations that represent physical processes. These equations are the basis for complex computer programs commonly used for simulating the atmosphere of Earth. High-resolution RCMs extract the meteorological information as input from gridded data generated by a Global Climate Model on global scale of coarse resolution and interpolate it on the Regional Climate Model’s domain of fine resolution.

Dispersion models, coupled with RCMs, are generally based on two modeling approaches which are Eulerian and Lagrangian. Eulerian based dispersion models solve advection diffusion equation to calculate average pollutant concentration at a particular instant in time and space. The most commonly used Gaussian Plume Model (GPM) uses Eulerian approach. The two major limitations of Gaussian Plume Model are consideration of spatially and temporally uniform wind field and non-consideration of wind shear. Still it has been used widely for regulatory purposes, under recommendation of international regulating agencies [IAEA, 1982; USNRC, 1982] because it is user friendly and theoretically simple. On the other hand, Lagrangian models are capable of incorporating spatial and temporal variations in
wind velocity and turbulence and that is why they offer better results than Gaussian Plume model (GPM) for both homogeneous and non-homogeneous conditions over flat or complex terrain [IAEA, 1987]. Some freely available Lagrangian dispersion models include FLEXPART (FLEXiblePARTicle) model [Stohl, 1998; Stohl, 1999; Stohl, 2005], CALPUFF (CALifornia PUFF) model [Scire, 2000 a,b], HYPACT (HYbrid Particle And Concentration Transport) model [Walko, 2001], ASHFALL [Turner, 2001] and HYSPLIT (HYbrid Single Particle Lagrangian Integrated Trajectory) Model [Draxler, 1997; Draxler, 1998; Draxler, 1999].

1.1.2 Atmospheric Chemistry in Lagrangian based Dispersion Model

Atmospheric chemical reactions transform primary air pollutants into secondary pollutants. The oxidation and transformation of sulfur dioxide (SO$_2$) and nitrogen dioxide (NO$_2$) to particulate sulfate and nitrates are the important characteristics of urban air photochemistry. This conversion plays an important role in controlling the ambient concentrations of these pollutants.

Some Lagrangian based particle dispersion models like FLEXPART do not consider the depletion of pollutants from atmosphere by chemical reactions. In order to enhance the precision and accuracy of modeling results, it is better to incorporate the chemical removal term for these pollutants into these models.

1.1.3 Experimental Validation of Predicted Results

Experimental validation of a computational model is obviously a mandatory requirement to examine the accuracy of predicted results of that model. As mentioned in section 1.1.1, RCMs used in dispersion studies are often derived by large scale synoptic analyses generated by GCMs instead of real meteorological data. They numerically solve the equations of atmospheric dynamics to determine local meteorological conditions. Moreover, different empirical correlations or parameterization schemes are used in these models to simulate diverse physical environmental processes. Various simulation studies performed using these models revealed that some empirical correlations failed to simulate the environmental parameters in some specific regions of the world indicating their dependence on climate and topographical features of specific region [Leung, 2003]. It is, therefore, necessary to compare model results with measured or observational meteorological
data of specific region for validation. Once meteorological model has been validated, it can be coupled with a specific Eulerian or Lagrangian dispersion model to investigate prevailing wind and other parameters required for dispersion analysis.

Along with a meteorological model, validation of the dispersion model is also equally important to determine performance and efficiency of the model. It is based on statistical comparison of model-predicted data with observed or measured data of ambient concentrations of different pollutants in environment. Data for validation purpose is normally collected by conducting field tracer experiments in which a controlled amount of a tracer is released from a source and its ambient concentration at different sampling locations is determined by different sampling and analyzing techniques. A number of tracer experiments have been conducted throughout the world. Subsequently datasets are compiled from such experimentation. These datasets may be used for validation of different dispersion models provided that the region under consideration has identical meteorological conditions and topography. In a typical topography of Pakistan where highest mountain peaks like K-2 and Nanga Parbat exist on one side and mean sea level on the other, with bi-annual bi-directional monsoon winds, no such tracer experiments have ever been conducted.

1.1.4 Post-Processing of Model Predicted Results

Many of the advanced dispersion models include a post-processor module for graphing the output data or plotting the area impacted by air pollutants on maps. For a specific accidental scenario, two dimensional graphs of affected areas are plotted by contours or isopleths showing the areas of low or high pollutant concentrations.

In order to trace out ‘the real time-three dimensional trajectory’ of a plume, powerful and fast post-processing is required as it is imperative to display the specific domain showing its geographical boundaries, topography, wind field and the trajectory of the plume dispersing with time in horizontal, lateral and vertical direction. The theme may be written in the form of subroutines incorporated in the graphic tools of any available software such as MATLAB (matrix laboratory), Visual Basic or NCAR Graphics etc. This post-processing enables to visualize the impending accidental scenario and assists in emergency planning, preparedness and decision making, regarding evacuation of large population towards refuge at safe regions. This type of
Chapter 1

Consequence assessment or emergency planning is mandatory under the regulations on management of a nuclear or radiological emergency [PNRA, 2008].

1.2 Introduction and Scope of this Research Work

As far as the scope of this dissertation is concerned, this work is focused on suggesting more accurate modeling tools for the analysis of plume dispersion and particle trajectories of specific hazardous air pollutants. These include toxic and chemical gaseous air pollutants such as sulfur dioxides (SO₂) etc. released from industrial sources. The scenarios of SO₂ can be replaced at any time by radioactive iodine, methyl or cesium iodide to analyze the radioactive pollutant dispersion. However, this cannot be experimentally validated as dispersion of radioactive iodine in atmosphere is extremely hazardous. Hence SO₂ or SF₆ may be used as tracers to predict the radioactive plume scenario in a conservative way.

The proposed modeling tools involve the use of coupled meteorological and dispersion models in conditions specific to Pakistan. The meteorological model that was employed generated the meteorological input for dispersion model. Before using its output in dispersion studies, the sensitivity of different empirical correlations in the Regional Climatic Model (RCM) was investigated to ensure and validate its potential use for Pakistani region as suggested by Sardar [Sardar, 2012a].

The general work in this area done previously by various researchers [Anfossi, 1998, 2006; Carvalho, 2002] was normally focused on computational modeling while its applicability was verified by raw data available in the literature from cluster of emission sources. The investigations also cover a combined effort for both computational modeling as well as dedicated and precise experimental data collection for model validation [Garcia, 1999]. No such combined computational modeling plus experimental validation studies have ever been performed for Pakistani region.

In present work, a sequential study was initiated from modeling of simple release scenario of toxic gases from the cluster of stacks of oil refineries and oilfields of Oman for which ground concentration data was available for validation [Abdul-Wahab, 2011; Abdul-Wahab, 2012]. In these studies a confidence was gained on the coupling of meteorology and dispersion codes.
The subsequent work was focused on Pakistani region where some emission sources may also be available. A brick kiln, a bit isolated from a cluster of brick kilns, of about 60 ft height was available in the sub-urban region of Islamabad. The missing links were the availability of emission data as well as ground concentration data. With lot of efforts and assistance of Federal EPA Islamabad, typical emission data from the isolated brick kiln was gathered by EPA stack analyzers and ground data were collected by a mobile air monitoring van for experimental validation.

In the brick kiln study, it was strongly felt that the contribution from other nearby brick kilns was significant. It was, therefore, more appropriate to use a single isolated stack, well separated by a distance of at least few kilometers from other sources. Moreover, the isolated stack should have a provision so as to get samples of gases at various elevations where temperatures and flow rates may also be determined. The exit velocity, temperature and concentration being the most important parameters should be well controlled and monitored so as to keep the source term constant during the experiments. In general, existence of such a stack with so many provisions was not expected to be available anywhere. Hence it was decided to design and fabricate a dedicated experimental stack at Pakistan Institute of Engineering and Applied Sciences (PIEAS), solely for experimental validation of a reliable dispersion model that can be employed for appropriate decision making in emergency scenarios (section 3.3.2.3).

After an extensive effort in designing and fabrication which is a part of this study, an appropriate experimental stack with all required provisions was installed at PIEAS. A hypothetical scenario of release of non-radioactive gas such as \( \text{SO}_2 \) from this stack was modeled along with computation of plume trajectory [Sardar, 2012b] as well as ground concentration at various locations near the emission point within few kilometers of the stack. Model predictions were validated by actual tracer experiments, releasing \( \text{SO}_2 \) as tracer gas from PIEAS experimental stack and collecting air samples by mobile ambient air quality monitoring van in the vicinity. Subsequently, the release height was further increased to 70 m and \( \text{SF}_6 \) used as a tracer gas was released and ground level concentrations were measured along six different arcs at varied distances. The same data is used for model validation at elevated source emission scenario. The results of all these studies are presented from section 5.1 to 5.2.
In order to simulate the particles’ trajectories, a three dimensional post-processor is developed to show the multilayered data of regional topography, geography, wind field and particles positions. This post-processor is capable of displaying the above mentioned streaming data in the form of a 3D animation or movie that is extremely helpful for visual analysis of accidental scenario and decision making by the disaster management authorities.

1.3 Thesis Layout

The first chapter of this thesis presents an introduction of the coupling approach in advanced dispersion studies. Some explanation of the experimental validation and post processing of the model-predicted results has also been included in this section giving due justification for performing atmospheric dispersion modeling for regulatory and general environmental impact assessment as well. Chapter 2 outlines the current status and information available in the literature regarding atmospheric dispersion modeling and tracer experimentation for the validation of computational dispersion modeling results. Third chapter gives a detailed description of the modeling methodologies and strategies as well as experimental setups and procedures including design, fabrication and installation of an experimental stack and tracer experiments conducted for collecting the experimental data for validation of modeling results. An experimental setup used to conduct a tracer experiment in a coastal region of Pakistan for finalizing preliminary safety analysis report of an industrial site is also thoroughly elaborated. Chapter four and five present and discuss in detail the modeling results and their experimental validation for regional meteorology and atmospheric dispersion of pollutants duly incorporating the developed post-processing computer program for visualization of dispersion and plume trajectories. The conclusions and suggestions for future work have been given in chapter six.
CHAPTER 2

Literature Review

Atmospheric dispersion modeling is basically an attempt to describe mathematically the atmospheric processes that are responsible to disperse the air pollutants emitted by a source. It is done with the help of computations that simulate pollutant dispersion by solving a set of mathematical formulations and algorithms numerically. Atmospheric dispersion modeling could be helpful in predicting health and environmental impacts of radioactive or toxic chemical pollutants that might be released during accidental scenario or routine operation of a nuclear or chemical plant [Beychok, 2005]. Dispersion modeling that predicts plume trajectories moving towards a particular region helps decision making authorities to manage and take necessary action to control any forthcoming situation that may arise as a result of accidental scenario. These measures may include timely evacuation of people from potentially threatened areas or announcement of emergency so that they may take refuge in some proper shelters for safety and security. Hence, the first section of this chapter reviews current status of usage of dispersion models and its applicability in regulating air quality monitoring and consequence analyses. This is followed by an elaboration of current approach of coupling of dispersion model with an appropriate meteorological model for realistic predictions. This coupling is required because meteorological models furnish more precise input parameters for dispersion model. These parameters include ambient temperature, wind field over the simulated region duly incorporating the regional topography. Dispersion model uses these parameters as an input and estimates spatially and temporally varying pollutant concentrations [Basit, 2009].

Atmospheric chemical reactions may convert primary pollutants into secondary pollutants which may be less harmful and, sometimes more toxic or even carcinogenic. For example, oxidation process in environment converts sulfur dioxide (SO₂) and nitrogen dioxide (NO₂) into particulate sulfate and nitrates that are benign. Photochemical reactions in the presence of ozone in urban environment result in formation of peroxy acetyl nitrate (PAN) which is a carcinogenic secondary pollutant. The conversion mechanism and reaction rates are important because they control the ambient concentrations of sulfur and nitrogen oxides [Khoder, 2002]. In order to
incorporate effect of chemical reactions on predictive ability of a dispersion model, removal term based on atmospheric chemistry should be incorporated for precision and accuracy in modeling predictions. Review of different dispersion models which deal with atmospheric chemistry of chemical pollutants is given in section 2.3.3.

Once modeling results are obtained, these are required to be verified and validated against some experimental data. This is normally collected by conducting field tracer experiments. In these experiments a tracer is released from a source under controlled conditions and the resulting ambient concentrations at different sampling points around the source are determined by using different sampling and analyzing techniques. Different studies have been conducted on model validation using the source terms of a single or multiple emission points. Subsequent measurements of tracer concentrations around the sources over extended sampling times are described in section 2.4.

The output results of a model can best be demonstrated and visualized by performing post-processing to exhibit plume trajectories moving in real topographic and geographic domain incorporating a specific wind field within which pollutants are emitted. Section 2.5 describes various post-processing modules that are incorporated in various dispersion software codes emphasizing their benefits and deficiencies.

### 2.1 Dispersion Modeling and Regulatory Requirements

There are multiple purposes to perform atmospheric dispersion modeling though it is most commonly used to predict air quality and verify it by comparing with the regulatory requirements. For maintenance of air quality at prescribed levels, every country has its national ambient air quality standards (NAAQS) that should not be exceeded. In many countries even for new industries with certain potential of atmospheric emissions it is necessary to obtain a permit for construction. This permit include commitment of the new facility that after completion and venturing into operation, it will not violate the air quality standards for any regulated pollutant. As it is not possible to make measurements of resulting air quality for a facility that has not yet been constructed, air quality dispersion modeling is the only way to estimate the future impact [Turner, 1994]. Hence models used in dispersion have a specific significance for governmental agencies which are involved in taking the protective safety impact analyses and managing air quality. Different countries use air quality
Chapter 2

standards defined by their regulatory bodies. For instance NAAQS in United States have been defined by US Environmental Protection Agency. These standards are included in title 40 of US Code of Federal Regulations part 50. In Bangladesh, applicability of Industrial Source Complex (ISC3) model [EPA, 1995] was employed for brickfield pollution [Ahmed, 2008]. The model was found to be very effective and appropriate both for gaseous and particulate pollutants from brick filed in specific region. Particulate matter was identified as the most important pollutant in that region which urgently needed to be taken care of. In India ‘Industrial Source Complex Short Term (ISCST2) model’ was employed in study to predict the effects of brick kiln emissions on surrounding ambient air quality. By stack monitoring exercise, source terms and ground level concentrations of Suspended Particulate Matter (SPM), SO₂ and NOₓ were measured to check the environmental impacts of brick kilns industry. Mitigation measures were suggested to minimize the emission level and ground level concentration [Bhanarkar, 2002]. A similar study was conducted to assess brick kiln emission impacts on air quality of Northern Vietnam [Le, 2009].

Atmospheric dispersion models are also used to assist in developing effective control strategies for mitigating harmful pollutant emissions. Public safety responders and emergency managers also use the results of dispersion modeling for emergency planning of any accidental chemical releases and conducting ‘Radiological Consequence Analysis’ of accidental releases of hazardous or toxic materials such as chemicals or radionuclides. For instance, on an accidental radioactive release which occurred on 11 March 2011 from Japanese Fukushima Reactor, a regional scale simulation study was made. Purpose of the study was to examine plume dispersion and its impact over 80 km radial distance around the reactor. Meteorological conditions were simulated using meteorological model WRF [Skamarock, 2008] and the plume dispersion and trajectory were simulated with Lagrangian particle dispersion models HYPACT [Walko, 2001] and FLEXPART [Stohl, 1998, 1999, 2005] using the accidental source term. Simulated seaward particle trajectories indicated that spread of radioactivity was over the sea under the influence of westerly winds on most days. Landward plume spread was observed on a few days under the influence of southeasterly, easterly and northeasterly flow. Comparison of models predicted results with observations showed that the plume pattern could be simulated reasonably and was in agreement with observations within margin of uncertainty in source term [Srinivas, 2012].
2.1.1 Conventional and Advanced Dispersion Models

Several dispersion models are used worldwide that include models as simple as box type to as complex as atmospheric computational fluid dynamics based. Suitability of a dispersion model under specific topographical and environmental conditions highly depends on scale of impact, complexity of meteorology and source characteristics. Gaussian-plume models [Sutton, 1947a] are widely used for regulatory applications. In medium-complex terrain and meteorological conditions, Gaussian-plume models are considered to generate reliable results. In case of more complex topography and meteorological conditions, advanced puff or particle models properly coupled with meteorological models are required to be used to generate more realistic modeling results [Bluett, 2004].

2.1.1.1 Gaussian Plume Models (GPM)

Work on air dispersion modeling started from 1930s and even earlier. Bosanquet and Pearson [Bosanquet, 1936] worked on derivation of an early plume dispersion equation without considering the assumptions of Gaussian distribution for vertical and crosswind plume dispersion and effect of ground reflection of the plume. Later on, an air pollutant dispersion equation was derived by Sir Graham Sutton in 1947 [Sutton, 1947b]. It was based upon the assumptions that concentration of pollutant in a plume follows ‘Gaussian Distribution’ by which its lateral and vertical spread can be measured. This assumption was not considered by Bosanquet and Pearson. With the introduction of ambient air quality standards and the formation of environmental protection agencies in the late 1960s, a tremendous increase in use of air pollutant dispersion calculations was observed. A lot of dispersion models in form of computer programs were developed during that era for simulation of atmospheric dispersion of air pollutants emitted from industrial sources. Most of the dispersion models were based on a single Gaussian equation, as presented below, for dispersion modeling of continuous and buoyant air pollutant plumes [Beychok, 2005; Turner, 1994].

\[
\chi = \frac{Q}{2\pi\nu\sigma_y\sigma_z} \exp\left\{-\left(\frac{y^2}{2\sigma_y^2} + \frac{(z+h)^2}{2\sigma_z^2}\right)\right\} + \exp\left\{-\left(\frac{y^2}{2\sigma_y^2} + \frac{(z-h)^2}{2\sigma_z^2}\right)\right\}
\]  (2.1)
Where ‘χ’ is pollutant concentration (g/m$^3$), ‘Q’ is emission rate of pollutant (g/sec), ‘v’ is wind speed at release point (m/sec). In this equation, ‘σ_x’ and ‘σ_z’ represent standard deviations of concentration distribution in cross and vertical wind directions (m) at downwind distance ‘x’ respectively, ‘h’ is plume effective height.

This equation is obtained by performing time integration of Gaussian puff equation for continuous release. Gaussian puff equation is obtained from the solution of Fickian diffusion equation with the assumptions of invariant wind field and homogenous turbulence [Stockie, 2011].

GPM has been employed widely for radiological consequence analysis and environmental impact assessment in case of nuclear accidents under recommendation of international regulatory agencies [IAEA, 1982; USNRC, 1982]. There are two major limitations of GPM. Vertical wind shear and variations in average wind speed over space and time are not treated by this model. Despite these limitations, GPM has extensively been used [Healy, 1984; Slade, 1968] because it is user friendly and theoretically simple. AUSPLUME [EPA, 2000], AERMOD [USEPA, 2004] and ISC3 [Schulman, 1997] are popular examples of GPMs [Sutton, 1932].

The primitive Gaussian model derived from the work of Sutton [Sutton, 1932] was not able to be employed for complex environmental or terrain conditions. Therefore, its use for hilly or coastal regions, urban atmosphere, long range transport (mesoscale), small wind speed, inversion conditions etc. generates misleading results [Benson, 1984; Sokhi, 1998; Thomson, 2001; Caputo, 2003; Basit, 2006].

2.1.1.2 Advanced Dispersion Models

In order to address the limitations of GPM, some advanced dispersion models have been developed and are subsequently being employed. These are generally meteorological data intensive and demand much higher computational resources than those of GPM. Advanced models may be grouped in two major categories depending on the way air pollutants are represented by the model. If pollutants are represented as puff then the category is termed as puff model whereas if pollutant is represented by certain number of particles then such models are termed as particle models.
(a) Puff Models

In puff models, pollutant emissions are represented by the number of puffs of that pollutant. These puffs are transported by the winds generated by a meteorological model. Each puff represents a discrete mass of pollutant. Volume of puff increases during transportation because of turbulent mixing of environment. Puff models have comparatively less computational requirements than particle models, but are not as realistic in their presentation of pollutant distribution as particle models. However, these models are often more than adequate and are used for regulatory purposes [Bluett, 2004]. Advanced puff models include dry or wet deposition and radioactive decay of radioactive particles. One of the most commonly used dispersion models is CALPUFF (CALifornia PUFF) model [Scire, 2000a,b].

CALPUFF model is a non-steady state, Lagrangian-Gaussian puff dispersion model consisting of data preprocessing, processing and post-processing modules. It uses meteorological data of surface and upper atmosphere for different meteorological parameters such as ambient temperature, wind speed, wind direction and precipitation etc. It processes geophysical data of land use and topography. It uses multilayered meteorological data and has a potential to simulate pollutants transportation and diffusion into atmosphere incorporating the impacts of spatially and temporally changing meteorological conditions. CALPUFF modeling system, which is also used in part of this research, is capable to simulate both instantaneous or continuous emissions over short distances of tens of meters to long distances of hundreds of kilometers. The model takes continuous release of pollutants puffs that are emitted from a source and entered into ambient air flow. Dispersion of pollutants follows Gaussian distribution within a puff and concentrations are calculated on the basis of contribution of individual puffs while passing near a receptor location. CALPUFF modeling system comprises of three main modules: CALMET, as a 3-D diagnostic meteorological model, CALPUFF as a dispersion model and CALPOST as a post-processor of the modeling package. CALMET develops hourly based three dimensional gridded meteorological data of temperature and wind fields on defined fine scale model grid. Input meteorological data for CALMET is provided either as observed data from surface meteorological stations, upper atmosphere stations, over water stations and precipitation stations or gridded three-dimensional data generated by prognostic meteorological models such as MM5, WRF, RAMS, etc. or even
combination of both types of data. CALMET combines geographical data of land use and topography with meteorological data to generate meteorological fields of winds and other environmental parameters such as ambient temperature etc. on a fine scale grid. The generated output file of CALMET also contains associated two-dimensional fields like surface characteristics, mixing height and dispersion properties. The model has capability to be run on higher spatial grid resolution than prognostic models to improve the simulation of meteorological fields. This is basically a simulation requirement in coastal and complex terrain regions [Klausmann, 2003, 2005].

Three-dimensional gridded meteorological data generated by CALMET is further used as an input to CALPUFF model. According to U.S. Environmental Protection Agency, CALPUFF may be used for regulatory purposes within less than 50 km spatial range i.e. near-field application, when spatial and temporal assumptions of steady state, straight-line pollutants transport are inappropriate [MacIntosh, 2010]. CALPUFF model includes modules for processing the variable metrological conditions on three-dimensional grid and effects of complex topography. Researchers used these modules and generated estimates of ambient concentrations, dry and wet depositions and transformation of chemical pollutants through different chemical reactions occurring in atmosphere. CALPUFF can also incorporate effects of other multiple processes in simulation such as effects of building downwash, plume-terrain interactions and dispersion over water or coastal region. The on-site measured turbulence data of Gaussian dispersion coefficients both in horizontal and vertical directions can be used in CALPUFF model. Moreover, these coefficients can also be obtained by running the model using similarity theory and data of micrometeorological variables that are derived from meteorological observations and surface characteristics [Scire, 2000a,b].

CALPUFF uses an algorithm for complex terrain in order to consider the effect of elevated land on ground-level concentration of emissions. A shoreline modeling approach is also incorporated in it to consider formation of thermal internal boundary layer due to differences in land–water temperatures. CALPUFF is well capable of simulating continuous or time varying emissions from different types of sources such as point, line, area, and volume sources. CALPUFF model deals a horizontal grid and multiple vertical levels. Two grids as meteorological and computational grids are defined in model. Meteorological parameters are defined at grid cells of
meteorological grid while concentration calculations are done on computational grid which may be same or may be a part of meteorological grid [Elbir, 2003].

CALPOST program, as a post-processor of CALPUFF modeling system is specially designed in order to display numeric averaged data from CALPUFF output file of pollutants concentration, wet or dry depositions and fluxes in graphical format making it easily understandable. In CALPOST module, different averaged sampling times can be selected and output results can be obtained in rank tables, exceedance tables and related plots [Oshan, 2006].

Basic formula [Scire, 2000a,b] to calculate concentration of a puff at a receptor location is given by:

\[
C = \frac{Q}{2\pi \sigma_x \sigma_y} \exp\left[-\frac{d_a^2}{2\sigma_x^2}\right] \exp\left[-\frac{d_c^2}{2\sigma_c^2}\right]
\]

(2.2)

Where ‘C’ is ground level concentration (g/m³), ‘Q’ is pollutant mass (g) in the puff, ‘\(\sigma_x\)’, ‘\(\sigma_y\)’, ‘\(\sigma_z\)’ are standard deviations (m) of Gaussian distribution in along, cross and vertical wind directions, ‘\(d_a\)’, ‘\(d_c\)’ are distances (m) from puff centre to receptor in along and cross wind direction, ‘\(g\)’ is vertical term (m) of Gaussian equation expressed as below:

\[
g = \frac{2}{(2\pi)^{1/2}\sigma_z} \sum_{n=-\infty}^{\infty} \exp\left[-\frac{(H_e + 2nh)^2}{2\sigma_z^2}\right]
\]

(2.3)

Where ‘\(H_e\)’ is effective height (m) above ground up to the puff center and ‘\(h\)’ is mixing layer height (m). Summation in vertical term ‘\(g\)’ accounts for multiple reflections off the mixing lid and the ground.

For a horizontally symmetric puff, with \(\sigma_x = \sigma_y\) equation (2.2) reduces to:

\[
C(s) = \frac{Q(s)}{2\pi \sigma_z^2(s)} \exp\left[-\frac{R^2(s)}{2\sigma_z^2(s)}\right]
\]

(2.4)

Where ‘\(R\)’ is distance (m) from center of puff to receptor and ‘\(s\)’ is distance (m) travelled by the puff. Distance dependence of variables in above equation is indicated (e.g. \(C(s), \sigma_y(s)\) etc.).

Integrating equation over distance of puff travel ‘\(ds\)’ during sampling step ‘\(dt\)’ yields time averaged concentration ‘\(\bar{C}\)’
Where ‘s_o’ is the value of ‘s’ at beginning of sampling step. An analytical solution to this integral can be obtained if it is assumed that most significant - dependencies during sampling step are in ‘R(s)’ and ‘Q(s)’ terms. Figure 2.1 illustrates movement of a puff from coordinates (x_1, y_1) to (x_2, y_2).

Assuming trajectory segment is a straight line, and transforming ‘s’ to a dimensionless trajectory variable ‘p’, radial distance to receptor at (x_r, y_r) is

\[ R(s) = [(x_1 - x_r + pdx)^2 + (y_1 - y_r + pdy)^2]^{1/2} \]  

Exponential variation of ‘Q’ due to removal and chemical transformation processes is expressed as a linear function of sampling interval:

\[ Q(s) = Q(s_o) + p\{Q(s_o + ds) - Q(s_o)\} \]  

Using equation (2.7) and transforming to ‘p’ coordinates, equation (2.5) becomes:

\[ \bar{c} = \frac{1}{ds} \int_{s_o}^{s_o + ds} \frac{Q(s)}{2\pi \sigma^2} g(s) \exp \left[ -R^2(s)/\left(2\sigma^2(s)\right) \right] ds \]  

\[ \bar{c} = \frac{g}{2\pi \sigma^2} \{ Q(s_o) \int_0^1 \exp \left[ -R^2(p)/(2\sigma^2) \right] dp + \{Q(s_o + ds) - Q(s_o)\} \int_0^1 \exp \left[ -R^2(p)/(2\sigma^2) \right] dp \} \]
Solution of integrals in equation (2.8) is expressed in terms of error functions and exponentials:

\[
\bar{C} = \frac{\sigma_y}{2\sqrt{\pi}} \left[ Q(s_0)I_1 + \{Q(s_0 + ds) - Q(s_0)\}I_2 \right] \tag{2.9}
\]

\[
I_1 = \left[ \frac{\pi}{2a} \right]^2 \exp \left[ \frac{b^2}{2a} - \frac{c}{2} \right] \left\{ \text{erf} \left[ \frac{a+b}{\sqrt{2a}} \right] - \text{erf} \left[ \frac{b}{\sqrt{2(2a)}} \right] \right\} \tag{2.10}
\]

\[
I_2 = \frac{-b_1}{a} + \frac{1}{a} \exp \left[ \frac{b^2}{2a} - \frac{c}{2} \right] \left\{ \exp \left[ \frac{b^2}{2a} \right] - \exp \left[ -\frac{1}{2} (a + 2b + \frac{b^2}{a}) \right] \right\} \tag{2.11}
\]

\[
a = (dx^2 + dy^2)/\sigma_y^2 \tag{2.12}
\]

\[
b = [dx(x_1 - x_r) + dy(y_1 - y_r)]/\sigma_y^2 \tag{2.13}
\]

\[
c = [(x_1 - x_r)^2 + (y_1 - y_r)^2]/\sigma_y^2 \tag{2.14}
\]

**Particle Models**

Particle models are based on Lagrangian modeling approach. Thomson worked on developing theoretical base of particle models [Thomson, 1987]. Further significant works in this regard were carried out by various researchers [Zannetti, 1990; Uliasz, 1994; Wilson, 1996]. In these models, emission of pollutants is simulated by a large number of discrete particles released by model (even if the pollutant is a gas) [IAEA, 1987; Wilson, 1996]. Once these particles are released, they are influenced by wind field and their transportation and diffusion in environment occur by averaged and fluctuating components of wind velocity respectively. Using Monte Carlo method, Lagrangian models compute eddy fluctuations by generating random numbers and calculate particle positions [Wang, 1992].

Lagrangian type particle models generate better results than Gaussian plume models for shorter distances generally and for longer distances particularly (i.e. greater than 10 km) [Chino, 1988]. The reason is that these models incorporate spatial and temporal variation in wind velocity and turbulent effects and are therefore independent of sigma curves of GPM. They evaluate dispersion coefficients such as \( \sigma_y \) and \( \sigma_z \) from particle positions that are stored at each time step. These models are
equally used for homogenous and inhomogeneous terrain conditions such as flat and complex topography [Basit, 2006; Tsuang, 2003; Hurley, 2003; Venkatesan, 2002; Oettl, 2001]. As Lagrangian particle models are independent of computational grid, they depend upon the number of released particles and resolution of meteorological fields for generating results of fine resolution. Some examples of Lagrangian models are HYPACT (HYbrid Particle And Concentration Transport) model [Walko, 2001], HYSPLIT (HYbrid Single Particle Lagrangian Integrated Trajectory) Model [Draxler, 1997, 1998, 1999] and FLEXPART (FLEXiblePARTicle) dispersion model [Stohl, 1998, 1999, 2005]. Wind field data for these models is provided as observations recorded at meteorological stations or by typical empirical correlations having basis on experimental data or by coupling with numerical meteorological model [Zannetti, 1990; Wang, 1992].

FLEXPART is an improved version [Stohl, 2005] of previous Lagrangian type particle dispersion models. Using this model, a large discrete number of particles can be emitted and positions of individual particles are determined after each time interval to simulate particle dispersion [Stohl, 1998]. This model has been extensively employed to study particle transport ways and mechanisms [Seibert, 2004; Srinivas, 2005]. Meteorological input to this model can be provided by either reanalysis data of NCEP (National Center for Environmental Prediction) or data of the European Centre for Medium-Range Weather Forecast (ECMWF). FLEXPART model presents good simulation performance in case of large-scale transport of pollutants [Forster, 2001; Stohl, 2003]. It is very clear from previous studies that the accuracy of FLEXPART modeling results is highly dependent upon meteorological field’s resolution [Pagano, 2010]. Therefore, it is recommended to have greater resolution of meteorological fields for getting better results of particle dispersion.

Particle trajectories are calculated according to following expression [Stohl, 2000]:

\[
X(t + \Delta t) = X(t) + \Delta t [v (X, t)]
\]

(2.15)

Where:

\[
v = \bar{v} + \dot{v}
\]

(2.16)
Above equation is obtained by integration of following trajectory equation:

$$\frac{dx}{dt} = v \left[ X(t) \right]$$ \hspace{1cm} (2.17)

Where ‘t’, ‘Δt’ and ‘X’ are time, time increment and position vector respectively. ‘v’ is composed of wind vector ‘v’ obtained directly from meteorological model simulations and turbulent wind vector ‘v’ that describes the atmospheric turbulent diffusion of tracer [Zannetti, 1992]. Differential increment in wind velocity fluctuations along x-direction i.e. ú (t) is obtained from Langevin equation:

$$d\bar{u} = -\left( \frac{\bar{u}}{T_{L_u}} \right) dt + \sigma_u \left( \frac{2}{T_{L_u}} \right)^{1/2} \epsilon(t) dt$$ \hspace{1cm} (2.18)

Where ‘T_{L_u}’ and ‘ϵ(t)’ are Lagrangian time scale and Gaussian random number with zero mean and unity variance. ‘σ_u’ is standard deviation of wind along x-direction which is given by Hanna scheme [Hanna, 1982]. Solution of Langevin equation requires knowledge of ‘σ_u’ and ‘T_{L_u}’ at any time and any position of a particle trajectory. To determine the fluctuating components of wind velocity, Hanna proposed an empirical relation that is based on boundary layer parameters such as PBL height (h), Monin-Obukhov length (L), convective velocity scale (w_s), roughness length (z_0) and friction velocity (u_*) [Hanna, 1982].

In the following, subscripts ‘u’, ‘v’ and ‘w’ refer to along, cross and vertical wind components of turbulent velocities, ‘f’ is Coriolis parameter. Hanna’s empirical profiles of turbulence in unstable atmosphere are as follows [Hanna, 1982]:

$$\frac{\sigma_u}{u_*} = \frac{\sigma_v}{w_*} = \left( 12 + \frac{h}{2L} \right)^{1/3}$$ \hspace{1cm} (2.19)

$$T_{L_u} = T_{L_v} = 0.15 \frac{h}{\sigma_u}$$ \hspace{1cm} (2.20)

$$\frac{\sigma_w}{w_*} = \left[ 1.2 \left( 1 - 0.9 \frac{z}{h} \right) \left( \frac{z}{h} \right)^{2/3} + \left( 1.8 - 1.4 \frac{z}{h} \right) u_*^2 \right]^{1/2}$$ \hspace{1cm} (2.21)

For $\frac{z}{h} < 0.1$ and $z - z_0 > -L$

$$T_{L_w} = 0.1 \frac{z}{\sigma_w [0.55 - 0.38(z - z_0)/L]}$$ \hspace{1cm} (2.22)

For $\frac{z}{h} < 0.1$ and $z - z_0 < -L$
For neutral atmosphere, empirical profiles of turbulence are as follows [Hanna, 1982]:

\[
T_{L_w} = 0.59 \frac{z}{\sigma_w}
\]  
\[\text{For } h > 0.1 \]

\[
T_{L_w} = 0.15 \frac{h}{\sigma_w} \left[ 1 - \exp \left( -\frac{5z}{h} \right) \right]
\]

For neutral atmosphere, empirical profiles of turbulence are as follows [Hanna, 1982]:

\[
\frac{\sigma_u}{u_*} = 2.0 \exp(-3fz/u_*)
\]  
\[
\frac{\sigma_v}{u_*} = \frac{\sigma_w}{u_*} = 1.3 \exp(-2fz/u_*)
\]

\[
T_{L_u} = T_{L_v} = T_{L_w} = \frac{0.5z/\sigma_w}{1 + 15fz/u_*}
\]

For stable atmospheric conditions, empirical relations for turbulence are as follows [Hanna, 1982]:

\[
\frac{\sigma_u}{u_*} = 2.0 \left( 1 - \frac{z}{h} \right)
\]

\[
\frac{\sigma_v}{u_*} = \frac{\sigma_w}{u_*} = 1.3 \left( 1 - \frac{z}{h} \right)
\]

\[
T_{L_u} = 0.15 \frac{h}{\sigma_u} \left( \frac{z}{h} \right)^{0.5}
\]

\[
T_{L_v} = 0.07 \frac{h}{\sigma_v} \left( \frac{z}{h} \right)^{0.5}
\]

\[
T_{L_w} = 0.1 \frac{h}{\sigma_w} \left( \frac{z}{h} \right)^{0.5}
\]

In above expressions, \(\sigma_u\), \(\sigma_v\) and \(\sigma_w\) are root mean squared values of fluctuations along x, y and z axes respectively. \(T_{L_u}\), \(T_{L_v}\) and \(T_{L_w}\) are eddy lifetimes for corresponding fluctuations. Here \(h\) represents height of planetary boundary layer at which turbulence dies off. \(z_0\) is surface roughness length and is of the order of 1/10th of the height of obstacles (vegetation, trees etc). \(u_*\) is frictional velocity which can be determined experimentally [Plate, 1971], while typical values for different surfaces roughness \((z_0)\) can be found in literature. Pollutant’s concentration at specific time ‘t’ in a grid cell is evaluated by summing mass fractions of all particles within grid cell and dividing by cell volume.
\[ c = \frac{1}{V} \sum_{i=1}^{N} (m_i f_i) \]  

(2.33)

Where \( V \) is grid cell volume, \( m \) is particle mass, \( N \) is total number of particles, \( f_i \) is fraction of mass of particle \( i \) that is attributed to specific grid cell. This mass fraction is calculated for each particle and for each grid cell using a simple uniform kernel with bandwidths (\( \Delta x, \Delta y \)) where \( \Delta x, \Delta y \) are grid distances on longitude-latitude output grid.

Advanced dispersion models require precise meteorological parameters as input such as wind speed, wind direction, temperature, pressure, etc. Prevailing wind at any time can only be incorporated in dispersion by taking input from meteorological models. Hence advanced dispersion models are necessary to couple with meteorological models to get precise input of existing meteorological and atmospheric stability conditions.

### 2.1.2 Meteorological Models

Application of meteorological models to forecast atmospheric stability, low and high pressure regions, wind pattern and weather conditions started in twentieth century, when a Norwegian Physicist, Vilhelm Bjerknes claimed that such type of forecasting could be done on basis of calculations. His proposed forecasting technique was not fully successful due to unavailability of advanced computational resources and precise observational data. First Numerical Weather Prediction (NWP) system was developed in 1922 by Lewis Fry Richardson. His method [Richardson, 1922] was practically used in 1940s with help of digital computers. His computing method was based on division of grid into small cells for solving differential equations by finite difference methods. John von Neumann, one of the earliest computer pioneers, helped in use of computers for weather forecasting [Aspray, 1990]. Work on development of an Atmospheric General Circulation Model (AGCM) was initiated in 1955. Cecil Leith offered a working five-level atmospheric model that was executed on supercomputer in 1960 [Leith, 1965]. National Center for Atmospheric Research that was established in 1960 started his work on General Circulation models in 1964. This research center constructed two different series of models called as NCAR 1-3 and CCM 0-1. By early 1960s, Andrew Gilchrist and others at UK Meteorological Office had also begun building an AGCM and were ultimately successful [Gilchrist, 1979].
In order to simulate dispersion of air pollutants in some specific region, meteorology at regional scale is generally required rather than at global scale. In order to achieve this target, output from GCM in the form of a large scale meteorological data is used to derive limited-area meteorological model with a suitably high-resolution for simulating regional meteorology [Giorgi, 1991, 1999]. Limited area meteorological model could generate realistic meteorological information of high spatial and temporal resolution consistent with driving large-scale meteorological data. Large-scale data is provided by either reanalysis data or a GCM output. Because of their coarse resolution, General Circulation Models (GCMs) often perform poorly in simulating regional processes, especially in regions with local fine-scale forcing topography [Gates, 1992; Gao, 2002]. In order to accurately focus and predict local dispersion pattern based on wind field prevailing in smaller domains, Mesoscale or Regional meteorological models such as MM5 [Grell, 1995], WRF [Skamarock, 2008], RegCM [Dickinson, 1989; Giorgi, 1990; Giorgi, 1989], RAMS [Tripoli, 1982] etc. are usually employed. Mesoscale is generally referred to horizontal dimensions ranging from around 2 kilometers to 2000 kilometers. Mesoscale climate models were originally designed for climatic simulation of some specific convective environments in North America and Europe [Tadross, 2006]. However, nowadays, these models, with some modifications, are being employed for atmospheric simulation of various other regions of the world. Different empirical procedures, i.e. parameterization schemes, have been incorporated in these models in order to simulate diverse physical environmental processes. Appropriateness of a selected scheme for a region may be dependent on climate and topography of target region. Simulation studies conducted using different regional models revealed the fact that some parameterization convective schemes have not satisfactorily simulated environmental parameters in some specific regions of the world, including Asian monsoon regions [Leung, 2003; Lee, 2000]. One of the causes of failure of some convective schemes may be the scale interaction that is intensively complex in Asian monsoon regions [Holland, 1995] due to effects of Tibetan plateau, ocean–continent contrast and sea-air interactions. These specific features require special consideration in designing regional models to be used in this particular region [Sardar, 2012a].
2.1.2.1 Mesoscale Model (MM5)

The Fifth-Generation NCAR/Penn State Mesoscale Model (MM5) is a regional mesoscale model (available from ftp://ftp.ucar.edu/mesouser/MM5V3). This is an open source software and is a modified form of an old model developed by Anthes in 1970s [Anthes, 1978]. MM5 is applied for a wide range of applications like hypothetical, real-time and predictive simulation studies. Over smaller scales (2-200 km), MM5 can be applied for studying mesoscale convective systems, fronts, land-sea breezes and mountain-valley circulations. The model has a lot of supplementary pre and post-processors jointly referred as MM5 modeling system. This prognostic meteorological model comprised of different modules such as TERRAIN, REGRID and INTERPF etc. It is a limited-area, non-hydrostatic and terrain-following sigma coordinate mesoscale modeling system developed to simulate complex physical environmental processes taking place in atmosphere at mesoscale. The model is used for numerical forecasting having capabilities of multiple nesting and four dimensional data assimilation (x, y, z, and t). The model also incorporates different physical options called as parameterization schemes of clouds, planetary boundary layer, humidity, radiation and surface temperature [Grell, 1995]. The model employs Arakawa-B staggering of velocity vectors with respect to scalars such as temperature and relative humidity etc. Velocity vectors and scalars are defined at dot and cross points respectively [Ratnam, 2006]. A brief introduction of MM5 can be found in literature [Grell, 1995; Dudhia, 2005].

Governing equations of MM5 (nonhydrostatic model) in terms of terrain following coordinates (x, y, σ) for basic variables such as pressure, momentum and energy represent overall predictive algorithm of the code. Parameter ‘σ’ is a dimensionless quantity and each model level is defined by a value of σ between 0 (at model top level) and 1 (model surface).

\[ σ = \frac{(p_o - p_t)}{(p_s_o - p_t)} \]  

(2.34)

Where p_o, p_t and p_s_o are reference-state, top and surface pressures.

In the set of governing equations, pressure is given by the expression:

\[ \frac{dp}{dt} = \rho gw + \gamma p \nabla \cdot V = -V \cdot \nabla p' + \frac{\gamma T}{T_c} \left( \frac{Q}{\theta_c} + \frac{T_c}{\theta} D_0 \right) \]  

(2.35)
Where \( p' \) is perturbation pressure (Pa), \( t' \) is time (sec), \( \rho_s \) is reference state density (kg/m\(^3\)), \( g' \) is acceleration of gravity (9.8 m/sec\(^2\)), \( w' \) is vertical velocity (m/sec), \( \gamma \) is ratio of specific heats \( \left( \frac{C_p}{C_v} \right) \), \( p' \) is pressure (pa), \( V' \) is horizontal wind vector, \( T' \) is temperature (K), \( Q' \) is diabetic heating rate per unit mass (J/Kg.sec), \( c_p \) is specific heat at constant pressure of dry air, \( T_s \) is reference state temperature (K) and \( \theta \) is potential temperature (K).

For momentum (x, y and z-components), equations are:

\[
\frac{\partial u}{\partial t} + \frac{m}{\rho} \left( \frac{\partial p'}{\partial x} - \frac{\sigma}{p^*} \frac{\partial p'}{\partial \sigma} \right) = -V \cdot \nabla u + v \left( f + u \frac{\partial m}{\partial y} - v \frac{\partial m}{\partial x} \right) - \varepsilon \cos \alpha - \frac{uw}{r_{\text{earth}}} + D_u
\]  
(2.36)

\[
\frac{\partial v}{\partial t} + \frac{m}{\rho} \left( \frac{\partial p'}{\partial y} - \frac{\sigma}{p^*} \frac{\partial p'}{\partial \sigma} \right) = -V \cdot \nabla v - u \left( f + u \frac{\partial m}{\partial y} - v \frac{\partial m}{\partial x} \right) + \varepsilon \sin \alpha - \frac{uw}{r_{\text{earth}}} + D_v
\]  
(2.37)

\[
\frac{\partial w}{\partial t} + \frac{\rho_s g}{p^*} \frac{\partial p'}{\partial \sigma} + \frac{gp'}{\gamma p} = -V \cdot \nabla w + g \frac{p^* T^'}{p} - \frac{R_d p'}{c_p} - e(u \cos \alpha - v \sin \alpha) + \frac{u^2 + v^2}{r_{\text{earth}}} + D_w
\]  
(2.38)

Where \( u \) and \( v \) are components of wind velocity (m/sec) in eastward and northward directions respectively, \( m \) is map scale factor, \( p \) is density of air (kg/m\(^3\)). \( \sigma \) is dimensionless vertical coordinate of model. \( p^* \) is defined as \( p^* = p_s - p_t \). \( p_s \) is surface pressure, \( p_t \) is pressure at top of model, \( f \) is coriolis parameter. Here \( e \) is horizontal coriolis parameter defined as \( e = 2\Omega \cos \lambda \) and \( \alpha = \Phi - \Phi_c \). \( \Omega \) is angular velocity of earth \( (7.2722 \times 10^{-5} \text{ sec}^{-1}) \). \( \lambda \) is latitude. \( \Phi \) is longitude and \( \Phi_c \) is central longitude.
For energy, formulation is:

\[ \frac{\partial T}{\partial t} = -V \cdot \nabla T + \frac{1}{\rho c_p} \left( \frac{\partial p}{\partial t} + V \cdot \nabla p' - \rho c_g w \right) + \frac{Q}{\epsilon_p} + \frac{T^*}{\bar{u}_b} D_0 \]  

(2.39)

(a) Parameterization Schemes of MM5 Model

Grell scheme [Grell, 1995] is a simplified form of Arakawa and Schubert scheme [Arakawa, 1974]. It is one dimensional single cloud scheme. It includes a single updraft and downdraft couplet. Mixing of ambient air is allowed only at top and bottom of cloud. To predict rainfall, a quasi-equilibrium assumption is used in the scheme. It is assumed that convective clouds make environment stable as quickly as non-convective processes destabilize it. Precipitation is determined by this scheme as follows [Ratnam, 2006]:

\[ R = I_1 m_b (1 - \beta) \]  

(2.40)

Where ‘R’, ‘I_1’, ‘m_b’ and (1 – \beta) are amount of precipitation, normalized updraft condensation, cloud base mass flux of updraft and precipitation efficiency respectively. Details of the scheme can be found in literature [Grell, 1995].

KF scheme [Kain, 1990] was derived from Fritsch and Chappell convective scheme [Fritsch, 1980]. This is one-dimensional entraining/detraining plume model based on Lagrangian parcel method [Simpson, 1969; Kreitzberg, 1976]. It includes vertical momentum dynamics with mass flux conservation to evaluate possibility of occurrence of instability in environment. This scheme includes both updrafts and downdrafts. Mixing is allowed throughout entire depth of the cloud. Convective precipitation in KF scheme is determined by multiplication of precipitation efficiency with total vertical fluxes of both vapor and liquid at about 150 hPa above condensation level [Wang, 1997]. A detailed description of scheme can be found in literature [Kain, 1993].

Anthes-Kuo scheme [Anthes, 1977] is a modified form of old Kuo scheme [Kuo, 1965]. Cloud dynamics as updrafts and downdrafts are not included in the scheme. Amount of convection is evaluated only from vertically integrated moisture convergence. Moisture convergence at grid-scale divides into two parts. One part is responsible to generate precipitation at ground and other causes moistening of air column.
According to Anthes [Anthes, 1977], following relation describes fractional part of moisture convergence that produces precipitation [Kerkhoven, 2006]:

\[
\alpha = \frac{RH_{\text{mean}} - RH_c}{1 - RH_c} \quad 0 \leq \alpha \leq 1
\]  

(2.41)

Where ‘\(\alpha\)’, ‘\(RH_{\text{mean}}\)’ and ‘\(RH_c\)’ are fraction of moisture convergence to precipitation, mean relative humidity in troposphere and critical relative humidity respectively. For initiation of convection, sufficient amount of energy available and moisture supply is required by the scheme.

Betts-Miller scheme [Betts, 1986b] is a convection adjustment scheme. It simply adjusts ambient temperature and moisture to a stable state without using a cloud model. Convection is triggered in scheme as instability creates in atmosphere and continues until the restoration of stability in environment. Limitation of the scheme is that a single stable reference profile is used. The scheme may not be suitable for severe convective environment, as it does not deal with updrafts and downdrafts in clouds. In this scheme environmental temperature and moisture profiles are constrained to a stable reference profile of these parameters [Kerkhoven, 2006].

\[
\frac{\partial T}{\partial t} = \frac{T_{\text{stable}} - T_{\text{current}}}{t_{\text{convective}}}
\]  

(2.42)

\[
\frac{\partial q_v}{\partial t} = \frac{(q_{v_{\text{stable}}} - q_{v_{\text{current}}})}{t_{\text{convective}}}
\]  

(2.43)

Where ‘\(t_{\text{convective}}\)’, ‘\(T\)’ and ‘\(q_v\)’ represent time scale, temperature and specific humidity respectively. Subscripts ‘stable’ and ‘current’ indicate stable reference profile and state of the model at current time step. Empirically derived reference profiles are defined as stable profiles. A detailed description of the scheme can be found in literature [Betts, 1986 a,b].

Several simulation studies using MM5 model indicated dependancy of model predictions especially for rainfall parameter on convective parameterization scheme selected in model. A simulation study was conducted using MM5 [Wang, 1997] for sensitivity analysis of parameterization schemes namely as Anthes–Kuo, Betts–Miller, Grelland Kain–Fritsch (KF) schemes. Rainfall patterns over continental USA for cold and warm seasons were simulated. Conclusions drawn were that KF scheme generated improved results as compared to others, although there was no single
scheme showing excellent performance consistently. A study was performed for numerical forecasting of quantitative precipitation during warm period of 2005–2007 over Greece. Kain–Fritsch, Grell and Betts–Miller convective schemes were used in this study for nested grids [Mazarakis, 2009].

Results from fine resolution nested grid i.e. 8 km showed underestimation for high amount of rainfall and overestimation for light to moderate amounts of rainfall for all convective schemes. Kain–Fritsch scheme remained successful in showing more consistent performance to simulate the rainfall quantitatively. Another study was carried out [Kerkhoven, 2006] in east China to evaluate performance of five convective schemes namely as Anthes–Kuo, Betts–Miller, Fritsch–Chappell, Kain–Fritsch and Grell. Purpose of study was to simulate light, moderate and heavy phases of precipitation events during summer monsoon season. It was concluded that Grell scheme showed superior agreement with observations in simulating rainfall of all intensities and overall spatial scales. Kain–Fritsch scheme remained good for simulation of moderate rainfall rates. Additionally when schemes with downdrafts were used with schemes incorporating no downdrafts, a clear improvement was observed in model predicted results. A modeling study was conducted by Ratnam to investigate dependance of monsoon depressions upon two convective parametrization schemes as Grell and Kain–Fritsch schemes of MM5 model [Ratnam, 2006]. It was found that Grell scheme generated overestimated results for rainfall, while Kain–Fritsch scheme seemed to be successful in capturing distribution of rainfall comparable to observations, although location of peak rainfall was not exact.

Dependency of model predicted results in case of rainfall simulation on model spatial resolution was also observed. Ferretti simulated several rainfall events during June 1990 in Alpine region using different convective schemes [Ferretti, 2000]. Fair estimation of rainfall intensity was achieved either with Grell or with Kain–Fritsch scheme. On the other hand, Anthes–Kuo scheme seemed to show a strong overestimation in model predicted results for rainfall. Colle made a comparative simulation study using different schemes of MM5 for northeastern region of United States simulating rainfall of cold and warm seasons of 1999–2001 and 2000, respectively [Colle, 2003]. It was observed during warm season that Kain–Fritsch scheme generated overestimated results for rainfall over coastal area while underestimated inland over Appalachians.
In view of above discussion, it is concluded that selection of a convective scheme of MM5 should be according to topography, rainfall intensity of region of interest and model’s spatial resolution. Subsequently, MM5 model may be coupled with a dispersion model to execute diagnostic models [Pfender, 2006; Yang, 2006; Tonnesen, 2007]. South Asian region especially Pakistan contains very complex topographical features with high mountains such as K2, Nanga Parbat etc on one side, plateau in middle, and desert with Arabian sea on other side. As such, no study to evaluate suitable parameterization scheme has ever been conducted for Pakistani region. Hence, an investigative study is worth conducting to test which convective scheme would be suitable for this region [Sardar, 2012a]. The convective parameterization schemes are not only part of MM5 model, rather they are also used in other regional and mesoscale models such as RegCM, WRF and RAMS, etc.

### 2.1.2.2 Weather and Research Forecasting Model (WRF)

Weather research and forecasting (WRF) model is a widely used new-generation non-hydrostatic mesoscale meteorological model which solves compressible non-hydrostatic Euler equations cast in flux form on a mass-based terrain-following vertical coordinate system and provides meteorological fields for study of regional air pollutant transport [Michalakes, 2001]. Prognostic variables include horizontal and vertical wind components, various microphysical quantities, perturbation potential temperature and surface pressure of dry air. The model uses Runge–Kutta 3rd order time integration scheme and 2nd–6th order advection schemes in both horizontal and vertical directions. A complete description of WRF modeling system can be found in literature [Skamarock, 2008].

The governing equations of WRF are given as:

\[ p = \rho \left( \frac{R_d}{\rho_0} \right)^\gamma \]  

(2.44)

Equation 2.44 is the equation of state where ‘\( p \)’, ‘\( \rho_0 \)’, ‘\( R_d \)’, ‘\( \theta \)’, ‘\( \alpha \)’ and ‘\( \gamma \)’ are pressure, reference pressure (typically \( 10^5 \) Pascal), gas constant for dry air, potential temperature, inverse density and ratio of the heat capacities for dry air.
Momentum equations in perturbation form are:

\[ F_u = \partial_t U + m_x \left[ \partial_x (Uu) + \frac{\partial y}{\partial y} (Vv) \right] + \partial_\eta (\Omega u) + \left( \frac{m_y}{m_x} \right) \left( \frac{\partial y}{\partial y} \right) \left[ \mu_d \partial_x \phi' + \alpha_d \partial_x p' + \alpha_d \partial_x \bar{\rho}' + \partial_x \phi \left( \partial_x \bar{\rho}' - \mu_d \right) \right] \]  

\[ F_v = \partial_t V + m_y \left[ \partial_x (Uv) + \frac{\partial y}{\partial y} (Vv) \right] + \left( \frac{m_y}{m_x} \right) \partial_\eta (\Omega v) + \left( \frac{m_x}{m_y} \right) \left( \frac{\partial y}{\partial y} \right) \left[ \mu_d \partial_x \phi' + \alpha_d \partial_x p' + \alpha_d \partial_x \bar{\rho}' + \partial_x \phi \left( \partial_x \bar{\rho}' - \mu_d \right) \right] \]  

\[ F_w = \partial_t W + \left( m_x m_y / m_y \right) \left[ \partial_x (Uw) + \frac{\partial y}{\partial y} (Vw) \right] + \partial_\eta (\Omega w) - m_y^{-1} g (\frac{\partial y}{\partial y}) \left[ \partial_\eta \bar{p}' - \bar{\mu}_d (\partial^2 \bar{\rho}') + \bar{\mu}_d \partial_\eta \left( \partial_\eta \bar{\rho}' \right) \right] \]  

Mass conservation equation is:

\[ \partial_t \mu_d' + m_x m_y \left[ \partial_x \mu' + \partial_y \nu \right] + m_y \partial_\eta \Omega = 0 \]  

Geopotential equation is:

\[ \partial_t \phi' + \mu_d^{-1} \left[ m_x m_y \left( U \partial_x \phi + V \partial_y \phi \right) + m_y \partial_y \phi \partial_\eta \partial_\eta - m_y g W \right] = 0 \]  

Conservation equations for potential temperature and scalars are:

\[ \partial_t \Theta + m_x m_y \left[ \partial_x (U \Theta) + \frac{\partial y}{\partial y} (V \Theta) \right] + m_y \partial_\eta (\Omega \Theta) = F_{\Theta} \]  

\[ \partial_t Q_m + m_x m_y \left[ \partial_x (U q_m) + \frac{\partial y}{\partial y} (V q_m) \right] + m_y \partial_\eta (\Omega q_m) = F_{Q_m} \]  

Where ‘\( \alpha_d \)’ is the inverse density of the dry air and ‘\( \alpha \)’ is the inverse density, ‘\( \mu_d \)’ is mass of the dry air in column,‘\( m \)’ is map scale factor, ‘\( p \)’ is perturbation pressure, ‘\( Q_m \)’ is generic coupled moisture variable, ‘\( U \)’ is coupled horizontal component of velocity in x-direction, ‘\( \Theta \)’ is horizontal component of velocity in x-direction, ‘\( V \)’ is horizontal component of velocity in y-direction, ‘\( \nu \)’ is horizontal component of velocity in y-direction, ‘\( \Theta \)’ is coupled potential temperature, ‘\( \theta \)’ is potential temperature.

In above equations for isotropic projections where \( m_x = m_y = m \),

\[ F_u = + \left( f + u \frac{\partial m}{\partial y} - v \frac{\partial m}{\partial x} \right) V - e W \cos \alpha_r - \frac{u W}{r_e} \]  

\[ F_v = - \left( f + u \frac{\partial m}{\partial y} - v \frac{\partial m}{\partial x} \right) U + e W \sin \alpha_r - \frac{v W}{r_e} \]  

\[ F_w = + e \left( U \cos \alpha_r - V \sin \alpha_r \right) + \left( \frac{u u + v v}{r_e} \right) \]
Where $\alpha_r$ is the local rotation angle between y-axis and meridians, ‘e’ is cosine component of coriolis term, ‘f’ is sine component of coriolis term, ‘F’ is forcing term of ‘U’, ‘V’, ‘W’, ‘$\Theta$’ and ‘$Q_m$’, ‘$r_e$’ is radius of earth.

\[
f = 2\Omega_e \sin \psi \tag{2.55}
\]

\[
e = 2\Omega_e \cos \psi \tag{2.56}
\]

Here ‘$\Omega_e$’ is angular rotation rate of earth, ‘$\psi$’ is latitude.

Once suitable mesoscale meteorological model with requisite provisions is chosen, next step is to ‘pipe’ its output wind field and other needed meteorological parameters into a versatile advanced dispersion model. This ‘piping’ of ‘output’ data at all grid nodes of meteorological model in appropriate compatible format into that of dispersion model as ‘input’, is termed as coupling. In subsequent section, this coupling of dispersion model with a mesoscale meteorological model is elaborated and status of research that has been performed in this direction is reviewed.

### 2.2 Coupling of Dispersion with Meteorological Models

Several studies have been conducted using coupling of above mentioned meteorological models such as MM5 or WRF with dispersion models like CALPUFF or FLEXPART.

#### 2.2.1 Coupling of MM5 with CALPUFF Dispersion Model

Approach to use a dispersion model (CALPUFF) with a prognostic meteorological model (MM5) is well recognized and has been practiced internationally in several studies for prediction of ground level concentration of atmospheric pollutants [Irwin, 2001; Elbir, 2003; Im, 2004; Wang, 2006; Tayance, 2007]. A modeling study was conducted with CALPUFF/MM5 modeling system by Macintosh to estimate long term averaged patterns of fine particles deposition in near-field under complex topography and wind conditions [Macintosh, 2010]. Indumati employed same coupled models to examine atmospheric pollutant dispersion over land–water–land interface [Indumati, 2009]. Results of the study provided a clear indication regarding influence of water body on ground level pollutants concentration. Coupled strategy was used by Ainslie to identify influenced regions of city of Prince George, British Columbia, Canada from burning of isolated masses of mountain pine [Ainslie, 2009]. Purpose of
study was to evaluate impact of burning of slash piles located around the city on local concentration levels of PM$_{2.5}$. To run the dispersion model, hourly meteorological input data of parameters of temperature, wind speed and wind direction was obtained from six surface stations and one upper air station. Modeling results revealed that location and coverage of affected areas was highly dependent upon meteorological parameters such as wind speed, direction and atmospheric stability.

A modeling study was conducted in Chongqing, China to investigate ambient air quality effects related with release of SO$_2$ from elevated point sources [Yang, 2008]. It was elaborated in study that concentration patterns were not homogeneous indicating significant topographical and climatic variations over spatial and temporal scales for short distances. Choi used coupled modeling system in order to investigate air quality impacts of agricultural fires on local and regional scales [Choi, 2007]. In this study, dispersion of PM$_{10}$ particulates was simulated from agricultural fires in the Yuma/San Luis area along U.S./Mexico border. A dispersion modeling study was conducted by Yang in 2006 in China to compute exposure of accidental release of H$_2$S from a sour well [Yang, 2006]. By comparing the model predicted results with observations, it was concluded in this study that model performance in estimating H$_2$S exposure was quite satisfactory. Chandrasekar investigated the possibility and effectiveness of ingesting model output in terms of wind and mixing ratio from coarsest prognostic meteorological model MM5 as input to a diagnostic meteorological model CALMET. CALMET is a module of CALPUFF modeling system to get a more accurate data of meteorological wind field for further using it in air quality modeling studies [Chandrasekar, 2003]. Results of the study revealed that this modeling technique remained successful in generating more accurate meteorological inputs for air quality modeling studies.

A simulative study was conducted to get estimates of fractional intakes of fine particles, sulfur dioxide, sulfate and nitrate released from a power plant in Beijing, China [Zhou, 2003]. Aim of this study was to determine adverse impacts of these air pollutants on human health by using long range air pollution dispersion model CALPUFF. Results showed that intake fraction of primary fine particles was roughly on the order of 10$^{-5}$, while intake fractions of sulfur dioxide, sulfate and nitrate were on the order of 10$^{-6}$. Estimated fraction of SO$_2$ was found in good agreement with observed values. Another study on same line was conducted which employed
CALPUFF modeling system to examine and assess combined adverse air quality impacts of six power plants generating total capacity of 2920 MW in Beijing area [Hao, 2007]. Intake fractions for SO\textsubscript{2}, NO\textsubscript{x} and PM\textsubscript{10} releases from power plants were determined for years 2000 and 2008 keeping in view existing mitigation measures and health risks related to exposure of toxic pollutants released from plants.

### 2.2.2 Coupling of WRF with FLEXPART Dispersion Model

Coupling of Weather Research and Forecasting (WRF) model with Lagrangian particle dispersion model FLEXPART was used to investigate reason of plume shapes which were sometimes observed during Hanford 67 tracer experiments. In first step, simulations of meandering wind flow at sub-mesoscale range i.e. 10 km spatial and less than one hour temporal were conducted using WRF. Subsequently model predicted wind field was used as input of FLEXPART by using coupling approach for plume simulation. Results of study confirmed that plume pattern was due to nocturnal sub-mesoscale meandering of wind over valley terrain [Sandeepan, 2013].

A modeling study was performed using trajectory model, FLEXPRT and regional meteorological model, WRF during Cal-Mex 2010 project. This US-Mexico collaborative project was started in 2010 to investigate cross-border transport of emissions in California-Mexico border region. WRF model was used to provide meteorological daily forecasts. These forecasts were verified using observational data obtained from analysis of surface and vertical measurements taken by radiosonde, ceilometers and tethered balloon. Based on WRF-FLEXPART simulations, four representative plume transport patterns were identified as “plume-southeast”, “plume-southwest”, “plume-east” and “plume-north”, indicating downwind direction of the plume. Plume transport directions were generally consistent with prevailing wind directions on 850 hPa. Low level (below 800 m) wind, temperature, and moisture characteristics were different for each plume transport category according to measurements from tethered balloon. Studies (such as using data assimilation and ensemble forecasts) were still in progress by investigators to improve temperature, wind and Planetary Boundary Layer (PBL) simulations [Naifang, 2012].

An anticyclonic weather system taking place at synoptic scale in northern China was simulated by WRF/FLEXPART modeling system [Peng, 2011]. Simulations were also conducted to trace out trajectories of PM\textsubscript{10} particles in anticyclone to explore its
effects on regional ambient air quality. Using air pressure data and PM$_{10}$ concentration measurements, pressure changeability was quantitatively linked with PM$_{10}$ concentration change within different sections of anticyclone. A linear correlation between PM$_{10}$ variation per unit area in mixing layer and pressure variation within a time interval was obtained. Several sections of anticyclone were associated to different linear regression equations. From this study, a parameter known as PM$_{10}$ variation rate was then determined for application of regional air pollution control and management [Peng, 2011].

Meteorological models have parameterization schemes dependent on topography and other region specific meteorological factors. When they are coupled with even an advanced dispersion model, acceptability of results is dependent on output of meteorological model. Above mentioned studies have been performed at various regions using coupled meteorological and dispersion models whereas no such coupled modeled studies have ever been conducted for Pakistani region for dispersion of any chemically toxic gaseous pollutant.

Many of the dispersion models do not consider removal term due to atmospheric reactions that are occurring with other possible species normally present in air. Concentration may therefore be overestimated by the model and may lead to increased sensitivity of situation. This is specifically true for dispersion model FLEXPART and some other similar dispersion models. Hence it is necessary to introduce removal term based on reactions occurring in atmosphere so as to estimate more realistic concentrations of pollutant.

### 2.3 Inclusion of Atmospheric Chemistry in Dispersion Models

Chemical reactions occurring in atmosphere convert primary air pollutants into secondary pollutants. Typical example is oxidation of some inorganic chemical pollutants such as sulfur dioxide (SO$_2$) and nitrogen dioxide (NO$_2$).

#### 2.3.1 SO$_2$ Removal due to Atmospheric Reactions

Oxidation of sulfur dioxide generates sulfuric acid which is further converted into sulfate particles. Oxidation rate is directly dependent upon relative humidity involving OH production. A large amount of SO$_2$ is converted into sulfite by heterogeneous
reaction: \( \text{SO}_2 + \text{H}_2\text{O} = \text{H}_2\text{SO}_3 \). Oxidation of sulfite to Sulfuric acid occurs either directly by reacting with ozone and \( \text{H}_2\text{O}_2 \) or with catalytic metals. \( \text{H}_2\text{SO}_4 \) can be formed directly from \( \text{SO}_2 \) by reaction with \( \text{OH} \) radical or \( \text{H}_2\text{O}_2 \). Oxidation of Sulfur dioxide to \( \text{H}_2\text{SO}_4 \) may occur by homogeneous gas phase reactions. Through these reactions, condensation of \( \text{H}_2\text{SO}_4 \) occurs onto already present particles and transformed into new particles reacting with \( \text{NH}_3 \). Sulfate is produced as \( \text{H}_2\text{SO}_4 \) mist by homogeneous nucleation processes in \( \text{H}_2\text{SO}_4 – \text{H}_2\text{O} \) system, followed by transition to \((\text{NH}_4)_2\text{SO}_4\) and/or \(\text{NH}_4\text{HSO}_4\) through reaction with gaseous \(\text{NH}_3\) [Khoder, 2002].

### 2.3.2 NO/NO\(_2\) removal due to atmospheric reactions

In troposphere, life of nitrogen oxides is less than one day in summer season at mid-latitudes but it may extend to several days in absence of active photochemistry. Oxidation of nitrogen oxides in atmosphere generates nitric acid, which further converts into nitrate particles. Formation of nitric acid occurs through either homogeneous reaction of \( \text{NO}_2 \) with \( \text{OH} \) radical, reaction of \( \text{NO}_3 \) with aldehydes or hydrocarbons or hydrolysis of \( \text{N}_2\text{O}_5 \) in atmosphere. During daytime, reaction of \( \text{NO}_2 \) with \( \text{OH} \) radical plays an important role while \( \text{N}_2\text{O}_5 \) hydrolysis is considered an important source of \( \text{HNO}_3 \) during night. Prime influence upon nitric acid concentrations are expected to be ambient temperature, relative humidity and ammonia concentrations at sites where \( \text{NH}_4\text{NO}_3 \) is formed. Ammonium nitrate being unstable under normal atmospheric conditions exists in reversible phase equilibria with gaseous precursors. Dissociation constant of equilibria is decided by conditions of ambient temperature, relative humidity and the chemical composition of aerosols and gases [Stelson, 1982a, b; Khoder, 2002].

Conversion mechanisms and rates for formation of secondary pollutants in atmosphere are of considerable interest, as conversion rates are important factors in controlling concentrations of these pollutants in atmosphere. There are different Eulerian approach based chemistry transport models which are used to simulate pollutants dispersion taking into account their chemical removal in atmosphere at global, regional and urban scales. Details of some models are presented onwards.
2.3.3 Atmospheric Chemistry Models

Regional Air Quality Modeling System (RAQMS) is used for simulation of air quality issues at global scale. This model has been developed to fulfill atmospheric chemistry modeling requirements of NASA, National Oceanic and Atmospheric Administration (NOAA) and Environmental Protection Agency (EPA). There are some multi-scale Eulerian chemistry transport models such as CMAQ and CHIMERE which are used for regional (several thousand kilometers) and urban scaled (100-200 Km) air quality issues as tropospheric ozone, fine particles, toxics and acid deposition. CMAQ modeling system is capable of simulating different physical and chemical processes that play important role in atmospheric pollutant transformation and distribution [Appel, 2008]. CHIMERE model was mainly developed for daily forecasts of ozone, aerosols and other pollutants and for making long-term simulations over seasons and years for emission control scenarios. Both models can be run with meteorological data input from a meso-scale model like MM5 [Zhang, 2006; Monteiro, 2007].

STEM-I is a three dimensional grid model that incorporates the spatial and temporal changes in topography, wind field, mixing layer heights, chemical transformation, dry deposition and eddy diffusivities [Dronamraju, 1988]. A Comprehensive Acid Deposition Modeling system (CADM) is also employed for applications of long-range transport of air pollutants and regional acidic deposition processes. CADM modeling system is consisted of a numerical atmospheric model (RAMS) and an Eulerian chemistry/transport/deposition model [Park, 2005]. Greenhouse Gas and Air Pollution Interactions and Synergies (GAINS) model was launched in 2006. It is employed for assessment of cost-effective response strategies that diminish releases of numerous air pollutants and greenhouse gases at least costs. It helps in reducing negative impacts of emissions upon public health, ecosystems and climate change. GAINS model is integrated with EMEP Eulerian model for emission inventories. EMEP incorporates more than a hundred chemical reactions relating 70 chemical species including several non-linear mechanisms [Simpson, 2003].

Some Lagrangian-Gaussian puff models also include chemical removal term for a few inorganic air pollutants such as SO₂ and NOₓ. Examples of such models are CALPUFF and MESOPUFF-II models. No such chemical depletion of chemical pollutants is treated in Lagrangian particle models such as FLEXPART.
Conversion mechanisms and rates for air pollutants in atmosphere are of considerable importance, as these are important factors in controlling concentrations of primary pollutants in atmosphere. It is better to incorporate chemical removal term in particle models to enhance degree of accuracy in modeling predictions.

Any modeling strategy or coupling methodology may be employed but model predictions are dependent in all cases on set of mathematical equations involving certain constants and parameters. These parameters are reliant on theoretical concepts involving certain assumptions. Hence, predictions cannot be reliable until validated by actual ground based observed data. Meteorological models have to be verified by meteorological data such as temperature, precipitation, wind velocity, wind direction, pressure, humidity etc. A review of the work in this regard is already given in section 2.1.2.1 (a). Once meteorological model is validated by observational data, one has the confidence that input to dispersion model is reliable. Next step is validation of dispersion model itself. If output of dispersion model is not verified by comparing it with ground concentration data collected through experiments, one is not confident regarding prediction of dispersion models and decision making in emergency accidental scenario based on such dispersion model may not be correct. Hence, it is necessary to validate final results with factual concentration data collected on ground by experiments using some tracer gas. A review of the status of such validation tracer experiments are presented in following sections.

2.4 Historic Perspective of Tracer Experiments

A number of tracer experiments have been conducted worldwide using different types of tracers to collect experimental data for development, testing and validation of different dispersion models.

2.4.1 Early Military Tracer Experiments

Initially tracer experiments were conducted for military purposes. Many short and long range tracer experiments up through about 1965 were mainly focused on releases from chemical or nuclear weapons. A large interest could be seen in spread of atomic bomb debris in two or three decades after World War II. A few experiments of generally large size i.e. greater than 200 km were conducted (at some elevation) on effective diffusivity of atomic bomb clouds at one thousand to two thousand miles
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[Wilkins, 1954]; diffusion of smoke in stratosphere [Kellogg, 1956] and worldwide travel of atomic debris clouds [Machta, 1956]. A lot of defense and nuclear related tracer experiments were conducted at ground level using point sources for flat, rural terrain and short distances i.e. less than 1 km. These experiments include Prairie Grass experiments [Barad, 1958; Record, 1958; Haugen, 1959], Green Glow experiments [Barad, 1962], Hogstrom experiment [Hogstrom, 1964] and Hanford experiments [Fuquay, 1964]. ‘Hanford Experiments’ were among earlier tracer experimental campaigns under which greater than 300 tracer experiments were conducted from 1959 to 1974 on Hanford site in Washington using single or dual tracers released from ground and elevated sources [Ramsdell, 1985].

2.4.2 Tracer Experiments for Dispersion Studies of Industrial Pollutants

Some early experiments were conducted to study diffusion and deposition of aerosols [Chamberlain, 1953; Bowne, 1969], relative diffusion of smoke puff [Gifford, 1957], Ocean Breeze/Dry Gulch diffusion [Haugen, 1963] and dispersion of windborne material from industrial sources [Pasquill, 1974]. With establishment of environmental agencies in late 1960s and introduction of ambient air quality standards, work on environmental issues started and attention was diverted to dispersion scenario (air pollution) of different sort of air pollutants released from industrial stacks. Many ‘stack plume experiments’ were performed at short distances for flat, rural and complex terrain like coastal region as well. Examples are buoyant plume rise experiments [Briggs, 1969], power plant dispersion experiment [Hanna, 1989], Cameron, Ventura, and Carpenteria overwater/coastal experiments [Hanna, 1985], dispersion experiment in convective conditions [Kaimal, 1986], several power plant experiments in rural and urban terrain [Hanna, 1993], stack plume flat terrain, complex terrain and overwater field experiments [Chang, 2004]. In 1960s, some dispersion experiments were conducted at urban scale [McElroy, 1968; Hilst, 1966].

2.4.3 Dispersion Experiments Performed in Hilly Terrain

In history of tracer experiments, a few studies can be found to be performed on hills. Experimental data collected from these experiments has a great significance because those modeling studies which simulate dispersion phenomena of pollutants in hilly
areas must incorporate effects of hills and there is a need of experimental data for model verification.

Effect of hills on dispersion of pollutants can be studied using wind tunnel at laboratory scale under controlled flow conditions in some cases. But for prediction of dispersion in real atmosphere, experimental data at full scale is required to validate models. A few experiments were reported by Lavery [Lavery, 1982a, b] and Spangler [Spangler, 1982]. Such experiments were performed at Cinder Cone Butte in United States under stable conditions. Maryon also reported that a set of experiments were conducted in 1982 at a hill, Blashaval under near-neutral stability conditions [Maryon, 1986]. In these experiments, tracer was emitted on hill slope within the region in which the hill causes mean flow distortion and influences the turbulence structure. Similar dispersion experiments were conducted at Nyland Hill in October 1984 for study of air flow and turbulence over the hill. Dispersion trials were limited to conditions of near-neutral stability [Mylne, 1989].

2.4.4 Long Range Tracer Experiments

Many experiments were planned to investigate dispersion of tracers on mesoscale and regional scales. For long range applications, some special tracers like perfluorocarbon were developed which could be detected with very low concentration at long distances from source [Ferber, 1981]. Initially, this scale was studied by Lagrangian tracers such as balloons (tetroons) [Angell, 1960]. Also special consideration was given to dispersion of pollutants in regions of complex topography. Moreover issues of dry and wet deposition and chemical removal of air pollutants while dispersing in environment were also considered.

Classic big tracer experimental campaigns at larger scale are CAPTEX [Ferber, 1986], ANATEX [Draxler, 1989] and ETEX [JRC, 1998]. Cross Appalachian Tracer Experiment (CAPTEX) was a joint project initiated in 1983 in north eastern United States and southeastern Canada by collaboration of Atmospheric Environment Service of Canada with several other U.S and Canadian agencies. These experiments were planned to test use of an inert organic tracer for long range atmospheric transport [Hoff, 1985]. An SO\(_2\) tracer project was started in parallel with CAPTEX study using tall stack of International Nickel Company of Canada (INCO) to trace long range transport of SO\(_2\). Additional cost for conducting this study was evaluated and it was
found that it was very small compared to costs of other tracer experiments. Thus it was concluded that in future use of correlation spectrometers (COSPEC) with SO$_2$ sources might be considered for long range transport projects [Millan, 1977]. ANATEX experiment was the largest scale experiment conducted in 1987 [Draxler, 1989]. European Tracer Experiment (ETEX) was initiated in 1992 selecting release location of tracers in western part of France to establish experimental database of perfluorocarbon tracer as a unique tool for models developments in future [Van Dop, 1998]. Another important experimental project was TRANSALP under which three experiments were jointly conducted in southern Switzerland by research centre of European Commission, Italy, Switzerland and Germany in years 1989, 1990 and 1991 under main project TRACT (Transport of pollutants over Complex Terrain). Main purpose of study was identification of main transport channels for assessment of dispersal extent of pollutants to enhance understanding of dynamics of environmental processes overriding long range mesoscale transport of pollutants over very complex Alpine topography from western valley in northern Italy to Swiss plateau and vice versa. These experiments contributed in developing understanding of dispersion characteristics in very complex terrain [Ambrosetti, 1998].

Mesoscale and Regional air quality problems such as acid rain and ozone transport began to be studied with large field experiments at urban scale from 1980s to present time. Attention to this issue was given in 1970s with realization that acid rain, ozone, small particles, mercury and other pollutants were an urban through regional-scale phenomenon. Emissions are scattered broadly and chemical reactions and deposition are important. Field experiments on this scale are very expensive and need many research groups and instrumental equipments. Examples are South Central Coast Cooperative Aerometric Monitoring Program, SCCCAMP [Hanna, 1991] and Texas Air Quality Study (TexAQS) conducted in 2000.

**2.4.5 Tracer Experiments to Simulate Accidental Toxic Emissions**

Some tragic accidental events like Three Mile, Bhopal, Chernobyl and Fukushima accidents have developed a special interest in conducting the dispersion field tracer experiments on the accidental releases of hazardous gases especially denser gases.

Three Mile nuclear accident occurred in 1979 at Three Mile Island in USA. In this accident, TMI-2 nuclear power plant was destroyed because of cooling malfunction
causing partial core melt down. Fortunately, no injuries or adverse health effects were reported in Three Mile Island accident. A small amount of radioactivity was released a few days after the event, but it imparted back ground level dose [Clark, 1989].

In 1984, another tragic accidental event occurred in which several thousand people lost their lives. It was the worst industrial accident in the world due to the leakage of methyl isocyanate (MIC) gas. It occurred at the Union Carbide India Limited (UCIL) pesticide plant located inside the city of Bhopal in India. Over 500,000 people were directly exposed to the MIC gas and other chemicals. The government of Madhya Pradesh reported 3,787 casualties due to the gas release [Chouhan, 2005].

The nuclear accident of Chernobyl occurred in 1986 due to a serious flaw in reactor design. The other reason was that the reactor was operated poorly by trained staff. The consequences of the accident appeared in the form of steam explosion and fires. At least 5% of the radioactive material from reactor core was released into the atmosphere in this terrible event. Two workers at Chernobyl plant died immediately on the night of accident, and further twenty eight people expired within a couple of weeks because of the acute radiation poisoning [Munipov, 1992].

Fukushima-Daiichi Nuclear Power Plant met an accident on March 11, 2011 due to power failure and loss of cooling. Accident was triggered by a massive earthquake followed by a tsunami. Earthquake and tsunami hit other ten reactors but cold shutdown of reactors was brought with the cooling availability. The radioactivity about 15% of that in Chernobyl accident was released into environment and resulted in the evacuation of people around the plant. Land and sea area contamination around the plant was as serious as living and fishery are prohibited [Baba, 2013].

From 2000s to this date, many large urban dispersion experiments have been conducted for military concerns and general public health as well. The more dangerous gases are denser than air and are emitted as a gas-aerosol mixture. Impacts are generally greatest in the near field (less than about 1 km). The data from many of these experiments have been collected in Modelers Data Archive [Chang, 2004].

2.5 Post-Processing of Modeling Results

As meteorological and dispersion models generate very complex three-dimensional numerical output, it is generally required to bring the data into visualized form. Some
appropriate graphical tools in this regard are generally helpful in performing such kind of work. This activity is called as ‘post-processing’ of the computational results. It helps in developing quick understanding of the modeling predictions indicating potentially most vulnerable areas affected by the dispersing plume.

There are some computer packages which are normally used for the purpose of post-processing the numeric data. The examples are GrADS, SURFER and VIS5D. Grid Analysis and Display System (GrADS) is an effective graphical tool for manipulation and visualization of numeric data. Using the software, data may be processed and displayed using a variety of graphical techniques such as line and bar graphs, scatter plots, smoothed or shaded contours, wind vectors, streamlines, grid and shaded grid boxes. GrADS supports many data file formats, including Binary, GRIB (Gridded Information in Binary Form), NetCDF (Network Common Data Format), HDF (Hierarchical Data Format) and BUFR (Binary Universal Form for the Representation). Some dispersion models have their own post-processing modules and graphical tools such as CALPUFF, ALOHA and HOTSPOT etc.

Considering the versatility of the available post-processing packages available it seems that little effort has been made on three-dimensional (3D) visualization software packages for dispersion simulation of industrial stack releases. In a dispersion study, a MATLAB program was presented for three-dimensional dispersion simulations of different pollutant releases from an industrial stack [Fatehifar, 2006]. The pollutants include SO₂, NOₓ etc. The overall purpose of this MATLAB program was to study the effects of different meteorological and stack parameters on the dispersion of pollutants like wind velocity, ambient temperature, stability class, exit temperature, exit velocity, concentration and stack height. In addition to the guidance one may have for reducing maximum ground level concentrations, it also acts as a post-processor and the output results of this program could be visualized in 3D graphical form.

A system was designed and presented for the real time modeling of the hazardous emissions from multiple industrial stacks [Bais, 1989]. The system consisted of a u. v. vector anemometer and the sensors for measuring ambient temperature, relative humidity and source term. The system was interfaced with a microcomputer. The output signals of the anemometer were fed into an interface. The software of system had an independently running routine that red the interface ports five times every 3
sec and calculated and displayed the wind speed and direction. At 10 minutes sampling intervals, the mean vector wind speed and direction as well as standard deviation of the wind direction were calculated. The concentrations of pollutants were calculated both at ground level and at various heights from ground using Gaussian puff model. This system had been installed in three major industrial plants in Greece. The authors compared the real time estimates of SO\textsubscript{2} concentrations from the system with those measured with a commercial analyzer in order to validate the system. It was concluded that the system could be used as a tool for real time visual simulation of pollutant concentration from industrial stacks.

The computer packages discussed above are generally used to display the numeric data into contours but mostly the general graphical tools and available in the open domain only provide 2D view. Hence, an efficient three-dimensional post-processor is required to display the multilayered streaming data of geographical boundaries, topography, wind field and particle positions in a plume in a single window in the form of real time or even faster 3D animation or movie that is extremely useful for the management for decision making in accidental scenario.

### 2.6 Summary

A detailed review is presented covering current and advanced atmospheric dispersion modeling strategies, their effectiveness, validity and application from the viewpoint of regulatory as well as administrative and decision making processes. It elaborates the upgraded provisions and superiority of Puff and particle models over conventional Gaussian Plume model (GPM). The features like prevailing wind field, effect of surface shear, topography and meteorological parameters that are usually addressed by a coupled meteorological and dispersion model are not very well addressed by GPMs reflecting a need of coupling advanced dispersion model by a meteorological model. Moreover literature also emphasize that due consideration should also be given to various parameterization schemes used in meteorological models i.e. prior to couple any meteorological model with a dispersion model, its selected parameterization scheme is required to be thoroughly validated for the region under consideration.

The review revealed some successful attempts of coupling meteorological model such as MM5, WRF with advanced dispersion models such as CALPUFF or FLEXPART
indicating their potential for use in south Asian region. The conversion rates of primary pollutants are worth considering as they play an important role in the removal of air pollutants from the atmosphere. Literature review in this regard suggests incorporating the chemical removal term in particle models to enhance the degree of accuracy in modeling predictions.

Model predictions anyway are dependent on set of mathematical equations involving certain constants and parameters that are based on theoretical concepts involving various assumptions. Hence, the modeling predictions cannot be reliable until model is validated by actual ground based observed data. Meteorological models have to be verified by meteorological data such as temperature, precipitation, wind velocity, wind direction, pressure, humidity etc. Once the meteorological model is validated by factual data, it’s computed meteorological parameters at grid points fed to dispersion model would be considered as ‘reliable’. On the same logical grounds, it is necessary to validate ‘dispersion model’ by comparing its final result with factual concentration data collected on ground by tracer experiments at the specified location. This implies that tracer experiments need to be conducted on specific locations where any industrial site or emission source is being located. Once coupled model is validated for the site, the prediction by the model may be used for tracing plume trajectories and ground level concentration.

The post processors generally available in the open domain only provide 2D view or can only display the numeric data into contours in third dimension. Hence, an efficient three dimensional post processor warrants its effectiveness if it displays the multilayered streaming data of geographical boundaries, topography, wind-field and particle positions (plume trajectory) in a single window in the form of real time or even faster 3D animation or movie. Such type of post processor is expected to be extremely useful for the disaster management and evacuations in accidental scenario.
CHAPTER 3

Computational and Experimental Setups

This chapter is divided into two main sections. First is related to computational model configuration and procedures for simulation work whereas second part is concerned with experimental setups and methodologies for experimental validation. Computational resources such as high performance computation facilities and clusters were employed and procedures were adopted for predicting plume concentration and trajectories using coupled meteorological and dispersion models. While performing computations, initial part is related to description of meteorological models and procedures used for simulation of meteorology of region under consideration. This is followed by description of coupling meteorological model with a Lagrangian based dispersion model under scenarios of toxic gas released from different sources. Prime importance remains validity of such predicted results obtained by computational modeling. Hence, an experimental set up was required that should incorporate precise control, not only on emission source term, but also on temperature, exit velocity, pressure etc. at which gas is emitted. In this regard detailed description of design and fabrication work to develop an experimental facility at PIEAS is given in subsequent section. Procedures followed to conduct dispersion experiment using sulfur dioxide (SO₂) and sulfur hexafluoride (SF₆) as tracer gas are also elaborated including sampling methodology for accurate measurement of ground concentration of tracer gas in ambient air to compare the same with computational results for validation.

3.1 Computational Requirements for Simulations

Ultimate aim of this research was to accurately predict plume trajectory and resulting ground level concentration in an accidental scenario for declaring general emergency, evacuation and making other important decisions. In this regard coupled meteorological and dispersion models e.g. MM5+CALPUFF and WRF+FLEXPART were to be used. For meteorological models, domain size is usually in hundreds of kilometers in length and breadth whereas vertical dimension is normally taken in kilometers. For instance if a model domain of 2220 km × 2220 km is selected with a spatial resolution of 30 km while vertically 24 layers are considered, then total nodes
at which calculation has to be performed per time step would be $75 \times 75 \times 24$ i.e. 1,35,000. If simulation has to be run for hourly average of one month taking a time step of three minutes, computational time and resources would increase tremendously. Moreover, calculations have to take care of topographical and geographical data at surface domain as well. It also involves calculation of wind field within which plume is injected. Calculation of plume trajectory involves bulk motion of toxic pollutant with wind and diffusion in lateral and vertical direction due to concentration difference. Hence these calculations go beyond the capability of personal computers even if high specification Personal Computer prevailing in the market is used. Thus present research required advanced computational resources for quick and colossal production of output results. This situation led to take initiative for deploying a computer cluster to accelerate pace of simulation work. Later, these models were also executed on a High Performance Computing (HPC) machine available at PIEAS. Procedure for setting up a Linux based cluster is described herein details.

### 3.1.1 Deployment of PC Cluster and HPC Facility

A cluster of 16 computers was established for execution of simulation codes used in present work. Based on execution requirements of specific computer codes, cluster is generally developed for serial or parallel processing. Keeping in mind, requirement of massive execution of various jobs at the same time, batch processing cluster was found to be most suitable solution. To serve this purpose, sixteen high spec computers (Intel (R), core 2 Duo CPU) with 4.0 GB RAM and 3.0 GHz speed were selected for deploying the cluster. The server (core 4, Intel (R), Xeou (R)) to distribute work to these nodes had 2.33 GHz processing speed and 8.1 GB RAM. A Gigabit switch (4200G, 24-port, model No. 3CR17661-91) was used for creating network infrastructure based upon Fast Ethernet. Scientific Linux was installed on each computer as a prerequisite for deployment of cluster, and then some free open source packages were installed under Linux environment.

A complete suit containing cluster components as Open PBS (Portable Batch System) /Torque/Maui was used to create complete batch-processing environment. Open PBS was used for creating basic framework for batch processing. Open PBS consisted upon two components. One component was installed on the machine that acted as a PBS server while other component PBS client was installed on all other nodes called worker
nodes. PBS server acted as master node for controlling working nodes, managing resources, housekeeping and scheduling jobs. Jobs submission, monitoring and controlling was responsibility of PBS server, while worker nodes acted as slaves for providing computing power. PBS package provided a special scripting language for defining environment for submitting jobs in batch queue. The PBS script was used to define various parameters/activities for jobs execution. Torque package was used to extend the facility of resources management. Maui scheduler was responsible for jobs control such as management, monitoring, scheduling and execution.

A common shared disk storage area in cluster was declared called storage element that was made accessible to all nodes in cluster, using Network File System (NFS). The NFS server was installed on server having direct access to shared disk storage devices and logically defined it mountable by other nodes in cluster. Each node mounted this mountable point, which ultimately gave fast, seamless sharing across network. Working nodes were able to have access to local hard disk as well as NFS shared storage. All useful codes/data was kept in shared storage area so that they were accessible to all working nodes for executing jobs. Shared storage area was used for installing all common software packages such as compilers, editors, libraries and graphic tools etc. Advantage of that area was that only one copy of software was required for installation and could be used by all working nodes.

Once job is submitted it is queued and PBS keeps on watching available resources on the cluster and submits job to a free node. On arrival of job on a particular machine, script copies all its input files from shared storage to user area on local hard disk. This step is called stage-in. Once execution is finished, output files can be copied to user directory in storage area. This step is called stage out. This stage-in and stage-out step is performed to optimize performance of system. Shared area is accessed by all nodes and sharing is done via NFS using Local Area Networking (LAN).

### 3.2 Computational Procedures and Strategies

Overall computational and research work performed in this thesis may be divided into nine major parts. First part involved use of MM5 to verify sensitivity of convective parameterization schemes on model predicted results with subsequent comparison with observed data. Several computational runs of MM5 were executed on sixteen PC cluster to compute the summer monsoon precipitation for July and August of 1998.
and 2001. In second part, bi-weekly runs were executed on twenty-four hourly average basis to evaluate the performance of coupled MM5-CALPUFF system for simulating stack releases from an oil refinery. In subsequent part, air quality assessment was performed within and near an industrial area by comparing predicted pollutant concentration by MM5-CALPUFF modeling system with limits prescribed by World Health Organization (WHO) and local regulatory bodies. Next three parts were related to simulation of SO2 releases from ground, brick kiln and experimental stack using coupled MM5-CALPUFF system and further comparing it with experimentally collected data. Seventh part was focused on inclusion of chemical removal term in Lagrangian based model as FLEXPART. The next part was related to six-hourly simulation of plume trajectory from an experimental facility at PIEAS to identify potential areas that may be affected in case of inadvertent release of any hazardous gas. This was done using coupled WRF-FLEXPART modeling system. The final part of computational research work involved validation of coupled MM5-CALPUFF modeling system using sulfur hexafluoride (SF6) as a tracer gas released from a proposed industrial site.

3.2.1 Computational Strategy for Sensitivity Analysis of MM5 Convective Parameterization Schemes

An investigative study was performed for Pakistani South Asian region to evaluate performance of a selected convective parameterized scheme in a mesoscale model (MM5). Results of this study are presented in section 4.2. As mentioned earlier that MM5 employs various parameterization schemes. It was imperative to decide which parameterization scheme suits South Asian regions, specifically the parts that are geographically included in Pakistan. Once a specific parameterized scheme of MM5 was finalized for the region and time interval, trans-boundary pollution dispersion studies could be carried out by coupling mesoscale model with a specific advanced dispersion model.

A model domain was selected from 20 to 40° N and 60 to 80° E with spatial resolution of 30 km to focus on Pakistani South Asian region for simulation of precipitation. Global dataset of USGS (United States Geological Survey) for land use and topography with 10 minutes spatial resolution were used as input to the model. For initial and boundary conditions, archive of analyzed data produced by United States National Centre for Environmental Prediction (NCEP) at 2.5° of spatial
resolution and 12h of temporal resolution downloaded from the website http://dss.ucar.edu/datasets/ds083.0/data/ was used. As mentioned previously, there are different parameterization options (cumulus, planetary boundary layer, humidity, radiation, surface temperature) available in MM5. In this study main emphasis was on cumulus schemes in the model that were tested to identify suitable convective scheme to predict summer monsoon precipitation for July and August of 1998 and 2001 over the region of interest.

Next step was selection of other physical options with a specific cumulus convective scheme. There may be several combinations available for selection. This open choice of selection of a model configuration makes it difficult to choose an appropriate combination of these schemes for simulating local climate of target region. Even if such a cumbersome and lengthy strategy is followed, it cannot be compared with other studies done in nearby regions available in literature. Therefore, a unique set of other physical options [Sardar, 2012a] with a cumulus convective scheme was selected for present study that was commonly used in other studies conducted in nearby regions [Kerkhoven, 2006; Ratnam, 2006]. In addition, ‘Simple ice scheme’ [Schultz, 1995] was selected under option of ‘Explicit moisture scheme’. This scheme deals with rain water and ice cloud processes as well, without any requirement of additional memory. Moreover, this simple microphysical scheme does not include graupel or hail properties and may be suitable to reduce complexity of analysis. Subsequently under heading of ‘Planetary Boundary Layer Scheme’, ‘Medium Range Forecast Model’ was selected which was implemented in National Centre for Environmental Prediction (NCEP) medium range forecast model by Hong [Hong,1996]. This scheme was selected due to its computational efficiency in order to incorporate atmospheric vertical diffusion processes due to turbulence in an unstable environment. Under option of ‘Radiation Scheme’, ‘Cloud Radiation Scheme’ [Dudhia, 1989] was selected which is based on interaction of both short and long wave radiation with environmental air and cloud, by considering absorption and scattering processes in atmosphere. In addition, this scheme also considers surface radiation fluxes. Finally ‘Five layer soil model’ was selected under option of ‘Surface Scheme’ [Dudhia, 1996]. For prediction of ground temperature, soil temperature and soil moisture etc., this multilayered surface scheme takes into account five soil layers of approximate thicknesses at 1, 2, 4, 8 and 16 cm with a fixed substrate located
below. In order to investigate influence of different convective parameterization schemes on some other meteorological parameters such as ambient temperature, potential temperature, relative humidity and moist static energy, simulations were performed with spatial resolution of 90 km for model domain. Reason for selecting coarse spatial resolution of 90 km in this case was only scarcity of data of resolution as fine as 30 km for validation purpose. Reanalysis data of United States National Centre for Environmental Prediction (NCEP) which was available at the website http://www.esrl.noaa.gov/psd/data/gridded/data.ncep.reanalysis2.pressure.html were used to validate predicted results for vertical profiles of these parameters.

Since results given in section 4.2 reveal satisfactory validation of model studies with observed data, this strategy was finalized and used in all subsequent cases wherever Mesoscale Meteorological model (MM5) was used.

3.2.2 Modeling Procedure for Predicting SO₂ Emission from an Oil Refinery

A simulation study was performed using integrated CALPUFF-MM5 modeling system for predicting SO₂ emission from an oil refinery. Results of this simulation are presented in section 5.1.2.2. Description regarding CALPUFF and MM5 employed can be found in sections 2.1.1.2 (a) and 2.1.2.1 respectively. Modeling procedure and strategy used for this study is elaborated here.

Model domain was set to cover area of 60 km × 60 km taking location of oil refinery as the center of domain. In order to account for earth curvature, Lambert Conformal Conic (LCC) map projection was chosen with a grid spacing of 1 km. Eleven vertical layers for modeling domain were selected at heights of 0, 20, 40, 80, 160, 320, 700, 1300, 1700, 2300 and 3000 meter. Observational meteorological data from a surface station located at 24.467° N, 56.641° E within study area was available but upper air observations were not available for the domain. Thus hourly three-dimensional meteorological data was input as initial guesses for diagnostic model, CALMET was provided by running MM5 model for a period of 15 days from June 1, 2008 to June 15, 2008. Initial and lateral boundary conditions were taken from Final Analyses (FNL) data provided by National Center for Environmental Prediction (NCEP). NCEP data archived at NCAR (National Center for Atmospheric Research) contains
spatial resolution of one degree and temporal resolution of 6 hours. Terrestrial data of land use and topography for model execution was obtained from MM5 website (ftp://ftp.ucar.edu/mesouer/MM5V3/TERRAIN_DATA).

An interface utility named CALMM5 was used to convert meteorological data of MM5 into a format compatible with CALMET. Before running CALMET, a geophysical file comprising of information regarding land use, topography and surface parameters of domain under investigation was generated. CALMET was run to interpolate coarse grid data of MM5 onto a fine scaled grid. CALMET was executed for a period of 15 days (June 1–15, 2008) with MM5 output as well as surface observations obtained from surface station. In next step, CALPUFF dispersion model was executed for entire period. Information about source emission and locations of eleven stacks of oil refinery used to execute CALPUFF model can be found in Appendix-I. A post-processor of CALMET named PRTMET was used to analyze and display meteorological parameters from binary CALMET output file. Finally CALPOST was used to process files from CALPUFF, generating a summary of simulation results in tabulated as well as in gridded form.

3.2.3 Computational Methodology for Assessing Impacts of Flaring Activities on Air Quality

An integrated modeling system comprising of mesoscale model, MM5 and dispersion model, CALPUFF was used in present study to assess impacts of flaring activities in an oilfield on nearby ambient air quality.

Site specific meteorological data at oilfield was not available, that is why meteorological input as initial guesses for diagnostic model CALMET was provided by running MM5 model. MM5 was executed selecting two nested domains containing spatial grid resolutions of 12 and 4 km centered at 18.695° N and 55.487° E.Domains had a number of grid points as 40×40 and 49×49 and 36 vertical levels. For initialization of MM5 model, input meteorological data of surface and upper air were provided from final analyses (FNL) data, provided by National Center for Environmental Prediction (NCEP). Model was run for one month from June 1 to 30, 2010. Data output was obtained from model after 1 hour. An interface utility was used to convert output from MM5 to CALMET. Model domain of CALMET was set to cover area of 70 km × 70 km selecting location of production station as central point.
of domain. Information about map projection, grid spacing and vertical layers height is same as described in section 3.2.2 para 2. CALMET automatically interpolates MM5 model grid system to its own grid. CALMET was executed for period of one month i.e. June, 2010 to produce micrometeorological data for CALPUFF. Information about emission rates, characteristics and location of production station as well as two flares can be found in Appendix II. To assess status of air quality, 10 sampling locations were selected within study area. Locations of receptors were selected in range of 100 m to 5 km from flaring sources. Locations were situated at both upwind and downwind areas of studied domain. Using data of meteorology from CALMET and source characteristics shown in Appendix II, CALPUFF model was executed to determine the SO$_2$ ground level concentrations at discrete receptors. CALPOST module was employed to get average and report model predicted concentrations based on output data file from CALPUFF. Peak values of concentrations data for different average sampling periods were generated using this module at each discrete receptor points. Schematic configuration of CALPUFF modeling system and meteorological model MM5 is given in Appendix III.

### 3.2.4 Strategy for Dispersion Modeling of Ground Release of SO$_2$

SO$_2$ emission in ground experiment was simulated using MM5-CALPUFF modeling system for comparing predicted ground level SO$_2$ concentrations with measured ones during experimentation. Results of this study are presented in section 5.1.1. Model configuration used in this simulation is elaborated here.

Location of emission point (33.654° N and 73.266° E) was taken as domain center of CALPUFF model. Meteorological data generated by MM5 were used as initial guesses to diagnostic model CALMET of CALPUFF model. For initialization of MM5 model, archived data of United States, National Centre for Environmental Prediction (NCEP) containing spatial resolution of 1°and temporal resolution of 6h were used. Data of source characteristics i.e. source height, diameter and emission rate etc. and locations of discrete receptor points used in this simulation can be found in section 3.3.2.1 which provide details of experimental part of this study. As air samples were collected by mobile van at a height of about 16 feet, same height from ground was used for all receptor points selected in model simulations. Release and
averaged sampling time was selected as 1 hour. Simulations were made by CALPUFF model for same period as involved in conducting experiments for sake of comparison.

### 3.2.5 Modeling Strategy for Simulation of Brick Kiln Releases

A simulation study was performed using integrated MM5-CALPUFF modeling system for predicting SO$_2$ emission from an isolated brick kiln. Results of this simulation are presented in section 5.1.2.1. Description regarding modeling procedure used in this study is presented here.

A specific location was selected as an observation site near “Tarlai Kalan” in north-eastern side of capital city of Pakistan i.e. Islamabad. An isolated coal fired brick kiln was selected to assess impact of its releases on nearby air quality. Due to lack of site-specific meteorological data, MM5 simulations were used as initial guess fields for diagnostic meteorological package CALMET of CALPUFF modeling system. MM5 generated data were further used to simulate wind fields with finer resolution over region of interest. MM5 was executed with input data for global topography and land use of 2 minutes spatial resolution (approximately equal to 4 km). Global meteorological dataset as Final Analyses (FNL) of National Center for Environmental Prediction (NCEP) with 1 degree spatial and 6hr temporal resolution was used for initial and boundary conditions of MM5 model. CALPUFF model was employed with a single model domain centered at latitude 33.614° N and longitude 73.153° E. There were 11 grid points selected in each ‘X’ and ‘Y’ direction with a grid spacing (domain resolution) of 1 km and 10 vertical layers were selected. Map projection of Lambert Conformal was applied. Finally post-processor CALPOST of CALPUFF model was used to obtain a summary of simulation results.

### 3.2.6 Modeling Strategy for Higher PIEAS Stack and Larger Receptor Distances

Experimental releases of SO$_2$ from PIEAS stack were simulated by using MM5-CALPUFF modeling system. Results of simulations are presented in section 5.1.3. with comparison of concentration data collected during experimentation. Modeling procedure used in the study is presented here.

Stack location (33.65° N, 73.26° E) was taken as central point of the model domain. To derive meteorological module as CALMET of CALPUFF model, data were
provided by running MM5 mesoscale model. MM5 model was initialized with data of Global topography, land use and meteorology. CALPUFF model was executed with source characteristic and emission data as mentioned in section 3.3.2.3 (d) in which experimental details of tracer experimentation has been provided. Release period and sampling time was selected as 1 hour. Concentrations were predicted by the model at different receptors selected within one kilometer distance from experimental stack.

### 3.2.7 Inclusion of Chemical Removal Term in Lagrangian Model

Atmospheric chemical reactions transform primary pollutants into secondary air pollutants. These reactions decide ambient concentrations of SO\(_2\) and NO\(_2\) in a chemical plume. In order to account for impact of chemical removal of SO\(_2\) and NO\(_2\) on resultant ground level concentrations from Lagrangian model FLEXPART, few subroutines based on empirical correlations representing chemical transformation rates were included in the model. Same formulation was originally developed and used in dispersion model MESOPUFF II. Later on, these expressions were also used in dispersion model CALPUFF. A photochemical box model was used to generate transformation rates on hourly basis. Simulation work has been performed by various researchers regarding dispersing a plume of SO\(_x\) and NO\(_x\) in ambient air containing ozone and reactive hydrocarbons (RHC) [Scire, 2000b]. Considering diversity of environmental conditions including different solar radiation intensities, temperatures, dispersion conditions, emissions times and background concentrations of ozone, reactive hydrocarbons, NO\(_x\) of plume, hourly transformation rates of SO\(_x\) and NO\(_x\) generated by box model were statistically analyzed. Finally, parameterized expressions were obtained by curve fitting to hourly conversion rates predicted by photochemical model for day time. These conversion rates are expressed as:

\[
k_1 = 36 \, R^{0.55} \, [O_3]^{0.71} \, S^{-1.29} \, + \, 3 \times 10^{-8} \, RH^4 \quad (3.1)
\]

\[
k_2 = 1206 \, [O_3]^{1.5} \, S^{-1.41} \, [NO_x]^{-0.33} \quad (3.2)
\]

Where ‘\(k_1\)’ is SO\(_2\) to SO\(_4\) \(-\) transformation rate (percent per hour). ‘\(k_2\)’ is NO\(_x\) to HNO\(_3\)+PAN transformation rate (percent per hour).‘\(R\)’ is total solar radiation (Kw/m\(^2\)). ‘\(O_3\)’ is background ozone concentration (ppm). ‘\(S\)’ is a stability index ranging from 2 to 6 (Pasquill-Gifford-Turner (PGT) class A and B=2, C=3, D=4, E=5, F=6). ‘\(RH\)’ is relative humidity in percent. ‘\(NO_x\)’ is concentration of NO\(_x\) in released
plume. Though these expressions were included in FLEXPART model, but because of limited time of research, modeling work and validation of computational results has been suggested as future recommendation. Subroutines included in model are given in Appendix-IV.

3.2.8 Modeling Procedure for Simulation of Plume Trajectories

Dimensions of model domain were set as 360 km × 360 km × 15 km taking central point of domain at 33.66° latitude and 73.27° longitude. Coordinates of central point coincide with location of release point. Number of grid cells in x, y and z directions was selected as 30, 30 and 24 respectively considering grid resolution of 12 km. Eulerian–Lagrangian modeling system (WRF+FLEXPART) was employed to simulate plume trajectory by calculating positions of emitted particles in plume. Wind fields were calculated with Weather Research and Forecasting (WRF) model. For initialization of the meteorological model (WRF), meteorological data (http://dss.ucar.edu/datasets/ds083.2/data/) of one degree spatial and 6h temporal resolution were used from archive of analyzed data produced by US National Centre for Environmental Prediction (NCEP). Data of land use type and terrain elevations (2 min. spatial resolution) were provided by USGS (United States Geological Survey). Trajectory of particles was traced out using Lagrangian particle dispersion model as FLEXPART for about 6 hours. It was assumed that a single puff with 1000 particles was released at about 00:00 h on June, 2, 2009 from a 30 m high experimental stack at 33.66° latitude and 73.27° longitude. Initial velocity of released particles was assumed to be zero. No chemical reactions were considered. Gravity effect was also neglected considering very small size and weight of particles.

3.2.9 Modeling Procedure for Dispersion Simulation of SF₆ Tracer

A simulation study was performed using MM5+CALPUFF modeling system for simulating dispersion of SF₆ tracer in a coastal region of Pakistan. SF₆ was released at 70 m height from a meteorological tower. Results of this study are presented in sections 5.1.4. Modeling procedure for this study is presented here.

Dimensions of modeling domain were selected as 30 km × 30 km taking location of meteorological tower (24° 51' 10.8" N and 66° 47' 10.5" E) as the center of domain. Lambert Conformal Conic (LCC) map projection was selected. Horizontal grid
spacing for domain was chosen as 1 km. Eleven vertical layers with variable heights were selected in such a way that distance between lower levels was kept small as compared to that for upper levels. Meteorological data is a key input data that is required for running dispersion model CALPUFF. Hourly three-dimensional gridded meteorological data input for CALPUFF dispersion model were provided by running MM5 model for a day on April 29, 2013. Initial and lateral boundary conditions to execute meteorological models were taken from Final Analyses (FNL) data provided by National Centre for Environmental Prediction (NCEP) archived at NCAR. NCEP data contains spatial and temporal resolutions of one degree and 6 hours respectively. Source height and diameter were selected as 70 m and 5/16". Release rate of SF$_6$ was 6.7 g/sec for a period of 1 hour. Six arcs as Arc-A to Arc-F were marked for collecting SF$_6$ samples within a radius of 10 km. Arcs were marked at different distances of 0.7, 1.5, 3, 5, 7 and 10 km. Number of sampling points selected in Arc-A to Arc-F was 24, 26, 26, 19, 17 and 16 respectively in each arc. Other details regarding distance and coordinates of each sampling point are presented in Appendix V. Three samples for 10 minutes time period were collected with interval of 5 minutes among consecutive sampling activities.

3.3 Methodology for Experimental Validation

All MM5+CALPUFF and WRF+FLEXPART model results using above mentioned modeling strategies as described in section 3.2.1 to 3.2.9 have to be verified by experimental data. This experimental validation is done in two respects. One is validation of meteorological model itself, and other is validation of results of ‘coupled meteorological and dispersion model’.

3.3.1 Validation of Meteorological Model

Meteorological models are validated by data of meteorological parameters that are observed and collected at ground based meteorological stations or collected through satellites. In present research this validation is performed by data collected from a meteorological station near oil refineries. Moreover, precipitation data collected by Pakistan Meteorological Department was employed as well as satellite derived data for Pakistani region was also used for validation purposes. Reanalyses data from NCEP including ambient temperature, potential temperature, humidity and moist static energy for Pakistani region was also used for meteorological model validation.
3.3.1.1 Observed Data from Surface Met Station near Refineries

Hourly data of ambient temperature, wind speed and wind direction collected at surface met station located near oil refinery was employed to validate meteorological model MM5. This validated MM5 coupled with dispersion model CALPUFF was used subsequently for modeling pollutant dispersion from oil refinery. Methodology of this modeling is already described in sections 3.2.2 and results are given in section 4.1.1.

3.3.1.2 TRMM Satellite Derived Rainfall Data

As extent of rainfall plays an important role in scavenging pollutants from atmosphere, if physical and chemical removal of pollutants is to be incorporated in overall dispersion modeling, it is essential to simulate trends of precipitation. Once a specific parameterized convective scheme of MM5 is finalized for the region and time interval, trans-boundary pollution dispersion studies may be carried out by coupling mesoscale model with a specific Eulerian-or Lagrangian dispersion model. Hence to validate MM5, TRMM satellite derived rainfall data was used. Tropical Rainfall Measuring Mission (TRMM) is a joint mission between National Aeronautics and Space Administration (NASA) and Japan Aerospace Exploration Agency (JAXA) designed to monitor and study rainfall in tropical and sub-tropical regions of Earth. TRMM is an Earth-observation satellite that provides important precipitation information using several space-borne instruments. Gridded TRMM Satellite derived rainfall data (3B43RT) was used to validate MM5 model predicted results of monthly accumulated rainfall in summer season in South Asian region. Spatial resolution of data was 0.25 × 0.25 degree. This data can be downloaded from the web link which is mentioned as [http://disc.sci.gsfc.nasa.gov/precipitation/documentation/TRMM_README/](http://disc.sci.gsfc.nasa.gov/precipitation/documentation/TRMM_README/)

3.3.1.3 Pakistan Meteorology Department Data for Validation

Surface synoptic observed data of Pakistan Meteorological Department (PMD) for South Asian region was also employed for validation of meso-scale model MM5 by comparing its predicted results of monthly accumulated rainfall in summer monsoon season from July to August of 1998 and 2001.
3.3.1.4 NCEP Collected Data for South Asian Region

In addition to rainfall, other meteorological parameters such as temperature, humidity and moist static energy etc. were also used to validate meteorological model. Reanalysis data of US National Centre for Environmental Prediction (NCEP) were used to validate MM5 model-predicted results for vertical profiles of ambient temperature, potential temperature, relative humidity and moist static energy. NCEP data were used for specific location of the city of Islamabad (33.6° N, 73.1° E) for month of August, 1998. Data available at NCEP side is of various spatial and temporal resolutions such as 1°, 2.5° with daily averaged or monthly averaged basis. In this modeling, monthly averaged data with 1° resolution was employed. Datasets of any mentioned resolution can be downloaded from the web link mentioned as http://www.esrl.noaa.gov/psd/data/gridded/data.ncep.reanalysis2.pressure.html.

3.3.2 Validation of Dispersion Models

As mentioned earlier in section 1.1.3, validation of ‘coupled meteorological and dispersion’ modeling system is of prime importance to determine performance and efficiency of predicted results. There may be two methods of doing these validations. One is to get available observed data of pollutant concentration from any system of pollutant emission sources and use identical conditions of source term to model scenario by coupled MM5-CALPUFF or WRF-FLEXPART system to verify its validation. If predicted results compare well with observed dataset of pollutant concentration, the model is said to be validated. Second option may be to conduct field tracer experiments locally in which a controlled amount of tracer is released from a source and its ambient concentration at different sampling locations is determined on site by different sampling and analyzing techniques.

In present work, first option was used for validation of coupled MM5-CALPUFF modeling system by modeling a simple release scenario of SO$_2$ from cluster of stacks of oil refineries of Oman for which ground concentration data was available for validation given in Table 5.9. In these studies a confidence was gained on coupling of meteorology and dispersion codes.

A number of tracer experiments have been conducted internationally and datasets are compiled from such kind of experimentations. These datasets may be used for
validation of different dispersion models provided that the region under consideration has identical meteorological conditions and topography. Such tracer experiments have never been conducted in typical meteorological and topographical conditions of Pakistan. Hence no ground level ambient pollutant concentration datasets are available as such in Pakistan to validate modeling results.

In present research work, a sequential study was initiated from modeling of simple release scenario of tracer gases from an emission source. Initiating from source elevation as low as 30 ft and emission-receptor distances as 165 ft to source elevation as high as 230 ft and emission-receptor distances of 33,000 ft. These tracer experiments may further be extended to even higher stacks and emission-receptor distances of hundreds of kilometers covering a broader region and trans-boundary dispersion in future. More elevated releases and greater distances are beyond the scope of this thesis research and are therefore suggested as future work.

Present research work may be divided into four sets of experiments. First set involves simple dispersion/diffusion experiments at a very short scale horizontally and vertically. Over a flat ground, a support system was erected and SO₂ gas was released at a height of 30 ft through a six inch internal diameter conduit and air samples were taken in prevailing wind direction at few sampling points on each of three arcs at varied radii from 165 ft to 495 ft. In second set of experimental work, height was increased to double i.e. 60 ft which is the usual height of brick kilns while samples were collected at sampling points covering larger distances. Clusters of emission sources were also considered. In third set of experimentation, 100 ft stack was used and air samples were collected at four sampling points in different directions at varied distances ranging from 1050 ft to about 2871 ft. In final set of experiments, SF₆ gas was released at height of 230 ft through a conduit of 5/16 inch internal diameter and samples were taken at 37 sampling points at distances ranging from 2300 ft to about 33000 ft. Sampling points were fixed depending upon prevailing wind direction and accessibility.

Two tracers used in these experiments are sulfur dioxide (SO₂) and sulfur hexafluoride (SF₆). Initial three sets of experiments were performed with SO₂ as tracer. Reason behind using SO₂ was the inspiration that tracer experiments were initiated by Prairie Grass Experiments [Barad, 1958] in which SO₂ was used as tracer gas. SO₂ is a very common and easily available gas and analytical ultra-pure
SO₂ cylinders were not only easily obtainable from local market but cylinders of various concentrations can also be prepared by dilution. In second set of experiments in which stack of brick kiln was considered, coal as a fuel was being used which always has certain sulfur content and on combustion produces sulfur dioxide in flue gases. Hence there was a tracer that was automatically being formed and emitted from brick kilns stack for dispersion studies thus eliminating any requirement of cylinders. In third set of experiments, apart from directly blowing SO₂ from a cylinder in air, an alternative economical option of a combustion rig was available that was attached to stack. Any calculated amount of sulfurous compound added to the flame would produce required concentration of sulfur dioxide in flue gases that can be verified by stack gas analyzers within combustion rig as well as at exit of stack. Moreover, sampling and analysis at parts per billion level concentration of SO₂ in ambient air was simple and easy, specifically with availability of highly sophisticated ambient air quality monitoring mobile van that was very generously offered by Pakistan Environmental Protection Agency (Pak-EPA) whenever requested.

There were some limitations in using SO₂ as tracer gas for atmospheric dispersion modeling studies. It is an environmentally noxious gas and could not be emitted through stack beyond certain prescribed limits. Moreover, there are many sources of SO₂ emission that are frequently emitting this gas hence one cannot be sure whether the SO₂ measured in ambient air at certain location is actually coming from PIEAS experimental stack or it has some local origin. This model validation work was being carried out in a sub-urban area called Nilore, located about thirty kilometers from main city with no local brick kilns or any noticeable larger SO₂ emitting source. Hence, to a certain level of confidence, measured ambient air concentration of SO₂ could be definitely correlated to the source term maintained and controlled at PIEAS experimental stack.

3.3.2.1 Experiments with Ground Release of SO₂

Small scale dispersion experiments were conducted in sports ground at PIEAS. Dimensions of ground are 150 m × 110 m and its central point coordinates are 33.65° N and 73.26° E. A supporting structure of 30 ft height was erected in ground. SO₂ was released through a 6” internal diameter PVC pipe of 30 ft height and
fastened with supporting structure as shown in Figure 3.1. Fifty liter Gas cylinder with 10% (i.e. $10^5$ ppm) \( \text{SO}_2 \) in nitrogen filled at 2200 psi weighing 1.9 kg was used in the experiment. Tracer was planned to be released during day time from 10:00 am to 05:00 pm. 100 ppm of \( \text{SO}_2 \) gas was released during experiments with release rate of 0.05 g/s for release period of one hour. For diluting the cylinder gas from $10^5$ ppm to 100 ppm, a blower of 400 cfm was attached with lower end of PVC pipe. Flow rate of 11 liter/min of cylinder gas was entered into PVC pipe through a tee-joint in centre of pipe.

![Figure 3.1: Supporting Structure for Releasing SO\(_2\) through PVC Pipe](image)

This flow rate was maintained by mass flow controller duly verified by a flow meter. Source term at exit was continuously monitored by a portable \( \text{SO}_2 \) stack gas analyzer by taking suction of samples of air exiting from upper end collecting the gas through a multi-nozzle sampler into the inlet of analyzer. It was important to keep this source term constant and this was ensured by keeping flow rates from gas cylinder and blower at a fixed value. Wind speed and its direction during experiments were thoroughly monitored with the help of wind anemometer and wind vane installed on top of EPA van. A flag as a wind barb was also fastened with supporting structure for indicating wind direction. Decision of releasing tracer was based on observed wind data. Experimental arrangements are depicted in Figure 3.2.

Sampling locations were marked on each of three semicircular arcs drawn at 50, 100 and 150 m from source in prevailing wind direction. Sampling locations were selected on basis of collected wind characteristic data of some previous days. Sampling points selected at each arc were designated as A1 to A4 in Arc-A, B1 to
B2 in Arc-B and C in Arc-C. Distribution of sampling locations is presented in Figure 3.3.

![Sampling Point Distribution in Different Arcs around SO2 Source](image)

Figure 3.3: Sampling Point Distribution in Different Arcs around SO2 Source

Mobile van of Pakistan Environment Protection Agency (PAK-EPA) was used to collect and analyze ambient samples of SO2 from selected sampling locations. Data of metrological parameters were collected with help of meteorological instruments installed on top of mobile van.

![Meteorological Instruments Installed on Van](image)

Figure 3.4: (a) Ambient Air Monitoring Van (b) Meteorological Instruments Installed on Van

Meteorological instruments include sensors for ambient temperature, humidity and radiation intensity. Wind speed and direction are measured by anemometer and wind vane (Figure 3.4). For continuous collection of samples of ambient air, sampling unit
is installed on top of mobile van at height of 16 feet from ground level. Samples are collected through this sampling unit in a common glass header installed inside the van (Figure 3.5). Subsequently, sampling input from this header goes to individual analyzers through different sampling probes.

Mobile van contains sophisticated analyzers to measure ambient concentration in parts per billion (ppb) of different pollutants such as SO$_2$ (model APSA-370), NO, NO$_2$ and NO$_x$ (model APNA-370). Moreover there are provisions to measure other pollutants such as atmospheric ozone, particulates PM$_{10}$ & PM$_{2.5}$, CO, Hydrocarbons etc. but apart from SO$_2$, other pollutant concentrations were not measured as these were not relevant and were not in the scope of this work.

![Figure 3.5: (a) Analyzers in Mobile Van (b) SO$_2$ Analyzer (c) Glass Header for Air Sampling](image)

Numerical results of analysis are digitally displayed on screen panels of each analyzer and also stored in a data logger. Saved data can be downloaded from data logger through a software package installed in a PC of mobile van. Through this software, plots of instantaneous or averaged data can be visualized (Figure 3.6). Before start of experiment, three averaged readings over 10 minutes interval at each sampling point were taken for measuring background concentration of tracer. During experiments, measurements for 10 minutes within an hour were made and finally a mean of all six readings was taken to get experimental hourly average concentration at each sampling location.
In next step, tracer experiments at relatively higher stacks (60 ft) were planned. This was not possible to conduct in PIEAS ground as installation of support structure for further elevated emission source was difficult. Moreover, if roofs of certain buildings were used, nearby office and hostel buildings and other elevated obstacles in dispersion might lead to engulfing, deposition and removal of tracer gas. Hence, existing SO$_2$ sources such as brick kilns that were remotely located in a flatter terrain were explored. Information was also available in literature regarding similar studies performed elsewhere in the world for comparison [Le, 2009; Ahmad, 2008; Bhanarkar, 2002].

3.3.2.2 Investigations on Brick Kiln Releases

A brick kiln cluster of multiple stacks was available in remotely located area with relatively flatter topography in Islamabad region. Field experiments were conducted by selecting an isolated brick kiln as source and emission and ground level concentration data of SO$_2$ were collected for experimental validation of modeling results at different sampling locations.

Brick kilns were found operating with similar operating conditions having average stack height of sixty feet. Twenty five out of thirty four brick kilns were operational on observation days. Observation site with locations of operational and non-operational brick kilns is shown in Figure 3.7. Data of stack flue gases concentrations for SO$_2$ were collected using a compact stack analyzer (PG-250) of EPA. Temperature and velocity of stack flue gases were measured using k-type thermocouple and S-shaped pitot tube along with a digital manometer respectively.
Pitot tube was connected to stack and dynamic and static pressures of flue gases were measured using manometer. Data of stack characteristics and emission rate of SO$_2$ released from brick kiln are presented in Table 3.1.

Table 3.1: Stack Characteristics and Emission Rate of SO$_2$ released from Brick Kiln

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Measured</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stack height</td>
<td>19.8 m</td>
</tr>
<tr>
<td>Exit diameter</td>
<td>0.76 m</td>
</tr>
<tr>
<td>Exit velocity of flue gas</td>
<td>1.9 m/sec</td>
</tr>
<tr>
<td>Exit temperature of flue gas</td>
<td>333.35 K</td>
</tr>
<tr>
<td>Flow rate of flue gas</td>
<td>3182 m$^3$/hr</td>
</tr>
<tr>
<td>SO$_2$ emission rate from stack</td>
<td>0.30 g/sec</td>
</tr>
</tbody>
</table>

To convert atmospheric pollutant concentration from ppm$_v$ to mg/m$^3$, following expression [Beychok, 2005] has been used;

\[
[mg/m^3] = (\text{ppm}_v) \times (12.187) \times (\text{MW}) / (273.15 + °C) \quad (3.3)
\]

Where: ‘mg/m$^3$’ are milligrams of gaseous pollutant per cubic meter of ambient air ‘ppm$_v$’ is volume of gaseous pollutant per $10^6$ volumes of ambient air ‘MW’ is molecular weight of gaseous pollutant, °C’ is ambient air temperature in degrees centigrade

Equation used to determine emission rate of gaseous pollutant in g/sec is:

\[
E \ (\text{g/sec}) = \left\{C(\text{mg/m}^3) \times Q \ (\text{m}^3/\text{hr})\right\} / \{(3600) \times 1000\} \quad (3.4)
\]
Where: ‘E’ is emission rate of pollutant in mg/hr, ‘C’ is concentration in mg/m$^3$, ‘Q’ is flow rate of flue gas in m$^3$/hr.

For collecting ambient data of ground level concentrations of SO$_2$, six sampling locations at various downwind directions from brick kiln were selected. Mobile ambient air monitoring van was used to measure ground level concentration at selected sampling points.

Figure 3.8: Sequential Steps from ‘a’ to ‘g’ to Collect Data for Ambient Ground Level SO$_2$ Concentration

Figure 3.8a to 3.8g show the sequence of steps in which ground level pollutant concentration data is collected. The plume approaches from stack in prevailing wind direction (figure 3.8a to 3.8c) where mobile van is stationed and sample is collected through sampler. Subsequently it is collected in sample header from where it is fed into various analyzers and entire data acquisition may be done by a dedicated PC within mobile van (figure 3.8d to 3.8g). Initially averaged concentration data values for 10 minutes interval were collected and subsequently 1-hour averaged values were calculated based on 10 minute averaged data.

In entire work completed with brick kilns, contributions in concentration values were observed from other brick kilns nearby. Hence, it was concluded that to validate any model, it was more appropriate to use a single isolated stack, well separated by a distance of at least few kilometers from other sources. Moreover, isolated stack should have a provision so as to get samples of gases at various elevations where temperatures and flow rates may also be determined. Concentration, velocity and
temperature at exit of stack being most important parameters, should be well controlled and monitored so as to keep source term constant in the duration of experiments. In general, existence of such a stack with so many provisions was not expected to be available anywhere. Hence it was decided to design and fabricate a dedicated experimental stack at PIEAS, solely for experimental validation of a reliable dispersion model that can be employed for appropriate decision making in emergency scenarios. After an extensive effort in designing and fabrication which is a part of this work, an appropriate experimental stack with all required provisions was installed at PIEAS, details of which are given in the following section.

3.3.2.3 PIEAS Experimental Stack and Related Experiments

Decision to install a dedicated experimental stack during this Ph.D. research was a crucial one as it was within itself a full-fledged project that involved detailed design calculations, time and cost. Considering the extreme sensitivity attached to a reliable and experimentally validated dispersion model that may assist in decision making in accidental scenarios, proposal was forwarded and thoroughly discussed. A facility was already being established within PIEAS for Hazardous Air Pollutant (HAPs) Characterization and Control that also required a stack for general exhaust. Moreover, there was a requirement of a tower for placement of meteorological sensors for continuous acquisition of data for meteorological parameters. Another research project involving simulation of coal combustion and subsequent post-combustion flue gas treatment for removal of NOx and SOx also required a vertical plug flow reactor attached to a combustion facility. Proposed stack could be designed to serve this purpose as well. Based on all these requirements, proposal for a dedicated multipurpose experimental stack was approved. Very first step in this regard was to decide about parameters such as height, base and exit diameters etc. along with all requisite experimental provisions to be incorporated in this unique R & D facility. Requirements may be listed considering four themes for which proposal was approved i.e. facility should:

(i) have all provisions for ‘Atmospheric Pollutant Dispersion Studies’
(ii) act as ‘Meteorological Tower’ for placement of Meteorological Sensors’
(iii) act as a ‘Vertical Plug Flow Reactor’ for investigation of progress of reaction between reactive gases
(iv) provide ‘General Exhaust’ for HAPs Laboratory.
Chapter 3

As the stack has to provide general exhaust facility to HAPs Laboratory, site was selected near HAPs Lab. To optimize land requirement, the idea to support steel stack by guy wires was dropped, as it would require an additional circular area of diameter of same order as that of stack height and hence a self-supported stack was proposed. For economy, material selected for stack was chosen as A-36 mild steel to provide protection against corrosion.

Stack mechanical design includes considerations of stack height, exit diameter, stack dead load, seismic and wind loads, buckling and bending moments etc. The code or standard used in designing of stack is ASME STS-1-2006 as it applies to those stacks where primary supporting shell is made of steel.

Location and height of a stack is generally selected on real knowledge of location, size and arrangement of nearby buildings, nature of geography and consideration of possibility of downwash due to local terrain or adjacent structures. Formula for good engineering practice determination of minimum height requirement of stack is as follows [USEPA, 1985]:

\[ H_g = H + 1.5L \]  

(3.5)

Where ‘\( H_g \)’ and ‘\( H \)’ are respective good engineering practice stack height and height of nearby structure(s) measured from ground level elevation at base of stack. ‘\( L \)’ is the lesser dimension height or projected width of nearby structure. Since the stack was proposed near HAPs laboratory, where nearby buildings had an average height of about 30ft and the width of just adjacent HAPs laboratory itself is 36 ft, therefore, using the height of nearby buildings (\( H \)) as 30 feet and the lesser dimension (\( L \)) as 30 feet in above equation, ‘\( H_g \)’ was calculated as 75 feet. Based upon above calculation and data analysis of 34 European industries [Pregger, 2009] (in which average of mean heights of their stacks was found as 100 ft), stack height of 100ft was selected. However, its plume height may be increased by increasing exit velocity by a proposed centrifugal blower that may be attached with experimental stack.

Stacks are generally fabricated in cylindrical shape for structural stability efficiency and economical point of view. Cylindrical shapes may vary in diameter throughout the height of stack. However, diameter changes should not be exceeding 30 degree from vertical. In selection of stack exit diameter, consideration of volume of process
gas flowing, available draft and structural stability play an important role. According to general engineering practice, any size selection based on mechanical criteria must be maintained as tentative until a structural analysis can confirm its acceptability. Natural draft for experimental stack was calculated as:

$$\Delta P = \text{C}ah \left( \frac{1}{T_0} - \frac{1}{T_1} \right)$$  \hspace{1cm} (3.6)

Where ‘ΔP’, ‘C’, ‘a’, ‘h’, ‘T₀’ and ‘T₁’ are available pressure difference, discharge coefficient, atmospheric pressure, stack height, ambient temperature and flue gas temperature respectively [Pregger, 2009]. Substituting values of respective parameters as 0.0342, 1.01 × 10⁵ Pa, 30.484 m, 303 K and 373 K in above equation, ‘ΔP’ was calculated as 65.21 Pa.

Smaller exit diameter also increases the exit velocity of tracer gases which avoid adjacent deposition and settlement of emitted pollutant outside of stack on lee side. Exit diameter of stack was calculated on basis of the requirement of general exhaust from HAPs lab. Maximum possible flow rate of gases exhausted from HAPs Lab was determined as 3000 cfm summing individual flow rate of 300 cfm from each of 10 fume hoods to be installed in HAPs lab. Considering 10% excess for future margin, exit diameter may be calculated from continuity equation

$$Q = Av$$  \hspace{1cm} (3.7)

$$D = \sqrt{\frac{4Q}{\pi v}}$$

Where ‘Q’ and ‘v’ are total exhaust flow from HAPs lab and exit velocity respectively. Substituting values of above parameters as 3300 cfm or 1.56 m³/s for flow rate and 10 m/s for exit velocity in above equation, value of exit diameter of stack 'D' was calculated as 0.445 m which is finally approximated to 0.45 m.

Since widened section of stack at base reduces unit stresses in steel at base of stack. Therefore the loads acting on steel stack are transferred to foundation easily by widened section. In the light of this criterion, lower portion of steel stack has been kept widened in order to provide a large base and greater stability. Base diameter and vertical angle were selected as 1050 mm (> 450) and 26(<30) degree respectively. Thickness of stack was reduced vertically from bottom to top. A minimum structural plate thickness criterion for steel stack is 0.125 inch [ASME STS-1-2006]. Including
corrosion allowance and safety factor as 1/12 inch and 1.5 respectively, plate thickness was selected as \((0.125 + 0.08) \times 1.5 = 0.31\) inch.

Experimental stack installed at PIEAS can be seen in Figure 3.23 with all its accessories. Other details of structural and foundation design of stack are given in Appendix-VI and Appendix-VII. As the experimental stack was designed to meet multifaceted research objectives, various experimental provisions were incorporated in its design as discussed below.

**(a) Experimental Facilities Required to be Incorporated in Stack Design**

Some provisions which were especially incorporated in design of experimental stack are as follows:

(i) **Manhole:** A manhole with inner diameter of 1.63 ft (496 mm) was required to serve basically two purposes. First was to provide man access to the inside of stack for inspection and maintenance purpose. Second purpose was attachment of a blower with stack through this manhole to control exit velocity of stack gases during conduction of dispersion experiments. It was planned that a blower ducting of 1 ft (305 mm) diameter would be flanged with manhole cover using a reducer of 1.63 ft-1 ft. Drawing of manhole is given in Figure 3.9.

(ii) **Inlet Openings:** As experimental stack was required to act as general exhaust for HAPs Lab, proper ducting was necessary to attach the stack with building of HAPs Lab. To fulfill this future requirement, two inlet openings of 1 ft (305 mm) diameter were provided at predetermined heights of 14.27 ft (4350 mm) and 21.29 ft (6490 mm) from the base of stack for entrance of exhaust gas pipes from HAPs lab. Drawing of inlet openings is given in Figure 3.10.

(iii) **Platforms:** To make use of experimental stack as a meteorological tower, it was necessary to install various sophisticated instruments at different heights. In this regard, four semicircular platforms were required at 25ft, 50ft, 75ft and 100ft of stack heights for working and maintenance purpose. Sturdy guard rails were also provided for safety purpose. Another important consideration was that platforms should have strength to bear load of three or four persons (working at the same time and involved in installation related activities) standing at these elevated platforms. Platform drawing is given in Figure 3.11.
(iv) Secure caged ladder: As access to different heights of stack and platforms was required for installation and maintenance of different instruments, a secure ladder was needed on windshield of stack extending right from bottom to top of stack for making stack inspections easier. A cage was also attached with ladder for safety purpose. Drawing of ladder and cage is given in Figure 3.12.

(v) Sampling ports: As stack was planned to be used as a vertical plug flow reactor as well, fifteen sampling ports were required for insertion and collection of gaseous samples at different stack elevations so that vertical profile of reactants concentration could be observed from time to time for sample analysis. For this purpose, it was necessary that all ports should be located on a single vertical axis of stack and accessible from semi-circular platforms and monkey-ladder. Three threaded holes of different sizes were drilled into the cap of each port. Two holes were required for insertion of temperature and velocity measuring instruments such as thermocouple and hot-wire anemometer. One central hole in each port of ¾ inch diameter was required for gas insertion and/or collection of sample for analysis. Inlet openings’ drawing is given in Figure 3.13.

(vi) Canopy and drain point: A removable canopy or cover was required on top end of stack. Requirement was that this would be in place normally so that general exhaust can be emitted from sideways keeping stack interior safe from rain water. It would be removed only when dispersion experiments would be planned or when HAPs Lab. gases had to be exhausted. Moreover, a drain point was required as a single exit point at bottom of stack for routing rain water out of stack base (Figure 3.14).

(vii) Stack Vertical Alignment Nuts: Although an initial alignment at the time of installation is carefully ensured but there are chances that due to wind or seismic loads this alignment may be disturbed. In such a scenario overall integrity or entire stack may be jeopardized. Hence with each J-bolt, a screw and nut arrangement was recommended so as to maintain the alignment even after installation of stack whenever disturbed (Figure 3.15). For this reason, special spanners were also requested with longer arm to move these bolts up or down according to requirement.
Figure 3.9: Manhole

Figure 3.10: Inlet Openings

Figure 3.11: Platform
Figure 3.12: Caged Ladder

Figure 3.13: Sampling Ports

Figure 3.14: Drain Point

Figure 3.15: Alignment Nuts
(b) Stack Fabrication and Installation

After inclusion of all above mentioned experimental facilities in design of experimental stack, its fabrication was initiated at HMC-3 (Heavy Mechanical Complex-3). Different fabrication stages can be observed in Figure 3.16.

![Figure 3.16: (a) Fabrication of a Shell of Experimental Stack at HMC-3 (b) Flange Welding with Stack Shell](image)

The stack was fabricated into four shells each of length 25 feet (7.62 m). Finally it was brought to PIEAS where it was erected after assembling different segments. Stages of stack assembling and erection are presented in Figure 3.17.

![Figure 3.17: (a) Alignment of Stack Shells on Ground at PIEAS (b) Erection of Experimental Stack Segments](image)

(c) Accessories Attached for Experimental Dispersion Studies

Parameters of stack exit temperature, exit velocity and pollutants concentration were of prime importance and should be precisely measured experimentally to conduct dispersion studies. In order to make measurements of these parameters during tracer experiments, some experimental arrangements were made including installation of
thermocouples, centrifugal blower, anemometer, automatic weather stations and arrangements for stack gas sampling. Details of each are presented below:

(i) **Thermocouples**: Instrumentation was required to measure exit temperature of stack gas. A k-type thermocouple was installed at top of stack. Digital display of temperature from this thermocouple was obtained in HAPs Lab. Moreover, thermocouples were also inserted into small holes in cap of each sampling port to measure vertical temperature profile of gases within experimental stack. Figure 3.18 shows K-type thermocouple with digital display unit.

![Figure 3.18: (a) K-type Thermocouple Used for Measuring Temperature of Stack Gas (b) Display Unit of Thermocouple](image)

(ii) **Centrifugal blower**: During dispersion studies, it was planned to perform experiments with an exit velocity of tracer gases in a wide range from 1.0 to 10 m/sec. To adjust and maintain the required exit velocity, a centrifugal blower along with a variable frequency derive was attached with experimental stack. Design details of blower are presented in Appendix-VIII. Attachment of blower and installation of VFD in electrical panel are shown in Figure 3.19.

![Figure 3.19: (a) Blower Attached with Stack (b) Variable Frequency Drive Installed in Electric Panel](image)
(iii) **Anemometer**: Exit velocity of stack flue gas is an important parameter in dispersion studies and it should be experimentally measured. A portable, digital anemometer was installed inside the stack for this purpose about one foot below its top end. Its low friction ball bearing design allows free vane movement, resulting in accuracy at both high and low velocities. A sensitive balanced vane wheel rotates freely in response to airflow. It includes a strong light weight plastic housing case. It measures velocity in range from 0.4 to 30 m/sec. Figure 3.20 shows installation of anemometer within experimental stack at exit point.

![Figure 3.20: (a) Anemometer with Display Unit (b) Anemometer Installed in Stack](image)

(iv) **Automatic weather stations**: Meteorology of a region under investigation during dispersion studies is a key input to any dispersion model. One of the sources for meteorological data is surface stations where data of different meteorological parameters are collected. As experimental stack was required to act as meteorological tower also, that is why two automatic weather stations (6162C Cabled Vantage Pro2™ plus manufactured by Davis) were installed at two platforms of stack located at 50 and 100 feet height. These weather stations along with data acquisition system were installed to get site specific meteorological data during experimentation (Figure 3.21). Various sensors installed in automatic weather station in order to collect the data of different meteorological parameters include three cup anemometer, wind vane, temperature & humidity sensors, pyranometer, barometer and rain collector. The collected data is displayed on the console of each weather station and this data can be transmitted to PC with the use of a device called ‘Weather Link’. A data logger in console is used to store the meteorological data even when it is not connected to a PC.
(v) **Gas insertion and collecting system:** As the stack would be used as vertical plug flow reactor, a system was required for gas insertion or collection from different elevations of stack to investigate concentration profile of different reactants during chemical reaction. Pipes of different lengths (Figure 3.22a) were passed through central holes of each port in such a way that their inner ends with expanders would be concentric with stack’s vertical axis (Figure 3.22b). Outer ends of these pipes approaching to nearest platform would be attached with flexible pipes of ¾ inch diameter through control valves. Ultimately, these flexible pipes were attached through a suction pump to a common header where analysis could be performed using stack gas analyzer.
(vi) **System to make constant gaseous release:** An experimental arrangement was made to draw gaseous samples from top of stack and collect into a common sampling header placed at ground near stack. For suction of gaseous sample, four pipes were fitted at stack’s top in such a way that their inner ends of 1 ft length with expanders were positioned inside the stack at different radial locations at same elevation. Their outer ends were attached with flexible pipes of ¼ inch diameter routed and attached with common header with control valves. Concentration of gaseous sample collected in header was determined using stack gas analyzer. Mass flow controller and flow meter attached to tracer gas cylinder were adjusted to desired fixed source term while measurements were taken repeatedly to verify constant emitted gas concentration at exit of stack.

(vii) **Centrifugal blower attached with stack:** To dilute the concentration of released gas through experimental stack and get its constant exit flow rate, a centrifugal blower was attached with stack using a round ducting of 12 inches diameter. It is single-stage blower in which air does not take many turns and hence it is more efficient. Blower consists of a centrifugal fan, an electric motor, a drive system, ducts or piping, flow controls and measuring devices. An induction type, belt driven motor of 10 Hp was attached with blower. Fan and motor are mounted on a single pedestal floor. A butter fly wafer damper was provided near the blower exhaust to protect the blower from the undesirable flow of corrosive gas from stack towards blower, when blower is not running. Three inlet openings of the diameter of 4, 6 and 8 inches were provided in the ducting after isolating damper for entering any tracer or pollutant into stack. A wafer (wedge seat round damper) damper was placed in the branch outlet for flow bypass and another wafer damper was used in the main stream line to vary the blower flow rate manually. A motor control centre (Penal) wall type was used to supply the electric power to blower and protection against any electric surge. It includes overload relay, ampere meter, volt meter, power indication lights, on and off push switches, phase sequencer, electrical connectors, circuit breaker, time delay relay and the starter of star delta type. A Variable Frequency Drive (VFD) was also installed in control panel to control the speed of blower motor and ultimately change the exit velocity of released gases through stack for experimental purposes.
Figure 3.23: Experimental Stack Installed at PIEAS with All its Accessories
(d) Experimental Methodology of Stack Release for Dispersion Studies

Third set of tracer experiments were conducted using experimental stack. The stack is located at 33° 39' 16.1” N and 73° 15' 51.7” E adjacent to Hazardous Air Pollutants Characterization Laboratory (HAPs lab) at PIEAS. Tracer used in stack experiments was sulfur dioxide (SO₂). Primary feature of experimental stack design that makes it different from brick kilns stacks was that a constant source term could be maintained and verified at all times (see section 3.3.2.3(c)-(iv)). Fifty liter Gas cylinder with 10% (i.e. 10⁵ ppm) SO₂ in nitrogen filled at 2200 psi weighing 1.9 kg was used in the experiment. Gas release rate of 0.6 g/sec was kept constant during one hour release period by using a mass flow controller and was verified by sample collection manifold header collecting and analyzing samples of gases sucked from exit of stack. Mass flow controller and flow meter arrangement with cylinder and subsequent verification was necessary because decreasing pressure inside gas cylinder may result in cooling thereby causing fluctuations in gas flow rate. To set constant stack emission level of SO₂ at 150 ppm, 140 liter/min of 10 % SO₂ cylinder were diluted by mixing with the air flow of 3300 cfm from centrifugal blower attached with stack. Gas from cylinder was inserted into the stack through one of the sample points which was near to first platform of experimental stack.

Figure 3.24: Diagram Indicating Components of Experimental Setup and Direction of Tracer Flow
Sixteen sampling locations as 1 to 16 were selected around the stack on ground at different distances and directions for collecting SO$_2$ samples. Due to complex topography, it was impossible to select sampling locations on equidistant circles around the source. So scattered but accessible sampling points were selected where mobile van could be easily moved for taking measurements. Point distribution is presented in Figure 3.25.

Figure 3.25: Sampling Locations Distribution around Experimental Stack

Initially a thorough background scan was done taking three ambient air concentration measurements of SO$_2$ at all sampling points to exclude any intervening effect of existing nearby SO$_2$ source. Subsequently continuous instantaneous measurements of SO$_2$ ambient concentration in ppm were taken for 10 minutes time period at each sampling location using EPA mobile van. A walkie-talkie contact between stack team and sampling team was always maintained to ensure any changes in wind direction as well as other source term conditions. Although different points were marked around the source but measurements were taken only at a few points that were in direction of prevailing wind at the time of experiment. Decision on selection of specific sampling
points was taken on real meteorological data information obtained from weather stations installed at experimental stack.

As mentioned earlier, fourth set of experimentation was planned to cover a longer source-receptor distance with more elevated release point employing greater quantity of an ‘inert harmless tracer’ which surely had no other source of emission nearby from any industry or transport.

Literature reveals that several different tracers have been used in various short and long range tracer experiments. Some classic tracer experiments were conducted with aerosols and particulates as tracers including fluorescein acid [Bultynck, 1972], zinc sulfide and cadmium sulfide [Eggleton, 1961; Mulholland, 1980], uranine dye [Islitzer, 1961; Singer, 1966], soluble fluorescent dyes such as fluorescein and rhodamine [Ramsdell, 1985] oil fog smoke [Raynor, 1975], spores [Hay, 1957], metal oxides [Shum, 1975] and enriched rare earth isotope of neodymium (Nd) [Ondov, 1992]. Some major issues with use of these particulate tracers were generation of aerosols, their capture by soil, tree leaves and pine-needles, dissolution in water and loss of fluorescence because of action of sunlight. So use of these tracers became obsolete with time. In few early experiments, radioactive gases such as $^{85}\text{Kr}$, $^{133}\text{Xe}$ and $^{41}\text{Ar}$ were also used as tracers [Eggleton, 1961; Singer, 1966; Draxler, 1979; Ramsdell, 1985]. Release of such radioactive tracers is hazardous for general public health hence most of such tracer experiments were conducted using already available sources of radioactive species such as routine releases of Krypton-85 during nuclear fuel reprocessing operation in nuclear facilities [Roland, 1979]. Efforts have been made by researchers to develop sophisticated inert perfluorocarbon tracers such as $\text{C}_6\text{F}_{12}, \text{C}_7\text{F}_{14}$ and $\text{C}_8\text{F}_{16}$ to study long range (mesoscale) transport of pollutants in atmosphere [Martin, 2010; Petersson, 2010; Carvalho, 2002; Anfossi, 1998]. Per fluorocarbons have been used for long (up to 100 km) [Draxler, 1979] and for very long-range dispersion experiments (500-1000 km) [Kallend, 1981; Ferber, 1981]. Some problems associated with these tracers include time consuming and more complication gas chromatographic analyses. Moreover, their emission is also more difficult because they are present in liquid phase at ambient temperature. Some laboratory-made heavy methanes such as $^{12}\text{CD}_4, ^{13}\text{CD}_4$ have been used for long-range experiments [Draxler, 1979; Roland, 1979; Ferber, 1981; Lovelock, 1982].
In most of recent tracer experiments, inert gases containing halogen elements have been preferred to be used as tracers. One of the reasons is that these gases containing fluorine, chlorine or bromine can be easily detected and measured even with very low ambient concentration. Most commonly used tracer in this category is sulfur-hexafluoride gas (SF₆). Earlier experiments conducted to test use of SF₆ in large scale urban dispersion studies revealed that its use is relatively inexpensive and this gas may be taken as an excellent tracer for studying dispersion of pollutants for urban areas [Peter, 1974]. SF₆ is a colorless and odorless gas at temperatures well below ambient. It is insoluble in water and has low ambient background levels, that is why it is detectable in ppt range in air. It is easy to emit at a constant rate and readily commercially available. Also, it is chemically inert and non-toxic, even with 80 % by volume concentration level [Verschueren, 1978]. Many of dispersion studies have been conducted with SF₆ gas as a tracer. Examples are large scale tracer experiments [Yersel, 1983; Brian, 1990], mesoscale experiments with multiple tracers [Roland, 1979; Fowler, 1983], Short-range diffusion experiments in unstable conditions over non-homogeneous terrain [Gryning, 1978], three tracer experiments conducted in a narrow mountain valley region [Richard, 1983], series of fifteen dispersion experiments conducted from 213 m high meteorological mast [Durren, 1980]. In light of mentioned information, SF₆ was selected as a tracer for conducting experiments in a complex coastal region.

3.3.2.4 SF6 Tracer Experiments

An atmospheric dispersion related tracer experiment was conducted at a coastal site during this research work. The experimental procedure can be divided into three major parts as follows:

(a) Release of SF₆ Gas

A meteorological tower of 102 meter height was used as a supporting structure for sulfur hexafluoride (SF₆) release. Meteorological tower was located at 24° 51' 10.8" N and 66° 47' 10.5" E bearing five platforms at 10, 30, 50, 70 and 100 m as shown in Figure 3.26.
SF₆ was released from 70 meter height of this tall meteorological tower through a special rubber pipe (YATAI) with internal diameter of 5/16" and pressure limit of 17.5 megapascal (MPa) attached with tower up to above mentioned height. Other end of this pipe was attached with SF₆ gas cylinder placed on ground. 40.8 liter cylinders filled with pure SF₆ at 13 kilopascal (kPa) pressure were used. Talking in terms of mass, weight of empty cylinder was 50 kg whereas gas itself in it was also 50 kg making total weight of SF₆ and cylinder as 100 kg.

Tracer was planned to be released during day time on April 29, 2013 under favorable wind conditions. Tracer release period was selected as one hour. Gas release rate of 2 kg/5min (6.7 g/sec) was kept constant during one hour release period by adjusting control valve of SF₆ cylinder repeatedly because decreasing pressure inside gas cylinder resulted into cooling and consequently varying gas flow rate. A digital weighing balance was placed under SF₆ cylinder with a digital display unit. Gas release rate was measured with the help of digital weight balance placed under SF₆ cylinder and a stop watch.
(b) Sampling of SF₆ Gas

Six arcs, Arc-A to Arc-F were marked for collecting SF₆ samples within a radius of 10 km. Arcs were marked at distances of 0.7, 1.5, 3, 5, 7 and 10 km in prevailing wind direction. Distance and direction of sampling locations were selected on basis of topography and prevailing wind conditions of specific region. Because of complex terrain and low wind speed, arcs near the source were kept closer as compared to others.

Details about distance and coordinates of each sampling point are presented in Appendix-V. Points where readings were taken as a part of this research are shown in
These points were considered sufficient for experimental validation of coupled meteorological & dispersion models. Studies were continued for other points as well, at the time of completion of this thesis and therefore were not included in this work. On the points shown in figure 3.31(b), three samples for 10 minutes time period were collected with interval of 5 minutes among consecutive sampling activities. Samples were collected in 2 liter sampling bags which were made of gas foil polymer composite. These sampling bags had high tightness, low absorption characteristics and ppm level of sample in bags could be maintained for six months. Sampling bags were filled at a constant flow rate of 0.2 liter/min for 10 minutes with the help of a small sized portable sampling pump. Samplers (TWA-300) used were made in Shanghai by Xinganzhuo Environmental Protection Technology Co. Ltd. The instrument is equipped with low power steady flow pump, flow control valves and electronic control circuit.

Some practical aspects experienced during conduction of experiments are worth mentioning here. Firstly, it seemed difficult to collect samples at all sampling locations simultaneously as it involves considerable man-hours. Other important thing was that the role of local wind field characteristics in releasing and sampling processes was very dominant. Decision on start of SF₆ releasing process and selection of specific sampling arc points was highly dependent upon existing wind speed and wind direction. Wind field observations were collected from ground station at experimental site. Moreover, five platforms were located at solar power operated ‘met tower’ at heights of 10, 30, 50, 70 and 100 meter carrying instruments for measuring ambient temperature, wind speed and wind direction at each height. Meteorological
data from all instruments installed on platforms of meteorological tower and ground station were displayed and stored by a micro data logger (CR-3000) installed in a portable, rugged, powerful data acquisition system at ground-station.

![Figure 3.34: Micro Data Logger](image)

(c) Laboratory Analysis of SF₆ Samples

A gas chromatograph of LUHONG Company, model GC-2000, was used to analyze SF₆ samples in a chemical analysis laboratory especially developed for that purpose. Electron Capture Detector (ECD) was used in GC and each sample took about 3 minutes for analysis. Chromatographic data was obtained in the form of a chromatogram representing detector response on y-axis and retention time of analyte in samples on x-axis. This graph shows peak of SF₆. Area under the peak of SF₆ is proportional to the amount of SF₆ gas. Recording area under peak and using a calibration curve, concentration of SF₆ gas in original sample was determined. For the purpose of calibration, 10 ml sample of SF₆ gas containing known concentration of 1.0 x 10⁻⁶ was taken in a syringe and mixed with 90 ml of air resulting in concentration of 1.0 x 10⁻⁷. This sample was loaded in gas chromatograph. Two peaks appeared in output of gas chromatograph. Larger peak represents oxygen concentration in sample and smaller peak represents SF₆ gas. Area under the curve of SF₆ peak was noted. Procedure was repeated for diluted concentration of SF₆ repeatedly.
Using above readings, a curve was drawn and slope of curve was determined as $1.0 \times 10^{-14} / (\text{mV} \times \text{time})$ called ‘K factor’. To determine the concentration of SF$_6$ gas, sample was evaluated by the following expression

$$\text{Concentration (g/m}^3) = \frac{K \times \text{Area under curve} \times 1000 \times \text{molar weight of SF}_6}{\text{molar volume of SF}_6 \text{ at STP}}$$  \hspace{1cm} (3.8)$$

Where molar mass of SF$_6$ gas is 146.047 g/mol and molar volume at STP is 22.414 dm$^3$/mole.

### 3.4 Summary

The entire work is directed initially on computational modeling methodology for precise atmospheric dispersion of toxic pollutants and subsequently towards practical setups, procedures and experimentation for model validation.

Computational resources such as high performance computation facilities and clusters were employed and procedures were adopted for predicting plume trajectories and ground level pollutant concentration using coupled meteorological and dispersion models such as MM5+CALPUFF and WRF+FLEXPART. Initially an investigative study was performed for Pakistani South Asian region to evaluate performance of a selected convective parameterized scheme in a mesoscale model [MM5]. Once a specific parameterized scheme of MM5 was finalized for the region and time interval, pollution dispersion studies could be carried out by coupling mesoscale model with a specific advanced dispersion model. Subsequently, modeling procedure and strategy used was elaborated for simulation studies that were performed using integrated MM5-CALPUFF modeling system for predicting SO$_2$ emission from an oil refinery.
and assessment of impacts of flaring activities in an oilfield on nearby ambient air quality. This is followed by description regarding modeling procedure using same modeling system for predicting SO$_2$ emission from an isolated brick kiln. Eulerian–Lagrangian modeling system (WRF-FLEXPART) was employed to simulate plume trajectory by calculating positions of emitted particles in a hypothetical plume that was assumed to be emitted from PIEAS experimental stack for which high performance computing machine having provision of 32 dual core processors was used. Computing strategy and methodology for plume dispersion simulation is thoroughly described using coupled CALPUFF-MM5 modeling system for simulating dispersion of SF$_6$ tracer in a coastal region of Pakistan in which SF$_6$ was released at 70 m height of a meteorological tower.

Later part of experimental validation is further comprised of validation of ‘meteorological model’ itself and validation of results of ‘coupled meteorological and dispersion model’.

Meteorological models are validated by data of meteorological parameters that are observed and collected at ‘ground based meteorological stations’ or collected through ‘satellites’. In present research this validation is performed by data collected from a meteorological station near oil refineries. Moreover data collected by Pakistan Meteorological Department as well as TRMM satellite derived data for Pakistani region was used for validation purposes. Re-analyses data from NCEP including ambient temperature, potential temperature, humidity and moist static energy for Pakistani region was also used for meteorological model validation. Results of all these meteorological modeling and validation are given in forthcoming sections of chapter four.

Validation of ‘coupled meteorological and dispersion modeling system’ is of prime importance to determine performance and efficiency of overall predicted results. There may be two methods of doing these validations. One is to get ‘available observed data’ of pollutant concentration from any system of pollutant emission sources and use identical conditions of source term to model the scenario by coupled MM5-CALPUFF or WRF-FLEXPART system to verify its validation. If predicted results compare well with observed data set of pollutant concentration, model is said to be validated. Second option may be to conduct on site ‘field tracer experiments’ in which a controlled amount of a tracer is released from a source and its ambient
concentration at different sampling locations is determined on site by different sampling and analyzing techniques. In present work, first option was used for validation of coupled MM5-CALPUFF modeling system by modeling a simple release scenario of SO\textsubscript{2} from cluster of stacks of oil refineries for which ground concentration data was available for validation. In these studies a confidence was gained on coupling of meteorology and dispersion codes.

A number of tracer experiments have been conducted internationally and datasets are compiled from such kind of experimentation. These datasets may be used for validation of different dispersion models provided that the region under consideration has identical meteorological conditions and topography. Such tracer experiments have never been conducted in typical meteorological and topographical conditions of Pakistan. Hence no ground level ambient pollutant concentration datasets are available as such in Pakistan to validate modeling results. In present research work, a sequential study was initiated from modeling of simple release scenario of tracer gases from an emission source. Initiating from as low source elevation as 30ft and emission-receptor distances as 165ft to as high source elevation as 230 ft and emission-receptor distances of 33,000 ft (6.25 miles).

Experimental setups, procedures and methodology of ‘four sets of tracer experiments’ conducted in present research work are elaborated in this chapter.

First set involved simple dispersion/diffusion experiments at a very short scale horizontally and vertically. Over a flat ground, a support system was erected and SO\textsubscript{2} gas was released at a height of 30ft through a six inch internal diameter conduit and air samples were taken in prevailing wind direction at sampling points on each of three arcs at varied radii from 165 ft to 495 ft.

In second set of experimental work, height was increased to double i.e. 60 ft which is the usual height of brick kilns while samples were collected at sampling points covering larger distances. Cluster of emission sources were also considered. In entire work completed with brick kiln and cluster of stacks, it was concluded that prior to validate any model by a cluster of sources, it was more logical to use a single isolated stack, well separated by a distance of at least few kilometers from other sources. Moreover, isolated stack should have a provision so as to get samples of gases at various elevations where temperature and flow rate may also be determined.
Concentration, velocity and temperature at exit of stack being most important parameters, should be well controlled and monitored so as to keep source term constant in duration of experiments. In general existence of such a stack with so many provisions was not expected to be available anywhere. Hence, it was decided to design and fabricate a dedicated experimental stack at PIEAS, solely for experimental validation of a reliable dispersion model that can be employed for appropriate decision making in emergency scenarios. After an extensive effort in designing and fabrication which is a part of this work, an appropriate experimental stack with all required provisions was installed at PIEAS, details of which are given in this chapter.

*In third set of experimentation*, 100 ft PIEAS experimental stack was used to emit SO\textsubscript{2} as tracer and air samples were collected at few sampling points in different directions at varied distances ranging from 1000 ft to about 3000 ft. There were some limitations in using SO\textsubscript{2} as tracer gas for atmospheric dispersion modeling studies. It is an environmentally noxious gas and could not be emitted through stack beyond certain prescribed limits. Moreover, there are many sources of SO\textsubscript{2} emission that are frequently emitting this gas hence one cannot be sure whether SO\textsubscript{2} measured in ambient air at certain location is actually coming from PIEAS experimental stack or it has some local origin. SF\textsubscript{6} is colorless, odorless, insoluble in water, gas at temperatures well below ambient, low ambient background levels, detectable in ppt range in air, easy sampling, easy to emit at a constant rate and readily commercially available. Also, it is chemically inert and non-toxic, even with 80 % by volume concentration level. Many of dispersion studies have been conducted with SF\textsubscript{6} gas as a tracer.

*Hence, in final set of experiments*, SF\textsubscript{6} gas was released at a height of 230 ft through a conduit of 5/16 inch internal diameter and samples were taken at 36 sampling points simultaneously at distances ranging from 2300 ft to about 33000 ft (6.25 miles). Sampling points were fixed depending upon prevailing wind direction and accessibility.

Results of all experimental validation studies of coupled meteorological and dispersion modeling through various sets of tracer experiments are presented in chapter five.
CHAPTER 4
Results and Discussion
Modeling and Validation of Mesoscale Meteorology for Dispersion

This chapter is mainly focused on computational results of meso-scale meteorological model MM5 and its validation. This was needed for its subsequent coupling with an advanced dispersion model. Data used in experimental validation is that of Pakistan and its nearby region Oman. Initially MM5 modeling was performed for three parameters i.e. ambient temperature, wind speed and wind direction and results were validated against observed data of a surface station of Oman. Based upon encouraging results thus obtained, work was focused on Pakistani region. In order to tune up meso-scale meteorological model MM5 for Pakistan specific region, sensitivity of different parameterized schemes generally used in MM5 such as Grell, Kain–Fritsch, Anthes–Kuo and Betts–Miller were investigated. Suitability of each scheme was verified by performing computations using each scheme, and then comparing them by factual data for various meteorological parameters such as ambient temperature, potential temperature, moist static energy, humidity and precipitation in Pakistan.

4.1 Validation of MM5 Modeling Results with Observed Data of Oman

A simulation study was performed using integrated CALPUFF-MM5 modeling system for predicting SO$_2$ emission from an oil refinery of Oman. Prior to use output of MM5 in dispersion model CALPUFF, simulated results have to be validated by comparing with available observed data from a surface station in the same region. Modeling procedure has already been described in section 3.2.2. Simulated results and their validation for meteorological data are presented in following section whereas results of ground level SO$_2$ concentration are discussed in section 5.1.2.2.

4.1.1 Modeling of Surface Level Meteorological Parameters

A comparison of MM5 model-predicted meteorological variables at 4 m from ground level was made against observed data of corresponding parameters at similar height of
a meteorological tower. Simulation time covers entire period from June 1–15, 2008 during peak summer season in Oman. This was done on hourly basis for each day for fifteen days. Results presented here are specifically for those four days (June 6–8 and 12, 2008) in which more variation in meteorological conditions prevailed.

Figure 4.1(a–d) shows a comparison of modeled and observed variation of time averaged ambient temperature for 24 h of selected days. It may be inferred from these plots that modeled values agree well with observed temperature.

![Graphs showing ambient temperature comparison](image)

**Figure 4.1:** Comparison of model predicted ( ) and observed ( ) data of ambient temperature for (a) June 6, 2008 (b) June 7, 2008 (c) June 8, 2008 (d) June 12, 2008

Variation in numerically calculated and observed wind speed of selected days is depicted in Fig. 4.2 (a–d). Though trend in all cases is similar but exact agreement in case of wind speed is difficult because of strong localized perturbation due to man-made ground features within four meters elevation.

Modeled and observed wind direction is plotted in Figure 4.3 (a–d). Predicted wind direction agrees within ±15% deviation from 6th - 8th June 2008 whereas on 12th June deviation was more indicating towards atmospheric instability.

It is noticed from analysis of these results that deviation between modeled and observed results of wind speed and direction is more as compared to ambient
temperature. This is most likely due to large perturbation (i.e., fluctuations in wind variables).

Figure 4.2: Comparison of model predicted (---) and observed (----) data of wind speed for (a) June 6, 2008 (b) June 7, 2008 (c) June 8, 2008 (d) June 12, 2008

Figure 4.3: Comparison of model predicted (---) and observed (----) data of wind direction for (a) June 6, 2008 (b) June 7, 2008 (c) June 8, 2008 (d) June 12, 2008
Since temperature does not experience abrupt changes generally during solar cycle of a day, that is why results of temperature seem much stable than that of wind variables. Other reason for more variation in case of wind speed and direction may be attributed to surrounding human-made features including meteorological station itself and presence of several stacks. These features located close to meteorological tower might have contributed to alteration of wind direction at such low level. This ground level perturbation has also been observed in other similar studies elsewhere [Basit, 2008]. These man-made features are not normally accounted for in any numerical model calculations and may cause deviation in model results. Discrepancy in wind speed and direction may also be attributed to influence of model grid resolution [Yang, 2008]. Despite these discrepancies mentioned above, overall qualitative trend in modeled wind speed and direction with that of actual observed data is in general agreement with one another. Hence overall performance of MM5 model in generating meteorological fields for CALPUFF is acceptable.

4.2 Validating MM5 for Pakistan Specific Topography

Compared to Oman where general geography involves a plane desert, Pakistan has a complex and variable geographical features as well as surface topography. An investigative study was performed for Pakistani South Asian region to evaluate performance of a selected convective parameterized scheme in a mesoscale model (MM5). Computational Strategy for study is presented in section 3.2.1. To validate ‘model-predicted monthly accumulated rainfall’, results of MM5 were compared with satellite derived rainfall data (3B43RT) of Tropical Rainfall Measuring Mission (TRMM) and synoptic data of Pakistan Meteorology Department (PMD).

As extent of precipitation plays an important role in scavenging pollutants from atmosphere, if physical and chemical removal of pollutants is to be incorporated in overall dispersion modeling, it is essential to simulate the trends of precipitation. Once a specific parameterized scheme of MM5 is finalized for a particular region and time interval, trans-boundary pollution dispersion studies may be carried out by coupling mesoscale model with a specific Eulerian- or Lagrangian dispersion model such as CHIMERE, CALPUFF or FLEXPART.

For specific location of ‘Islamabad’ within the domain studied, reanalysis data of US National Centre for Environmental Prediction (NCEP) was employed. This was done
for validation of model-predicted results for vertical profiles of ambient temperature, potential temperature, relative humidity and moist static energy. Results of entire simulations covering four parameterized schemes of Grell, Kain–Fritsch, Anthes–Kuo and Betts–Miller for months of July and August of years 1998 and 2001 are discussed in following sections. Reason for selection of specific years for this study is that beginning of year 1998 brought a severe famine in the region, which lasted up to year 2000 and then year 2001 brought a wet summer monsoon season. This drought left hazardous impacts on agricultural yield of region and, hence, the extremes of this time interval i.e. year 1998 and year 2001 are worth considering. Month of July and August are selected because summer monsoon season usually lasts from June to September whereas July and August are peak months of this season.

4.2.1 Comparison of Modeled and Observed Precipitation Data

Figures 4.4 and 4.5 present satellite derived and PMD recorded data of total monthly precipitation for July of years 1998 and 2001, respectively. Climatology facts of precipitation pattern over this area are obvious from these figures. First thing in this regard is indication of less precipitation in July 1998 and comparatively higher rainfall in the same month in 2001, which indicates that years 1998 and 2001 experienced dry and wet summer monsoon seasons, respectively. Second thing is higher amount of precipitation over northern mountainous areas compared to southern plain areas of simulated region. Such precipitation patterns were expected due to the reason that winds coming from adjacent oceans to south Asian region in summer monsoon experience extensive uplift when approaching high mountain ranges of northern areas, and produce heavy rainfall over there.

It can be observed that for July 1998, satellite data (Figure 4.4a) showed rainfall with intensity of 100 mm over a broad northern area located at (32–34° N, 70–74° E) and peak rainfall with intensity of 200 mm over a small area located at (33° N, 74° E). For same month, PMD data showed two peaks of rainfall with intensity 300 mm (Figure 4.5a), one located at (32-34° N and 72-74° E) and other at (32-34° N and 74-76° E).

Comparing modeled results of Grell scheme (Figure 4.6a) for same month of same year with satellite and PMD data, it was observed that Grell scheme captured precipitation well over the northern areas though with underestimation showing precipitation with intensity of 100 mm over a comparatively small area. Location of
Figure 4.4: Map showing satellite derived (3B43RT) total monthly rainfall (mm) in Pakistan for (a) July, 1998 (b) July, 2001

Figure 4.5: Map showing PMD data of total monthly rainfall (mm) in Pakistan for (a) July, 1998 (b) July, 2001

Figure 4.6: Modeled ‘accumulated monthly rainfall (mm) in Pakistan for July, 1998’ with (a) Grell scheme (b) KF scheme
peak rainfall was at the same location as displayed in satellite and PMD data. This scheme showed better performance for southern plain areas by capturing precipitation contours of 25 and 50 mm of satellite and PMD data.

Moreover, Grell scheme clearly demonstrated a greater amount of rainfall over northern mountainous areas of the region and comparatively less rainfall over southeastern plain areas that are in good qualitative and quantitative agreement with satellite derived and PMD data.

On the other hand, Kain–Fritsch scheme (Figure 4.6(b)) overestimated results for both northern and southern areas of simulated region, showing peak rainfall intensity of 400 mm though at same location as in satellite data. KF scheme captured rainfall peaks with intensity of 300 mm in PMD data very well at almost same locations as in observed data, though showing a bit higher intensity of about 400 mm. It may be noted that, as with the Grell scheme, the Kain–Fritsch scheme, irrespective of rainfall intensity, seemed to be successful in capturing the location of peak rainfall as well as following the trend of higher precipitation over northern areas and less precipitation in plain areas as displayed in both data types. Colle also showed overestimated results by Kain–Fritsch scheme and lesser precipitation by Grell scheme, though Colle investigated patterns of total monthly precipitation over coastal region of United States [Colle, 2003].

Figure 4.7: Accumulated monthly rainfall (mm) for July, 2001 in Pakistan with (a) Grell scheme (b) KF scheme
For July, 2001, comparison of model-predicted data with that of satellite and PMD illustrated that Grell scheme (Figure 4.7(a)) largely underestimated peak rainfall over northern area displayed in satellite and PMD data with intensity of 400 mm and 500 mm respectively at (32–34° N, 72–74° E).

The scheme showed precipitation with intensity of only 50 mm though at the same location. For southern areas, this scheme was again successful showing peak rainfall with intensity of 100 mm centered at (24-25° N and 68-71° E) which is somewhat in quantitative agreement with both observed data types.

On the other hand, Kain–Fritsch scheme (Figure 4.7(b)) showed a comparable trend with satellite data showing maximum precipitation of 400 mm over northern areas located at (32–34° N, 72–74° E) and (32–34° N, 74–76° E), which is in good agreement with satellite data. With slightly underestimated results, KF scheme showed also comparable results with PMD data. Scheme captured peak intensity and locations of observed two precipitation contours centered at 32-34° N, 72-74° E and 32-34° N, 74-76° E of intensity 500 mm and 400 mm respectively in PMD data. For plain areas, this scheme again provided overestimated results.

It may be noted here that Kain–Fritsch scheme showed overestimated results over northern region for month of July 1998 which was a dry month and comparatively little precipitation was observed over mountain region. This strange behavior of KF scheme may be due to performance dependence of convective schemes on precipitation intensity. This dependence has been studied by Mukhopadhyay who investigated overestimated and underestimated behavior of same convective scheme for different intensity levels of precipitation [Mukhopadhyay, 2010].

Figures 4.8 and 4.9 present satellite derived and PMD recorded data of total monthly precipitation for August of years 1998 and 2001, respectively.

For August 1998, comparing Figure 4.10 (a) with Figures 4.8 (a) and 4.9 (a), it may be noticed that Grell scheme (Figure 4.10(a)) captured very well the intensities and locations of two precipitation contours over southern plain areas centered at 26–29° N, 66–68° E and 24–26° N, 68–71° E of intensities 25 and 50 mm respectively, showing an excellent qualitative and quantitative agreement. This scheme showed underestimated results for northern mountainous areas showing peak rainfall with intensity of 100 mm over same place (32–34° N, 72–74° E) as displayed in PMD data (Figure 4.9(a)).
Figure 4.8: Map showing satellite derived (3B43RT) total monthly rainfall (mm) in Pakistan for (a) August, 1998 (b) August, 2001

Figure 4.9: Map showing PMD data of total monthly rainfall (mm) in Pakistan for (a) August, 1998 (b) August, 2001

Figure 4.10: Modeled ‘total monthly rainfall (mm) in Pakistan for August, 1998’ with (a) Grell scheme (b) KF scheme
On the other hand, Kain–Fritsch scheme (Figure 4.10(b)) again presented overestimated results for both mountainous and plain areas, indicating peak rainfall with intensity of 400 and 100 mm centered at 30–32° N, 74–76° E and 26–29° N, 66–68° E, respectively, when compared with satellite data (Figure 4.8(a)) and PMD data (Figure 4.9(a)).

It may be noted that Grell scheme seemed to be successful in capturing precipitation patterns over plain areas. This is in line with findings of Kerkhoven who also found that Grell scheme is the most robust for region of east China plains for summer monsoon precipitation [Kerkhoven, 2006].

Satellite data (Figure 4.8(b)) and PMD data (Figure 4.9(b)) of August 2001 reveal that most of the areas of simulated region experienced very small amount of precipitation throughout the month. A single peak of rainfall for total month was observed over north at 32–34° N, 72–74° E with intensity of 100 mm displayed in satellite derived data or 200 mm displayed in PMD data.

Comparing satellite derived precipitation in Figure 4.8(b) with that predicted by Grell scheme in Figure 4.11(a) for August 2001, it was noted that Grell scheme captured peak of rainfall with intensity of 100 mm, though over a very smaller area compared to that displayed in satellite and PMD data, but at the same place in both data types. On the other hand, this scheme provided satisfactory results for southern plain areas with slight overestimation indicating peaks of rainfall of intensity of 50 mm at scattered locations when compared with satellite data. There was indication of rainfall with intensity of 50 mm over southern areas in PMD data but locations of rainfall in model-predicted and PMD data were found in mismatch. Here it may be noted that Grell scheme indicated slightly overestimated results for plain areas for the first time in this study. The reason for this behavior may be attributed to the fact that in this month very little amount of precipitation was observed over the plain areas.

This is consistent with findings of Mukhopadhyay who concluded that Grell scheme gives overestimated results for lighter precipitation. On the other hand, Kain–Fritsch scheme (Figure 4.11(b)) showed slightly overestimated results for both northern mountainous and southern plain areas in comparison with satellite derived data indicating a single peak of rainfall with intensity of 200 mm at exact location of maximum rainfall with intensity of 100 mm as displayed in satellite data (Figure 4.8(b)).
On the other hand, behavior of KF scheme seemed to be in better agreement with PMD data for northern areas by capturing peak rainfall with intensity of 200 mm centered at 32-34° N and 72-74° E as displayed in PMD data.

On similar lines, intensity and pattern of precipitation for July and August of 1998 and 2001 were also investigated for Anthes–Kuo and Betts–Miller schemes. When compared with satellite data, both the schemes were unable to provide appropriate results over region of interest, showing either under-predicted precipitation or over-estimated contours of rainfall patterns, while locations of rainfall were also found to be substantially out of phase. For this reason, only typical figures are being referred to here instead of including all of them. For instance, Figures 4.12 (a) and 4.12 (b) show accumulated monthly precipitation in millimeters for August 1998 as predicted by Anthes–Kuo and Betts–Miller schemes, respectively. Both schemes predicted 200 mm precipitation contours at locations extending from 68 to 72 ° E and from 28 to 32 ° N that are quantitatively as well as qualitatively in disagreement with satellite (Figure 4.8(a)) and PMD data (4.9(a)).

Previous studies of Wang and Ferretti also showed poor performance of Anthes–Kuo and Betts–Miller schemes in capturing precipitation patterns over Alpine region of Italy and continental region of USA [Wang, 1997; Ferretti, 2000]. In both studies Kain–Fritsch scheme showed better performance in capturing both intensity and location of maximum precipitation.
To find out exact reasons responsible for superiority of one convective scheme over others is not the objective of present study. However, plus point that seems to favor better performance of Grell scheme may be its close assumption that mixing in deep convection occurs at cloud top rather than through its sides in plume-like fashion, hence interaction of cloudy air with environmental air occurs only at top of cloud [Reuter, 1986]. On the other hand, feature which may support Kain–Fritsch scheme is probably the inclusion of entrainment and detrainment processes in formation of cloud. Other reason for better performance of Kain–Fritsch scheme, especially over high mountainous regions, may be the triggering factor of scheme related to uplift, which in a region of complex topography may play a major role. Failure of Betts–Miller scheme may be due to use of a single stable moisture profile in scheme which is based on observations of tropical storms that prevents its application to other environments. Anthes–Kuo scheme is also unable to show better performance, probably due to its assumptions regarding nature of atmospheric convection. In view of above, Anthes–Kuo and Betts–Miller schemes may not be suitable for complex terrain of south Asian region.

### 4.2.2 Ambient Temperature & Potential Temperature Profiles

In order to evaluate variation in ambient temperature and potential temperature with increasing height, monthly averaged vertical profiles of these parameters were plotted.
for August 1998 and compared with Reanalysis data of US National Centre for Environmental Prediction (NCEP) for corresponding month. Simulations were conducted taking model domain with spatial resolution of 90 km. Specific location (33.6° N, 73.1° E) of city of Islamabad was selected for the purpose of validation. This is because selected area was always observed to be receiving peak rainfall throughout the analysis. Figure 4.13(a) illustrates a comparison of monthly averaged ambient temperatures predicted by different convective schemes (lines) at different vertical heights with that of NCEP data (dots) for August 1998.

This figure 4.13 depicts an overall decreasing trend in temperature with increasing height. A close agreement can be seen between observed and model-predicted temperatures. Other noticeable thing is that results of the Grell and Betts–Miller schemes are closer to observed ones as compared to those by other schemes, though it is difficult from Figure 4.13(a) to distinguish curves of different schemes because plot covers a wide range of data presented for whole vertical domain. Figure 4.13(b) shows vertical variation in monthly averaged potential temperatures predicted by different schemes (lines) with increase in height for August 1998.

Figure 4.13: A comparison of model-predicted (lines) monthly averaged (a) ambient (b) potential temperature (°C) profile with NCEP data (dots) at the location of Islamabad City for the month of August, 1998. ■ NCEP data  
Grell  
KF  
Kuo  
BM
As potential temperature is a dynamically important quantity more than actual temperature, model simulated results for this parameter are also presented and compared with NCEP data (dots). Potential temperature is a useful measure of static stability of atmosphere. For a stable atmosphere, potential temperature increases with height, while it decreases with height for an unstable convective atmosphere. One thing that is obvious from Figure 4.13(b) is presence of a steep potential temperature gradient in upper atmosphere and a very small temperature gradient, almost zero, at lower heights. This trend indicates that upper atmosphere is more stable than lower. Approximately constant value of potential temperature at lower heights is indicative of weak convection, as expected, due to fact that year 1998 had experienced little convective precipitation throughout summer monsoon season. Comparison of model-predicted results with observed data of NCEP also show that results of Grell and Betts–Miller schemes are closer to observed data compared to other schemes.

4.2.3 Vertical Variation in Relative Humidity and Moist Static Energy

Figure 4.14 illustrates comparison of monthly averaged relative humidity predicted by different schemes (lines) with that of observed data of NCEP (dots) for August 1998. Comparing simulated results with NCEP data, it was observed that both Grell and Betts–Miller schemes were again successful in capturing overall trend of vertical variation in relative humidity with increasing height, although neither scheme was able to generate values of humidity in close agreement to those of NCEP data. Some deviation of model-predicted results from NCEP data is most likely due to difference between spatial resolutions of model domain and NCEP dataset.

Figure 4.15 depicts comparison of model-predicted vertical profiles of monthly averaged moist static energy for different convective parameterization schemes (lines) with that of data of NCEP (dots) for August 1998. It is again clear from Figure 4.15 that both Grell and Betts–Miller schemes seemed to be successful in capturing well the overall trend of vertical variation in moist static energy with increasing height compared to other convective schemes.

In light of above discussion on results of precipitation, ambient temperature, potential temperature, relative humidity and moist static energy, it is substantially reflected that Grell scheme performed well for all meteorological parameters over both resolutions for specific month of August 1998.
Figure 4.14: A comparison of model-predicted (lines) monthly averaged (a) relative humidity (%) (b) moist static energy (kJ kg\(^{-1}\)) profile with NCEP data (dots) at the location of Islamabad City for the month of August, 1998. ■ NCEP data Grell KF Kuo BM

On the other hand, Betts–Miller scheme, which produced overestimated results with 30 km resolution for same period in case of precipitation, seemed to be successful in generating reasonable results with 90 km model resolution for dynamic variables of temperature, relative humidity and moist static energy. Results thus indicate dependence of a convective scheme on spatial resolution of model. This dependence has also been reported previously by some investigators [Kerkhoven, 2006; Ratnam, 2006].

### 4.3 Summary

Meso-scale meteorological modeling using MM5 is validated to confidently couple it with an advanced dispersion model. Initially ambient temperature, wind speed and wind direction data of Oman was used in model validation. Within an acceptable margin of deviation, overall qualitative trend of modeled ambient temperature, wind speed and direction was found to be in general agreement with that of actual observed data demonstrating MM5 to be a prospective model for generating meteorological fields for coupling it with an advanced dispersion model. For further tuning it up for
Pakistan specific region, sensitivity of different parameterized schemes generally used in MM5 such as Grell, Kain–Fritsch, Anthes–Kuo and Betts–Miller were investigated. Suitability of each scheme was verified by performing computations using each scheme, and then comparing them by factual data acquired from TRMM and PMD for ambient temperature, potential temperature, moist static energy, humidity and precipitation in Pakistan. The aim was to finalize a specific parameterized scheme of MM5 for Pakistani region so that pollutant dispersion studies may be carried out by coupling it with an advanced dispersion model.

Among the schemes, Grell scheme generated better results for all parameters and resolutions but for lesser precipitation intensity. On the other hand, Kain–Fritsch scheme captured rainfall patterns and intensity reasonably well over northern mountainous region for heavy precipitation. Anthes–Kuo remained unable to produce realistic results indicating its unsuitability in this region. Betts–Miller scheme which remained unable to capture precipitation well with model resolution of 30 km gave some reasonable results for meteorological parameters with model resolution of 90 km indicating its dependence on spatial resolution of selected model domain. These investigations assisted in finalizing the decision to select Grell scheme in MM5 for performing further computations using coupled MM5-CALPUFF dispersion modeling.
CHAPTER 5

Results and Discussion

Experimental Validation of Coupled Meteorology and Dispersion Modeling

Once meteorological model such as MM5 is validated and parameterization schemes are finalized, it can be coupled with a dispersion model. By term ‘coupling’ means that meteorological parameters obtained as an output of mesoscale model can be directly used as input of a dispersion model such as CALPUFF. Final results of this entire coupling would then be acquired as concentration of pollutant at desired locations. Since all these efforts of modeling are being made for decision making and accident management, it is obviously important that modeling results be validated by extensive experimentation. This chapter is, therefore, mainly directed towards presentation of these modeling results and their experimental validation commencing from smaller flat terrain with lower release height followed by involving larger dispersion area and increasing release heights. Within this sequence, results of experiments involving effects of multiple or cluster of stacks would also be discussed. Last section would discuss post processing for tracing released pollutant particle trajectories.

5.1 Tracer Dispersion Experiments

Present research work may be divided into four sets of experiments. First set involves simple dispersion/diffusion experiments at a very short scale horizontally and vertically. Over a flat ground, a support system was erected and SO\textsubscript{2} gas was released at a height of 30 ft through a six inch internal diameter conduit and air samples were taken in prevailing wind direction at sampling points on three arcs of varied radii. In second set of experimental work, the height was doubled i.e. 60 ft, which is usual height of brick kilns while samples were collected at sampling points covering larger distances upto 1640 ft. Cluster of emission sources was also considered. In third set of experimentation, a 100 ft stack was used and air samples were collected at sampling points in different directions at varied distances ranging from 1000 ft to about 3000 ft. In final set of experiments, SF\textsubscript{6} gas was released at
height of 230 ft through a conduit of 5/16 inch internal diameter and samples were taken at various sampling points at distances ranging from 2300 ft to about 33000 ft (6.25 miles). Sampling points were selected considering prevailing wind direction and accessibility.

5.1.1 Results of Tracer Experiments with Ground Release of SO₂

Sulfur dioxide gas was continuously released at a constant rate of 0.05 g/s for entire duration of about seven (07) hours from 1000 hrs to 1700 hrs while concentration at any sampling point was measured continuously. Thus sampling was done for ten minutes and the average concentration was noted. Finally a mean of six readings was taken to get experimental hourly average concentration at that point. Moreover, wind parameters were also measured at all sampling locations. Among these, most important parameter was wind direction as it was influencing the bulk motion of released SO₂. It is important to mention here that though these directions were also computed by models but as observed in figure 4.3, experimentally observed wind was expected to elaborate prevailing SO₂ dispersion more realistically. For comparison of both modeled as well as experimentally measured wind directions, values are shown in tables adjacent to each of the time series profiles. Details of all experimental arrangements have already been given in section 3.3.2.1.

Experimental as well as modeled concentrations as a function of time are shown in Figure 5.1. Though overall trend of both is almost similar but experimental curve lies above modeled curve indicating that model is somewhat underestimating the SO₂ concentration. As entire observational readings lie above modeled values, this reflects that in experimental measurements there is an added background of SO₂ that keeps experimental curve above modeled curve. Lower positioning of modeled curve specifies that model as such does not accommodate prevailing effects of other sources that may contribute to background at that location. Hence, prior to recording any concentration reading at a certain sampling point, a background observation was also noted every day. Despite similar trend, some discrepancies at start of day and at evening time can be noticed. For a few mid-day readings minor error may be due to fluctuations in reading related to electronic noise of analyzer. Relatively more difference in experimental and modeled readings at morning i.e. 1000 hrs and at
Table 5.1: Temporal Variation in Model Predicted and Measured Direction of Wind at A1

<table>
<thead>
<tr>
<th>Time (hrs)</th>
<th>1000 hrs</th>
<th>1100 hrs</th>
<th>1200 hrs</th>
<th>1300 hrs</th>
<th>1400 hrs</th>
<th>1500 hrs</th>
<th>1600 hrs</th>
<th>1700 hrs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dir(modeled)</td>
<td>+22.8</td>
<td>+9.4</td>
<td>+6.8</td>
<td>+2.3</td>
<td>-0.3</td>
<td>-23.8</td>
<td>-8.7</td>
<td>+35.2</td>
</tr>
<tr>
<td>Dir(exp.)</td>
<td>+21.3</td>
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<td>+23.0</td>
<td>+22.3</td>
<td>+10.4</td>
<td>-2.2</td>
<td>-0.9</td>
<td>+9.9</td>
</tr>
</tbody>
</table>

Figure 5.1: Variation of Experimentally Measured and Modeled Concentrations of SO$_2$ at A1

evening i.e. 1700 hrs may be due to the SO$_2$ emitted from pick and drop transport fleet. These experiments were conducted in PIEAS which is located in Nilore Complex that is about thirty kilometers from main cities Islamabad and Rawalpindi. There is a transport fleet for pick and drop of all staff from main city to Nilore complex and back. Most of these vehicles are buses and vans using diesel fuel and some are cars that run on petrol. Entire fleet reaches Nilore around 0830 hrs. While dropping the employees at various offices in different establishments at Nilore Complex, vehicular engines keep on combusting diesel emitting SO$_2$ as a by-product in the form of flue gases. The effect, therefore, may prevail for some time resulting in relatively higher background prevailing even at 1000 hrs onwards. This trend breaks in the afternoon when vehicular traffic is generally minimum hence differences between experimental and modeled curves seem decreasing and remain almost negligible from 1300 hrs to about 1500 hrs. Same scenario happens again when entire fleet comprising mostly of buses starts from PIEAS premises and other establishments to pick staff from Nilore Complex and drop them back to their residences. This might have resulted in increased background thus bringing experimental results on higher side compared to predicted values on the curve around 1700 hrs.

Table 5.1 shows temporal variation in hourly averaged direction of wind predicted by model and measured by meteorological instruments installed on mobile monitoring
station during experimental period from 1000 hrs to 1700 hrs. Temporal change in concentrations of SO₂ measured at sampling location A1 may be attributed to continuous alteration of wind direction. During initial hours of experimental day i.e. Feb 24, 2013, wind was observed blowing towards sampling location i.e. wind direction remained within 3.5° above or below actual direction where mobile van was positioned (22.5° w.r.t. South). Thus relatively higher concentrations were observed during these specific hours. A decreasing trend in SO₂ concentration was observed in afternoon i.e. after 1300 hours. This may be explained on the basis of change in wind direction that started shifting its direction away from location of sampling point. Significant SO₂ concentration was noted at 1400 hrs of the day though wind had diverted by about 12° from sampling location. Despite shift in wind direction, existence of about 12.9 ppb of SO₂ at sampling location A1 may be due to physical phenomenon of lateral dispersion in SO₂ plume.

At 1500 hrs, wind was blowing far away from sampling location thus concentration was dropped to background level. A rise in concentration was again observed during evening time, when wind started to change its direction and took its course back towards location of mobile van.

Similar trends may be observed in Figure 5.2, though it shows a slight initial increase in SO₂ concentration in morning time of experimental day i.e. February 14, 2013, indicating that wind was slowly shifting its direction towards location of sampling point A-2. A peak value of SO₂ concentration was observed in afternoon i.e. at 1300 and 1400 hrs, when direction of wind was almost towards sampling location as can be seen from Table 5.2. Subsequently wind moved further away towards south, resulting in decreasing trend observed in SO₂ concentration till 1500 hrs. A slight increase in experimental value of SO₂ concentration in evening may again be due to an increased background observed in evening due to transport exhaust.

Figure 5.3 shows increasing trend in concentration of SO₂ measured at A3 on Feb 15, 2013 during period from 1000 hrs to 1100 hrs. Peak value of concentration was observed at 1100 hrs and which decreased. After 1500 hrs, an increase was again observed in concentration. This temporal variation in SO₂ concentration may be explained by experimental data of wind direction in Table 5.3. Directional change in wind towards sampling location at 1000 hrs as well as at 1500 hrs supports increasing trend of SO₂ concentration.
Table 5.2: Temporal Variation in Model Predicted and Measured Direction of Wind at A2

<table>
<thead>
<tr>
<th>Time</th>
<th>1000 hrs</th>
<th>1100 hrs</th>
<th>1200 hrs</th>
<th>1300 hrs</th>
<th>1400 hrs</th>
<th>1500 hrs</th>
<th>1600 hrs</th>
<th>1700 hrs</th>
</tr>
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<tbody>
<tr>
<td>Dir (modeled)</td>
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<td>+49.1</td>
<td>+40.2</td>
<td>+30.4</td>
<td>+21.6</td>
<td>+17.9</td>
</tr>
<tr>
<td>Dir (exp.)</td>
<td>+60.5</td>
<td>+56.7</td>
<td>+59.5</td>
<td>+46.3</td>
<td>+43.4</td>
<td>+27.3</td>
<td>+19.8</td>
<td>+17.2</td>
</tr>
</tbody>
</table>

Figure 5.2: Variation of Experimentally Measured and Modeled Concentrations of SO₂ at A2

Table 5.3: Temporal Variation in Model Predicted and Measured Direction of Wind at A3

<table>
<thead>
<tr>
<th>Time</th>
<th>1000 hrs</th>
<th>1100 hrs</th>
<th>1200 hrs</th>
<th>1300 hrs</th>
<th>1400 hrs</th>
<th>1500 hrs</th>
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<tbody>
<tr>
<td>Dir (modeled)</td>
<td>+57.6</td>
<td>+61.6</td>
<td>+63.6</td>
<td>+62.6</td>
<td>+60.6</td>
<td>+58.6</td>
<td>56.7</td>
<td>+61.3</td>
</tr>
<tr>
<td>Dir (exp.)</td>
<td>38.3</td>
<td>+66.1</td>
<td>+50.0</td>
<td>+63.3</td>
<td>+37.1</td>
<td>32.0</td>
<td>41.2</td>
<td>60.3</td>
</tr>
</tbody>
</table>

Figure 5.3: Variation of Experimentally Measured and Modeled Concentrations of SO₂ at A3
During afternoon, wind started moving away from sampling location resulting in decrease in concentration. Concentration that prevails during this interval may be due to diffusion of SO\textsubscript{2} in lateral direction as wind is within 10\textdegree of sampling point A3. A synergistic effect of favorable wind towards A3 as well as increase of background at these times due to exhaust of mobile sources is reflected by final gradual upward rise in SO\textsubscript{2} concentration after 1500 hrs.

Table 5.4: Temporal Variation in Model Predicted and Measured Direction of Wind at A4

<table>
<thead>
<tr>
<th>Time (Hrs)</th>
<th>1000 hrs</th>
<th>1100 hrs</th>
<th>1200 hrs</th>
<th>1300 hrs</th>
<th>1400 hrs</th>
<th>1500 hrs</th>
<th>1600 hrs</th>
<th>1700 hrs</th>
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<tr>
<td>Dir(modeled)</td>
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<td>+53.4</td>
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<td>-5.5</td>
<td>-48.8</td>
<td>-49.1</td>
<td>-41.4</td>
<td>+23.1</td>
</tr>
<tr>
<td>Dir(exp.)</td>
<td>+87.2</td>
<td>+68.7</td>
<td>-8.6</td>
<td>-13.0</td>
<td>-22.2</td>
<td>-25.5</td>
<td>-20.8</td>
<td>+9.6</td>
</tr>
</tbody>
</table>

Figure 5.4: Variation of Experimentally Measured and Modeled Concentrations of SO\textsubscript{2} at A4

During experimentation on Feb 20, 2013, significant concentration of SO\textsubscript{2} was observed at sampling location A4 only for a single initial hour i.e. 1000 hrs. For rest of the experimental day, wind direction was away from sampling location (Table 5.4) and as a result, only background level concentration of SO\textsubscript{2} was observed during entire period of experimentation as can be seen in figure 5.4.

Figure 5.5 shows similar trend as observed for sampling point A2. Here, it may be noted that both points were positioned in same direction oriented at 45\textdegree SW but at different arcs. This experimentation was done on Feb 20, 2013 to assess effects of increased distance with respect to point of emission. Though trend is similar, concentrations are higher at B1 as compared to A2. This can be explained on basis of the fact that under certain atmospheric stability conditions, point of maximum concentrations follows a certain pattern. Ground level concentration due to plume
emitted at certain height initially increases, attains a maximum concentration at specific distance and then decreases [Slade, 1968].

Table 5.5: Temporal Variation in Model Predicted and Measured Direction of Wind at B1

<table>
<thead>
<tr>
<th>Time</th>
<th>1000 hrs</th>
<th>1100 hrs</th>
<th>1200 hrs</th>
<th>1300 hrs</th>
<th>1400 hrs</th>
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<tbody>
<tr>
<td>Dir (modeled)</td>
<td>+56.6</td>
<td>+27.3</td>
<td>+15.7</td>
<td>+17.6</td>
<td>37.4</td>
<td>56.1</td>
<td>61.3</td>
<td>+71.3</td>
</tr>
<tr>
<td>Dir (exp.)</td>
<td>+35.3</td>
<td>+24.0</td>
<td>+23.0</td>
<td>+30.7</td>
<td>+42.1</td>
<td>+50.2</td>
<td>+60.3</td>
<td>+77.1</td>
</tr>
</tbody>
</table>

Figure 5.5: Variation of Experimentally Measured and Modeled Concentrations of SO$_2$ at B1

One may assume that concentration was following similar pattern and was rising from point A2 to B1 according to expected pattern but not yet reached a distance of maximum concentration. Had there been some more readings in same direction at various distances and had the wind prevailed in same direction, concentration could have reached at a point of maxima. This indicates that more experiments may be required to examine effect of distance on the pattern a concentration may follow, if plume is released at certain height [Lamarsh, 1968].

The crossing of experimental time series profile falling below model profile as shown in Figure 5.6 indicates an error in measurement as it is simply not possible. This probability is ruled out due to the fact that model never considers existing background concentration while experimental observation always includes in it the prevailing background and hence should remain above modeled profile. Figure 5.6 elaborates that concentration of SO$_2$ remained at background level most of the time during experimental day on Feb 21, 2013. Reason may be that wind was never in direction of sampling location B2 throughout the day as shown in Table 5.6. Rise in concentration was observed only at 1100 hrs and 1600 hrs of the day, when wind was observed blowing towards B2 within 20° to 25°.
Table 5.6: Temporal Variation in Model Predicted and Measured Direction of Wind at B2

<table>
<thead>
<tr>
<th>Time</th>
<th>1000 hrs</th>
<th>1100 hrs</th>
<th>1200 hrs</th>
<th>1300 hrs</th>
<th>1400 hrs</th>
<th>1500 hrs</th>
<th>1600 hrs</th>
<th>1700 hrs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dir(modeled)</td>
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<td>+95.6</td>
<td>+111.1</td>
<td>+109.5</td>
<td>+102.9</td>
<td>+96.7</td>
<td>88.1</td>
<td>+81.9</td>
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<tr>
<td>Dir(exp.)</td>
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<td>+88.1</td>
<td>+88.5</td>
<td>+90.0</td>
<td>+80.4</td>
<td>+88.3</td>
</tr>
</tbody>
</table>

Figure 5.6: Variation of Experimentally Measured and Modeled Concentrations of SO₂ at B2

Though wind was not exactly in same direction of sampling location but significant contribution of released plume to concentration of SO₂ was observed at sampling location during both times. Concentration at 1000 hrs as well as at 1700 hrs may be due to lateral diffusion from other location.

Table 5.7: Temporal Variation in Model Predicted and Measured Direction of Wind at C

<table>
<thead>
<tr>
<th>Time</th>
<th>1000 hrs</th>
<th>1100 hrs</th>
<th>1200 hrs</th>
<th>1300 hrs</th>
<th>1400 hrs</th>
<th>1500 hrs</th>
<th>1600 hrs</th>
<th>1700 hrs</th>
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</thead>
<tbody>
<tr>
<td>Dir(modeled)</td>
<td>+68.7</td>
<td>+68.9</td>
<td>+73.8</td>
<td>+76.6</td>
<td>+74.4</td>
<td>+69.3</td>
<td>63.4</td>
<td>+68.4</td>
</tr>
<tr>
<td>Dir(exp.)</td>
<td>64.2</td>
<td>68.3</td>
<td>83.5</td>
<td>89.7</td>
<td>80.3</td>
<td>67.0</td>
<td>57.4</td>
<td>66.0</td>
</tr>
</tbody>
</table>

Figure 5.7: Variation of Experimentally Measured and Modeled Concentrations of SO₂ at C
Other contributing factor may be transport fleet as mentioned in previous discussion because both peaks of concentration were observed near to arrival and departure times of transport fleet.

Relatively higher concentrations of \( \text{SO}_2 \) were measured at point C during the experimental day on Feb 26, 2013. Three peaks of concentration were observed at 1100 hrs, 1500 hrs and 1700 hrs. This sampling point is at farthest distance from source i.e. 150 m. Reason for higher concentration at this point may be that wind direction was favorable and remained directed towards the location of sampling point C almost throughout entire duration from 1500 hrs to 1700 hrs (Table 5.7).

In short, among these ground level experiments, it was observed that coupled meteorological & dispersion model (MM5+CALPUFF) predicted concentrations that were generally in agreement with experimental results within an error range of prevailing background concentration of tracer. These experiments demonstrated the phenomenon of bulk motion of \( \text{SO}_2 \) as a tracer along wind and to some extent lateral diffusion. Though this set of basic experiments provided encouraging results that matched with model trends, yet data could not reflect variation of ground level concentration with respect to emitter-receptor distance and release height. Moreover, collection of data from a cluster of stacks located within a small area was expected to be useful for validation of (MM5+CALPUFF) model results under identical scenario. Hence, next set of experiments was planned to assess effect of increased stack height and corresponding ground level maxima of concentration at relatively larger receptor distances from a single or cluster of stacks.

5.1.2 Results with Higher Stacks and Larger Emitter-Receptor Distances

Coupled CALPUFF+MM5 modeling system was employed to model ground level concentration and was then compared with experimentally collected or observed data of \( \text{SO}_2 \) released from a relatively isolated brick kiln chimney as well as from cluster of stacks of an oil refinery. Modeling and experimental procedures for \( \text{SO}_2 \) emission from brick kiln are given in section 3.2.5 and 3.3.2.2. Similarly procedure of modeling stack cluster of oil refinery and flaring activities on oil wells is given in section 3.2.2 and 3.2.3 respectively. Results of both of these studies are presented in following sections.
5.1.2.1 SO$_2$ Emission from Isolated Brick Kiln

Predicted results of SO$_2$ concentrations were validated against that of experimental data collected using Mobile Ambient Air Quality Monitoring van. Experimental data were recorded at different downwind distances from a single emission source i.e. an isolated brick kiln.

Table 5.8 shows comparison of predicted and experimentally measured hourly averaged SO$_2$ concentration for three hours of two consecutive experimental days of March, 2013. Difference between predicted and measured concentrations varied from 10.7 to 29.9 %.

Table 5.8: Comparison of Hourly Average Predicted and Measured Concentration of SO$_2$ Emitted from Single Brick Kiln under Stability Condition ‘B’

<table>
<thead>
<tr>
<th>Distance (m)</th>
<th>50</th>
<th>100</th>
<th>200</th>
<th>300</th>
<th>400</th>
<th>500</th>
</tr>
</thead>
<tbody>
<tr>
<td>Predicted conc. (ppb)</td>
<td>1.7</td>
<td>8.6</td>
<td>7.0</td>
<td>5.4</td>
<td>3.1</td>
<td>1.9</td>
</tr>
<tr>
<td>Observed conc. (ppb)</td>
<td>2.0</td>
<td>7.3</td>
<td>5.7</td>
<td>7.7</td>
<td>2.8</td>
<td>2.2</td>
</tr>
<tr>
<td>Difference (%)</td>
<td>15.0</td>
<td>17.8</td>
<td>22.8</td>
<td>29.9</td>
<td>10.7</td>
<td>13.6</td>
</tr>
<tr>
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<td>1000</td>
<td>1200</td>
<td>1400</td>
</tr>
</tbody>
</table>

Ground level SO$_2$ concentration ‘χ’ was measured at a number of downwind distances from brick kiln in prevailing wind direction. Sampling time was taken as 10 minutes and subsequently averaged out on basis of 1-hour. Since turbulent structure of atmosphere influences dispersion behavior, all concentration measurements were taken under same stability class to avoid its impact on concentration values. It was observed that stability class ‘B’ prevailed during experimental period i.e. from 1000 hrs to 1400 hrs and it changed into Class ‘C’ after 15:00 hrs for both experimental day times. This is in agreement with observation in dispersion experiments that showed similar atmospheric behavior over sub-urban areas during day time [Pooler, 1965].

In order to further investigate atmospheric diffusion predicted and measured values of a parameter, χ v/Q (i.e. relative ground level concentration times wind speed) were plotted against downwind distances on a log-log scale as shown in Figure 5.8.

Model predicted curve of Figure 5.8 indicates a decreasing tend for SO$_2$ concentration after attaining point of maximum concentration i.e. 8.6 ppb at downwind distance.
around 100 meter. Predicted dispersion behavior is in agreement with that presented in literature indicating ground level concentration in terms of \((\chi v/Q)\) with distance for similar height as of brick kiln (H) and stability class B [Turner, 1972].

![Figure 5.8: Experimental and Modeled SO\(_2\) Concentrations at Different Receptor Locations from Source](image)

As compared to predicted results, Figure 5.8 indicates that experimentally measured SO\(_2\) concentration values showed underestimated results at some distances and overestimated results at some others. This may be due to presence of other brick kilns not nearby but still contributing to variable background. Domestic heating was also not accounted for in CALPUFF results, which may also be adding discrepancies in comparative results. Moreover, emission rate of brick kiln has been taken constant during one hour release period. However, practically it varies during operating period of brick kiln. This variation in flow rate may also be a source of creating deviation between modeled and measured concentration which is also observed in previous studies on brick kilns [Ahmed, 2008; Le, 2009].

### 5.1.2.2 Model Validation for Cluster of Stacks Considering SO\(_2\) as Tracer Gas

CALPUFF has an option of modeling multiple sources of pollutant. Hence, a scenario was considered where there was cluster of eleven stacks ranging from 25 ft to 480 ft in height, stack exit diameter from 1.0 m to 3.6 m, exit gas temperature from 60\(^\circ\) C to 400\(^\circ\) C, emission rates from 0.01 g/s to 50 g/s and exit velocity from 0.3 m/s to 193 m/s.). Observed recorded data of meteorology and concentration was available from a ‘met station’ as well as from a mobile monitoring station respectively provided by the
Ministry of Environment and Climate Affairs (MECA) Oman. This part of research work was done in collaboration with Department of Mechanical and Industrial Engineering, College of Engineering, Sultan Qaboos University, Muscat, Oman.

Coupled MM5+CALPUFF model validation was done by comparing model predicted results with that of observations. Observed values of SO$_2$ are 24 hourly averaged, recorded at Mobile Van–Sohar monitoring station close to Sohar refinery. Since recorded data available was in units of µg/m$^3$, comparisons in Table and Figure are shown in this unit. Equation 3.3 gives relation between mg/m$^3$ and ppm.

**(a) Comparison of Model Predicted Daily Averaged Concentrations of SO$_2$ with Observed Values**

24-hourly averaged concentrations of SO$_2$ as predicted by CALPUFF and observed from monitoring station are summarized in Table 5.9. It is reflected from Table 5.9 that model underestimated or overestimated observed values for a few days in duration of study i.e. June 1–15, 2008 while maximum deviation remained within 35.60%. Observed mismatch may be explained by the fact that Sohar city is an industrial hub of Oman and many industries are located in the city along with Sohar refinery. Contributions of nearby sources of SO$_2$, comprising of local industries and domestic heating, were recorded by sensors in monitoring van. Furthermore, effects of high buildings in and around study area were not accounted for in CALPUFF results, which may be responsible of discrepancies in results. Involvement of such factors in modeling results has been reported in previous studies [Elbir, 2003; Yerramilli, 2009]. Hence these factors though affected observed data but influence of such local details and sources was not considered by the model and therefore not reflected in predicted curve. Despite these deviations one may notice from Figure 5.9 that same general trend of both modeled prediction as well as observed data prevailed validating model results (Figure 5.9).
Table 5.9: A Comparison of 24-Hourly Measured and Predicted Levels of SO$_2$

<table>
<thead>
<tr>
<th>Day (June, 2008)</th>
<th>Measured SO$_2$ (µg/m$^3$)</th>
<th>Predicted SO$_2$ (µg/m$^3$)</th>
<th>Difference (µg/m$^3$)</th>
<th>Difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Not Available</td>
<td>7.73</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>7.03</td>
<td>5.75</td>
<td>1.28</td>
<td>18.20</td>
</tr>
<tr>
<td>3</td>
<td>7.41</td>
<td>6.67</td>
<td>0.74</td>
<td>9.99</td>
</tr>
<tr>
<td>4</td>
<td>6.66</td>
<td>6.20</td>
<td>0.46</td>
<td>6.91</td>
</tr>
<tr>
<td>5</td>
<td>6.18</td>
<td>7.50</td>
<td>-1.32</td>
<td>21.36</td>
</tr>
<tr>
<td>6</td>
<td>7.38</td>
<td>8.97</td>
<td>-1.59</td>
<td>21.54</td>
</tr>
<tr>
<td>7</td>
<td>7.67</td>
<td>9.98</td>
<td>-2.31</td>
<td>20.60</td>
</tr>
<tr>
<td>8</td>
<td>7.50</td>
<td>10.17</td>
<td>-2.67</td>
<td>35.60</td>
</tr>
<tr>
<td>9</td>
<td>6.56</td>
<td>7.68</td>
<td>-1.12</td>
<td>17.03</td>
</tr>
<tr>
<td>10</td>
<td>8.52</td>
<td>9.72</td>
<td>-1.20</td>
<td>14.08</td>
</tr>
<tr>
<td>11</td>
<td>6.49</td>
<td>6.15</td>
<td>0.34</td>
<td>5.24</td>
</tr>
<tr>
<td>12</td>
<td>8.18</td>
<td>8.10</td>
<td>0.08</td>
<td>0.98</td>
</tr>
<tr>
<td>13</td>
<td>6.41</td>
<td>5.99</td>
<td>0.42</td>
<td>6.55</td>
</tr>
<tr>
<td>14</td>
<td>6.03</td>
<td>5.90</td>
<td>0.13</td>
<td>2.16</td>
</tr>
<tr>
<td>15</td>
<td>5.51</td>
<td>5.58</td>
<td>-0.07</td>
<td>1.27</td>
</tr>
<tr>
<td>Maximum</td>
<td>8.52</td>
<td>9.72</td>
<td>-1.20</td>
<td>14.08</td>
</tr>
</tbody>
</table>

Figure 5.9: Variation of Observed and Modeled Concentrations of SO$_2$

(b) Maximum SO$_2$ Concentrations for Hourly Averaged, Daily Averaged and Average of Entire Simulation Period

Four highest values of SO$_2$ concentration as predicted by CALPUFF for averaging period of 1-h, 24-h, and total period are tabulated in Table 5.10. The maxima of hourly, daily and total period averaged concentrations are 85.50, 10.17, and 3.34 µg/m$^3$ respectively. These highest ranked values of SO$_2$ concentration were estimated on 6, 7, 8, and 12 June, 2008. Maximum of 24-hourly averaged ground level concentrations of SO$_2$ was predicted on July 8, 2008. This particular day is
characterized by such meteorological conditions, which are quite suitable for increased concentration levels.

Table 5.10: Ranked Values of Predicted SO\textsubscript{2} Concentrations

<table>
<thead>
<tr>
<th>Receptor Coordinates (km)</th>
<th>Peak value (µg/m\textsuperscript{3})</th>
<th>Period (Day, Start time)</th>
<th>Rank</th>
<th>Average period</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1.17, -1.50</td>
<td>85.50</td>
<td>0800 (12 June 2008)</td>
<td>Highest 1</td>
<td>hourly</td>
</tr>
<tr>
<td>-13.83, 14.50</td>
<td>76.22</td>
<td>0200 (8 June 2008)</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>-13.50, 14.17</td>
<td>67.78</td>
<td>0300 (8 June 2008)</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>-13.50, 14.50</td>
<td>62.68</td>
<td>0400 (8 June 2008)</td>
<td>Lowest 4</td>
<td></td>
</tr>
<tr>
<td>-12.17, 12.83</td>
<td>10.17</td>
<td>8 June 2008</td>
<td>Highest 1</td>
<td>Daily</td>
</tr>
<tr>
<td>-12.50, 2.83</td>
<td>9.98</td>
<td>7 June 2008</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>-11.50, 11.83</td>
<td>8.97</td>
<td>6 June 2008</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>-0.83, -1.83</td>
<td>8.10</td>
<td>12 June 2008</td>
<td>Lowest 4</td>
<td></td>
</tr>
<tr>
<td>-0.83, -1.50</td>
<td>3.34</td>
<td></td>
<td>Total Period</td>
<td></td>
</tr>
</tbody>
</table>

Wind speed in early hours of the day was not exceeding 2.83 m/s (Fig. 4.2(c)) with a predominant direction towards northwest (Fig. 4.3(c)). There was an increase in wind speed up to 5.35 m/s in noon and afternoon period with a change of direction towards west of sources, due to introduction of sea-breeze which was reinforcing synoptic wind. Decrease in wind speed up to 1.23 m/s was observed in evening and night time along with change in direction towards southwest. This region was under effect of low pressure field in range of 995.5 mb early in the morning and up to 998.5 mb in the noon and again up to 995.2 mb in the evening and night time. Relative humidity of the day was in range of 67 to 80%. Prevailing meteorological conditions of the day played a key role in prediction of results.

(c) Isopleths Plots of Maximum Daily Averaged Concentrations of SO\textsubscript{2}

Figure 5.10 shows isopleths plot of maximum 24-hourly averaged ground level concentration of SO\textsubscript{2} at communities located in surrounding of Sohar refinery. Concentration isopleths indicate spatial and temporal variations of SO\textsubscript{2} in study area. Predominant directions of plume variations are: northwest and southwest. Contour lines spreading in direction of northwest are concentric and homogeneous in shape while shape of concentration levels directing towards west and southwest are distorted in shape. This is due to the fact that variations in terrain elevations towards northwest of sources parallel to coastal boundary are less as compared to the area in west and
southwest of sources. Comparatively flat terrain containing less number of obstacles (High buildings, etc.) causes less distortion in shape of extending plume. Area in direction of west and southwest to sources is characterized by complex terrain including mountains and valleys. Dispersal pattern of pollutant cloud becomes irregular in shape on its interaction with mountains or any other obstacles in path of plume. This is in accordance to a previous study conducted by Fisher who reported that complex topography can directly influence plume dispersion and dilution as plumes may strike hillsides or become trapped in valleys [Fisher, 2003].

![Wind Concentration Distribution](image)

**Figure 5.10: 24-Hourly Averaged Rank-1 Ground Level Concentration Distribution of SO₂**

Resulting effect will be splitting of a dispersing plume into two major portions based on kinetic energy. Upper portion will rise vertically upon contact with elevated terrain, while lower portion of the plume will spread horizontally or laterally around the obstacle. Strength of wind and wind field variations are very prominent in Figure 5.10. Wind field along the coast line is stronger while wind is weak away from coastal region as indicated by size of wind vectors. Direction of wind is variable throughout the domain. Sea breezes from coastal region are playing their part in strengthening wind field of the region. Temporal variation in plume spread is following the alteration in direction of wind according to varying wind flow pattern. Winds originating from seaside are responsible for diverting direction of SO₂ cloud towards
residential area of Sohar city. Iso-concentration contours having higher magnitudes are not extending far away from sources as compared to that one with lower values. Concentration level having value of 0.2 \( \mu g/m^3 \) extends to large downward distances from sources indicating a low polluted area away from coastline. This is a clear indication of coastal boundary effects on ground level concentrations of SO\(_2\) in study area. Estimated results of model on this particular day are towards higher side as compared to that of observed. Complex topography and prevailing meteorological conditions may be one of the reason of overestimation. Due to unavailability of background data, no transformation mechanism was included during execution of CALPUFF modeling system for present study; this might lead to overestimation of the results.

![Wind Concentration Map](image)

**Figure 5.11: 24-Hourly Averaged Rank-2 Ground Level Concentration Distribution of SO\(_2\)**

Second rank value of 24-hourly averaged concentration of SO\(_2\) is noticed on June 7, 2008 as shown in Fig. 5.11. Magnitude of concentration in this case is 9.98 \( \mu g/m^3 \). Plume is extending towards west and northwest directions. Temporal and spatial distribution of concentrated plume is heterogeneous due to terrain diversity and wind field variations. Wind from sea side is transporting the plume again towards residential areas.
Figure 5.12: 24-Hourly Averaged Rank-3 Ground Level Concentration Distribution of SO₂

Figure 5.12 depicts patterns and magnitudes of SO₂ concentrations for 3rd rank. Model made this prediction on June 6, 2008 with a value of 8.97µg/m³. Leading directions for distribution of concentration isopleths are towards northeast and southwest.

Figure 5.13: 24-Hourly Averaged Rank-4 Ground Level Concentration Distribution of SO₂
Nature of isopleths is again irregular due to differences in terrain elevations. Flow of wind from seaside is once again responsible to divert polluted plume towards the area in proximity of refinery. 4th highest value (8.10 \( \mu g/m^3 \)) of ground level concentration of \( SO_2 \) was observed on June 12, 2008. Allocation of concentration patterns along with their magnitudes is illustrated in Figure 5.13. Prominent direction of concentration plume is towards southeast and plume is changing its orientation in accordance with spatial variations in wind field.

**(d) Isopleths Plot of Maximum 1-hourly Averaged Concentrations of \( SO_2 \)**

Maximum 1-hourly averaged ground level concentration of \( SO_2 \) was also estimated on June 12, 2008 at 0800 hrs. Figure 5.14 depicts patterns and magnitudes of the maximum 1-hourly averaged \( SO_2 \) concentration in and around the refinery. Meteorological conditions of this day were very much favorable for atmospheric dispersion of pollutants. Synoptic flow during entire day was very weak.

Due to weak synoptic flow, local thermal circulations began to develop later in the day. Development of thermal circulations played a very decisive role in dispersion of atmospheric pollutants due to result of a complex wind field also reported by Kotroni [Kotroni, 1999]. In present case, wind speed prior to noon was in the range of 0.62–1.65 m/s (Fig. 4.2(d)) and was blowing in direction of southeast (Fig. 4.3(d)). These calm conditions supported development of a sea breeze towards land in noon and afternoon with a magnitude in the range of 4.32–6.89 m/s. In evening and night time, there was sudden decrease in wind speed up to 0.51 m/s along with change of direction from land to sea indicating a land-breeze phenomenon. Average relative humidity for whole day was around 58.38 %. The region was under low pressure field in the range of 999.6 to 996.5 mb at various times of day. Therefore, meteorological conditions of day, in conjunction with topography of studied area, are very much suitable for dispersion of \( SO_2 \) in and around the refinery rather than away from it. It is true for the case under discussion; as maximum ground level concentration of \( SO_2 \) averaged on basis of 1-hour is seen at distance of 1.5 km approximately from sources. Magnitudes of pollutant concentration drop rapidly as distance from sources is increased which is clear from concentration levels in Fig. 5.14. This is in accordance with already reported trend [Turner, 1972]. Predominant direction of concentration
isopleths is toward south and southeast. Direction of contours is changing in accordance with wind field.

![Wind Concentration Distribution of SO₂](image.png)

**Figure 5.14: Maximum of 1-Hourly Averaged Ground Level Concentration Distribution of SO₂**

The 2nd, 3rd and 4th rank values of 1-hourly averaged were 76.22, 67.78, and 62.68 μg/m³, respectively. These magnitudes of concentration were noticed on second, third and fourth hour of June 8, 2008. Night time along with calm wind conditions and variable terrain was significant factor making this day with highest concentration values. Above quoted maximum concentrations of SO₂ were predicted during night time with low wind speeds and stable atmospheric conditions. Findings of current study reveal that dispersion patterns of SO₂ were influenced by various factors including wind speed and direction, type of terrain and land sea breeze. From analysis of predicted results, it is concluded that CALPUFF-MM5 modeling system provided reasonably correct estimates of SO₂. It was also found that levels of predicted concentration of SO₂ in surrounding areas of Sohar refinery were lower than ambient air quality limit (125 μg/m³) specified by Ministry of Environment and Climate Affairs (MECA) in Oman.
5.1.3 Tracer Experiments Results with PIEAS Experimental Stack

In brick kilns study, it was observed that discrepancies occurred due to presence of other brick kilns nearby despite being a few kilometers away. Hence it was felt more appropriate to use a single isolated stack, well separated by a distance of at least ten kilometers from other sources. Moreover, as amount of coal burnt in Kiln was of different quality and quantity, it was not sure whether the release rate (source term) remained constant at 0.3 g/s from the single stack considered in Brick Kiln experiment in section 5.1.2.1. Dilution rate was observed to be quite frequently changed and hence exit velocity and temperature of flue gases coming out of stack was varying. Plume rise which is dependent on these parameters was therefore fluctuating as buoyancy was continuously changing. Such type of variation in release rate and temperature of flue gas has also been noticed in previous studies on brick kilns conducted by Ahmed and Le [Ahmed, 2008; Le, 2009]. Hence, for reliability of experiments, exit velocity, temperature and release rate being the most important parameters should be well controlled and monitored so as to keep source term constant during experiments. To monitor these parameters isolated stack should have a provision to get samples of gases at various elevations where temperature and flow rate may also be determined. In general, existence of such a stack with so many provisions and experimental facilities was not expected to be available anywhere. In Literature, several studies have been published on SO\(_2\) emission from multiple stacks of power plant, desalination plant etc. [Al-Azmi, 2008; Alameddine, 2005] but dispersion studies using single isolated stack of SO\(_2\) like the study done by Utah was found to be very rare [Utah, 2012].

Keeping in view all above mentioned factors and other requirements, it was decided to design and fabricate a dedicated experimental stack at PIEAS, solely for experimental validation of a reliable dispersion model that can be employed for appropriate decision making in emergency scenarios.

After an extensive effort in designing and fabrication which is a part of this study, an appropriate experimental stack with all required provisions was installed at PIEAS. Details of design, fabrication and mounted experimental facilities are given in section 3.3.2.3. Logical step in parallel to the installation of stack was to model a hypothetical scenario of release of non-radioactive gas from this stack such as SO\(_2\) and model its
Chapter 5

plume trajectory [Sardar, 2012(b)]. Subsequently experimental validation of results of the model using PIEAS experimental stack was planned.

Following section describes tracer experiments performed using this physically isolated PIEAS experimental stack for determination of real (i.e. experimentally determined) ground concentration at various locations near emission point within few kilometers of stack while keeping source term along with all parameters constant.

For precise experimental validation of any model, it is generally necessary to design a comprehensive experimental plan that spreads over entire year, all seasons, different times of day specifically including morning, noon, afternoon, evening, night and dawn to cover different stability conditions that prevail at different times of the day. Moreover, all possible directions according to wind rose should be included and an entire area of several kilometers should be covered around the stack (figure 3.25). Only a few similar studies were conducted for whole year such as by Al-Azmi who performed such detailed study including model validation for two fuel-oil power plant emissions in Kuwait [Al-Azmi, 2008]. In limited period of this Ph.D. research, only four such points were studied (figure 5.15). Since, PIEAS experimental stack has now been developed in this work, research may be continued in future to cover entire experimental plan. A proposal in this regard is included in future recommendations section 6.2.

Considering the prevailing wind direction by wind rose of the area (Appendix-IX) as well as by plume trajectory modeling [Sardar, 2012(b)], four points were initially selected as receptor locations for sampling. These points are explicitly shown in figure 5.15. As can be seen in Figure 5.15 that these points were accessible and mobile ambient air quality monitoring station could easily be taken to these points. Moreover, some effect of varying distance on ground concentration could also be assessed by these points.

‘Sampling point 15’ is located 320 m away and at -45° SE w.r.t. south from the stack. SO$_2$ concentration was measured on March 06, 2013 from 1000 hrs to 1700 hrs using mobile ambient air quality monitoring station.
Figure 5.15: Four Sampling Locations around Experimental Stack Selected in this Study

Figure 5.16 compares model profile and experimental profile as a function of time for ‘sampling point 15’. A general agreement in overall trend can be observed while experimental curve retains its upper location due to addition of background concentration which is not considered by the model.

Table 5.11: Temporal Variation in Model Predicted & Measured Wind Direction at SP-15 on 6-3-13

<table>
<thead>
<tr>
<th>Time</th>
<th>10 hrs</th>
<th>11 hrs</th>
<th>12 hrs</th>
<th>13 hrs</th>
<th>14 hrs</th>
<th>15 hrs</th>
<th>16 hrs</th>
<th>17 hrs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stability class</td>
<td>B</td>
<td>B</td>
<td>C</td>
<td>C</td>
<td>C</td>
<td>C</td>
<td>C</td>
<td>D</td>
</tr>
<tr>
<td>Dir(modeled)</td>
<td>-13.7</td>
<td>-31.2</td>
<td>-35.1</td>
<td>-39.1</td>
<td>-43.2</td>
<td>-48.9</td>
<td>-51.1</td>
<td>27.4</td>
</tr>
<tr>
<td>Dir (exp.)</td>
<td>-25.3</td>
<td>-28.6</td>
<td>-19.1</td>
<td>-33.6</td>
<td>-42.1</td>
<td>-52.0</td>
<td>-44.7</td>
<td>13.2</td>
</tr>
</tbody>
</table>

Figure 5.16: Variation of Measured and Modeled Concentrations of SO₂ at SP-15 on 6-3-13
Increasing trend from 1200 hrs till 1600 hrs can be explained by wind direction that gradually changed its direction towards ‘Sampling Point 15’ as can be seen in table 5.11. A slight deviation in general trend at 1200 hrs and at 1500 hrs can also be noticed where a dip in profile indicating comparatively lower concentration was observed. This deviation may be due to statistical fluctuation in analyzer’s readings as well as localized change in wind direction.

Comparing profiles in figure 5.16 with that of ground release scenario in figure 5.7, it is worth considering that despite the fact that ‘Sampling Point 15’ is at a distance of 300 m, still a noticeable SO\textsubscript{2} concentration i.e. 10 to 13 ppb was observed while stability conditions during experiments remained within category B and C. This is an obvious indication of the effect of increased release height (i.e. 100 ft) and larger release rate (i.e. 0.6 g/s) along with favorable wind direction that provided an access of greater SO\textsubscript{2} at relatively larger distance. This is also in accordance with the fact that for higher stacks, the point of maximum ground concentration shifts away from emission point under same stability conditions [Turner, 1972; Utah, 2012].

The fact that SO\textsubscript{2} is now being released from PIEAS experimental stack at 100 ft and at a constant rate of 0.6 g/s which is larger compared to previous two cases i.e. ground experiments (release height 30 ft, release rate 0.05 g/s) and brick kiln experiments (release height 60 ft, release rate 0.3 g/s), it was logical to further study effect of increasing distance from stack in same direction as that of ‘Sampling Point 15’. Hence, another accessible point at a distance of 830 m was selected as a receptor and was named as ‘Sampling Point 14’.

Figure 5.17 shows modeled and experimental ground level concentration profile at ‘sampling point 14’ whereas Table 5.12 shows modeled and experimental wind direction w.r.t time along with prevailing stability class at respective times. It can be seen from Figure 5.17 that a lesser concentration prevails during entire period of experiment as compared to previous results at ‘Sampling Point 15’ which may be attributed to greater distance from PIEAS experimental stack. Similar variations in behavior of SO\textsubscript{2} concentration with increasing downwind distance from source were also observed and reported by Alameddine under different stability classes for near-field and far-field receptors [Alameddine, 2005].
Another noticeable fact is the closeness of model and experimental curve indicating lesser difference between predicted and experimentally measured values of SO₂ concentrations during morning and evening times in contrast to what was observed previously. It may be due to the fact that ‘Sampling Point 14’ is at a remote location farther from route of mobile SO₂ sources. Peak of concentrations in modeled and measured data were observed when wind retained its direction towards sampling location.

Table 5.12: Temporal Variation in Modeled & Measured Wind Direction at SP-14 on 07-03-2013

<table>
<thead>
<tr>
<th>Time</th>
<th>1000 hrs</th>
<th>1100 hrs</th>
<th>1200 hrs</th>
<th>1300 hrs</th>
<th>1400 hrs</th>
<th>1500 hrs</th>
<th>1600 hrs</th>
<th>1700 hrs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stability class</td>
<td>B</td>
<td>B</td>
<td>B</td>
<td>B</td>
<td>B</td>
<td>C</td>
<td>C</td>
<td>D</td>
</tr>
<tr>
<td>Dir(modeled)</td>
<td>+37.6</td>
<td>-18</td>
<td>-35.2</td>
<td>-41.6</td>
<td>-46.6</td>
<td>-49.4</td>
<td>-45.3</td>
<td>+35.2</td>
</tr>
<tr>
<td>Dir (exp.)</td>
<td>+15.3</td>
<td>-25.0</td>
<td>-31.1</td>
<td>-34.5</td>
<td>-32.6</td>
<td>-46.1</td>
<td>-30.8</td>
<td>+20.6</td>
</tr>
</tbody>
</table>

Figure 5.17: Variation of Measured and Modeled Concentrations of SO₂ at SP-14 on 7-3-13

Figure 5.18 shows comparison of model predicted and experimentally measured SO₂ concentrations at ‘sampling point 9’ on experimental day of March 9, 2013. The peak of concentration was observed at 1500 hrs, as wind direction was towards sampling location (Table 5.13). Model predicted results show close agreement with experimentally measured data for SO₂ concentrations.

It may be due to comparatively stable wind conditions during experimental day. Wind seemed to remain within southwest quadrant most of time during experimentation as can be seen from Table 5.13. Maximum concentrations observed at this point are lesser than 10 ppb which is an indicative of greater distance of ‘sampling point 9’ from source i.e. 875 m.
Table 5.13: Temporal Variation in Modeled & Measured Wind Direction at SP-9 on 09-03-2013

<table>
<thead>
<tr>
<th>Time</th>
<th>1000 hrs</th>
<th>1100 hrs</th>
<th>1200 hrs</th>
<th>1300 hrs</th>
<th>1400 hrs</th>
<th>1500 hrs</th>
<th>1600 hrs</th>
<th>1700 hrs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stability Class</td>
<td>D</td>
<td>C</td>
<td>C</td>
<td>C</td>
<td>D</td>
<td>D</td>
<td>D</td>
<td>D</td>
</tr>
<tr>
<td>Dir(modeled)</td>
<td>+82.7</td>
<td>+92</td>
<td>+96.8</td>
<td>+98.8</td>
<td>+96.8</td>
<td>+89.5</td>
<td>+73.6</td>
<td>+59.7</td>
</tr>
<tr>
<td>Dir (exp.)</td>
<td>+80.2</td>
<td>+94.1</td>
<td>+95.8</td>
<td>+94.2</td>
<td>+99.7</td>
<td>91.3</td>
<td>+77.5</td>
<td>+71.0</td>
</tr>
</tbody>
</table>

Figure 5.18: Variation of Measured and Modeled Concentrations of SO$_2$ at SP-9 on 9-3-13

This explanation is further strengthened by the fact that similar concentration levels were observed at ‘sampling point 14’ which is also located at approximately same distance from stack. Separation between model and experimental curve may again be explained on the basis of background SO$_2$ level due to contribution of vehicular emissions as this sampling point is located exactly on the entry/exit road from Tumair entrance. Relatively lesser separation at 1400 and 1500 hrs compared to that at 1000 and 1600 hrs would further support this background concentration contribution argument as the transport fleet in morning as well as in evening follows same route taking this entry/exit road.

Figure 5.19 depicts model predicted and measured SO$_2$ concentrations at ‘sampling point 16’ on March 13, 2013. Highest concentration was observed at 1400 hrs, when wind direction was towards sampling location as can be seen in Table 5.14. Again Figure 5.19 shows greater difference in magnitudes of model predicted and experimentally measured concentration values for morning and evening hours of experimental day indicating contribution of background. Generally experimental curve shows higher concentrations in favorable wind conditions for point 16 as compared to other curves for points which are positioned at greater distance from experimental stack.
Table 5.14: Temporal Variation in Modeled & Measured Wind Direction at SP-16 on 13-03-2013

<table>
<thead>
<tr>
<th>Time</th>
<th>1000 hrs</th>
<th>1100 hrs</th>
<th>1200 hrs</th>
<th>1300 hrs</th>
<th>1400 hrs</th>
<th>1500 hrs</th>
<th>1600 hrs</th>
<th>1700 hrs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stability Class</td>
<td>C</td>
<td>C</td>
<td>C</td>
<td>C</td>
<td>D</td>
<td>D</td>
<td>D</td>
<td></td>
</tr>
<tr>
<td>Dir(modeled)</td>
<td>+59.3</td>
<td>+59.9</td>
<td>+57.6</td>
<td>+49.9</td>
<td>+44.3</td>
<td>+40.8</td>
<td>+38.9</td>
<td>+39.5</td>
</tr>
<tr>
<td>Dir (exp.)</td>
<td>+54.1</td>
<td>+57.3</td>
<td>+62.4</td>
<td>+51.4</td>
<td>+47.2</td>
<td>+39.4</td>
<td>+43.2</td>
<td>+37.5</td>
</tr>
</tbody>
</table>

Figure 5.19: Variation of Measured and Modeled Concentrations of SO$_2$ at SP-16 on 13-3-13

To evaluate model performance, statistical comparison was performed between predicted and measured concentrations of SO$_2$ by plotting scatter plots [Figure 5.20, 5.21, 5.22, 5.23] and calculating statistical parameters such as coefficient of correlation (r) and index of agreement (d). Same method was used by previous researchers as well [Mahapatra, 2011; Khamsimak, 2012; Le, 2009]. Coefficient of determination, correlation coefficient and index of agreement for predicted and measured SO$_2$ concentrations at different sampling locations are given in table 5.15.

Correlation coefficient measures strength and direction of a linear relationship between two variables. A correlation greater than 0.8 is generally described as strong, whereas a correlation less than 0.5 is generally described as weak. In present work, range of correlation coefficients was observed from 0.74 to 0.91 which indicates good correlation between predicted and measured SO$_2$ concentrations. Index of agreement varied from 0.40 to 0.64 indicating moderate degree of agreement between predicted results and measured data of SO$_2$ concentration. Overall, statistical analysis showed that model performance was satisfactory for predictions of ground level SO$_2$ concentration.
Figure 5.20: Scatter Plot between Predicted and Measured Concentrations (ppb) for SP-15 on 6-3-13

Figure 5.21: Scatter Plot between Predicted and Measured Concentrations (ppb) for SP-14 on 7-3-13

Figure 5.22: Scatter Plot between Predicted and Measured Concentrations (ppb) for SP-9 on 9-3-13

Figure 5.23: Scatter Plot between Predicted and Measured Concentrations (ppb) for SP-16 on 13-3-13
Table 5.15: Statistical Parameters for Predicted and Measured SO$_2$ Concentrations at Four Sampling Points around Experimental Stack

<table>
<thead>
<tr>
<th>Sampling locations</th>
<th>SP-15</th>
<th>SP-14</th>
<th>SP-9</th>
<th>SP-16</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coefficient of determination</td>
<td>0.80</td>
<td>0.55</td>
<td>0.83</td>
<td>0.71</td>
</tr>
<tr>
<td>Correlation coefficient</td>
<td>0.89</td>
<td>0.74</td>
<td>0.91</td>
<td>0.84</td>
</tr>
<tr>
<td>Index of agreement</td>
<td>0.63</td>
<td>0.63</td>
<td>0.40</td>
<td>0.64</td>
</tr>
</tbody>
</table>

Spatial extent of stack experiments was limited to only some specific receptor points because of topography and type of tracer released from stack. Hazardous nature of tracer in stack experiments and presence of nearby residential areas prevented to release a greater amount of pollutant from stack to study dispersion over comparatively longer distances around the source. SF$_6$ gas is an option if larger source term is required to be used in future. Thus tracer experiment with further increased source height was conducted with release of SF$_6$ gas (Section 3.3.2.4 (a)). Results of last part of experiment described below involves a tracer experiment performed using SF$_6$ released at a height of 230 ft while ground concentrations at various arc points around emission point were collected simultaneously within few kilometers. Selection of receptor points were done on the basis of prevailing wind direction which was continuously observed at surface meteorological station at experimental site. Modeling procedure is already described in detail in section 3.2.9 while results of experiment and coupled MM5+CALPUFF model are compared and discussed in following section.

5.1.4 Results with SF$_6$ as Tracer Gas at Larger Release Height

Main aim of this last part of research work was to conclude experimental validation of ‘coupled mesoscale & dispersion model’ by eliminating restrictions such as limited release (small source term), lesser height and to cover relatively larger receptor distances while doing sampling simultaneously at all important receptor points. SF$_6$ being inert gas is released at a rate of about 7.0 g/s in contrast to 0.05, 0.3 g/s and 0.6 g/s earlier release rates in cases of ground SO$_2$ experiments, Brick Kiln Experiments and PIEAS stack experiments respectively. Similarly, release height in this experiment is taken as 230 ft compared to respective 30 ft, 60 ft and 100 ft considered in previous experiments. Moreover, a team work was performed to collect simultaneous samples at a specified rate in sampling bags instead of ‘one
point continuous sampling’ by ambient air monitoring van. With greater source term and release height, maximum receptor distance covered was about 10,000 m compared to 150 m, 500 m, 875 m selected in previous experiments.

Different receptor points were marked on six arcs, Arc-A to Arc-F for collecting SF$_6$ samples within the radius of 10 km. Arcs were positioned at distances of 0.7, 1.5, 3, 5, 7 and 10 km. Distance and direction of sampling locations were selected on the basis of topography and prevailing wind conditions of specific region. Experiment was performed at a coastal site where a possible nuclear power plant was being planned to be located. Because of complex terrain and low wind speed, arcs near source were kept closer to each other as compared to others. Further details have already been given in section 3.3.2.4.

Three samples with 10 minutes sampling time for each were collected during one hour period of SF$_6$ release on April 29, 2013. Results of maximum ground level SF$_6$ concentrations predicted by model as well as measured from laboratory analysis out of three SF$_6$ samples at each receptor point are presented in Table 5.16. The significant figures in the table are indicative of the fact that gas chromatography with electron capture detector (ECD) is a more sensitive and accurate technique as compared to using SO$_2$ analyzer in mobile van based on the Ultra Violet Fluorescence (UVF) method. Most of previous tracer experiments were conducted using SF$_6$ and gas chromatography with electron capture detector because SF$_6$ gas can be determined in air with high sensitivity in ppt range due to presence of halogen element [Dietz, 1973; Peter, 1974; Gryning, 1978].

The UVF based sensors use fluorescence in UV cell where sample gas is irradiated by UV source exciting a portion of SO$_2$. The de-excitations to ground state generate fluorescent radiations that are detected by a photomultiplier tube (PMT) such that the detected fluorescent intensity has a relationship with SO$_2$ concentration in the cell. As a result, SO$_2$ concentration is calculated from the PMT output. In contrast, Electron Capture Detector (ECD) involves electrons from a radioactive nickle-63 or tritium beta ($\beta$) emitter that causes ionization in the nitrogen used as carrier gas. In the absence of sampling compound, a constant current is maintained between two electrodes while with the introduction of sampling compound, the current decreases significantly as the functional groups attached to the compound capture the electrons. ECD has the high selectivity and sensitivity towards certain species with
electronegative functional groups such as halogens etc. hence this method is best suited in applications where trace quantities of chemicals containing electronegative atoms are to be detected. As can be seen from table 5.16 the highest SF$_6$ concentration of 4.19 ppb could be measured at sampling point A-15 at about 700m which is of the order of background concentration observed in SO$_2$ experiments. This is indicative of the fact of negligible ambient background concentration of SF$_6$ as compared to SO$_2$ and higher sensitivity and lower detection limit of ECD technique.

Table 5.16 shows a gradual decrease in measured and predicted SF$_6$ concentrations at sampling locations on the same arc from a point of maxima. This behavior indicates occurrence of lateral diffusion over both sides of plume central axis. Considering table 5.16 in combination with the figure 5.25 on each arc A, B, C, D, E and F, a centre line corresponding to maximum ground level concentration of SF$_6$ can be observed which extends from A-15 to F-10 passing through points B-19, C-20, D-9, E-10 and F-10. One may observe a lateral diffusion that is obvious from the concentrations on both sides of the point of maxima along each arc. For instance on arc-A, the point of maxima is 4.19 ppb at A-15 which diffuses on both sides as indicated by a decrease in concentration to 0.66 ppb at A-16, 0.23 ppb at A-18 and 0.05 ppb at A-20 along the northern side of the arc. Similarly concentration decreases to 0.83 at A-14 and 0.03 at A-12 on the other side. A similar trend may be observed on both sides of point of maxima on the other arcs as well. Due to limited number of participants in conduction of experiment, experimental data for other side of plume centerline at arc-D could not be collected. Lateral diffusion within SF$_6$ plume was well elaborated in previous studies especially conducted to estimate lateral dispersion parameter from the concentration measurements [Gryning, 1978; Durren, 1980].

Comparison of maximum measured and predicted ground level SF$_6$ centre line concentrations at different downwind distances from source is presented in Figure 5.24 (a). Both curves followed almost same trend of decreasing concentration with increase in downwind distance up to 10 km. Similar effect of increasing distance on pollutant concentration was observed and discussed for SO$_2$ release from brick kiln and experimental stack in sections 5.1.2.1 and 5.1.3.
Table 5.16: Measured and Predicted SF₆ Ground Level Concentration on April 29, 2013

<table>
<thead>
<tr>
<th>Arc points</th>
<th>Distance (km)</th>
<th>Dir. from North (degree)</th>
<th>Conc. (ppb)</th>
<th>Predicted points</th>
<th>Dir. from North (degree)</th>
<th>Conc. (ppb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A-20</td>
<td>0.749</td>
<td>44</td>
<td>0.05</td>
<td>A’-20</td>
<td>60</td>
<td>0.26</td>
</tr>
<tr>
<td>A-18</td>
<td>0.768</td>
<td>50</td>
<td>0.23</td>
<td>A’-18</td>
<td>66</td>
<td>2.12</td>
</tr>
<tr>
<td>A-16</td>
<td>0.702</td>
<td>56</td>
<td>0.66</td>
<td>A’-16</td>
<td>72</td>
<td>5.70</td>
</tr>
<tr>
<td>A-15</td>
<td>0.741</td>
<td>59</td>
<td>4.19</td>
<td>A’-15</td>
<td>75</td>
<td>6.69</td>
</tr>
<tr>
<td>A-14</td>
<td>0.746</td>
<td>64</td>
<td>0.83</td>
<td>A’-14</td>
<td>80</td>
<td>4.89</td>
</tr>
<tr>
<td>A-12</td>
<td>0.768</td>
<td>70</td>
<td>0.03</td>
<td>A’-12</td>
<td>86</td>
<td>1.35</td>
</tr>
<tr>
<td>B-24</td>
<td>1.63</td>
<td>40</td>
<td>0.79</td>
<td>B’-24</td>
<td>61</td>
<td>0.13</td>
</tr>
<tr>
<td>B-22</td>
<td>1.52</td>
<td>46</td>
<td>0.96</td>
<td>B’-22</td>
<td>67</td>
<td>1.26</td>
</tr>
<tr>
<td>B-19</td>
<td>1.52</td>
<td>55</td>
<td>1.99</td>
<td>B’-19</td>
<td>76</td>
<td>4.24</td>
</tr>
<tr>
<td>B-18</td>
<td>1.51</td>
<td>58</td>
<td>1.96</td>
<td>B’-18</td>
<td>79</td>
<td>3.66</td>
</tr>
<tr>
<td>B-17</td>
<td>1.52</td>
<td>61</td>
<td>1.56</td>
<td>B’-17</td>
<td>82</td>
<td>2.39</td>
</tr>
<tr>
<td>B-16</td>
<td>1.52</td>
<td>64</td>
<td>0.15</td>
<td>B’-16</td>
<td>85</td>
<td>1.18</td>
</tr>
<tr>
<td>C-24</td>
<td>3.11</td>
<td>41</td>
<td>0.01</td>
<td>C’-24</td>
<td>71</td>
<td>0.82</td>
</tr>
<tr>
<td>C-22</td>
<td>3.1</td>
<td>47</td>
<td>0.64</td>
<td>C’-22</td>
<td>77</td>
<td>0.94</td>
</tr>
<tr>
<td>C-20</td>
<td>2.89</td>
<td>53</td>
<td>0.98</td>
<td>C’-20</td>
<td>83</td>
<td>1.64</td>
</tr>
<tr>
<td>C-18</td>
<td>2.93</td>
<td>59</td>
<td>0.49</td>
<td>C’-18</td>
<td>89</td>
<td>0.15</td>
</tr>
<tr>
<td>C-17</td>
<td>2.97</td>
<td>62</td>
<td>0.45</td>
<td>C’-17</td>
<td>92</td>
<td>0.04</td>
</tr>
<tr>
<td>C-16</td>
<td>2.98</td>
<td>65</td>
<td>0.01</td>
<td>C’-16</td>
<td>95</td>
<td>0.00</td>
</tr>
<tr>
<td>D-12</td>
<td>4.43</td>
<td>46</td>
<td>0.14</td>
<td>D’-12</td>
<td>70</td>
<td>0.12</td>
</tr>
<tr>
<td>D-10</td>
<td>4.46</td>
<td>53</td>
<td>0.19</td>
<td>D’-10</td>
<td>77</td>
<td>0.63</td>
</tr>
<tr>
<td>D-9</td>
<td>4.97</td>
<td>56</td>
<td>0.44</td>
<td>D’-9</td>
<td>80</td>
<td>0.72</td>
</tr>
<tr>
<td>D-7</td>
<td>5.33</td>
<td>62</td>
<td>-</td>
<td>D’-7</td>
<td>86</td>
<td>0.33</td>
</tr>
<tr>
<td>D-6</td>
<td>5.34</td>
<td>65</td>
<td>-</td>
<td>D’-6</td>
<td>89</td>
<td>0.13</td>
</tr>
<tr>
<td>D-4</td>
<td>5.47</td>
<td>72</td>
<td>-</td>
<td>D’-4</td>
<td>96</td>
<td>0.00</td>
</tr>
<tr>
<td>E-14</td>
<td>7.92</td>
<td>45</td>
<td>0.02</td>
<td>E’-14</td>
<td>70</td>
<td>0.01</td>
</tr>
<tr>
<td>E-10</td>
<td>7.86</td>
<td>57</td>
<td>0.16</td>
<td>E’-10</td>
<td>82</td>
<td>0.42</td>
</tr>
<tr>
<td>E-9</td>
<td>7.82</td>
<td>60</td>
<td>0.02</td>
<td>E’-9</td>
<td>85</td>
<td>0.37</td>
</tr>
<tr>
<td>E-8</td>
<td>7.78</td>
<td>63</td>
<td>-</td>
<td>E’-8</td>
<td>88</td>
<td>0.22</td>
</tr>
<tr>
<td>E-7</td>
<td>8.57</td>
<td>66</td>
<td>-</td>
<td>E’-7</td>
<td>91</td>
<td>0.09</td>
</tr>
<tr>
<td>E-6</td>
<td>8.34</td>
<td>69</td>
<td>-</td>
<td>E’-6</td>
<td>94</td>
<td>0.02</td>
</tr>
<tr>
<td>E-4</td>
<td>7.23</td>
<td>74</td>
<td>-</td>
<td>E’-4</td>
<td>99</td>
<td>0.00</td>
</tr>
<tr>
<td>F-14</td>
<td>10.75</td>
<td>43</td>
<td>-</td>
<td>F’-14</td>
<td>69</td>
<td>0.00</td>
</tr>
<tr>
<td>F-13</td>
<td>10.54</td>
<td>46</td>
<td>0.03</td>
<td>F’-13</td>
<td>72</td>
<td>0.01</td>
</tr>
<tr>
<td>F-10</td>
<td>10.11</td>
<td>55</td>
<td>0.06</td>
<td>F’-10</td>
<td>81</td>
<td>0.25</td>
</tr>
<tr>
<td>F-7</td>
<td>9.95</td>
<td>64</td>
<td>0.02</td>
<td>F’-7</td>
<td>90</td>
<td>0.14</td>
</tr>
<tr>
<td>F-6</td>
<td>9.95</td>
<td>67</td>
<td>-</td>
<td>F’-6</td>
<td>93</td>
<td>0.07</td>
</tr>
<tr>
<td>F-4</td>
<td>9.81</td>
<td>73</td>
<td>-</td>
<td>F’-4</td>
<td>99</td>
<td>0.00</td>
</tr>
</tbody>
</table>

A close agreement between measured and predicted values of concentrations for the points at larger distances from source can be observed from Figure 5.24 (a). The correlation coefficient (r) of 0.988 as shown in figure 5.24 (b) showed good correlation between predicted and measured SF₆ concentrations. The reason of data
discrepancy for few points may be due to error in sample collection specifically any slight leakage during attaching and detaching sampling bags with the sampler, keeping constant flow rate at 0.2 litre per minute and measuring exact ten minute time interval for a single sample.

Figure 5.24: (a) Comparison of Measured and Predicted Maximum SF₆ Concentration on Plume Centerline (b) Scatter Plot of Measured and Predicted Maximum SF₆ Concentrations.

Figure 5.25 shows modeled spatial and temporal variations in pattern of SF₆ plume during release period of one hour. Plume movement remained along coastal boundary during entire simulation period under influence of prevailing wind conditions. Contour lines spreading in direction of east were found to be concentric and homogeneous in shape. Similar pattern was observed for SO₂ plume in simulations of oil refinery emissions (Figure 5.10) where possible reason of homogenous shape of plume was also discussed.

A slight deviation in the measured and predicted directions of plume can be observed from figure 5.25. This deviation may be attributed to the difference in predicted and real wind direction during sampling period. As sampling was done over a very short period of time i.e. 10 minutes, it may be expected that model remained unable in reproducing instantaneous behavior of wind at that specific time. This difference may be minimized, if real site-specific meteorological data are used along with MM5 generated data as a combined input to CALPUFF model or concentrations are averaged out on the basis of large sampling periods as hourly or daily averages. A comparison of centre lines of actual and modeled plume shown in figure 5.25 and 5.26 indicates that the predicted maximum concentrations have an error ranging from 37 to 76% whereas shift in location of maxima points was about 16° to 26°.
Figure 5.25: Isopleths Plot for the Dispersion of SF$_6$ Plume with the Wind Field over the Study Area
Figure 5.26: Experimental Results of Ground Concentrations of SF₆ Measured at Different Sampling Locations
This may be attributed to directional deviation observed in experimentally measured and model predicted wind directions. Possible deviation in wind direction may be due to fluctuations in wind field over 10 minutes sampling interval which might not have been captured by model predicted wind field data for such a short time interval. This difference between predicted and observed wind directions has been observed throughout the study including ground and stack experiments.

The predicted 2D plume dispersal pattern elaborated in figure 5.25 does not show features such as topography, regional boundaries and altitude wise wind field change. Application of an appropriate graphical tool is generally helpful to bring the data into 3D visualized form. This activity is called ‘post processing’ of computational modeling results. It helps in developing a quick understanding of modeling predictions indicating potentially most vulnerable areas affected by dispersing plume. Most of the graphical tools available in open domain only provide 2D view. Hence, an efficient three dimensional post processor was developed in MATLAB to display multilayered data of geographical boundaries, topography, wind field and particle positions in a plume in a single window in the form of real time or even faster 3D animation or movie that is extremely useful for management for decision making in accidental scenario. Computational results of a modeling study processed with MATLAB postprocessor are discussed in following section.

5.2 Simulation and Post-Processing of Particles Trajectories

A modeling study was carried out to simulate plume trajectory assuming hypothetical accidental release of Sulfur dioxide (SO$_2$) from experimental stack at PIEAS. Spatial trajectory calculations required wind field data over domain under consideration. This wind patterns over a specific location and time interval were obtained by employing WRF meteorological model. Particles trajectories were computed by coupling WRF with an advanced grid independent Lagrangian dispersion model FLEXPART and results were demonstrated by a three dimensional post processor in MATLAB developed during this research.
5.2.1 Visualization of Plume Trajectory by Post-Processing

MATLAB postprocessor is capable to create a 3D movie or animation of plume trajectory including displaying features of regional geography, topography and meteorology. This type of post-processing may be helpful for quick decision making regarding emergency handling and evacuation plan. Salient features of MATLAB programming done for visualization of plume trajectories are discussed in subsequent sections.

5.2.1.1 Geography of Simulated Region

Complete geographical information of region of interest including district’s boundaries and their names were displayed in a plane using MATLAB post-processor as shown in Figure 5.27. Figure shows selected model domain covering various cities located within the domain. Cities are denoted by blue dots at specific latitude-longitude coordinates with labels, while red dot identifies the location of emission point which is taken as PIEAS experimental stack.

![Figure 5.27: Geographical Boundaries of Different Cities of Simulated Region](image)

5.2.1.2 Topography of Simulated Region

The considered domain contains complex topographical features including plains, deserts, forests and mountains ranging from plain areas in south to high mountainous peaks in north. Northern mountainous area is comprised of parts of Hindu Kush,
Karakoram and Himalayas with peaks as high as Nanga Parbat (7980 m) and K-2 (8475 m, the second highest in the world) [Shamshad, 1988]. Topographical features of region can be observed from Figures 5.28(a) and 5.28(b). Maps in Figure 5.28(a) and 5.28(b) have been generated with use of SURFER and MATLAB post-processor respectively.

![Figure 5.28: (a) Surface Map Showing Topographical Features of Model Domain (b) Wireframe Map Showing 3-D View of Topography of Domain under Consideration](image)

### 5.2.1.3 Wind Field over Simulated Region

Spatial trajectory calculations required wind field data over area under study. Wind patterns over specific location and time interval were generated by employing a WRF meteorological model as shown in Figure 5.29.

![Figure 5.29: Wind Field over Simulated Region](image)
5.2.1.4 Particles Trajectories

Figure 5.30 (a) shows particles dispersion and wind field at time of release i.e. at 0000 hrs on June 2, 2009. It can be observed from figure that direction of wind at release site is from mountainous range at northern side moving towards plain areas. Wind speed at that time was relatively low about 1.8 m/sec. Figure 5.30 (b) illustrate particles trajectory two hours after release. Wind in the vicinity of emission point is coming from north east and under influence of this wind field, particles moved towards south–west direction and covered a distance of 45 km in this direction.

![Figure 5.30: Particle Dispersion and Wind field (30 m above ground level) on June 2, 2009 (a) at 0000 hrs (b) 0200 hrs, 2 hours after release](image)

Figure 5.31 (a) represents particle positions and wind vectors after 4 hours of release. At this moment particles can be seen traveling in south-west direction while part of them have started moving towards northwest direction because the direction of wind is gradually changing in this direction as can be seen by small vectors at plume front. This non-uniform and asymmetric dispersion cannot be predicted with use of Gaussian plume model (GPM).

Figure 5.31(b) shows particle positions 6 hours after release. This figure shows a reversal trend in wind direction. This change causes the particles to transport in south-east direction and extending branches of plume may be observed turning back in same direction.
Figure 5.31: Particle Dispersion and Wind Field (30 m above Ground Level) on 2 June 2009 (a) at 0400 hrs, 4 hours after Release (b) 0600 hrs, 6 hours after Release

Figure 5.32 shows a 3-D view of particle trajectory along with topography and windfields. Figure indicates plume spread towards plain areas of simulated region during entire simulation period. It is due to influence of wind filed that remained directed towards plain areas.

Figure 5.32: 3-D View of Particle Trajectory and Wind Field (30 m above Ground Level) at 0600 hrs on June 2, 2009, 6 hours after Release

In short, 3D MATLAB based post-processor developed in this research was observed to be a good tool for visualization of particle trajectories simulated by coupled FLEXPART-WRF modeling system. Irregular shaped ‘potential vulnerable area’
covered by plume predicted by ‘coupled model’ was observed to be quite different from expected straight line plume dispersion generally predicted by Gaussian Plume Model (GPM). The 3D visualization may help in decision making regarding emergency evacuation of population from ‘potential vulnerable areas’ thereby shifting them to places that are surely safe according to more accurate predictions made by these coupled models.
Hazardous air pollutants whether emitted accidentally or by routine releases may be damaging if not monitored, assessed and controlled. Atmospheric dispersion modeling of toxic pollutants released from industrial sources is an essential regulatory requirement. It may help in decision making regarding emergency evacuation of population from affected areas in accidental scenario or emission reduction in specific situations when air quality is deteriorating unacceptably. Present research is directed towards accurate prediction of ground level concentrations and trajectories of air pollutants released into atmosphere involving large doses to general public. Suggested solution is the use of ‘coupled meteorological and dispersion models’ as the most effective modeling technique. Validation and visualization of modeling results are mainly focused. Two tracer gases, SO$_2$ and SF$_6$ were selected for experimentation to collect concentration data for validation purpose. Following conclusions may be drawn from the work undertaken:

- Present work showed the ability of mesoscale meteorological model MM5 to predict meteorological parameters such as precipitation pattern, ambient temperature, potential temperature, relative humidity, moist static energy and wind field, provided that the convective parameterization schemes used in it are thoroughly investigated according to regional topography and local meteorology.

- Sensitivity analysis of four parameterized schemes in MM5 model for Pakistani region indicated that Grell scheme generated better results for all parameters and resolutions for lesser precipitation intensity. Kain–Fritsch scheme captured rainfall patterns reasonably well over northern mountainous region for heavy precipitation. Anthes–Kuo and Betts–Miller scheme were found to be unable to produce realistic results indicating their unsuitability in this region in general. These investigations assisted in finalizing the decision to select ‘Grell scheme’ in MM5 for performing further computations using coupled MM5-CALPUFF dispersion modeling.
• The deviation observed between modeled and observed results of wind speed and direction was more as compared to that for ambient temperature. Sources of large perturbation in wind parameters were attributed to surrounding human-made features and influence of model grid resolution. Despite these discrepancies, overall performance of MM5 model in generating wind fields was acceptable.

• Coupled meteorological and dispersion modeling predicted the dispersion behavior in isolated brick kiln emissions well as observed by its agreement with ‘relative concentration versus distance curve’ presented in literature. Average variation of about 20% may be due to presence of other nearby brick kilns, domestic heating and variation in SO\textsubscript{2} emission rate.

• SO\textsubscript{2} emission from cluster of stacks of oil refinery using coupled CALPUFF-MM5 model was quite satisfactory with an average variation of only 13%. The maximum daily averaged concentration did not exceed 10 µg/m\textsuperscript{3} which was within daily permissible limit of 125 µg/m\textsuperscript{3} for SO\textsubscript{2} specified by local regulatory authority.

• Coupled CALPUFF-MM5 model predicted the impacts of flaring activities in Al-Noor oilfield on ambient air quality well as reflected by range of variation in measured and modeled SO\textsubscript{2} concentration from 2 to 22%.

• Designing and fabrication of PIEAS experimental stack in this research work was a very useful asset for validation of dispersion modeling results using tracer experiments. Overall trends of time series plots of measured and modeled SO\textsubscript{2} concentrations using PIEAS experimental stack were found to be in reasonable agreement. This can be seen by the correlation coefficients ‘r’ and Index of agreement ‘d’ ranging from 0.74 to 0.91 and 0.40 to 0.64 respectively showing that coupled model performance was satisfactory for predictions of ground level SO\textsubscript{2} concentration.

• Tracer experiment using SF\textsubscript{6} released at a height of 230 ft with a larger release rate of about 7 g/s with simultaneous sampling at 37 points on six arcs
covering a radial distance from 0.7 to 10 km were conducted. These tests demonstrated the cross-wind diffusion as well as down-wind dispersion well. A slight deviation in directions of plume and sampling point locations was observed due to difference in predicted and real wind directions. The model seemed to have limited capability in reproducing instantaneous behavior of wind over such a short sampling period of 10 minutes.

- 3D MATLAB based post-processor developed in this research was used for trajectory simulation of hypothetical SO$_2$ release from PIEAS experimental stack using coupled FLEXPART-WRF modeling system. Irregular shaped ‘potential vulnerable area’ covered by plume predicted by ‘coupled model’ was observed to be quite different from expected straight line plume dispersion generally predicted by Gaussian Plume Model (GPM).

- As an overall conclusion it may be stated that use of ‘coupled meteorological and dispersion models’ may help in decision making regarding emergency evacuation of population from ‘potential vulnerable areas’ thereby shifting them to places that are surely safe according to more accurate predictions made by these coupled models.

Recommendations for further work that may be carried out are:

- Due to limited period of PhD research, experimental data was collected at only four sampling points around PIEAS experimental stack for validation of modeling results. Research may be continued in future to cover an entire year covering all seasons and stability conditions that prevail at different times of day i.e. morning, noon, afternoon, evening, night and dawn. Moreover, all possible directions according to wind rose and larger area in kilometers may be covered around the stack.

- One of the reasons for discrepancies between predicted and observed SO$_2$ concentrations was found to be deviation in respective data of wind direction. Real site-specific meteorological data along with mesoscale model generated
data may therefore be used in CALPUFF dispersion model. Site specific wind field data may be collected by SODARs (Sonic Detection and Ranging System) whereas upper atmospheric data may be collected by balloon launching.

- Present work was done using meteorological data of past days generated by mesoscale model for coupled dispersion model. Simulation work may be recommended by using meteorological data of next few days prediction generated by meteorological model for ‘all-time standby alert’ conditions in case of possible accidental release and its dispersion mitigation.

- Subroutines on formulation of chemical removal of SO\textsubscript{2} and NO\textsubscript{2} from resulting ground level concentrations of a plume were written for inclusion in FLEXPART model source program during this research. Testing and validation of this work could not be done due to limitation of time. Continuation of this work is highly recommended to take into account chemical removal of pollutants in Lagrangian particle model.

- In present work, a sequential study was initiated from modeling of simple release scenario of tracer gases from an emission source. Initiating from as low source elevation as 30 ft and emission-receptor distance as 165 ft to as high source elevation as 230 ft and emission-receptor distance of 33,000 ft (6.25 miles). These tracer experiments may further be extended to even higher stacks and emission-receptor distances of hundreds of kilometers covering a broader region and trans-boundary dispersion in future.

- MATLAB post-processor developed during this research may be interfaced with a hardware system for getting real time streaming inputs from nearby meteorological stations thus displaying in the control room ‘all-time’ plume dispersion pattern based on ‘coupled models’.
References


References


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References


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Spangler, T. C. and Taylor, G. H. (1982). Flow Simulation Techniques Used In the Small Hill Impaction Study. 3rd Joint Conference on Applications of Air Pollution Meteorology, A.M.S., Boston, MA.


USEPA. (1985). Guideline for Determination of Good Engineering Practice Stack Height. EPA-450/4-80-023R.


References


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<table>
<thead>
<tr>
<th>No.</th>
<th>Unit</th>
<th>Tag number of the furnace/incinerator</th>
<th>Service of the furnace/incinerator</th>
<th>Stack height m</th>
<th>Diameter m</th>
<th>Emission rates g/s</th>
<th>Gas flow speed m/s</th>
<th>Exit flue gas temp. K</th>
<th>X coord. m</th>
<th>Y coord. m</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>Area-200 RXn-Regn. section</td>
<td>F-2002</td>
<td>Steam super heater</td>
<td>147.2</td>
<td>2.26</td>
<td>0.856</td>
<td>0.30</td>
<td>578</td>
<td>0</td>
<td>0</td>
</tr>
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<td>2</td>
<td>Area-100 CDU</td>
<td>F-1101</td>
<td>Crude oil heating</td>
<td>35.0</td>
<td>3.00</td>
<td>0.0105</td>
<td>0.30</td>
<td>643</td>
<td>-161.66</td>
<td>1394.26</td>
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<td>Area-200 Flue gas section</td>
<td>SK-2301</td>
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<td>85.0</td>
<td>3.60</td>
<td>50.580</td>
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<td>333</td>
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<td>-59.91</td>
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<td>F-3201</td>
<td>Combined feed heater</td>
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<td>1.22</td>
<td>0.0212</td>
<td>6.03</td>
<td>573</td>
<td>87.97</td>
<td>56.72</td>
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<td>F-4201</td>
<td>Finishing HDT reactor feed heater</td>
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<td>1.17</td>
<td>0.0131</td>
<td>4.05</td>
<td>673</td>
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<td>63.8</td>
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<td>Area-400 HGU</td>
<td>F-3301</td>
<td>Natural gas steam reforming to H2</td>
<td>40.0</td>
<td>3.05</td>
<td>3.2900</td>
<td>19.55</td>
<td>450</td>
<td>163.24</td>
<td>-1691.96</td>
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<td>7</td>
<td>Area-400 TGTU thermal incinerator</td>
<td>F-3704</td>
<td>H2S oxidizing into SO2</td>
<td>39.8</td>
<td>1.07</td>
<td>2.4300</td>
<td>5.03</td>
<td>603</td>
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<tr>
<td>8</td>
<td>Utility</td>
<td>B-5401 A</td>
<td>Utility boiler</td>
<td>30.0</td>
<td>2.00</td>
<td>0.7068</td>
<td>15.00</td>
<td>453</td>
<td>-166.88</td>
<td>-1481.56</td>
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<td>Utility</td>
<td>B-5401 B</td>
<td>Utility boiler</td>
<td>30.0</td>
<td>2.00</td>
<td>0.7068</td>
<td>15.00</td>
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<td>-1485.96</td>
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<tr>
<td>10</td>
<td>Utility</td>
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<td>Waste heat boiler</td>
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<td>2.75</td>
<td>6.8300</td>
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<td>-166.88</td>
<td>-1459.46</td>
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<td>WHB-5101 B</td>
<td>Waste heat boiler</td>
<td>40.0</td>
<td>2.75</td>
<td>6.8300</td>
<td>76.66</td>
<td>503</td>
<td>-164.42</td>
<td>-1466.65</td>
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Table 1: Flare Characteristics and Emission Rates of SO\textsubscript{2}

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<thead>
<tr>
<th>S. No.</th>
<th>Source Name</th>
<th>X (Km)</th>
<th>Y (Km)</th>
<th>Flare Height (m)</th>
<th>Base Elevation (m)</th>
<th>Flare Dia. (m)</th>
<th>Exit Gas Velocity (m/sec)</th>
<th>Exit Gas Temp (K)</th>
<th>Emission Rates (g/sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>High Pressure (HP) Flare</td>
<td>1.876</td>
<td>-0.753</td>
<td>60.5</td>
<td>4</td>
<td>0.46</td>
<td>20</td>
<td>1342</td>
<td>47.61</td>
</tr>
<tr>
<td>2</td>
<td>Low Pressure (LP) Flare</td>
<td>1.876</td>
<td>-0.758</td>
<td>60.5</td>
<td>4</td>
<td>0.76</td>
<td>20</td>
<td>1342</td>
<td>209.26</td>
</tr>
</tbody>
</table>

Fig. 1: Location of Study Area, Al-Noor Production Station
Appendices

Appendix-III

Fig. 1: Schematic Configuration of CALPUFF Modeling System and Meteorological Model MM5

Appendices

Appendix-IV

Steps for inclusion of chemical removal term of SO₂ or NOₓ in FLEXPART model

1. Place two subroutines, ‘readchem.f’ and ‘chem..f’ as given below in ‘src’ directory of FLEXPART model. Subroutine ‘readchem.f’ reads input data from formatted input file ‘CHEM’, while subroutine ‘chem..f’ calls the subroutine ‘readchem.f’ for acquiring all input data and subsequently calculates the transformation rates for SO₂ or NOₓ.

2. Make changes in ‘makefile’ of model by introducing the names of “readchem” and “chem” subroutines with extension ‘.o’.

3. Compile FLEXPART model with changed ‘makefile’. Successful compilation will generate two object files as “readchem.o” and “chem..o” in same directory.

4. Place the formatted input file ‘CHEM’ as given below in ‘options’ directory of FLEXPART. Subsequently, edit this file by providing input data regarding all input parameters which are necessary required to compute transformation rates for specific pollutants.

5. Make following changes in subroutine ‘conccalc.f’ of FLEXPART model in order to calculate the ground level pollutant concentration. For performing calculations, ‘conccalc.f’ collects the information of transformation rates of SO₂ or NOₓ from the output of subroutine ‘chem.f’.

   i. Addition in integer defining is ‘integer il, ind, indz, indzp, chemode’

   ii. Addition in real number defining is ‘real rhoprof(2), rhoi, r(2), dt, flosss, flossn, frests, frestn’

   iii. Addition under title “C Estimate concentration at receptor” is

       callchem(chemode,r)

       dt=itime/3600

   iv. Changes under title ‘r2=xd*xd+yd*yd+zd*zd’

       if (r2.lt.1.) then
xkern=factor*(1.-r2)
if (chemode.eq.0)then
  do 45 k=1,nspec
  45   c(k)=c(k)+xmass1(i,k)*xkern/h
else
  if (chemode.eq.1)then
    do 46 k=1,nspec
    46      flosss=(1.-exp(-r(1)*dt))
    frests=1.0-flosss
    46      c(k)=c(k)+xmass1(i,k)*frests*xkern/h
  else
    do 47 k=1,nspec flossn=(1.-exp(-r(2)*dt)) frestn=1.0-flossn
    47      c(k)=c(k)+xmass1(i,k)*frestn*xkern/h
endif
endif
endif
continue

Makefile
SHELL = /bin/csh
MAIN = flexpart_wrf
INCF = incl*

FC=/usr/pgi/linux86/6.1/bin/pgf90
#FFLAGS = -s -fast -byteswapio
#FFLAGS = -s -g -C -byteswapio -I$(NETCDF)/include
#note -- "-s" strips symbol table, so cannot debug
#FFLAGS = -g -C -Ktrap=fp -byteswapio -I$(NETCDF)/include
FFLAGS = -s -fast -byteswapio -I$(NETCDF)/include

#LDFLAGS = -s -L/files1/d3j082/flexpart/emoslib -emos
LDFLAGS = -L$(NETCDF)/usr/local/lib -lncdf -lm

# OBJECTS = assignland.owriteheader.o \
calcpar.o part0.o \
caldate.opotdep.o \
coordtrafo.opsih.o \

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raerod.o \n
drydepokernel.orandom.o \n
erf.oreadavailable.o \n
ew.oreadcommand.o \n
advance.oreaddepo.o \n
releaseparticles.opsim.o \n
dexpart_wrf.oreadlanduse.o \n
getfields.oinit_domainfill.o \n
interpol_wind.oreadoutgrid.o \n
interpol_all.oreadpaths.o \n
getrb.oreadreceptors.o \n
getrc.oreadreleases.o \n
getvdep.oreadspecies.o \n
interpol_misslev.oreadwind.o \n
conccalc.orichardson.o \n
concoutput.oscalev.o \n
pbl_profile.o \n
juldate.otimemanager.o \n
interpol_vdep.ointerpol_rain.o \n
verttransform.opeartoutput.o \n
hanna.owetdepokernel.o \n
mean.owetdepo.o \n
hanna_short.owindalign.o \n
obukhov.ogridcheck.o \n
hannal.o initialize.o \n
cmapf1.0.o gridcheck_nests.o \n
readwind_nests.ocalcpar_nests.o \n
verttransform_nests.ointerpol_all_nests.o \n
interpol_vdep_nests.ointerpol_misslev_nests.o \n
readageclasses.oreadpartpositions.o \n
calcfluxes.ofluxoutput.o \n
qvsat.oskplin.o \n
convmix.ocalcmatrix.o \n
convect43c.o redist.o \n
sort2.o distance.o \n
centerofmass.opeartetraj.o \n
openouttraj.ocalcprv.o \n
calcpv_nests.o distance2.o \n
clustering.ointerpol_wind_short.o \n
interpol_wind_short_nests.o shift_field_0.o \n
shift_field.ointergrid_init.o \n
openreceptors.oboundcond_domainfill.o \n
partoutput.ointergridoutput_nest.o \n
outgrid_init.owetdepokernel_nest.o \n
drydepokernel_nest.o \n
read_ncwrfout.omap_proj_wrf.o \n
map_proj_wrf_subaa.o chem.o \n
readchem.o

$(MAIN): $(OBJECTS)

$(FC) -o $(MAIN) $(FFLAGS) $(OBJECTS) $(LDFLAGS)

$(OBJECTS): $(INCF)
CHEM (Input file)

*****************************************************************
* CHEM Input file for FLEXPART model                           *
* Please select your options                                    *
*****************************************************************
1. _____  3X, I1
   1
CHEMODE  0 FOR NO CHEMISTRY, 1 FOR SOx CHEMISTRY, 2 FOR
NOx CHEMISTRY

2. _____  3X, I5
   1
COZPPB  BACKGROUND OZONE CONCENTRATION (ppb)

3. _____  3X, I5
   1
QSW    INTENSITY OF SHORT WAVE RADIATIONS (watt/m²)

4. _____  3X, I5
   1
RHUM   ATMOSPHERIC RELATIVE HUMIDITY (%)

5. _____  3X, I5
   1
CNOXPPB CONCENTRATION OF NOx IN PLUME (ppb)

6. _____  3X, I5
   1
ISTAB  ATMOSPHERIC STABILITY CLASS

**************************************************************************
subroutinereadchem(chemode,cozppb,qsw,rhum,cnoxppb,istab)

**************************************************************************
*readchem subroutine reads the user specifications for the
*chemistry run                                              *
**************************************************************************
* Variables:                                                *
* chemode          option for chemistry inclusion in model    *
* cozppb           concentration of background ozone in ppb    *
* qsw              intensity of short wave radiations          *
* rhum             relative humidity in air                    *
* cnoxppb          concentration of NOx in plume in ppb        *
*
* istab               atmospheric stability class
*
* Constants:
* unitcommand       unit connected to file CHEM
*
******************************************************************************
include 'includepar'
include 'includecom'
real coozppb, gsw, rhum, cnoxppb, istab
integer chemode
character*50 line
logical old

C Open the CHEM file and read user options
******************************************************************************

open(unitcommand, file=\"CHEM\", status=\"old\",
    +err=999)

C Check the format of the CHEM file (either in free format, C or using formatted mask)
C Use of formatted mask is assumed if line 10 contains the word 'CHEMODE'
******************************************************************************
*
* call skplin(9,unitcommand)
read (unitcommand,901) line
*
*
901 format (a)
if (index(line,'CHEMODE') .eq. 0) then
  old = .false.
else
  old = .true.
endif
rewind(unitcommand)
*
*
C Read parameters
**********************
*
* call skplin(7,unitcommand)
if (old) call skplin(1,unitcommand)
*
*
read(unitcommand,*) chemode
if ((chemode.ne.0).and.(chemode.ne.1).and.(chemode.ne.2)) goto 10
*
*
if (old) call skplin(3,unitcommand)
read(unitcommand,*) cozppb
*    
   if (old) call skplin(3,unitcommand) 
read(unitcommand,*) qsw
*    
   if (old) call skplin(3,unitcommand) 
read(unitcommand,*) rhum
*    
   if (old) call skplin(3,unitcommand) 
read(unitcommand,*) cnoxppb
*    
   if (old) call skplin(3,unitcommand) 
read(unitcommand,*) istab
*    
close(unitcommand)
*    
return
*

999write(*,*) '#### FLEXPART MODEL ERROR! FILE "CHEM" ####'
*    
write(*,*) '#### CANNOT BE OPENED IN THE DIRECTORY ####'
*    
write(*,'(a)')path(l)(1:len(l))
*    
10write(*,*) '#### FLEXPART MODEL ERROR! FILE "CHEM" ####'
*    
write(*,*) '#### DOES NOT HAS CORRECTLY CHOSEN ####'
*    
write(*,*) '#### OPTION "CHEMODE" ####'
*    
stop
end

subroutinechem(chemode,r)
*****************************************************************
* subroutine chem calculates the transformation rates for SO2 and
* NOx.
*****************************************************************
* Inputs:
*    
* chemode option for chemistry inclusion in model
*    
* cozppb concentration of background ozone in ppb
*    
* qsw intensity of solar radiation in w/m**2
*    
* rhum relative humidity in atmosphere
* cnoxppb  concentration of NOx in plume in ppb
* istab  atmospheric stability class
* *
* Constants:
* * rnitel  Loss rate of SOx used for night
* * rnite2  Loss rate of NOx used for night
* *
* Outputs:
* * r(1)  Daytime Transformation rate of SOx
* * r(2)  Daytime Transformation rate of NOx
* *
******************************************************************************
  
  realcozppb,qsw,rhum,cnoxppb,istab
integerchemode
  real r(2)
  real rnitel,rnite2
  callreadchem(chemode,cozppb,qsw,rhum,cnoxppb,istab)
*
*
c---------nighttime transformation rates

  rnitel=1
  rnite2=1
*
c---------initializaion of transformation rates

  do 10 i=1,2
  r(i)=0.0
10  continue
*
*
c--------convert units of solar radiation from w/m**2 to Kw/m**2
tsr=0.001*qsw
c03ppm=0.001*cozppb
st=amax0(istab,2)
*
*
c ******************************************************************************
  C --- SOx Transformation Rate
C ******************************************************************************

  if(tsr.le.0.)then
  *
  c ------ usenighttime transformation rate
  r(1)=rnitel
  else
  *
* c -------- Compute daytime transformation rate
r(1)=36.*(tsr**.55)*(co3ppm**.71)/(st**1.29)
* c -------- Add heterogeneous component
rshet=3.E-8*(rhum**4)
rshet=amax1(rshet,0.2)
r(1)=r(1)+rshet
endif
* c ***********************************************************
c c --- NOx transformation rates
c c ***********************************************************
if(tsr.le.0.)then
c ------ Use nighttime transformation rate
r(2)=rnite2
else
*
*c ------ Compute daytime transformation rate
rnppm=0.001*cnoxppb
rnppm=amax1(cnppm,1.e-4)
r(2)=1206.*(co3ppm**1.50)/(rnppm**.329)/(st**1.41)
endif
write(*,*)"r1=",r(1),"(%/hr)"
write(*,*)"r2=",r(2),"(%/hr)"
return
end
### Table 1: Sampling Points Distribution in Arc-A

<table>
<thead>
<tr>
<th>Point</th>
<th>Direction (degree)</th>
<th>Distance(km)</th>
<th>Coordinate</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>296°</td>
<td>0.716</td>
<td>24°51'0.8&quot;N, 66°47'33.8&quot;E</td>
</tr>
<tr>
<td>A2</td>
<td>291°</td>
<td>0.693</td>
<td>24°51'2.6&quot;N, 66°47'33.6&quot;E</td>
</tr>
<tr>
<td>A3</td>
<td>288°</td>
<td>0.687</td>
<td>24°51'3.7&quot;N, 66°47'33.8&quot;E</td>
</tr>
<tr>
<td>A4</td>
<td>284°</td>
<td>0.676</td>
<td>24°51'5.3&quot;N, 66°47'33.9&quot;E</td>
</tr>
<tr>
<td>A5</td>
<td>281°</td>
<td>0.675</td>
<td>24°51'6.5&quot;N, 66°47'34.1&quot;E</td>
</tr>
<tr>
<td>A6</td>
<td>276°</td>
<td>0.678</td>
<td>24°51'8.5&quot;N, 66°47'34.5&quot;E</td>
</tr>
<tr>
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### Table 2: Sampling Points Distribution in Arc-B

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Table 3: Sampling Points Distribution in Arc-C

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<tr>
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### Table 4: Sampling Points Distribution in Arc-D

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## Table 5: Sampling Points Distribution in Arc-E

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Table 6: Sampling Points Distribution in Arc-F

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Appendices

Appendix-VI

Structural Details of Experimental Stack

The structural details of experimental stack designed, fabricated and installed at PIEAS are presented here including calculations for wind force, turning moment, earth quack load and stress analysis.

Design Calculation for Wind Force and Turning Moment

Design wind force for experimental stack was calculated using following expression

\[ F = q_z G_f C_f A_f \]  

(1)

Where \( C_f \) is force coefficient. Its value is calculated for individual sections of stack and depends upon cross section, surface type and ratio of \( \frac{h}{D} \) of the particular section. The projected surface area \( A_f \) is expressed as the product of equivalent diameter \( D_e \) and height \( h_z \) for each small section of the structure i.e. \( A_f = D_e \times h_z \).

When ladder, platforms and other accessories are incorporated in the design structure, the actual diameters are increased and are calculated as \( 2D_o \). \( D_o \) and \( h_z \) are the outer diameter and height of each small section.

The other important parameter \( q_z \) is external wind pressure on stack shell at elevation under consideration that is given as

\[ q_z = 0.00256V^2IK_{zf}K_z \]  

(2)

Where \( V \), \( I \), \( K_{zf} \) and \( K_z \) are the basic wind speed, importance factor, topographic factor and velocity pressure exposure coefficient evaluated at height \( z \).

The other important parameter is

\[ G_f = \frac{1+2gI_z\sqrt{Q^2+R^2}}{1+7I_z} \]  

(3)

Where \( g \) is gravitational acceleration and \( I_z \) is the intensity of turbulence at height \( z \), expressed as
\[ L_z = c \left( \frac{33}{z} \right)^{\frac{1}{6}} \]  

(4)

Where ‘c’ is a constant and ‘\( \bar{z} \)’ represents equivalent height of the stack calculated as

\[ \bar{z} = 0.6 \times h \]  

(5)

The expression for calculation of ‘\( Q^2 \)’ is as follows;

\[ Q^2 = \frac{1}{1 + 0.63 \left( \frac{D_e + h}{L_{z}} \right)^{0.63}} \]  

(6)

Where ‘\( h \)’, ‘\( D_e \)’ and ‘\( L_{z} \)’ represent the stack height, equivalent diameter and the integral length scale of turbulence at the equivalent height of stack, ‘\( \bar{z} \)’ expressed as

\[ L_{z} = I \left( \frac{z}{33} \right)^{\frac{2}{3}} \]  

(7)

Where ‘\( I \)’ and ‘\( \varepsilon \)’ are constants. The value of ‘\( R^2 \)’, was calculated as

\[ R^2 = \frac{R_s R_h R_b (0.53 + 0.47 R_d)}{\beta} \]  

(8)

Where ‘\( \beta \)’ is the structural damping coefficient depending upon the type of land. The expression for ‘\( R_n \)’

\[ R_n = \frac{7.465 N_l}{(1+10.302 N_l)^{\frac{2}{3}}} \]  

(9)

Where

\[ N_l = \frac{f L_{z}}{\bar{V} z} \]  

(10)

Where ‘\( f \)’, ‘\( L_{z} \)’ and ‘\( \bar{V} z \)’ are the natural frequency defined as\( 1/T \). ‘\( T \)’ is period of vibration which was calculated during the calculations of Earth quack load, the integral length scale of turbulence at the equivalent height and the mean hourly wind speed at the equivalent height ‘\( \bar{z} \)’, respectively. The mean hourly wind speed is expressed as
\[ \bar{V}_z = b \times \left( \frac{22}{33} \right)^{\alpha} \times V \times \left( \frac{22}{15} \right) \]  

(11)

Where \( \bar{V} \) is the basic design wind speed, ‘b’ and ‘\( \alpha \)’ are constants.

Here \( R_h \) is defined as

\[ R_h = \frac{1}{N_h} - \frac{1}{2 N_h^2} \left( 1 - e^{-2 N_h} \right) \]  

(12)

Where

\[ N_h = \frac{s \cdot h}{V_z} \]  

(13)

The expression for calculation of \( R_b \) is as

\[ R_b = \frac{1}{N_b} - \frac{1}{2 N_b^2} \left( 1 - e^{-2 N_b} \right) \]  

(14)

Where

\[ N_b = \frac{4.6 f D_e}{V_z} \]  

(15)

The expression for calculation of \( R_d \) is as

\[ R_d = \frac{1}{N_d} - \frac{1}{2 N_d^2} \left( 1 - e^{-2 N_d} \right) \]  

(16)

Where

\[ N_d = \frac{15.4 f D_e}{V_z} \]  

(17)

\( M \) is the overturning moment at base calculated as follows;

\[ M = \bar{F} \times \bar{d} \]  

(18)

As the force acts through the centre of gravity of a body and in the present case it lies in the centre of each small section of the stack. That is why \( \bar{d} \) was taken as the distance from ground level to centre of each section of stack. Finally summing over the thirteen sections of stack, the resulting overturning was calculated as

\[ \sum_{i=1}^{13} M_i = \sum_{i=1}^{13} \bar{F}_i \times \bar{d}_i \]  

(19)
**Design Calculation for Earthquake load**

The expression used for calculation of period of vibration is given as

$$T = \left(\frac{H}{100}\right)^2 \sqrt{\frac{\sum W_x \Delta \alpha + \sum W \beta / H}{\sum E(D/10)^2 t \Delta \gamma}}$$  \hspace{1cm} (20)

Where ‘T’ is the period of vibration, ‘H’ is the stack height, ‘\( W_x \)’ is the uniformly distributed load for each section and is represented by \( W_x = w / L \). Where ‘w’ and ‘L’ are the total weight and the length of the shell section of stack. ‘\( \Delta \alpha \)’ and ‘\( \Delta \gamma \)’ are the differences in values of ‘\( \alpha \)’ and ‘\( \gamma \)’ from top to bottom of a section. Where ‘\( \alpha \)’, ‘\( \beta \)’ and ‘\( \gamma \)’ are the co-efficients for given plane based on ‘\( h_x / H \)’. ‘\( h_x \)’ is the height from base to centre of a section. ‘t’ and ‘D’ are the thickness and outer diameter of shell section. ‘E’ is the modulus of elasticity at design temperature i.e. 29106 psi.

From time of vibration, the natural frequency ‘f’ can be calculated as it is the reciprocal inverse of time period.

$$f = \frac{1}{T}$$  \hspace{1cm} (21)

The expression for lateral force applied at each section is given as

$$F_x = (V - F_i)(W_x h_x) / (\sum W_x h_x)$$  \hspace{1cm} (22)

Where ‘\( F_i \)’ and ‘\( V \)’ represent the seismic force applied at the top of the stack and base shear calculated as

$$F_i = 0.07 \times T \times V$$  \hspace{1cm} (23)

$$V = \sum W_x \alpha_H$$  \hspace{1cm} (24)

Where ‘\( \alpha_H \)’, ‘\( W_x \)’ are maximum horizontal acceleration coefficient and the total weight of a section.

Moment at Plane under consideration is calculated as

$$M_i = F_i (H - h_i) + F_x (h_x - h_i)$$  \hspace{1cm} (25)

Where ‘\( h_i \)’ is the height from base to plane under consideration.
Appendices

Comparison of the moments of wind and earthquake revealed the fact that moments of wind were severe than those of earthquake, therefore further analysis was done considering the wind factor only.

Design Calculations of Stress analysis

The expressions for determining allowable stresses are applicable for cylindrical stacks provided that following equation is satisfied;

\[
\frac{t}{D} \leq \frac{10F_y}{E} \quad (26)
\]

Where ‘E’ and ‘F_y’ are the modulus of elasticity at design temperature and the yields strength of selected material of stack i.e. A-36 at 33000 Psi and 200°F. The equation no. 26 was found to be completely satisfied at all the specified sections. Since for stacks meeting the requirements of equation no. 26, the following four load cases must be satisfied. Therefore testing for each case was also performed.

Case 1: Longitudinal Compression.

The longitudinal compressive stress in cylindrical stacks (P/A) must not exceed the allowable limit ‘S_{cl}’

\[
\frac{P}{A} \leq S_{cl} \quad (27)
\]

Where ‘P’, ‘A’, and ‘S_{cl}’ represent the dead load of stack above elevation under consideration, the cross-sectional area of stack plate and allowable longitudinal compressive stress in shell.

Here one of the formulas is selected for ‘S_{cl}’ by making a check for

\[
S_{cl} = \frac{EtY}{4D(F.S.)} \text{ when } \frac{t}{D} \leq \frac{2.8F_y}{E} \quad (28)
\]

or

\[
S_{cl} = \frac{F_y(1-0.3K_s)Y}{(F.S.)} \text{ when } \frac{2.8F_y}{E} < \frac{t}{D} \leq \frac{10F_y}{E} \quad (29)
\]

And
Appendices

\[ Y = 1 \text{ when } \frac{L_e}{r} \leq 60 \text{ and } F_y \leq 50\text{ksi} \] (30)

Or

\[ Y = \frac{21,600}{18,000 + \left(\frac{L_e}{r}\right)^2} \text{ when } \frac{L_e}{r} > 60 \text{ and } F_y \leq 50\text{ksi} \] (31)

\[ K_s = \left(\frac{10F_y - t}{E} \frac{E}{7.2F_y} \frac{D}{D}\right)^2 \] (32)

Where ‘\( F_\text{s}.S. \)’ is factor of safety. ‘\( L_e \)’ is equivalent length. ‘\( Y \)’ is the coefficient used to calculate longitudinal compressive stress. ‘\( r \)’ is the weighted mean radius of gyration for elevation under consideration and is given as \( \sqrt{\frac{I_{\text{section}}}{A}} \). Where ‘\( I_{\text{section}} \)’ is the moment of inertia and ‘\( A \)’ is the cross-sectional area of a particular section. The moment of inertia for cylindrical body is expressed as ‘\( \pi R^2 t \)’. Here ‘\( t \)’ is thickness and ‘\( R \)’ is the mean radius of a section.

Results for the above calculations indicated that the condition of equation (27) is completely satisfied and the longitudinal compressive stress was within the limit.

**Case 2: Longitudinal Compression and Bending Combination**

The combined longitudinal compressive and bending stress in cylindrical stacks must not exceed the allowable stress, ‘\( S_{bl} \)’.

\[ \frac{P}{A} + \frac{MD}{2I_{\text{section}}} \leq S_{bl} \] (33)

The expressions for ‘\( S_{bl} \)’ are the same as used above for ‘\( S_{cf} \)’ provided ‘\( Y = 1 \)’ in any case. Results for the above calculations indicated that the requisite condition of equation (33) is satisfied.

**Case 3: Circumferential Stress**

The circumferential stress ‘\( f_c \)’ in the shell due to external wind pressure ‘\( q_z \)’ between stiffeners spaced at distance, ‘\( I_\infty \)’ was determined using
The circumferential stress must be less than the allowable stress, \( S_{cc} \), calculated as

\[
S_{cc} = \frac{1.30 EK \left( \frac{t}{D} \right)^{1.5}}{(F.S.)\left( \frac{t}{D} \right)}
\]  

(35)

When \( 0 \leq \frac{t}{D} \leq \frac{2.8 F_y}{E} \), \( K = 1 \)

(36)

When \( \frac{2.8 F_y}{E} < \frac{t}{D} \leq \frac{10 F_y}{E} \), \( K = 1.68 \frac{F_y D}{Et} + 0.465 - \frac{0.0232 Et}{F_y D} \)

(37)

Results for above calculations were indicative of the qualification of the above case.

**Case 4: Combined Longitudinal and Circumferential Compressive Stress**

The combined longitudinal and circumferential compressive stress in cylindrical stacks must satisfy the following criteria.

\[
\frac{P}{A} + \frac{MD}{2I_{section}} + \left( \frac{f_c}{S_{cc}} \right)^2 \leq 1.0
\]  

(38)

Results for above calculations were found indicative of the qualification of the above case.
Details of Foundation for Experimental Stack

Preparation steps for the stack foundation are presented here in details. Since the civil design of a foundation for a stack depends upon soil characteristics, availability of space and the amount of overturning at specific site, therefore foundation for experimental stack was especially designed by Works and Services Organization (WASO) to make it appropriate to the site of PIEAS considering the local wind, seismic and stack operating conditions.

For a safe and economical design of stack foundation, a thorough geotechnical survey of the site area was made by SOILCON Company. The purpose of investigation was to collect the geological information of the site regarding the major subsoil types and physical and chemical characteristics of soils and rocks beneath the site. Such type of information helped to calculate bearing capacity of the soil which is an important parameter for the design and construction of stack foundation.

Based upon the real knowledge of foundation loadings and the soil parameters obtained from the stack mechanical design and investigations of geotechnical survey respectively, ‘Pad type foundation’ was selected for self-supporting stack because of the design simplicity and economical point of view. Pad foundation is normally defined as an isolated foundation to spread a concentrated load. The footing area was calculated on the basis of bearing strength as follows:

\[
\text{Minimum area required for foundation} = \frac{\text{Total load to be transferred to soil}}{\text{Allowable bearing capacity}}
\]

Total load includes the loads from self-weights of stack, foundation (initially assumed for calculation) and the backfill. Allowable Bearing Capacity is defined as the load transferred to the soil on square feet of the ground surface area. Footing shape was selected square because it is more economical as compared to other footing shapes like octagonal shape.

The design area of footing was calculated as 31'×31' with the depth of 13'6" as shown in Figure1.
In the initial constructional stage of the stack foundation, a layer of Planned Cement Concrete (P.C.C) with thickness of 4"and ratio 1:4:8 was laid down. First reinforcement bar frame was built over P.C.C layer with each bar of 1" diameter and 4"centre to centre distance between consecutive frame bars. Second reinforcement bar frame was laid down with each bar of ¾" diameter and 5"center to center distance between consecutive bars. The gap between two frames was kept as 3' 6" as shown in Figure 2. A supporting column for stack running from bottom of the footing up to a height of 4' above the ground level was fabricated as shown in Figure 3.

24 M.S J-bolts of 1500 mm length and 50 mm thinness were imbedded in R.C.C foundation column. Two M.S template plates each with thickness of 10 mm
containing 24 holes were spot welded to the J-bolts and the structural steel bars. The template plate II was first placed and adjusted among the bars of vertical column with the help of chain pulley and folding. Subsequently, template plate I was adjusted after the insertion of 24 J bolts through the holes of template plate II as shown in Figure 4.

![Fig.4: Two Template Plates with 24 J Bolts](image)

Distance between two template plates was 675mm. The straight ends of the J-bolts extending upward were made threaded in order to hold the base plate and top-ring of the steel stack. The J-bolts were extending up to 500 mm above the top of template I. The purpose of template plates was to keep the J-bolts in position and in plumb so that the base plate of the stack could easily be inserted into all 24 J-bolts after the completion of RCC work. The pouring of the concrete in the footing steel frame structures was done to ensure that voids are minimized. Finally concreting of the foundation and the back filling of the soil was carried out using sufficient water to eliminate voids and loose pockets up to height of 10' as shown in Figure 5 and 6. The foundation was cured for 14 days (minimum) and thereafter left undisturbed for a period not less than 30 days.

![Fig.5: Concreting of Stack Foundation](image)  ![Fig.6: Back Filling of Foundation](image)
Details of Blower for Experimental Stack

To dilute the concentration of cylinder gas from $10^5$ ppm (10%) to 150 ppm inside the stack, air flow of 3300 cfm was provided using a centrifugal blower of Air-mech BFC series (model: BFC-20-FH). This system was especially designed to fulfill the experimental requirements. It consists of a centrifugal fan, an electric motor, a drive system, ducts or piping, flow controls and measuring devices. A 10 Hp belt driven motor was attached with blower. This motor is induction type (Y132M-4 380-420V) of class–B and draws the current of 14.6 amperes. Both motor and blower are linked together with a belt rotating on the pulleys of different sizes. The blower has been attached with stack using a round ducting of diameter of 12 inches fabricated by 20gauge G.I sheet. A Side change reducer round and rectangular in shape was used to connect blower outlet to ducting. A few isolators have been placed between the platform and blower base for providing vibration protection to the whole unit. A butter fly wafer damper was placed near the blower exhaust to prevent the undesirable corrosive gas flow from stack towards blower, when the blower is not running. Three inlet openings of the diameter of 4, 6 and 8 inches have been provided in the ducting after isolating damper for entering any tracer or pollutant into stack. A wafer (wedge seat round damper) damper was placed in the branch outlet for flow bypass and another wafer damper was used in the main stream line to vary the blower flow rate manually. Figures 1 and 2 illustrate the different components configuration in blower ducting system.

![Plane View of Blower Ducting System](image)

Fig. 1: Plane View of Blower Ducting System
Fig. 2: Sectional View of Blower Ducting System
Appendices

Appendix-IX

Fig. 1: Wind Rose at Height of 60m for the Year 1987