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Dispersion of Cd, Cr, Cu, Ni, Pb and Zn Particles in a Turbulent Air Flow

[1]M.N. Abbasi, [1]I. Ahmad and [2]M. Tufail

[1]Pakistan Institute of Engineering and Applied Sciences, Nilore, Islamabad, Pakistan
[2]Riphah International University, Islamabad, Pakistan

Abstract: From the prospective of air quality, the dispersion of heavy metal pollutants has gain importance in recent past. The pollutants disperse from the point of release to the distant areas transporting contaminants there. Heavy metal pollutants in the form of fine particulate matter can be harmful to human health through inhalation. In this study the lateral dispersion of heavy particles is predicted with the help of experimentally measured values of the dispersion for copper particles. The experimental values of the dispersion for copper particles are taken from the literature. The stochastic technique is used to develop a rigorous simulation model for the dispersion of the copper particles. This technique helped in the generation of random fluctuations for the fluid (air) as well as for the heavy particle, copper. The random behavior of copper particle is applied on other heavy metals belonging to the same class. In this study the lateral dispersion of various heavy metal particles is predicted on the basis of their densities and particle sizes. The results so obtained make good sense and relate well with the density and size of the heavy metal particles.

Key words: Heavy particles · Lateral dispersion · Particle size · Random fluctuations

INTRODUCTION

In order to monitor and develop better understanding of the air quality and dispersion phenomenon in the urban atmospheric boundary layer (ABL) environment, the application of computational fluid dynamics has become very interesting and important topic [1]. The estimation of the dispersion for toxic pollutants into the atmosphere requires the computation of the concentration of the pollutants. The dispersion of different pollutants, in the turbulent flow, released from the industries, chemical plants, Nuclear reactor and other pollution sources in the form of fine particles is an important atmospheric pollution study. These pollutants get transported from place to place in the form of very small micron size particles. These particles may be in the form of ash and smoke [2]. The micron size particles in the form of suspended dust, droplets, bubble etc produced by many natural phenomenons get advected into the incompressible turbulent atmospheric flow [3, 4]. The size, type and density of the particles describe transport of particles in the air as well as the deposition of these particles into the human body through respiratory tracks [5].

Various approaches have been adopted as cited in the literature for the dispersion estimation of the particles in air. Markov chain-Monte Carlo (MCMC) method has been used in a homogeneous turbulent flow for the dispersion measurement as well as simulating particle trajectories [6]. MCMC model has also been used for the particles dispersion and air concentration measurements in planetary boundary layer (PBL) under neutral atmospheric conditions from a continuous point source at the ground level and at a height of 100 m above the ground level [7]. The Lagrangian Model for concentration fluctuation 'LAGFLUM' is the mix up of the macro and micro schemes for the langrangian model for the passive tracer concentration [8].

Light and heavy particles have different flow trends with respect to the carrier fluid. Light particles follow nearly the same path as that of the carrier fluid however heavy particles having density different than that of the

Corresponding Author: M.N. Abbasi, Department of Physics and Applied Mathematics, Pakistan Institute of Engineering and Applied Sciences, P.O. Nilore, Islamabad, Pakistan.

carrier fluid do not follow the same path as that of the fluid [9]. The light particles behave just like the fluid points however the heavier particles having significant inertia show crossing trajectories effect [10]. The heavy particles because of inertia do not follow the highly frequent fluctuations of the fluid (air). If the particle has sufficient terminal velocity it will fall from one eddy to another and this phenomenon is named as 'corrosing-trejectories effect'. However the light particle representing the fluid point has no inertial impacts on the eddy and will remain in the same eddy for its life time [5]. The heavy metal trajectory model in the turbulent flows was presented in the uniform horizontal atmospheric surface. Dispersion of glass in the form of a sphere has been studied when released at a height of few meters above the ground level [7]. Particle velocities as well as trajectories have been computed with the help of lagrangian approach [11].

In the present study the lateral dispersion of copper particles is computed with an assumption that the particles do not collide with each other. The computational results for the dispersion of copper particles are obtained with the help of stochastic simulation technique which produces more rigorous results when compared with the experimental dispersion results for the copper particle [2]. The lateral dispersal trends for a number of heavy particles are predicted keeping the same random behavior as that of copper particles. The dependence of the lateral dispersion on the particle size as well as density of the particle is studied for various heavy metals that include Cd, Cr, Cu, Ni, Pb and Zn. It has been found that for each heavy metal, the greater the density of the heavy metal particle, the smaller is the lateral dispersion and vice versa. Also the greater the particle size of the heavy metal particle the smaller is the lateral dispersion and vice versa.

MATERIALS AND METHODS

In order to find out the particle motion in the lateral direction, we make use of the following equations as described by [2]:

$$\frac{du_x}{dt} = \frac{u_x - u_{xp}}{T_p} \quad (1)$$

where u_x is the lateral velocity fluctuation of fluid as a particle carrier and u_{xp} is the lateral particle fluctuation.

Time which describes the motion of a particle is T_p and is given by the following equation [2]:

$$T_p = \frac{M_p}{3\pi\mu F D_p} \quad (2)$$

M_p is the mass of the particle moving in a carrier fluid, μ is the kinematic viscosity of the fluid, D_p is the diameter of the spherical particle and F is the drag coefficient given by [2]

$$F = 1 + 015 Re_p^{\ 0.687} \quad (3)$$

Particle Reynolds number can be calculated from the following Equation [2].

$$Re_p = \frac{\rho D_p u_{rel}^{\ 2}}{u} \quad (4)$$

where ρ is the fluid density and u_{rel} is the relative velocity.

The fluid velocity fluctuations and so the particle velocity fluctuations are generated using the RAND function. For the generation of the velocity fluctuations, for a specific particle, the coefficient as well as the argument of the function has to be adjusted to get the accurate results. The mean lateral velocity of the particle is taken as zero [2]. The standard deviation is obtained from the randomly generated velocity fluctuations for the copper particle.

The time for which a particle remains in an eddy is known as eddy life time of the particle. The particle eddy may be calculated with the help of turbulent kinetic energy and dissipation rate of the kinetic energy [2, 10]. The solution of equation 1 is given as [2]:

$$u_{xp} = u_x - (u_x - u_{xpo})\ exp^{-t/Tp} \quad (5)$$

u_{xpo} is the value of particle velocity at t=0. where 't' is the small time interval whose value is chosen as 19.1 ms and this value is kept less than the eddy life time.

The computational results found for the copper particle has been used to find out the lateral dispersion $\overline{X^2}$ trends of the various heavy metals belonging to the same class of metals as copper. Six heavy metals are chosen and assuming the same random behavior of these metals as that of copper particle, the dispersion values are studied. The various input values relating the dispersion studies of the heavy metal particles are given in Table 1. In order to predict the dispersal behavior due to the size of a particle, seven particle sizes are selected for each metal and their dispersion trends are observed. The volume of each particle is measured from the size of the spherical particle. With the help of density of each particle, mass is calculated.

Table 1: Heavy metal particulates characterization and dispersion parameters.

Sr.No	Element Name	Particle Dia (µ m)	Particle Volume (m^3)	Particle Mass (Kg)	Rynolds Number	Dynamic time (s)	Particle Density (Kg/m^3)
1	Copper	30	$1.409*10^{-14}$	$1.262*10^{-10}$	$3.355*10^{-2}$	$3.552*10^{-2}$	8960
		35	$2.238*10^{-14}$	$2.005*10^{-10}$	$3.914*10^{-2}$	$4.830*10^{-2}$	
		40	$3.340*10^{-14}$	$2.993*10^{-10}$	$4.473*10^{-2}$	$6.299*10^{-2}$	
		45	$4.756*10^{-14}$	$4.262*10^{-10}$	$5.033*10^{-2}$	$7.961*10^{-2}$	
		46.5	$5.24*10^{-14}$	$4.671*10^{-10}$	$5.200*10^{-2}$	$8.438*10^{-2}$	
		60	$1.127*10^{-13}$	$1.010*10^{-9}$	$6.71*10^{-2}$	$1.409*10^{-1}$	
		75	$2.202*10^{-13}$	$1.973*10^{-9}$	$8.388*10^{-2}$	$2.193*10^{-1}$	
		90	$3.805*10^{-13}$	$3.409*10^{-9}$	$1.006*10^{-1}$	$3.147*10^{-1}$	
2	Cadmium	30	$1.409*10^{-14}$	$1.219*10^{-10}$	$3.355*10^{-2}$	$3.431*10^{-2}$	8650
		35	$2.238*10^{-14}$	$1.936*10^{-10}$	$3.914*10^{-2}$	$4.663*10^{-2}$	
		40	$3.340*10^{-14}$	$2.889*10^{-10}$	$4.473*10^{-2}$	$6.080*10^{-2}$	
		45	$4.756*10^{-14}$	$4.114*10^{-10}$	$5.033*10^{-2}$	$7.685*10^{-2}$	
		60	$1.127*10^{-13}$	$9.753*10^{-10}$	$6.71*10^{-2}$	$1.360*10^{-1}$	
		75	$2.202*10^{-13}$	$1.904*10^{-9}$	$8.388*10^{-2}$	$2.117*10^{-1}$	
		90	$3.805*10^{-13}$	$3.291*10^{-9}$	$1.006*10^{-1}$	$3.038*10^{-1}$	
3	Chromium	30	$1.409*10^{-14}$	$1.013*10^{-10}$	$3.355*10^{-2}$	$2.851*10^{-2}$	7190
		35	$2.238*10^{-14}$	$1.609*10^{-10}$	$3.914*10^{-2}$	$3.876*10^{-2}$	
		40	$3.340*10^{-14}$	$2.402*10^{-10}$	$4.473*10^{-2}$	$5.055*10^{-2}$	
		45	$4.756*10^{-14}$	$3.420*10^{-10}$	$5.033*10^{-2}$	$6.388*10^{-2}$	
		60	$1.127*10^{-13}$	$8.107*10^{-10}$	$6.71*10^{-2}$	$1.131*10^{-1}$	
		75	$2.202*10^{-13}$	$1.583*10^{-9}$	$8.388*10^{-2}$	$1.760*10^{-1}$	
		90	$3.805*10^{-13}$	$2.736*10^{-9}$	$1.006*10^{-1}$	$2.526*10^{-1}$	
4	Nickel	30	$1.409*10^{-14}$	$1.245*10^{-10}$	$3.355*10^{-2}$	$3.529*10^{-2}$	8900
		35	$2.238*10^{-14}$	$1.991*10^{-10}$	$3.914*10^{-2}$	$4.796*10^{-2}$	
		40	$3.340*10^{-14}$	$2.973*10^{-10}$	$4.473*10^{-2}$	$6.257*10^{-2}$	
		45	$4.756*10^{-14}$	$4.233*10^{-10}$	$5.033*10^{-2}$	$7.907*10^{-2}$	
		60	$1.127*10^{-13}$	$1.003*10^{-9}$	$6.71*10^{-2}$	$1.339*10^{-1}$	
		75	$2.202*10^{-13}$	$1.960*10^{-9}$	$8.388*10^{-2}$	$2.734*10^{-1}$	
		90	$3.805*10^{-13}$	$3.386*10^{-9}$	$1.006*10^{-1}$	$3.126*10^{-1}$	
5	Lead	30	$1.409*10^{-14}$	$1.599*10^{-10}$	$3.355*10^{-2}$	$4.501*10^{-2}$	11350
		35	$2.238*10^{-14}$	$2.540*10^{-10}$	$3.914*10^{-2}$	$6.118*10^{-2}$	
		40	$3.340*10^{-14}$	$3.791*10^{-10}$	$4.473*10^{-2}$	$7.978*10^{-2}$	
		45	$4.756*10^{-14}$	$5.399*10^{-10}$	$5.033*10^{-2}$	$1.008*10^{-1}$	
		60	$1.127*10^{-13}$	$1.279*10^{-9}$	$6.71*10^{-2}$	$1.784*10^{-1}$	
		75	$2.202*10^{-13}$	$2.499*10^{-9}$	$8.388*10^{-2}$	$2.778*10^{-1}$	
		90	$3.805*10^{-13}$	$4.319*10^{-9}$	$1.006*10^{-1}$	$3.988*10^{-1}$	
6	Zinc	30	$1.409*10^{-14}$	$1.004*10^{-10}$	$3.355*10^{-2}$	$2.826*10^{-2}$	7130
		35	$2.238*10^{-14}$	$1.595*10^{-10}$	$3.914*10^{-2}$	$3.842*10^{-2}$	
		40	$3.340*10^{-14}$	$2.382*10^{-10}$	$4.473*10^{-2}$	$5.013*10^{-2}$	
		45	$4.756*10^{-14}$	$3.391*10^{-10}$	$5.033*10^{-2}$	$6.334*10^{-2}$	
		60	$1.127*10^{-13}$	$8.039*10^{-10}$	$6.71*10^{-2}$	$1.121*10^{-1}$	
		75	$2.202*10^{-13}$	$1.570*10^{-9}$	$8.388*10^{-2}$	$1.745*10^{-1}$	
		90	$3.805*10^{-13}$	$2.713*10^{-9}$	$1.006*10^{-1}$	$32.505*10^{-1}$	

RESULTS AND DISCUSSIONS

The lateral dispersion $\overline{X2}$ of the various particles is assessed in two ways; first the dispersion is studied for each element by varying the particle size. In the second case the particle size is kept the same however elements are varied to observe for the lateral dispersion trends of the elemental particulates with respect to each other. The computational results for the dispersion of the element copper are obtained for the particle size 46.5 µm and are compared with the experimental dispersion results for copper [2]. The computational and experimental results show good agreement as indicated by a solid line and small circles in Figure 1(a). This element and the rest of the five elements have been computed for the lateral dispersion showing different behavior based on the density of the particle for the specific element. It has been observed that as the particle size decreases there is an increase in the lateral dispersion as shown in Figure 1(a-f). It is also observed that there is an increase in the difference between the two dispersed particles of an element as the particle size decreases.

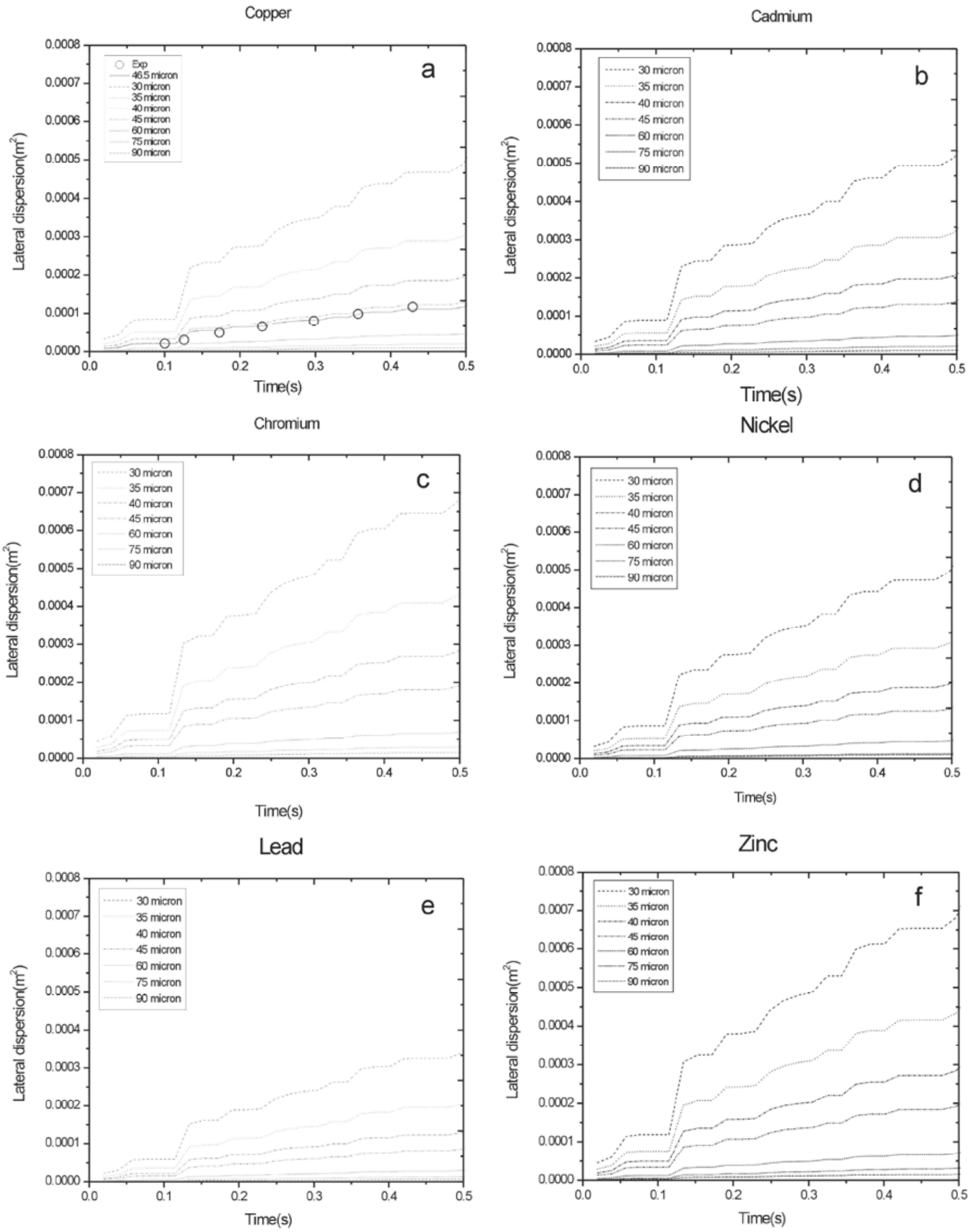

Fig. 1(a-f): Dispersion of the six elements. For each element the particle size is varied from 30 to 90 microns

In the second case studied for the lateral dispersion $\overline{x^2}$, the particle size is kept the same and the behavior of lateral dispersion is seen for all the six elements under study. This study shows that as the particle size of the heavy metal increases, the lateral dispersion decreases as shown in the Figure 1(a-f) and Figure 2(a-g). Also it is

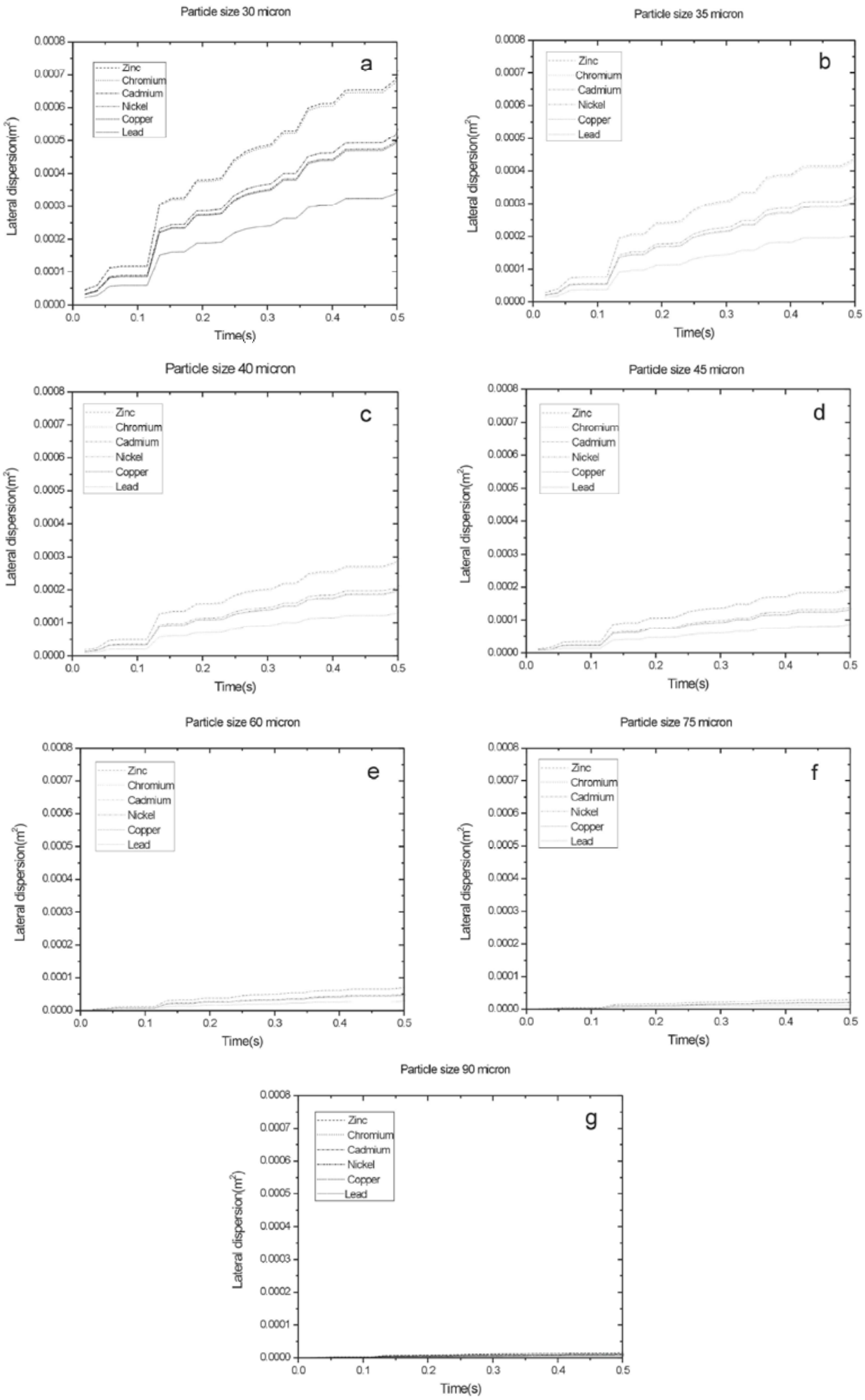

Fig. 2(a-g): Dispersion of the six elements. For each particle size the dispersion of all the six elements is observed

observed that the particles of the elements with the smaller densities are dispersed more than that with the high density values. The difference in the dispersion is comparable with the densities of the elements. The elements show the following lateral dispersion order:

$$\overline{X_{Zn}^2} > \overline{X_{Cr}^2} > \overline{X_{Cd}^2} > \overline{X_{Nt}^2} > \overline{X_{Cu}^2} > \overline{X_{Pb}^2} \quad (6)$$

The densities of the heavy metals are in the following order

$$\rho_{Pb} > \rho_{Cu} > \rho_{Ni} > \rho_{Cd} > \rho_{Cr} > \rho_{Zn} \quad (7)$$

It can be seen from the above two inequalities that there is an inverse relationship between the lateral dispersion and the densities of the elemental particles studied. One can also observe that there is an inverse relationship between the particle size and the lateral dispersion as seen in Figure 1(a-f).

CONCLUSIONS

Based on the stochastic numerical dispersion simulations conducted for wide range of heavy metal particles of various sizes, the following conclusions may be drawn.

- For Copper, the simulated values of lateral dispersion agree with the corresponding experimental data.
- By increasing the particle size, the values of lateral dispersion decreases.
- The lateral dispersion of the heavy metal particles exhibits inverse proportionality with the density of the metal.
- The dispersion process dilutes the heavy metal pollutant particles into the atmosphere.

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REFERENCES

1. Gorle, C., J.V. Beeck, P. Rambaud and G.V. Tendeloo, 2009. CFD modeling of small particle dispersion: The influence of the turbulence kinetic energy in the atmospheric boundary layer. Atmospheric Environment, 43: 673-681.
2. Avila, R. and M.A. Rodriguez-Meza, 2004. Velocity autocorrelation function of a dispersion of heavy particles in a turbulent flow: on the effect of inter-particle collisions. Revista Mexicana De Fisica, 50(2): 156-161.
3. Csanady, G., 1980. Turbulent Diffusion in the Environment. Geophysics and Astrophysics Monographs, D. Reidel Publishing Company.
4. Shaw, R.A., 2003. Particle turbulence interactions in atmospheric clouds. Annual Review of Fluid Mechanics, 35: 183-227.
5. Guha, A., 2008. Transport and deposition of Particles in a turbulent and laminar flow. Annual Review of Fluid Mechanics, 40: 311-41.
6. Avila, R., 1997. Simulacion numerica de la dispersion de una nube de particulas solidas liberada a la atmosfera, Ph.D thesis, Facultad de Ingenieria, Universidad Nacional Autonoma de Mexico.
7. Avila, R. and S.S. Raza, 2005. Dispersion of Particles Released into a Neutral Planetary Boundary Layer Using a Markov Chain–Monte Carlo Model. Journal of Applied Meteorology, 44: 1106.
8. Amicarelli1, A., P. Salizzoni, P. Monti, G. Leuzzi, L. Soulhac1and F.X. Cierco, 2010. Modelling concentration fluctuations in a turbulent boundary layer: Sensitivity of a lagrangian model to dissipation rates estimates. In the proceedings of the 13th Conference on Harmonisation within Atmospheric Dispersion Modeling for Regulatory Purposes.
9. Bec, J., L. Biferale, A.S. Lanotte, A. Scagliarini and F. Toschi, 2010.Turbulent pair dispersion of inertial particles. Journal of Fluid Mechanics, 645: 497-528.
10 Snyder, W.H. and J.L. Lumley, 1971. Some measurements of particle velocity autocorrelation functions in a turbulent flow. Journal of Fluid Mechanics, 48: 41-71.
11. Oliveira, L.A., V.A.F. Costa and B.R. Baliga, 2002. A Lagrangian Eulerian model of particle dispersion in a turbulent plane mixing layer. International Journal for Numerical Methods in fluids, 40: 639-653.