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## DEFENCE RESEARCH ESTABLISHMENT SUFFIELD <br> RALSTON ALBERTA

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AN INVESTIGATION OF PARTICULATE IMPACTION ON SPHERICAL AND CYLINDRICAL TARGETS (U)
by

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ABSTRACT


This project was a theoretical investigation of particulate impaction on spheres and cylinders. The motion model developed was implemented on a computer and yielded results focused on two main goals: first, the net effect of gravity on particulate impaction was determined; and second, a man simulation was conducted. This simulation calculated to a first approximation the amount of chemical that would impact on a man subjected to a chemical attack.

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## LIST OF SMMBOLS

| b | - constant |
| :---: | :---: |
| $C_{\text {D }}$ | - drag coefficient |
| F | - Froude number |
| $F_{\text {d }}$ | - drag force |
| $\mathrm{F}_{\mathrm{g}}$ | - gravity force |
| g | - acceleration of gravity |
| $\mathrm{g}^{\prime}$ | - non-dimensional gravity |
| G | - ground fraction |
| K | - inertia parameter |
| L | - target radius |
| m | - particle mass |
| $r$ | - distance from the origin |
| ${ }^{\prime}$ | - particle radius |
| Re | - local Reynold's number |
| $\mathrm{Re}_{0}$ | - free stream Reynold's number (based on particle size) |
| t | - time |
| u | - local fluid velocity |
| $u^{\prime}$ | - non-dimensionalized local fluid velocity |
| U | - free stream velocity (synonymous with windspeed) |
| $v$ | - particle velocity |
| $v^{\prime}$ | - non-dimensionalized particle velocity |
| $\mathrm{v}_{\mathrm{z}}$ | - terminal velocity |
| $B^{2}$ | - rotation angle of frame 1 re frame 0 |
| $\gamma$ | - rotation angle of frame 2 re frame 1 |
| $\theta$ | - position angle in frame 0 |
| $\rho_{a}$ | - air density |
| $\rho_{p}$ | - particle density |
| $\mu$ | - air viscosity |

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## INTRODUCTION

1. In assessing the hazard to troops from attacks with chemical agents in aerosol form, it is important to be able to predict the motion of the chemical agents as they disperse through the atmosphere and impact on various target objects (Figure 1). This project was conducted to investigate the impaction aspect of the overall motion problem specifically to provide an answer to the question, "How much chemical will hit a target.
2. Some theoretical studies have been performed in this area of aerosol impaction ${ }^{1}$. This project sought to upgrade the theoretical models used through the inclusion of the gravity force into the problem; in fact, the secondary purpose of the project was to quantify the error incurred when gravitational effects are ignored. The primary purpose of the project was to develop a model which would calculate the amount of chemical that a man received in relation to how much the ground received.
3. The complex nature of this fluid mechanical problem required a number of simplifying approximations in order to be tractable. Consequently, the results obtained are first approximations only, calculated on the basis of a theoretical model which required computer programs for implementation. The project results are seen as a foundation upon which to conduct experimental and/or improved theoretical research.
4. The project evolved significantly durings its lifetime. The initial phases were very much a learning phase during which the model was continuously tested and changed. Spherical targets were used for these initial tests, tests which also provided much data on the effect of gravity on the problem. This initial phase ended with the study of cylindrical targets during which the last gravity effect calculations were performed. The final phase of the project dealt with the man-target simulation.

BACKGROUND THEORY

## Fundamentals of Particulate Motion

5. The derivation of the aerosol particle motion equation follows directly from Newton's Second Law ${ }^{2}$. There are two forces present, namely gravity and aerodynamic drag:

$$
\begin{gather*}
F_{d}=c_{0}\left(\pi r_{p}^{2}\right)\left(\frac{1}{2} p_{a}|\underline{U}-\underline{y}|{ }^{2}\right)  \tag{1}\\
\underline{F}_{g}=m_{g} \tag{2}
\end{gather*}
$$

The particles are assumed to be spherical because of their small size ( $<2000 \mathrm{jm}$ radius). The resulting equation of motion is therefore:

$$
\begin{equation*}
\underline{m} \underline{v}=C_{D}\left(\pi r_{p}{ }^{2}\right)\left(\frac{1}{2} \rho_{a}|\underline{v}-\underline{v}|^{2}\right)+m \underline{g} \tag{3}
\end{equation*}
$$

Noting that;

$$
\begin{gather*}
m=\frac{4}{3} \pi r_{p}{ }^{3} \rho_{p}  \tag{4}\\
R e=\frac{2 r_{p} \rho_{a}}{\mu}|\underline{U}-\underline{v}| \tag{5}
\end{gather*}
$$

we can re-arrange equation [3] to produce:

$$
\begin{equation*}
\dot{\dot{v}}=\frac{3 \mu C_{D} \operatorname{Re}(\underline{U}-\underline{v})}{16 r_{p}^{2} \rho_{p}}+\underline{g} \tag{6}
\end{equation*}
$$

6. Equation [6] can be non-dimensionalized by using the free stream velocity $U$ and the characteristic target length $L$ :

$$
\begin{align*}
\underline{v}^{\prime} & =U^{-1} \underline{v}  \tag{7}\\
\dot{\underline{v}}^{\prime} & =L U^{-2} \underline{v}  \tag{8}\\
\underline{u}^{\prime} & =U^{-1} \underline{u}  \tag{9}\\
\mathrm{t}^{\prime} & =\mathrm{tUL}-1  \tag{10}\\
\underline{\underline{q}}^{\prime} & =L U^{-2} \underline{g}
\end{align*}
$$

If we define:

$$
\begin{gather*}
K=\frac{2 \rho_{p} r_{p}^{2} U}{9 \mu L}  \tag{12}\\
F=\frac{U^{2}}{L g} \tag{13}
\end{gather*}
$$

then equation [6] can be written in the following non-dimensional form:

$$
\begin{equation*}
\dot{\underline{v}}^{\prime}=\frac{C_{D} \operatorname{Re}\left(\underline{u}^{\prime}-\underline{v}^{\prime}\right)}{24 K}+\frac{1}{F} \tag{14}
\end{equation*}
$$

7. Clearly, the problem can be solved by either equation [6] or equation [14]. Traditionally, these problems have been solved in nondimensional form resulting in graphs of collection efficiency vs. inertia parameter for various Reynold's numbers (Collection efficiency is explained in the next section). In this problem, however, the inclusion of gravity adds another parameter, namely the Froude number. The graphical presentation of non-dimensional results now becomes quite complicated, and the physical interpretation of such results becomes obscure. It was felt that superior physical insight and applicability would result from analysis of the restricted case of motion in air under representative experimental situations. Equation [6] was therefore used in the model.
8. In reference frame 1 (Figure 2), equation [6] can be resolved into the following scalar equations:

$$
\begin{gather*}
\dot{v}_{x}=b C_{D} \operatorname{Re}\left(u_{x}-v_{x}\right)  \tag{15}\\
\dot{v}_{y}=b C_{D} \operatorname{Re}\left(u_{y}-v_{y}\right)  \tag{16}\\
\dot{v}_{z}=b C_{D} \operatorname{Re}\left(U_{z}-v_{z}\right)-g \tag{17}
\end{gather*}
$$

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$$
\begin{equation*}
\text { where } b=\frac{3 \mu}{16 r_{p}{ }^{2} \rho_{p}} \tag{18}
\end{equation*}
$$

9. The drag coefficient for spheres is defined in terms of the Reynold's number by the following equations ${ }^{3}$ :

For Res4,

$$
\begin{gather*}
\operatorname{Re}=\frac{C_{D} R^{2}}{24}-2.3363 \times 10^{-4}\left(C_{D} \operatorname{Re}^{2}\right)+2.0154 \times 10^{-6}\left(C_{D} \operatorname{Re}^{2}\right)^{3} \\
-6.9105 \times 10^{-9}\left(C_{D} \operatorname{Re}^{2}\right)^{4} \tag{19}
\end{gather*}
$$

For $3<\operatorname{Re} \leqslant 10^{4}, \log _{10} \operatorname{Re}=1.29536+9.86 \times 10^{-1}\left(\log _{10} C_{D} \operatorname{Re}^{2}\right)-4.6677$

$$
\begin{equation*}
\times 10^{-2}\left(\log _{10} C_{D} \operatorname{Re}^{2}\right)+1.1235 \times 10^{-3}\left(\log _{10} C_{D} \operatorname{Re}^{2}\right)^{3} \tag{20}
\end{equation*}
$$

10. Two assumptions were made regarding the initial condition of the aerosol particle. First, it was assumed that the particle was moving horizontally at the free stream velocity and that a starting position upstream would experience negligible flow perturbations caused by the target. Second, the particle was defined to be falling at its terminal velocity, because small aerosol particles quickly attain that speed. Consequently, the particle initially possessed a velocity given by its terminal velocity ( $v_{Z_{0}}$ ) and the free stream velocity, with a direction defined by the angle $\gamma$ to the $x$-axis:

$$
\begin{equation*}
r=\tan ^{-1}\left(\frac{v_{Z_{0}}}{u}\right) \tag{21}
\end{equation*}
$$

The terminal velocity was calculated by setting $\dot{v}=0$ and $U_{z}=0$ in equation [17], and solving for $\mathrm{v}_{\mathrm{Z}_{0}}$. The result was:

$$
\begin{equation*}
v_{z_{0}}=\left(\frac{8 r_{p} \rho_{p} g}{3 \rho_{a} c_{0}}\right)^{1 / 2} \tag{22}
\end{equation*}
$$

11. Therefore, simultaneous solution of [5], [22] and one of [19] or [20] yielded the terminal velocity.
12. The flow equations will be derived in paragraphs 15-24 for the various target geometries. All such equations were inviscid fluid equations. These were deemed applicable to the problem because real fluid flow is virtually ideal on the leading face of an object, which was the only face of interest in this particle impaction problem. It was also assumed that the chemical particles themselves did not perturb the fluid flow.

## Collection Efficiency

13. The concept of a collection efficiency is the primary means of quantifying the amount of chemical which impacts on a target (Figure 3). The collection efficiency is a number ranging from zero to one, and is defined by equation [23]:

$$
\begin{align*}
& \text { Collection }  \tag{23}\\
& \text { Efficiency }
\end{align*}=\frac{\text { Cross-sectional area of the envelope }}{\text { Cross-sectional area of the target }}
$$

The envelope is that region on the starting plane in which initial particle placement results in a trajectory which hits the target. Clearly, the absence of the fluid medium would result in a collection efficiency of one, because the particles would travel in straight lines, and massless particles would have a collection efficiency of zero, because the particles would follow fluid streamlines around the target without impaction.
14. The task at hand is to calculate the collection efficiency for any given test situation. This is done using a half-interval method to
find the boundaries of the envelope. A series of particles are considered, each of which begins on the starting plane with the same initial velocity (Figure 4). Two initial particle positions are required to start the procedure: an 'inside' one that results in target impaction (P2) and an 'outside' one that results in target miss (P1). A third position (P3) is calculated such that it lies halfway between the first two points; this particle is then tracked to the target. If it misses, the ( $P 3$ ) becomes the new 'outside' position and a new starting position is chosen at (P4). If it hits, then (P3) becomes the new 'inside' position, and a new starting position is chosen at (P5). The distance between the inside and outside positions is successively reduced by half, and it asymptotes to the envelope boundary. In this manner, the envelope boundary is defined, allowing its area to be calculated for use in equation [23]. Note that the boundary is generally a two-dimensional curve on the starting plane which requires a large number of boundary points before an accurate estimation of its shape and size can be made.

## Target Geometry For Spheres

15. The fluid velocity field around a sphere is given in terms of polar coordinates ${ }^{4}$ :

$$
\begin{gather*}
u_{r}=u \cos \theta\left[1-\left(\frac{L}{r}\right)^{3}\right]  \tag{24}\\
U_{\theta}=-U \sin \theta\left[1+1 / 2\left(\frac{L}{r}\right)^{3}\right] \tag{25}
\end{gather*}
$$

These equations are valid for any plane passing through the origin of the sphere and parallel to the $x$-axis of Frame 1 . Let us designate such a plane as Frame 0 with $x, n, \psi$ axes; Frame 1 is related to Frame 0 by the
rotation angle $\beta$ about the $x$-axis (Figure 5). In terms of Frame 0 cartesian coordinates, equations [24] and [25] become:

$$
\begin{gather*}
U_{x}=U \cos ^{2} \theta\left[1-\left(\frac{L}{r}\right)^{3}\right]+U \sin ^{2} \theta\left[1+1 / 2\left(\frac{L}{r}\right)^{3}\right]  \tag{26}\\
U_{n}=\frac{-3 U}{2}\left(\frac{L}{r}\right)^{3} \cos \theta \sin \theta  \tag{27}\\
U_{\psi}=0 \tag{28}
\end{gather*}
$$

Equation [28] is obtained by inspection. These three equations can be used to specify the velocity field at any point in space in Frame 1 via a suitable rotation of Frame 0 to align it with the position of interest. In matrix notation, the required velocity components are generated as follows:

$$
\left|\begin{array}{l}
u_{x}^{x}  \tag{29}\\
u_{x}^{y} \\
u_{z}^{y}
\end{array}\right|=\left|\begin{array}{llll}
1 & 0 & 0 & \\
0 & \cos \beta & -\sin \beta \\
0 & \sin \beta & \cos \beta
\end{array}\right|\left|\begin{array}{l}
u_{x} \\
u_{n}^{x} \\
u_{\psi}^{n}
\end{array}\right|
$$

Upon evaluation we get:

$$
\begin{gather*}
u_{x}=U \cos ^{2} \theta\left[1-\left(\frac{L}{r}\right)^{3}\right]+U \sin ^{2} \theta\left[1+\frac{L}{2}\left(\frac{L}{r}\right)^{3}\right]  \tag{30}\\
U_{y}=\frac{-3 U}{2}\left(\frac{L}{r}\right)^{3} \cos \theta \sin \theta \cos \beta \tag{31}
\end{gather*}
$$

$$
\begin{equation*}
U_{z}=\frac{-3 U}{2}\left(\frac{L}{r}\right)^{3} \cos \theta \sin \theta \sin \beta \tag{32}
\end{equation*}
$$

By definition, we obtain these auxiliary equations:

$$
\begin{gather*}
r=\left(x^{2}+y^{2}+z^{2}\right)^{1 / 2}  \tag{33}\\
\beta=\tan ^{-1}\left(\frac{z}{y}\right)  \tag{34}\\
\theta=\tan -1\left(\frac{y \cos \beta+z \sin \beta}{x}\right) \tag{35}
\end{gather*}
$$

16. Due to the wide range of initial particle velocities angles $\gamma$, it was decided that calculations would be simplified if done in a reference frame aligned at $\gamma$ to Frame 1. Consequently, Frame 2 was defined for each particle test such that the starting plane was perpendicular to the initial particle direction (Figure 6). All transformed into this frame by means of the following rotation matrix:

$$
C_{21}=\left|\begin{array}{ccc}
\cos \gamma & 0 & -\sin \gamma  \tag{36}\\
0 & 1 & 0 \\
\sin \gamma & 0 & \cos \gamma
\end{array}\right|
$$

17. The collection envelope for this sphere geometry was necessarily two-dimensional. Essentially, the half-interval method was used to calculate $z^{\prime}$ boundary values for a series of $y$ coordinates; the $y^{\prime}$ boundaries themselves were also calculated by means of the half-interval method. The set of boundary points ( $y^{\prime}, z^{\prime}$ ) were then connected by cubic splines and then the enclosed envelope area calculated.

## Target Geometry For Horizontal Cylinders

18. In reference Frame 1 (previously defined for spherical geometry) the fluid velocity field is given by the following equations ${ }^{5}$ :

$$
\begin{gather*}
u_{x}=u\left[1-\frac{L^{2}\left(x^{2}-z^{2}\right)}{r^{4}}\right]  \tag{37}\\
u_{y}=0  \tag{38}\\
u_{z}=\frac{-2 U x z L^{2}}{r^{4}}  \tag{39}\\
\text { where } \quad r=\left(x^{2}+z^{2}\right)^{1 / 2} \tag{40}
\end{gather*}
$$

It is readily deduced from these equations that the particle motion will be confined to the $x-z$ plane provided that the initial particle velocity in the $y$ direction is zero. That velocity was set to zero in accordance with the previously stated initial conditions; therefore, this problem was twodimensional.
19. As with the spherical geometry, Frame 2 was defined and used as the main frame in which all motion and envelope calculations were made. Due to the planar motion, the envelope was only one-dimensional, requiring only an 'upper' and a 'lower' boundary to be calculated (Figure 7). This case is consequently very much simpler than that of the spheres.

## Target Geometry For Vertical Cylinders

20. The theory here is essentially the same as in the horizontal
cylinder case. The only change involves the flow field which was changed to the $x-y$ plane from the $x-z$ plane in Frame 1 (Figure 8). The flow equations are:

$$
\begin{gather*}
U_{x}=U\left[1-\frac{L^{2}\left(x^{2}-y^{2}\right)}{r^{4}}\right] \\
U_{y}=\frac{-2 U x y L^{2}}{r^{4}}  \tag{41}\\
U_{z}=0  \tag{42}\\
\text { where } r=\left(x^{2}+y^{2}\right)^{1 / 2} \tag{43}
\end{gather*}
$$

21. The combination of an infinite vertical cylinder with the required five target radil starting position from the cylinder, removed the usefulness of Reference Frame 2. Therefore, Frame 1 was chosen as the frame for motion and envelope calculations. Due to the motion symmetry about the $x$-axis and the z-axis, only a $y$-boundary needed to be calculated for the envelope; clearly, any z-coordinate starting position will result in a similar trajectory that differs only by a fixed z-direction displacement.

## Target Geometry For Man Simulation

22. This simulation was rather crude, and it comprised many simplifying approximations (Figure 9). First, a vertical cylinder of approximate man dimensions was used since the determination of the flow field around a man was much too complicated a proposition for this project. Second, the flow field of an infinitely long cylinder was used because a calculation of end flow conditions around a finite cylinder was deemed too complicated for a first approximation model like this one. Third, the particles which impacted on the top of the cylinder were ignored.
23. A major component of this model was the inclusion of a wind gradient to mimic the Earth's own boundary layer. Essentially, the horizontal windspeed is a function of height above the ground. The equation used was:

$$
\begin{equation*}
u(Z)=U_{1}\left(\frac{Z}{Z_{1}}\right)^{1 / 7} \tag{44}
\end{equation*}
$$

The base point $\left(Z_{1}, U_{1}\right)$ scales the curve; for this application, the basis used was:

$$
\begin{gather*}
Z_{1}=5.0 \mathrm{~m}  \tag{45}\\
U_{1}=1.0,1.5,2.5,5.0 \text { and } 7.5 \mathrm{~m} / \mathrm{s}
\end{gather*}
$$

Therefore, five tests were conducted at five different reference windspeeds.
24. The flow equations for vertical cylinders, equations [40] to [42] were modified for this simulation by replacing the factor $U$ with $U_{(Z)}$ as defined in equation [44]. The resulting flow equations were:

$$
\begin{gather*}
U_{x}=U_{1}\left(\frac{Z}{5}\right)^{1 / 7}\left[1-\frac{L^{2}\left(x^{2}-y^{2}\right)}{r^{4}}\right]  \tag{47}\\
U_{y}=U_{1}\left(\frac{Z}{5}\right)^{1 / 7}\left[\frac{-2 x y L^{2}}{r^{4}}\right]  \tag{48}\\
U_{z}=0 \tag{49}
\end{gather*}
$$

25. As for the vertical cylinders, Reference Frame 1 is used for all motion and envelope calculations. The presence of the wind gradient destroys the problem symmetry in the z-direction; therefore, the envelope on the starting plane was necessarily two-dimensional. Its calculation was quite similar to that of the spherical targets. Specifically, the bounds in the $z$-direction were found by the half interval method, then the $y$ bounds were calculated for eleven equally spaced $z$-coordinates over this interval. The resulting boundary points $(z, y)$ were then integrated to yield the enclosed envelope area.
26. In order to relate the chemical concentration on a man to that which falls on the ground, an extra number was introduced, termed the ground fraction (G). It was defined by equation [50]:

$$
\text { Man Concentration }=\text { Ground Concentration } \times \mathbf{G}
$$

(This man concentration is based on frontal cross-sectional area, not surface area.)
Calculation of $G$ combined the factors of collection efficiency with the relative areas of impact regarding the target and the corresponding ground; the equation was:

$$
\begin{equation*}
G=\frac{\text { Collection Efficiency }}{\tan \alpha} \tag{51}
\end{equation*}
$$

In this equation, $\alpha$ is a representative trajectory angle of all particles in the envelope; note that the trajectories are not straight lines because of the wind gradient. The angle $\alpha$ is that between the horizontal and the line connecting the top of the 'man' to the top of the envelope.

## Computer Programs

27. During the course of the project, several computer programs were written. Four collection efficiency programs were written; one for each geometrical case. Two programs were written to tabulate and plot chemical particle trajectories for the sphere and horizontal cylinder cases; these programs were used primarily for verification of the motion model. Finally, a number of utility programs were written to tabulate and graph results. All programs were written in the Honeywell FORTRAN-77 language and executed on the Honeywell CP-6 computer at DRES.
28. The collection efficiency and trajectory plotting programs shared many features, most importantly, the initial condition and motion calculations. This redundancy, coupled with space limitations, has limited the program listing in this report to just two representative programs: AEROSOL-8 which performed the man simulation (Appendix A), and AEROSOL-6, which performed the trajectory plotting for horizontal cylinders (Appendix B). The only real difference between these programs and their sister programs was in geometry; different target geometries required different envelope calculations and sometimes different reference frames, as has been illustrated in the previous section. Implementation of the background theory on the computer was quite similar for the different geometries, and will now be explained in detail for programs AEROSOL-8 and AEROSOL-6.
29. AEROSOL-8 was designed to accommodate five sets of test conditions (the '700 loop', commencing line 50). The test conditions, namely windspeed, target radius and chemical particle density, were obtained from the data file AEROINFO. The program then proceeded to calculate collection efficiencies for a range of particle sizes which were stored in the array SIZE(10). This loop (the '650 loop', commencing line 63) comprised four main sections: calculation of initial conditions (lines

68-83), calculation of the 2-direction envelope boundaries (lines 86-138), calculation of the $y$-direction envelope boundaries (lines 141-161) and calculation of resulting collection efficiency (lines 164-172). The implementation of the background theory in these sections was relatively straightforward except for the following points. First, in order to implement the half-interval method, a starting position which results in particle impact must be found; in the 2 -direction, it was searched for (the '200 loop', commencing line 95), but in the $y$-direction it was assumed that $y=0$ resulted in impact since it lay on the target centerline and would experience no sideways drag force. Secondly, preliminary calculations showed that the y-bounds increased monotonically with increasing zcoordinate, therefore the previous y-boundary value (variable YMEM, line 143) was used as the 'inside' position for the ensuing half-interval calculation. Finally, note that the problem was symmetrical about the $y$ axis, requiring that only positive $y$-boundaries be calculated for the envelope.
30. The TRAJECTORY subroutine comprised all of the motion calculations from initial conditions to a determination of particle impact or miss. Upon receipt of the initial conditions, the subroutine sets up an iterative loop (the '10 loop', commencing on line 244) to 'move' the particle towards the target. The iteration involved five main steps: calculation of local flow velocity (lines 248-252), calculation of Reynold's number and Drag Coefficient (lines 254-279), solution of the differential equations of motion over a predetermined time interval (lines 284-291), testing for impact or miss (lines 291-297) and adjustment of the differential equation step-size if the iteration is to continue (1ines 303305). Note that the step-size is governed by the choice of the variable DT, not the IMSL routine DVERK, because the positional dependence of the flow velocity requires frequent updating. DVERK could not accommodate nonconstant coefficients, and in practice performed only one step per call due
to the choice of DT which determined the end condition TEND. This also meant that the DVERK accuracy parameter TOL was of no practical importance; its assigned value of 0.01 was arbitrary.
31. The remaining two program subroutines require no detailed explanation above the internal documentation notes. Note that a partial output is included with the program listing in Appendix A.
32. AEROSOL-6 was designed to plot particle 'streamlines' near a horizontal cylindrical target. It was restricted to one size of particle, which can be arbitrarily set, and one set of test conditions. The calculation of initial conditions (lines 64-84) was identical to that of AEROSOL-8, with the exception of the ability to perform in a no gravity environment; hence, this program could recognize and plot streamlines for a hypothetical no gravity situation. The motion analysis section (the '60 loop', commencing on line 105) was the same as that of AEROSOL-8.
33. The one aspect of AEROSOL-6 that differs from AEROSOL-8 was the trajectory plotting. To fully understand the details of this plotting, one must study the CALCOMP Electromechanical Plotters User's Manual (From California Computer Products, Inc.). As far as this project was concerned, CALCOMP provided a list of subroutines which could be called upon to draw graphs; separate subroutines could draw axes, plot lines, print titles and draw other graph elements. In AEROSOL-6, the arrays XVAL(500) and ZVAL(500) were used to store the $x$ and $z$ coordinates of each successive particle location. This data was then sent to the CALCOMP System and plotted (lines 211-241). Examples of these trajectory plots as given in Figures 10 and 11, and a sample output is included in Appendix $B$ with the program listing.

## RESULTS

34. The computer generated collection efficiency results for all four geometrical cases are listed in Tables I-VIII. Figures 10 and 11 show trajectory pictures generated by AEROSOL-6. Figures 12-15 show representative and comparative graphs based on the data contained in Tables I-VIII. Although a detailed analysis of these results will be conducted in the next section, the acquisition and content of these results require some explanations. Note that all results are in MKS units unless otherwise stated.
35. Sphere runs Sl to S 10 , and horizontal cylinder results Cl to C 10 were all performed under gravity and no gravity conditions to calculate the effect of gravity on the problem. These results are listed side by side in Tables I, II, IV and V. At the bottom of each double column are two sets of numbers labelled 'maximum positive change', and 'maximum negative change'. These are simply the greatest divergence values between the two sets of data, recorded as either a positive or a negative divergence relative to the gravity values. The numbers in brackets are the particle sizes corresponding to those divergences.
36. Because spheres were the first geometrical case to be studied, a few extra runs were conducted in order to evaluate the validity and the accuracy of the motion model. The accuracy test, run S11, used half the step-size as run S2 in order to check the numerical accuracy of the method. In actuality, several accuracy checks were conducted, resulting in many step-size modifications until the final accuracy level was achieved. The similarity test, runs S 12 and S 13 , was conducted in an attempt to validate the motion model. According to the principles of fluid mechanics, tests with the same set of non-dimensional numbers must yield identical results. Here, there are three non-dimensional numbers which describe the problem:
$C_{D}, \operatorname{Re}_{0}, F$. These were kept constant for runs $S 2, S 12$, and $S 13$, but the constitutive parameters ( $U, L, F, P, g$ ) were varied to learn whether or not the results would change. A change in the results would indicate that the motion model was flawed.
37. The computer time required for solution of test runs varied considerably with the problem geometry. The one-dimensional nature of the horizontal and vertical cylinder envelopes resulted in very little computer execution time, typically ten minutes or less per test. (By way of clarification, a 'test' refers to the calculation of collection efficiencies for all ten particle sizes under a given set of windspeed, target size and particle density values. Each column in Tables I-VIII represents one test.) The two-dimensional envelopes for the sphere cases typically required one and a half hours per test. The man simulation was somewhat peculiar. Because the particles travelled almost horizontally in test Ml , it required only twenty minutes; but the more vertical trajectories of test M4 and M5 resulted in much longer trajectories (note that the horizontal distance travelled remained constant so as to minimize the cylinder flow perturbation at start) and execution times of up to six hours per test. Actually, the collection efficiencies for the 2000 pm particle were not calculated for tests M4 and M5, and the 1000 mm particle collection efficiency was not calculated for M5. The reason was that hours of execution time would have been required for each particle, a cost which was not thought to be worthwhile. The absence of these three values is indicated in Tables VII and VIII by a negative value.
38. Finally, note that the graphs plotted in Figures 12-15 were done using small plotting programs written during the project. These programs are not listed in this report.

## DISCUSSION

39. The computed similarity and accuracy test results (Table III) verified the motion model and provided an indication of its accuracy. The accuracy test clearly showed that numerical accuracy improved with increasing particle size. This was because larger particles were less affected by drag forces, and it was the drag force which exhibited nonlinear behaviour with position, making it the most difficult aspect to numerically approximate. This also accounted for the observation that all errors were positive, because the total influence of the drag force (and hence the greatest particle deflection) will only be attained in the limit as the number of steps approaches infinity. Hence, the drag force was underestimated by this model. Since the overall collection efficiency was the chief result sought, the relative error was of less importance nere; that is to say, the large relative error of the smallest particles was made insignificant by the very small collection efficiencies involved. Based on the absolute errors tabulated, the maximum error present in the calculations was on the order of +0.003 for the collection efficiency $1+$ $0.3 \%$ for the values in Tables I-VII). It should be noted that the computer model worked to four significant digits in distance values $\mathbf{( 0 . 1} \mathbf{~ m m}$ or 100 $\mu \mathrm{m}$ ). Since the targets were generally 0.1 m in radius, 0.1 mm represents an accuracy to 0.1\%.
40. The results of the similarity test were within numerical error for all three runs, provided that one qualification to the collection efficiency error value of +0.003 be accepted; specifically, that the absolute collection error was a function of the target size in addition to step-size. It seems plausible that the relative magnitude of the step size to the target size would influence numerical accuracy, since an increase in the target size would attenuate the rate of change of the drag force over distance, allowing a greater accuracy for the same step size. As proof,
note that the $S 12$ and $S 13$ results are within .003 of each other, with the S13 values uniformly lower; this suggests that its larger target radius ( $L=0.15$ ) improved numerical accuracy, since the step sizes were equal. Conversely, the small target size of test S 12 seemed to have degraded numerical accuracy; the S 12 values were up to .008 higher than the S 2 values. In summary, the results of tests S2, S12 and S13 were deemed sufficiently close as to be judged the same to within numerical error.
41. Figures 10 and 11 qualitatively demonstrate many of the aspects of this motion problem. The smaller particle (Figure 10) showed a mostly horizontal trajectory which indicated low terminal velocity. Close to the cylinder, all trajectories were substantially deflected to the extent that only one particle impacted on the cylinder. This was an indication that the collection efficiency would be low for this small ( 50 mm ) particle. Figure 11 demonstrated the aspects of large particle motion. The trajectory was much steeper due to a higher terminal velocity. There was almost no particle deflection; consequently, one would expect a high collection efficiency for this large ( $250 \mu \mathrm{~m}$ ) particle. Reference to run C 4 which had the same test conditions as in Figures 10 and 11 , yielded the expected magnitude of collection efficiencies: a low $14.11 \%$ for 50 mm , and a high $93.70 \%$ for 250 mm . The qualitative model verification by these and many other trajectory pictures supported the similarity tests and led us to conclude that the motion model was valid.
42. The collection efficiency test results for spheres and cylinders yielded many noteworthy features, most of which will be discussed in the next few pages. We will start with the effect of gravity on the motion results.
43. All of the sphere and horizontal cylinder tests (S1 - S10 and C1 -C10) produced results similar to that shown in Figure 12. The sigmoidal
shape of the curve agreed with the previous theoretical work. ${ }^{7}$ The most notable feature of the double curve plot in figure 12 was the crossing of the two curves between $100 \mu \mathrm{~m}$ and $250 \mathrm{\mu m}$ particle sizes; this was thought to be due to the following reasons. For larger particles, gravity caused the particles to fall with a terminal velocity close to or greater than the horizontal free stream velocity. Hence, the particle's inertia was significantly greater, rendering the particle much less susceptible to deflection by the diverging fluid streamlines around the target. This resulted in a collection efficiency with gravity, as evidenced by the larger particles in Figure 12.
44. The gravity-decrease effect on the smaller particles was much more difficult to explain. First, the terminal velocity was low, virtually insignificant compared to the free stream velocity; therefore, the particle's inertia was not noticeably higher. This allowed a second factor to make a discernible impact on the motion; this factor was a motion asymmetry around the target due to gravitational effects. The envelope results for test C3 (Table 9) illustrate this asymmetry. It can be seen that gravitational effects decrease the upper bound more than they increase the lower bound for particles of $50-100 \mu \mathrm{~m}$, which was the range of the gravity decrease effect in Figure 12. The explanation of this asymmetry was as follows. Near the upper boundary, the fluid streamlines are deflected upwards by the target, in effect flowing crossways to the particle motion vector, thereby increasing the local Reynold's numbers and hence the drag force, resulting in a smaller boundary. At the lower boundary, however, the fluid streamlines are deflected in the direction of the particle motion vector (that is, diagonally downwards) thereby reducing the local Reynold's number and the drag force, resulting in a larger boundary. The non-linear nature of the problem was such that the former effect was greater than the latter effect, resulting in lower collection efficiencies for particles in this motion regime when gravity was included.
45. Generally, gravitational effects altered collection efficiencies in these tests by less than $\pm 3 \%$ (Tables I, II, IV, V). The exceptions were tests involving low windspeeds, speeds of $1.5 \mathrm{~m} / \mathrm{s}$ or less. The greatest difference was found in test 55 ; there, gravity added $21.2 \%$ to the collection efficiency of 100 um particles. Note that the crossover point between the gravity and no gravity curves in this test was not present; all differences were positive. Generally, the crossover point decreased in particle size with decreased windspeed.
46. In summary, the gravity effect on collection efficiencies was negligible except in cases of low windspeed. Other facets of the sphere and cylinder studies will now be explored.
47. Figure 13 compared the collection efficiencies of the vertical cylinder, the horizontal cylinder and cylinder no gravity cases, under the same test conditions. (Note that in the absence of gravity, the vertical and horizontal cylinders were geometrically equivalent.) The crossover of the no gravity and horizontal cylinder curves occurred at 500 m ; the gravity effect was minimal here as would be expected from the high windspeed. The vertical cylinder curve was lower than either of the other curves, except for a brief particle range around $100 \mu \mathrm{~m}$. The reduced collection efficiency was easily explained: as particles approached the cylinder, they initially deccelerated, thereby increasing the trajectory angle relative to the horizontal (the terminal velocity remains almost constant) and provided more time for the diverging fluid streamlines to deflect the particle. The exception at $100 \mu \mathrm{~m}$ was probably a result of the asymmetrical particle flow around the horizontal cylinder, postulated before as the explanation for the gravity-decrease effect. The vertical cylinder possessed symmetrical flow conditions and was therefore not affected. However, the steepening trajectory effect with vertical cylinders still lowered the collection efficiency relative to the no gravity case; the reduction was just marginally less than that of the horizontal cylinders.
48. Figure 14 compared the two cylinder geometries to spheres, under slightly different test conditions than in Figure 13. Spheres clearly possessed higher collection efficiencies than cylinders for all particle sizes. This can be understood in light of the fact that cylinders perturb the flow more than spheres, in the sense that cylinders represented a greater obstacle to the flow and thus cause faster fluid motion around the periphery. This larger fluid velocity represented a greater drag force which tended to deflect the particles away from the target; hence, the collection efficiencies were lower. The relationship between the vertical and horizontal cylinder curves was the same as in Figure 13 except that the difference here was smaller because of the smaller target size. It should be noted that figures 13 and 14 were representative of all of the test results listed in Tables I to VI, and were not just the product of those specific test conditions.
49. Some general observations on the sphere and cylinder studies will now be made. In all three cases, a decrease in windspeed resulted in reduced collection efficiency for any given particle size. Evidently, the reduced drag force was more than compensated for by the decrease in particle inertia. Increased particle density appeared to merely shift collection efficiency values from larger to smaller particles; equivalently, plots of collection efficiency vs log (particle radius) were translated left. The reason for this was that particle terminal velocity and inertia were increased, rendering the particles more difficult to deflect. A reduction in target size had the same effect as increased particle density. The explanation in this case, however, was that larger targets create more far-reaching flow perturbations, the net effect of which was subject to incoming particles to greater deflecting drag forces; conversely, smaller targets resulted in less deflecting drag forces.
50. The remaining discussion will focus on the man simulation results. Although the ground fraction values are of most importance here,
a brief comparison of the collection efficiency results in Tables VI and VII needs to be done. The only difference between the two tests was that the ' $M$ ' tests (Table VII) incorporated a velocity gradient from the ground up. This velocity gradient significantly lowered the collection efficiency for all particle sizes. The reason was that as the particles fell, the windspeed decreased which in turn decreased the particle's horizontal speed. As in all previous cases of reduced windspeed, this must result in reduced collection efficiency.
51. The ground fraction results demonstrated several noteworthy features. Most striking were the greater than unity ground fractions for some of the particles in high windspeed tests. This was due to almost horizontal particle trajectories for these cases; near horizontal trajectories will result in low ground concentration since the particles will be distributed over a large area. Clearly, objects standing vertically in such a situation could receive greater concentrations than the ground.
52. Figure 15 showed three curves corresponding to tests M1, M2 and M3. The central peak in each curve resulted from the interaction of two effects. For small particles, the collection efficiency was so small that the ground fraction was zero; for large particles, their near vertical trajectories meant that relatively few could impact on the vertical sides of the cylinder, so that the ground fraction was again near zero. Both ground fraction reducing effects decreased toward the opposite end of the particle size spectrum; therefore, the largest ground fractions occurred in the middle region, in which neither effect dominated. This peak migrated from $50 \mu \mathrm{~m}$ in the upper curve to $100 \mu \mathrm{~m}$ in the lower curve.
53. The tremendous effect of windspeed was well illustrated by figure 15. The lower windspeeds possessed very low ground fractions; note that a maximum ground fraction of 0.17 was calculated for the $1.0 \mathrm{~m} / \mathrm{s}$ windspeed
case. The reason for this was that particle trajectories were near vertical for such low windspeeds; hence, little particle impaction could occur on the vertical cylinder sides.
54. The man simulation model in this project was undoubtedly crude. Nevertheless, the essential aspects of this kind of man simulation problem were believed to have been demonstrated, even though the flow geometry was drastically simplified. Some speculative conclusions will now be drawn from the ground fraction data.
55. The curves of Figure 15 indicate that the largest aerosol particles are not suitable for impacting on a standing man; in fact, the best particle size is around $100 \mu \mathrm{~m}$. This must be viewed in light of two important qualifiers: first, the smaller particles will travel further from the dissemination point, resulting in lower ground concentrations to begin with; and second, aerosols from materials with some volatility will tend to evaporate as they move downwind, so that the smaller particles might disappear altogether. Note that the evaporative characteristics will also influence ground persistence of the chemical, which is another vital consideration. Nonetheless, these ground fraction results suggest that an upper limit for ideal particle size for impaction on a man may exist.
56. The subject of man motion under this kind of chemical particle bombardment was not considered in the project. Although authoritative comments will have to wait until detailed work is done, there is one speculation that needs to be recorded here. Specifically, if the man were walking in the direction of the wind, the particle trajectories would assume a more vertical shape in the man's frame of reference. This would be equivalent to a man-stationary, reduced windspeed problem such as was studied in this project; and according to those results, the ground fraction, and hence the man contamination, would be reduced. Incorporation
of a moving target into this simulation model is a logical next step for research, one that would help to resolve the speculation suggested above.

## CONCLUSIONS

57. The numerical tests conducted with spherical cylindrical targets indicated that gravitational effects altered the collection efficiencies insignificantly, on the order of $\pm 3 \%$ (absolute), provided that the free stream velocity was $2.5 \mathrm{~m} / \mathrm{s}$ or higher. Lower free stream velocities resulted in much greater gravitational effects, up to $21.2 \%$ (absolute) for $100 \mu \mathrm{~m}$ particles impacting on a spherical target. Changes in the particle density and target size were found to have a negligible effect on the importance of gravity in the problem.
58. The man simulation tests indicated that a man would receive the most chemical relative to the ground concentration for particles on the order of $100 \mu \mathrm{~m}$ radius. In fact, he could receive up to 6.9 times the ground concentration. Although there were mitigating factors, the analysis suggested that an upper limit may exist for the ideal particle size in considering impaction on a standing man.

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| TEST NLNBE¢ |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | 51 | $5 ?$ | S 3 | $\leq 4$ | S 5 |
| WJNOSF | 7.5 | 5.1 | 2. | 1. | 1.5 |
| RADTAN | 1 C | .15 | . 1 | 1 | -16 |
| DENFAK | 15 | 1005 | 1 CO | 1 C | 10 C |
| PARTICL GAOILS | $\triangle C$ | Aic | --1 | Mo | Nic |




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TABLE III
MISCELLANEOUS SPHERE RUNS

| ACCURACY TEST |  |  |  |  | SIMILARITY TEST |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | S2 | S11 | ABS. <br> ERROR | REL. <br> ERROR |  | S2 | S12 | S13 |
| U $\mathrm{L}$ $F$ P $g$ | $\begin{gathered} 5.0 \\ 0.1 \\ 25.5 \\ 1000 \\ 9.81 \end{gathered}$ | $\begin{gathered} 5.0 \\ 0.1 \\ 25.5 \\ 1000 \\ 9.81 \end{gathered}$ |  |  | $u$ L $F$ P $\mathrm{g}$ | $\begin{gathered} 5.0 \\ 0.1 \\ 25.5 \\ 1000 \\ 9.81 \end{gathered}$ | $\begin{gathered} 5.0 \\ 0.05 \\ 25.5 \\ 500 \\ 19.62 \end{gathered}$ | $\begin{gathered} 5.0 \\ 0.15 \\ 25.5 \\ 1500 \\ 6.54 \end{gathered}$ |
| PARTICLE RADIUS |  |  |  |  | PARTICLE RADIUS |  |  |  |
| 10 | . 00044 | . 00032 | . 00012 | 37.5\% | 10 | . 00044 | . 00156 | . 00020 |
| 15 | . 00640 | . 00515 | . 00125 | 24.3\% | 15 | . 00640 | . 01010 | . 00493 |
| 25 | . 11263 | . 11008 | . 00255 | 2.3\% | 25 | . 11263 | . 12058 | . 10988 |
| 50 | . 44986 | . 44751 | . 00235 | 0.5\% | 50 | . 44986 | . 45592 | . 44775 |
| 75 | . 63808 | . 63635 | . 00173 | 0.3\% | 75 | . 63808 | . 64261 | . 63666 |
| 100 | . 74054 | . 73904 | . 00150 | 0.2\% | 100 | . 74054 | . 74426 | . 73934 |
| 250 | . 92237 | . 92182 | . 00060 | 0.06\% | 250 | . 92237 | . 92443 | . 92158 |
| 500 | . 97778 | . 97771 | . 00007 | 0.007\% | 500 | . 97778 | . 97978 | . 97725 |
| 1000 | . 99656 | . 99656 | - | - | 1000 | . 99656 | . 99792 | . 99603 |
| 2000 | 1.00032 | 1.00032 | - | - | 2000 | 1.00032 | 1.00217 | 1.00001 |



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PARTICLE RADII ARE GIVEN IN MICRCNS


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TABLE IX

ENVELOPE RESULTS FOR TEST C3

| PARTICLE <br> RADIUS <br> (microns) | UPPER <br> BOUND <br> $(\mathrm{m})$ | LOWER <br> BOUND <br> $(\mathrm{m})$ | NO GRAVITY <br> BOUND <br> (m) |
| :---: | :---: | :---: | :---: |
| 10 | -.0003 | -.0005 | $\pm .0001$ |
| 15 | -.0008 | -.0010 | .0001 |
| 25 | -.0006 | -.0039 | .0016 |
| 50 | +.0162 | -.0299 | .0236 |
| 75 | +.0314 | -.0523 | .0439 |
| 100 | +.0435 | -.0668 | .0579 |
| 250 | +.0827 | -.0967 | .0873 |
| 500 | +.0971 | -.1004 | .0959 |
| 1000 | +.1004 | -.1009 | .0994 |
| 2000 | +.1019 | -.1019 | .1014 |

The boundary values 1 isted here are $z^{\prime}$ co-ordinates (Frame 2). The target was 0.1 m in radius.


Figure 1
OVERVIEW OF CHEMICAL MOTION PROBLEM


Figure 2


Figure 3
COLLECTION ENVELOPES


Figure 4
HALF-INTERVAL METHOD

FRAME $0 \rightarrow(x, \eta, \psi)$ FRAME $1 \rightarrow(x, y, z)$

THE X-AXIS IS OUT OF THE PAGE


Figure 5
SPHERE REFERENCE FRAMES 0 AND 1


SPHERE REFERENCE FRAME 2


HORIZONTAL CYLINDER GEOMETRY


Figure 8
VERTICAL CYLINDER GEOMETRY


Figure 9
MAN SIMULATION GEOMETRY


FIGURE 10<br>PARTICLE SIZE $=50$. MICRONS WINDSPEED $=1.5 M / S$

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FIGURE 11
PARTICLE SIZE $=250$ MICRONS WINDSPEED $=1.5 M / S$

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FIGURE 13
CYLINDER COMPARISON CURVE


$$
\begin{gathered}
\text { FIGURE } 14 \\
\text { CYLINDER-SPHERE COMPARISON CURVE }
\end{gathered}
$$



## APPENDIX A

## LISTING OF PROGRAM AEROSOL-8 (MAN SIMULATION) SAMPLE OUTPUT FOR

 FIRST SET OF TEST CONDITIONS (RUN 1)











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## APPENDIX B

LISTING OF PROGRAM AEROSOL-6
(TRAJECTORY PLOTS AROUND HORIZONTAL CYLINDERS) SAMPLE OUTPUT OF MINIMUM TABULATION RUN SAMPLE OUTPUT OF FULL TABULATION RUN (FIRST PAGE ONLY)







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11. SUPPLEMENTARY NOTES
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13. ABSTAACT
(U) This project was a theoretical investigation of particulate impaction on spheres and cylinders. The motion model developed was implemented on a computer and yielded results focused on two main goals: first, the net effect of gravity on particulate impaction was determined; and second, a man simulation was conducted. This simulation calculated to a first approximation the amount of chemical that would impact on a man subjected to a chemical attack.




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