ABSTRACT of

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Chemical or radioactive air pollutants whether emitted accidently 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 meteorolgical 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 groud level SO_2 concentrations from a cluster of stacks of oil refnery 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 simoultaneously 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'.