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CHARGE EFFECTS ON PARTICLE DEPOSITION IN THE HUMAN TRACHEOBRONCHIAL TREE

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Abstract—Electrification occurs in most aerosol generating processes. The unipolar charges carried by these particles can influence the deposition of inhaled particles in the lungs. Recently published studies using a hollow lung cast of a human larynx-tracheobronchial tree and *in vivo* experiments in human subjects have demonstrated that increased deposition was due to electrostatic charges on the particle. The electrostatic charge effect on deposition may be important in the assessment of hazards associated with charged particles and was therefore studied theoretically. A new model was developed to predict particle deposition in the bronchial airways due to the combined mechanisms of inertial and electrostatic image forces. The agreement between the predicted values and the experimental data suggests that the new theory can be used to estimate tracheobronchial deposition of charged particles in the human respiratory tract.

INTRODUCTION

AIRBORNE particles of either natural or anthropogenic origin can acquire electrostatic charges. Electric field forces and charged ions in nature can lead to the formation of charged particles in the atmosphere, whereas highly charged particles in the occupational environment are generated under high shear forces during grinding, sanding or similar operations. On a lesser scale, aerosols generated by atomization for therapeutic purposes and in inhalation studies can also be electrically charged. These mechanisms described are known as field charging, contact charging and charging by atomization. The upper particle charge limits for these different mechanisms are established theoretically and have been summarized by LIU and PUI (1974). The actual charge levels encountered are usually within these respective upper limits and the RMS charge levels at Boltzmann equilibrium (JOHN *et al.*, 1980; CHOW and MERCER, 1971).

The effect of charged particles on deposition in the human respiratory system may be important in industrial hygiene and aerosol therapy. Although earlier experiments (FRASER, 1966; FRY, 1970) have suggested that increased lung deposition due to charged particles under 'normal circumstances' would be insignificant, recent studies of MELANDRI *et al.* (1977) and CHAN *et al.* (1978) clearly demonstrated the need to re-examine the potential of increased lung deposition for charged particles smaller than 5 μm. MELANDRI *et al.* found an increase in lung deposition in human subjects for submicron aerosols between 0.3 and 1.1 μm having particle charges ranging from 30–110 elementary charges/particle. CHAN *et al.* observed a significant increase in deposition in the bronchial airways of a hollow human lung cast for particles of 2–5 μm

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with 360–1100 charges/particle. In addition, theoretical considerations of INGHAM (1980), CHEN (1978), YU and CHANDRA (1977, 1978) THIAGARAJAN and YU (1979) and DIU and YU (1980) have illustrated that increased deposition for the charged particles is possible under appropriate conditions. A recent review of the charge effect on deposition for freshly-generated aerosols was given by JOHN (1980).

In this study, a theoretical deposition model for charged particles is developed by considering the combined mechanisms of inertial and electrostatic image forces in a tube bend. Using appropriate bend angles for the bronchial airways, the theoretical calculations are compared with the charged particle deposition data obtained in a hollow human lung cast deposition study (CHAN *et al.*, 1978). Total tracheobronchial deposition during inspiration for inhaled particles of various particle diameters and charge levels are also computed. Upper particle charge limits for contact charging (HARPER, 1951) and atomization charging (SMOLUCHOWSKI, 1912) are used in some of the calculations. These limits are imposed to represent the 'worst case' estimates that might be encountered in an occupational environment or in respiratory treatment involving freshly generated aerosols.

THEORY

In a recent paper, DIU and YU (1980) presented a deposition theory for charged aerosols passing through a tube bend by considering the combined effect of inertial and electrostatic image forces. Deposition efficiencies were obtained numerically by calculating limiting particle trajectories. If the deposition efficiency is very small, an analytical expression can be found by superimposing the individual efficiencies due to separate mechanisms, i.e.

$$\eta = \eta_1 + \eta_2 \qquad \text{for } \eta \ll 1 \tag{1}$$

where η is the combined efficiency and η_1 and η_2 are, respectively, the efficiency by particle inertia and electrostatic image force.

The deposition efficiency of particles in a tube bend due to particle inertia only has been studied by a number of authors. YEH (1974), CHENG and WANG (1975) and DIU and YU (1980) assumed idealized flows while CRANE and EVANS (1977) included the more realistic secondary flows in their calculations. Although particle trajectories depend strongly upon the presence of secondary flows, the deposition efficiency was found to be affected only to a minor extent. Thus, it seems reasonable to assume an idealized flow field for the determination of efficiency. Using a rotational flow field, DIU and YU (1980) obtained the following expression:

$$\eta_1 = 1 - \frac{1+e^{-2I}}{\pi}[\sin^{-1} z + z(1-z^2)^{\frac{1}{2}}] + \frac{z}{\pi S}\left(1-e^{-2I}\right)\left(1+S^2-\frac{z^2}{3}\right) \tag{2}$$

where

$$z = \left[1 - S^2\left(1 - \frac{2}{1+e^I}\right)^2\right]^{\frac{1}{2}} \tag{3}$$

and

$$I = \theta(St)/S \tag{4}$$

where $St = \rho d_p^2 u/(18\mu a)$ is the Stokes number (ρ and d_p being particle mass density and diameter respectively, μ the fluid viscosity, a the pipe radius and u the axial fluid velocity), θ is the bend angle in radians, and S is the bend-to-pipe radius ratio. Since $S > 1$ always, equation (3) can be simplified to yield $z = 1$ if $\theta(St) \ll 1$. Thus, from equation (2), we have

$$\eta_1 = \frac{\theta}{S}\left[\frac{2}{\pi S}\left(\frac{2}{3} + S^2\right) + 1\right] St. \tag{5}$$

For a 90° bend with large bend-to-pipe ratio, $S \to \infty$ and $\theta = \pi/2$, equation (5) reduces to

$$\eta_1 = St. \tag{6}$$

The deposition efficiency for charged aerosols in a conducting tube due to electrostatic image forces alone was derived by YU (1977) in the following parametric form

$$\eta_2 = 1 - r^2 \tag{7}$$

and

$$E = \frac{1}{r} + 2 \ln r - r \tag{8}$$

where

$$E = \frac{n^2 \theta S e^2}{48\pi^2 \varepsilon \mu a^2 d_p u} = n^2 (E)_{n=1} \tag{9}$$

in which ε is the permittivity, e the electronic charge and n the number of unit charges per particle.

For small values of E ($r \to 1$; $\eta_2 \to 0$), PICH (1978) obtained a simplified expression for η_2 in the form of

$$\eta_2 = 2.88 E^{\frac{1}{3}}. \tag{10}$$

Adding equations (5) and (10), we obtain

$$\eta = \frac{\theta}{S}\left[\frac{2}{\pi S}\left(\frac{2}{3} + S^2\right) + 1\right] St + 2.88 E^{\frac{1}{3}}. \tag{11}$$

Equation (11) is an analytical expression for particle deposition efficiency due to the combined mechanism of inertial and electrostatic image forces. It provides a good approximation as long as $\eta \ll 1$.

To examine further the effect of electrostatic image forces on deposition, we may calculate the number of unit charges per particle, n^*, from equation (11) such that deposition by electrostatic image forces equals that by inertial forces. The result for n^* is

$$n^* = 0.205\left(\frac{\theta}{S}\right)^{\frac{3}{2}}\left[\frac{2}{\pi S}\left(\frac{2}{3} + S^2\right) + 1\right]^{\frac{3}{2}} (St)^{\frac{3}{2}} (E)_{n=1}^{-\frac{1}{2}}. \tag{12}$$

Thus, for $n \gg n^*$, deposition is dominated by electrostatic image forces.

It is also interesting to note from equation (11) that a deposition minimum exists at a particular particle size d_p^* since $St \sim d_p^2$ and $E \sim d_p^{-1}$. The value of d_p^* is found as

$$d_p^* = 1.05\left(\frac{n^2e^2\mu^2aS^4}{\rho^3\varepsilon u^4\theta^2}\right)^{\frac{1}{7}}\left[\frac{2}{\pi S}\left(\frac{2}{3}+S^2\right)+1\right]^{-3/7}. \tag{13}$$

When $d_p < d_p^*$, the electrostatic image force would be the dominant deposition mechanism. The deposition minimum observed here is analogous to the one resulting from the deposition due to the combined mechanism of sedimentation and diffusion.

The tracheobronchial tree of the human lung consists of 16 generations of bifurcating airways according to WEIBEL's model (1963). In order to apply equation (11) to these airways, we assume each airway to be a bend. For the ith generation airways, the bend angle θ_i is

$$\theta_i = l_i/(8a_i) \tag{14}$$

where l_i and a_i are respectively the length and radius of the ith generation airways. $8a_i$ is the radius of the bend so that $S_i = 8$ for all i. Using these results, we may obtain from equation (11) the following expression for η_i:

$$\eta_i = 0.768\theta_i(St)_i + 2.88E_i^{\frac{1}{3}} \tag{15}$$

where

$$(St)_i = \frac{\rho d_p^2 u_i}{18\mu a_i} \tag{16}$$

and

$$E_i = \frac{n^2\theta_i e^2}{6\pi^2\varepsilon\mu a_i^2 u_i d_p} \tag{17}$$

The total deposition efficiency in the tracheobronchial tree including the trachea during inspiration can be written as

$$\eta_{TB} = \eta_0 + \sum_{i=1}^{16}\prod_{i=1}^{16}(1-\eta_{i-1})\eta_i \tag{18}$$

where η_0 is the deposition efficiency in the trachea.

COMPARISON WITH EXPERIMENT

The experimental data used to validate the deposition theory for charged particles are quoted from the studies of CHAN *et al.* (1978) and CHAN and LIPPMANN (1980). In these studies, charged and uncharged particles were used to determine particle deposition efficiencies in the human bronchial airways. The experiments involved the 'inhalation' of monodisperse radioactive tagged iron oxide aerosols of known size through a hollow lung cast of a human tracheobronchial tree with an upstream larynx. Particles depositing in the individual airway branch were determined by γ-counting. Particles penetrating the hollow cast were also collected by a fallout collector and an absolute filter canister. Deposition efficiency for each airway branch and the mean deposition efficiencies for each airway generation were calculated by assuming the fraction of aerosols entering an airway branch to be proportional to the fraction of total bronchial airflow. Normally, a 20 mCi ^{85}Kr source was used to neutralize the aerosols generated from a spinning disc aerosol generator in experiments with particles at the RMS Boltzmann equilibrium charge levels. Removal of the ^{85}Kr neutralizer provided the negatively charged aerosols from the same generator at charge levels which were determined in a Whitby aerosol analyser (Thermosystems Inc. model 3000) by bypassing the ionizer and reversing the normal polarity of the high voltage collection rod.

Figure 1 illustrates a comparison between the calculated deposition and experimental data for charged aerosols in the trachea during inspiration. The charged aerosol used in the experiment was between 360 and 1100 negative unit charges per particle, and the particle diameters ranged between 2 and 7 μm. As an approximation, the calculated deposition was made for 4 μm aerosols with 400 unit charges per particle. The comparison of deposition data for both charged and uncharged aerosols are reasonable, since the trachea with an upstream larynx was modelled as a bend with a bend angle of 1.66 according to equation (14).

For neutralized aerosols, equation (15) can be simplified to give $\eta_i = 0.785\theta_i(St)_i$ for estimating particle deposition efficiency in the human bronchial airway. Figure 2 shows the comparison of this deposition equation designated as the DIU and YU model and the deposition equation proposed by YEH (1974) with the data of CHAN and LIPPMANN (1980) obtained from the first six airway generations of a lung cast. The calculated deposition is for an average bend angle of 0.837 radians. It is seen that the agreement between the data and the present theory is reasonable. Since some deposition due to sedimentation has not been included, the theoretical deposition curves lie within the lower limit of the 95% confidence band of the empirical deposition curve. Other computed depositions by CHENG and WANG (1975) and by CRANE and EVANS (1977) apply to 90° bends only and therefore are omitted from this comparison.

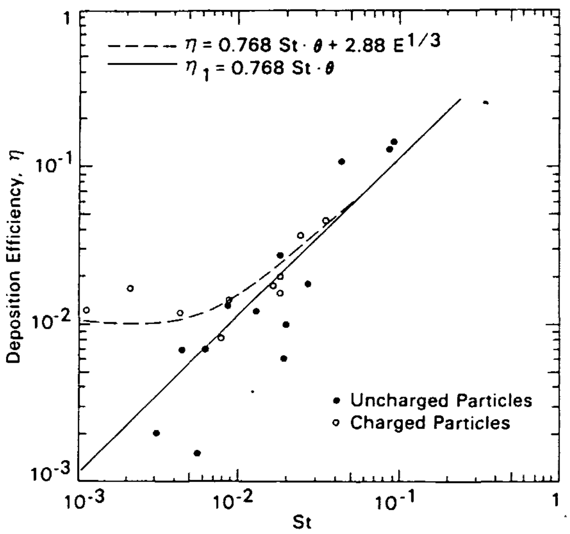

FIG. 1. Comparison of experimental data for charged particle deposition in trachea (CHAN *et al.*, 1978) to the predicted values for 4 μm particles with 400 elementary charges/particle.

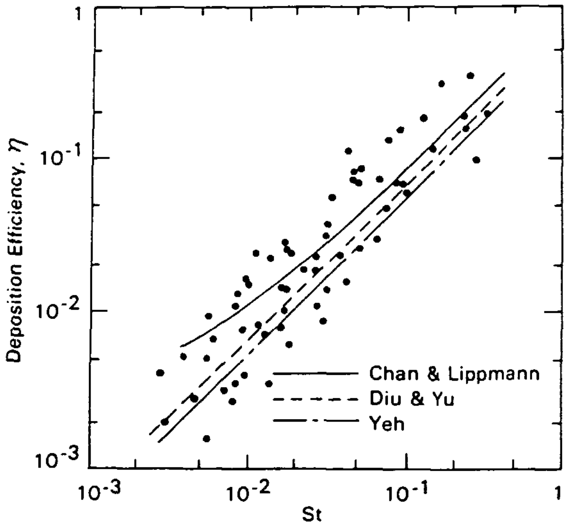

FIG. 2. Comparison of deposition efficiencies for neutralized particles in the first six airway generations reported by CHAN and LIPPMANN (1980). The impaction deposition equations proposed by YEH (1974) and equation (15) shown here as the DIU and YU (1980) model are included for an average bend angle 0.837 radians.

PREDICTION OF CHARGE EFFECT ON DEPOSITION

Using equation (15) and Weibel's airway morphometry model, deposition efficiencies during inspiration in each airway generation were computed for various particle sizes and charge levels at inspiratory flowrates 15 and 30 l. min^{-1}. The results are shown in Figs. 3 and 4. For 2 μm particles, significant increases with only 50 unit charges/particle are seen for all airway generations with dramatic increases beyond the fourth airway generation. Similar deposition patterns are observed for larger particle sizes. The total tracheobronchial depositions during inspiration for various particle sizes and charge levels at typical inspiratory flowrates are shown in Fig. 5. The charge effect on deposition increases with decreasing flowrate and smaller particle size. Again, the deposition of particles due to sedimentation is not considered in our calculations, since inertial impaction is the major deposition mechanism for the particle size and flowrates of interest.

Finally, we have calculated the total tracheobronchial deposition during inspiration for different particle sizes and flowrates using the upper particle charge limits for contact charging and atomization charging (see Fig. 6). These represent the 'worst case' estimates for depositions that may be encountered using freshly generated aerosols. The charge values at these upper charge limits were based upon the theories of HARPER (1951) and SMOLUCHOWSKI (1912). It is seen that particles at the upper charge limit for contact charging can lead to a deposition of at least 90% in the human tracheobronchial tree. For contact charging, particles with over 1000 unit charges per particle are not uncommon (JOHN *et al.*, 1980) and could result in significant increases in deposition in the lungs.

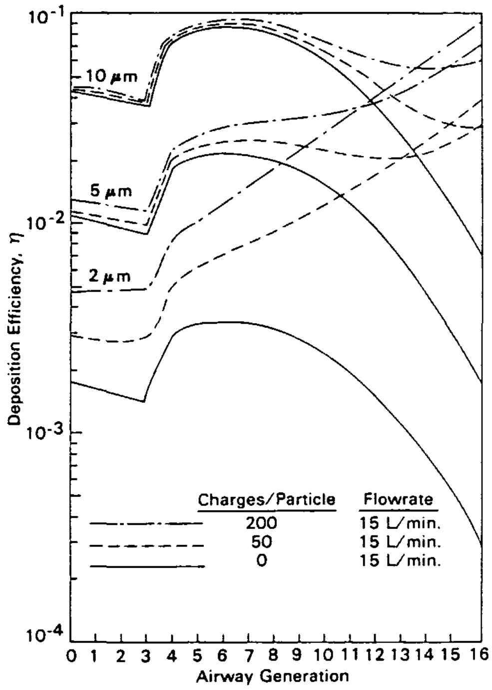

FIG. 3. Calculated deposition efficiency for charged particles at different airway generations for 2, 5 and 10 μm particles with different charge levels at steady inspiratory flowrate of 15 l. min^{-1}.

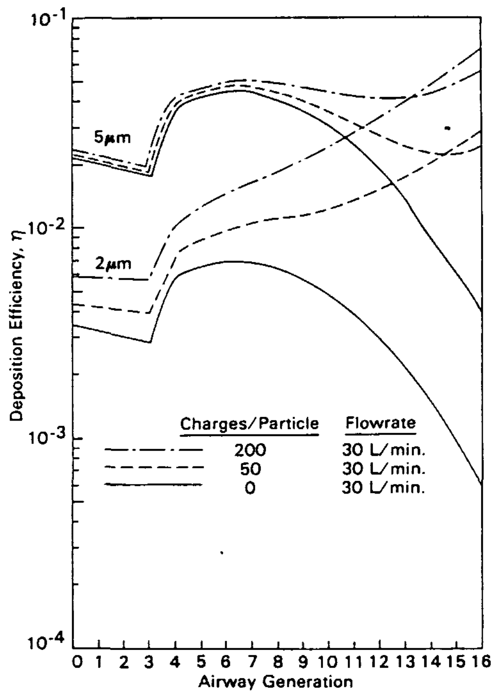

FIG. 4. Calculated deposition efficiency for charged particles at different airway generations for 2 and 5 μm particles with different charge levels at steady inspiratory flowrate of 30 l. min^{-1}.

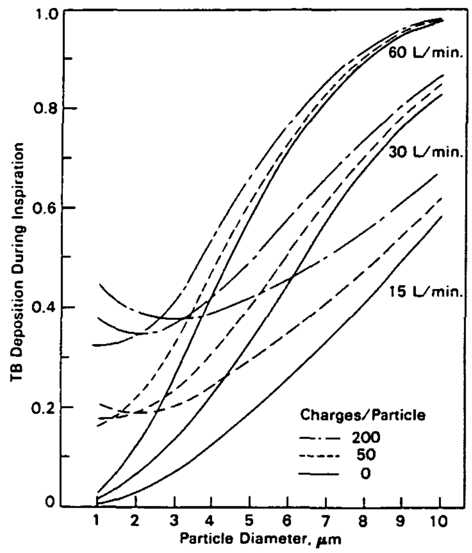

FIG. 5. Calculated total tracheobronchial deposition during inspiration for charged particles of 1–10 μm dia. at different charge levels and inspiratory flowrates.

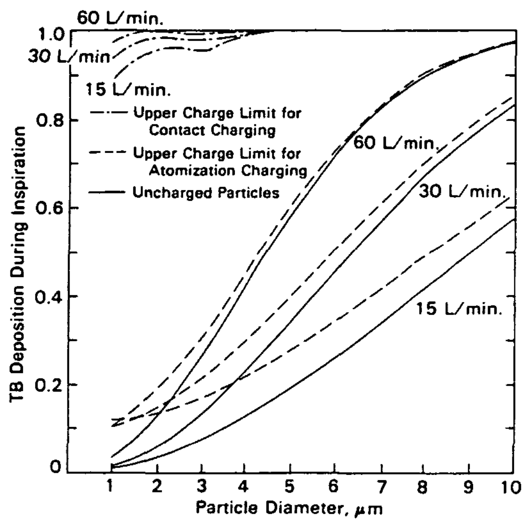

FIG. 6. Calculated total tracheobronchial deposition during inspiration for neutralized particles and charged particles at the contact charging and atomization charging limits.

SUMMARY AND CONCLUSIONS

Charged particles can lead to increased deposition in the lung. The deposition theory described in this paper has been shown to be consistent with the experimental findings of charged particle deposition in the human respiratory tract and can therefore be used as a predictive model for tracheobronchial (TB) deposition. Theoretical estimates of TB deposition values for charged particles in the 1–10 μm size range show significant enhancement in deposition. For example, inhaled particles having a mass median aerodynamic diameter of 2 μm and 200 elementary charges/particle will result in TB deposition of 39% compared with 3% for uncharged particles of the same size during inspiration.

We believe these findings can be interpreted in several ways. In the first place, charged particles in the workplace should be identified since they would represent an additional inhalation hazard. Thus, in assessing airborne health hazards associated with particles, the electrostatic charges on aerosols freshly generated by mechanical, electrical and thermal forces should be measured whenever possible. Besides, charged particles in the workplace should be recognized in the design of air cleaning equipment. Potential artifacts in inhalable and respirable mass sampling of charged particles in environmental health and industrial hygiene should also be addressed. This would be particularly important if non-conductive surfaces are used in the sampling train. Finally, the theory for charged particle deposition in the bronchial airways can be applied in aerosol therapy. Higher doses to the bronchial epithelium can be achieved by controlling the key variables in the dimensionless electrostatic deposition parameter, E. By optimizing the respiratory rate, tidal volume, particle size and particle charge, the unnecessarily high laryngeal deposition (Chan *et al.*, 1980) can be avoided and the full benefits of the therapeutic aerosols utilized effectively.

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DISCUSSION

J. H. VINCENT: My group has been concerned with the causes and effects of the static electrification of airborne asbestos fibres. Such dusts are highly polydisperse and the particles very irregular in shape. It seems inappropriate to describe the electrification of such an aerosol in terms of charge per particle. How would the authors suggest that it be characterized? In terms of surface charge per unit area of particle (Cm^{-2})?

Dr CHAN: One of the limitations of this model is that it is derived for spherical particles and may not apply to charged fibrous aerosols. The fibre cannot be modelled as a point charge and the electrostatic image forces can be very different. These forces can be analysed if the charge distribution on the fibre is known. In addition, the intertial and interception deposition mechanisms associated with the fibre should also be considered. Perhaps Professor Yu would care to comment?

Professor YU: A fibrous aerosol has a finite length. Therefore, the electrostatic charge on the fibre should be characterized by the charge distribution per unit length. In general, a charged fibre will be subjected to a net electrostatic force and a torque due to its interaction with the wall. To determine these forces, one can consider the fibre to be made up of small segments each of which can be treated as a point charge. The net force on the fibre is then the summation of the forces of all the segments. In some cases, the fibre may have no net charge, but a net force would still be present owing to its charge distribution.

P. V. PELNAR: Dr Gibbs and his colleagues at McGill University have studied the effect of electrical charge on the settling velocity of a chrysotile asbestos cloud. Laboratory experiments showed evidence of increased sedimentation, but field tests have been less successful. In a different context, electrically charged aerosols were investigated as a means of prevention of pneumoconiosis in German coal miners in the 1950s. The workers were exposed in an inhalation chamber before and after their working shift. Perhaps someone in the audience may remember the rationale of the method and how it relates to Dr Chan's presentation.

S. DEVIR: In the study you have described, particles in the size-range 2–7 μm carried from 360–1100 units of negative charge. Are charges of such magnitude found in reality on this size of particle either in ambient air or in occupationally produced dusts?

Dr CHAN: For atmospheric aerosols, the effect of electrostatic charge on particle deposition is relatively unimportant, since charge is lost during a long residence time in the atmosphere. However, charge effects associated with freshly generated aerosols in the workplace must not be ignored, since it may take from a few minutes to a few hours for the charge to decay to Boltzmann equilibrium levels. The results of studies performed years ago before the existence of modern refined instrumentation should not be taken as evidence that particles with significant charges do not exist in the occupational environment.

S. DEVIR: Accepting that highly charged particles are formed in the high-shear forces involved in grinding, blasting etc., I would like to know the magnitude of the charge and how long it would persist in the presence of mechanisms and processes (coagulation, precipitation on surfaces, ion-pair diffusion charging) all leading to rapid charge diminution.

Dr CHAN: The decay of laboratory-generated charged aerosols has been studied. However, very limited data on charged particles in the workplace are available. This is precisely the information we need.

P. A. VALBERG: An aerosol labelled with ^{99m}Tc is highly ionizing owing to the low-energy β particles emitted by decay of this isotope. As a consequence of its short half-life, aerosols of the isotope are often of high specific activity. To what extent can the ion-pairs from this source contribute to the dissipation of electrical charges on the aerosol particles?

Dr CHAN: ^{99m}Tc does not emit any β particles. However, about 10% of its radioactivity is in the form of low energy conversion electrons which do not lead to ion pair production. In contrast, ^{198}Au labelled aerosols, which do emit β particles, have been shown to possess some self-charging characteristics due to the loss of valence electrons (YEH *et al.*, *J. Aerosol Sci.* 1976, 7, 245–253). In general, isotopes of short half-lives do not necessarily imply high specific activity. The experimental data in Figs 1 and 2 were quoted from studies using ^{99m}Tc tagged particles having a specific activity of less than 10 dpm/particle. A 20 mCi ^{85}Kr source was used to neutralize the charge aerosols in some of those experiments.