SPACE RESEARCH COORDINATION CENTER

A STOCHASTIC MODEL STUDY OF THE MOVEMENT OF SOLID PARTICLES

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1. INTRODUCTION

"Stochastic Process" is a time dependent random phenomenon described by a probability distribution law. In general, physical phenomena can be classified into deterministic, random and hybrid processes. However, there are few physical phenomena which are pure deterministic or pure random processes. Instead, most of physical phenomena are hybrid processes which are the combination of deterministic and random processes.

Random walk is a kind of Markov chain which in turn is a particular type of stochastic process. The random walk model was first used by Karl Pearson[7] in 1905 in a study of random motion of a particle in space. Since then, it has been used by a great number of investigators. The random walk process, as described by Pearson, can very closely reproduce the diffusion process. In his book, Feller[8] states; "If the individual steps of a random walk are made extremely small and occoure in rapid succession, then at the limit the process will appear as a continuous motion. The point of interest is that in passing to this limit the formulae (describing the motion) remain meaningful and agree with physically significant formulae of diffusion theory..... This explains partly why the random walk model, despite its crudeness, describes diffusion process reasonably well ".

Random walk provides a solution to a continuum equation. Smoluchowski[2] has applied it to the solution of the one-dimensional diffusion equation. Another example is Knighting's[3] solution of the three-dimensional turbulent diffusion from an instantaneous point source near the boundary in a uniform velocity field.

The random walk model can be employed in solving differential equations of the continuum case by a method of random sampling. Sometimes, the method of random sampling is more effective than the analytical or numerical method. The method of random sampling, which is called "Monte Carlo" method, was first suggested by Fermi[4] for studying the Schrodinger equation. A typical example of the application of this method to fluid mechanics is the solution of the Laplace equation.

Random walk can also be used to simulate physical processes. In a direct simulation the features of a process are reproduced by imitating the behaviors of appropriate discrete entities, such as particles. This approach has proved effective in the studies of the diffusion and decay of nuclear particles.[6] For simulating a specific problem, the only requirement is to build a discrete model that gives a proper representation of the behaviors of the particles. The essential features which characterize the specific aspects of the process being investigated should be reproduced.

Bugliarello and Jackson[1] applied the random walk method to the molecular diffusion in convective flow fields. They showed that the use of a random walk technique yields solution to problems of molecular diffusion in a convective flow field. They stated, "It has been shown for the laminer flow that the random walk not only has the advantage of by-passing the analytical solution of the problem, but also allows for considerable insight into the physical process. Both of these properties render the method a tool of potentially great usefulness in the treatment of turbulent diffusion problems". Results of a random walk study of turbulent diffusion agreed very well with those given by Taylor's statistical theory of turbulent diffusion[1]. Random walk thus emerges as a good approach to the solution of the diffusion problem.

In this study, the transport of suspended solid particles under the influence of secondary flow will be studied in a three dimensional convective flow field in a corner of a straight rectangular channel. The secondary flow is a circulatory motion of the fluid around an axis parallel to the longitudinal axis of a channel, while the primary flow is a translation of the fluid parallel to the longitudinal axis of the channel. The combination of primary and secondary flows results in a spiral motion. There are two types of secondary flow: (1) secondary currents in straight, noncircular channel, and (2) secondary currents at bends of a channel. In the present study only the first type of secondary flow, as shown in Fig. 1-1, is considered.

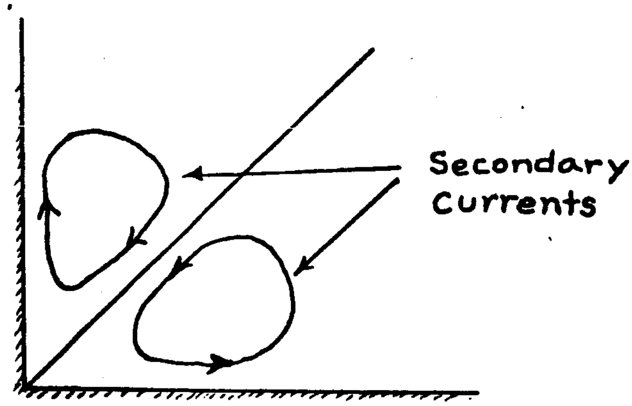


Fig. 1-1 Secondary Currents in a Corner of a Straight Rectangular Channel

There are two principal objectives in this study. The first objective is to build a stochastic model to represent the transport of suspended solid particles in corners of straight channels under the influence of secondary flow. The second objective is to solve the developed diffusion equation (equation (2-14)) of suspended solid particles by Monte Carlo method. The solution will give the concentration of suspended solid particles.

II RANDOM WALK AND MONTE CARLO

As stated previously, random walk can be used as a model of a physical phenomenon. Once the model is built the Monte Carlo method can then be employed to simulate the physical system and find solutions to a problem through the random sampling technique. Thus, a combination of random walk and Monte Carlo can provide solutions to complex problems in fluid mechanics which can not be solved by analytical methods.

A. Random Walk

Mathematically, a stochastic process can be written as a collection of time-dependent random variables as $\{X(t); t \in T\}$ that is, a sequence of time dependent random variables. A discrete parameter stochastic process $\{X(t), t = 0, 1, 2, \cdots\}$ or a continuous parameter stochastic process $\{X(t), t \geq 0\}$ is said to be a Markov process if, for $t_1 < t_2 < \cdots < t_n$

$$P[X(t_n) \leq X_n \mid X(t_1) = X_1, \cdots, X(t_{n-1}) = X_{n-1}]$$
$$= P[X(t_n) \leq X_n \mid X(t_{n-1}) = X_{n-1}] \qquad (2\text{-}1)$$

where P denotes a conditional probability function. A real number X is said to be a possible value, or a state, of a stochastic process if there exists a time t in T such that the probability $P[X-h < X(t) < X+h]$ is positive for an increment of X, h>0. The set of possible values of a stochastic process is called state space. A Markov process whose state space is discrete is called a Markov Chain.

A Markov process is described by a transition probability function, often denoted by $P(X, t_0; E, t)$ or $P(E, t | X, t_0)$, which represents the conditional probability that the state of a system will at time t belong to the set E, given that at time t_0 ($< t$) the system is in the state X. In order to specify the probability law of a discrete parameter Markov chain $\{X_n\}$, it suffices to state for all times $n \geq m \geq 0$, and states j and k, the probability mass function

$$p_j(n) = P[X_n = j] \tag{2-3}$$

and the conditional probability mass function

$$p_{jk}(m, n) = P[X_n = k | X_m = j] \tag{2-4}$$

The function $p_{jk}(m, n)$ is called the transition probability function of the Markov chain. The probability law of a Markov chain is determined by the functions in equations (2-3) d (2-4), since for all integers q, and any q times $n_1 < n_2 < \cdots < n_q$, and states $k_1, k_2, \cdots, k_q$

$$P[X_{n_1} = k_1, \cdots, X_{n_q} = k_q] = p_{k_1}(n_1)\, p_{k_1 k_2}(n_1, n_2)\, p_{k_2 k_3}(n_2, n_3) \cdots p_{k_{q-1} k_q}(n_{q-1}, n_q) \tag{2-5}$$

A Markov chain is said to be homogeneous in time or to have stationary transition probability if $P_{jk}(m, n)$ depends only on the difference n-m. Then,

$$p_{jk}(n) = P[X_{n+t} = k \mid X_t = j]$$

for any integer $t \geq 0$ .....(2-6) is the n-step transition probability function of the homogeneous Markov chain $\{X_n\}$. In words, $P_{jk}(n)$ is the conditional probability that a homogeneous Markov chain now in state j will move, after n steps, to state k. The one-step transition probability $P_{jk}(1)$ are usually written simply P_{jk}, or

$$p_{jk} = P[X_{t+1} = k \mid X_t = j] \qquad (2\text{-}7)$$

The transition probabilities of a Markov chain $\{X_n\}$ with state space $\{0, 1, 2, \ldots\ldots\}$ are best exhibited in the form of a matrix:

$$P(m,n) = \begin{bmatrix} p_{00}(m,n) & p_{01}(m,n) & \cdots & p_{0k}(m,n) & \cdots \\ p_{10}(m,n) & p_{11}(m,n) & \cdots & p_{1k}(m,n) & \cdots \\ \vdots & \vdots & & \vdots & \\ p_{j0}(m,n) & p_{j1}(m,n) & \cdots & p_{jk}(m,n) & \cdots \\ \vdots & \vdots & & \vdots & \end{bmatrix}$$

In which the elements of a transition probability matrix $P(m, n)$ satisfy the conditions

$$p_{jk}(m,n) \geq 0 \quad \text{for all } j, k \qquad (2\text{-}8)$$

$$\sum p_{jk}(m,n) = 1 \quad \text{for all } j \qquad (2\text{-}9)$$

A fundamental relation satisfied by the transition probability function of a Markov chain $\{X_n\}$ is the so-called Chapman-Kolmogorov equation; for any time $n > u > m \geq o$ and states j and k.

$$p_{jk}(m,n) = \sum_{\text{state } i} p_{ji}(m,u)\, p_{ik}(u,n) \qquad (2\text{-}10)$$

A random walk is a Markov chain $\{X_n, n=o,1,\ldots\}$ which consists of integer state spaces, with the property that if the system is in a given state k then in a single transition the system either remains at k or moves to one of the states immediately adjacent to k. For example, as in the one-dimensional case it can be represented by a transition probability matrix P as:

$$P = \begin{bmatrix} r_0 & p_0 & 0 & 0 & 0 & \cdots \\ q_1 & r_1 & p_1 & 0 & 0 & \cdots \\ 0 & q_2 & r_2 & p_2 & 0 & \cdots \\ 0 & 0 & q_3 & r_3 & p_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \end{bmatrix} \qquad (2\text{-}11)$$

where,

$$r_k + p_k = 1 \qquad \text{for } k = 0$$

$$q_k + r_k + p_k = 1 \qquad \text{for } k = 1, 2, \cdots$$

and

P (q) represents the probability that the particle moves in positive (negative) direction.

r represents the probability that the particle remain at the same place.

B. Random Walk Model of the Transport of Suspended Solid Particles

Let $P(x_1, x_2, x_3, t)$ be the probability that a particle, which at t_0 starts from the origin $(0, 0, 0)$, arrives at the position (x_1, x_2, x_3) at t. P will be called the probability function of displacement. Let P_j (q_j) denote the probability that a particle moves in the positive (negative) X_j -direction. Suppose in each step a particle travels a distance ΔX_j in the X_j -direction and the time interval between any two consecutive steps is τ.

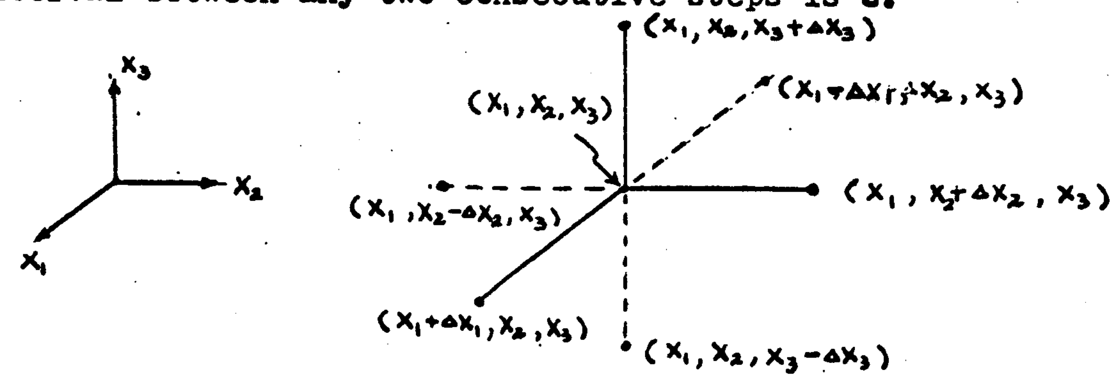


Fig 2-1. Schematic Diagram of Random Walk Model

Then, by total probability theorem;

$$P(X_1, X_2, X_3, t) = \sum \left[p_j P(X_j - \Delta X_j, t-\tau) + q_j P(X_j + \Delta X_j, t-\tau) \right] \quad (2\text{-}12)$$

where the index j refers to the coordinates which varies. For example, when $j = 2$, $P(X_j - \Delta X_j, t-\tau) = P(X_1, X_2 - \Delta X_2, X_3, t-\tau)$ After rearranging, equation (2-12) can be rewritten in the form of difference equation:

$$\frac{P(x_1,x_2,x_3,t)-P(x_1,x_2,x_3,t-\tau)}{\tau} = \sum_{j=1}^{3} \frac{(p_j+q_j)(\Delta x_j)^2}{2\tau} \Big[P(x_j+\Delta x_j,t-\tau) + P(x_j-\Delta x_j,t-\tau) - 2P(x_1,x_2,x_3,t-\tau)\Big] \Big/ (\Delta x_j)^2 + \sum_{j=1}^{3} \frac{(q_j-p_j)(\Delta x_j)}{\tau} \Big[P(x_j+\Delta x_j,t-\tau) - P(x_j-\Delta x_j,t-\tau)\Big] \Big/ (2\Delta x_j) \qquad (2\text{-}13)$$

In the limiting case, equation (2-13) becomes a differential equation of particles.

$$\frac{\partial P}{\partial t} = \sum_{j=1}^{3}\left[\epsilon_j \frac{\partial^2 P}{\partial x_j^2} + \left(\frac{\partial \epsilon_j}{\partial x_j} - V_j\right)\frac{\partial P}{\partial x_j}\right] \qquad (2\text{-}14)$$

where

$$\epsilon_j = \lim_{\tau\to 0} \frac{(p_j+q_j)(\Delta x_j)^2}{2\tau} = \frac{\sigma_j^2}{2\tau} = \text{the } x_j\text{-component of}$$

the diffusion coefficient. .....(2-15)

in which σ_j^2 represents the mean square displacement of particles in the X_j direction.

$$\frac{\partial \epsilon_j}{\partial x_j} - V_j = \lim_{\tau\to 0} \frac{(q_j - p_j)}{\tau} = \frac{\overline{\Delta X_j}}{\tau} \qquad (2\text{-}16)$$

which is the mean displacement of particles in the X_j-direction and is called the "drift coefficient".

Equation (2-16) is shown by Tchen[15].

In one dimensional case, equation (2-14) becomes a diffusion equation

$$\frac{\partial P}{\partial t} = \epsilon_1 \frac{\partial^2 P}{\partial x_1^2} + \left(\frac{\partial \epsilon_1}{\partial x_1} - V_{x_1}\right)\frac{\partial P}{\partial x_1} \qquad (2\text{-}17)$$

in the x_1-direction. Further more, if $p=q$, equation (2-14) becomes the classical diffusion equation

$$\frac{\partial P}{\partial t} = \epsilon_1 \frac{\partial^2 P}{\partial x_1^2} \qquad (2\text{-}18)$$

where ϵ_1 is called diffusion coefficient in an one dimensional flow. Equation (2-18) can be solved analytically to give

$$P(x_1, t) = \frac{1}{\sqrt{4\epsilon_1 \pi t}} e^{-x_1^2/4\epsilon_1 t} \qquad (2\text{-}19)$$

In a steady uniform flow in the x -direction, P is independent of x and t. Then the equation (2-14) becomes

$$-\epsilon_2 \frac{\partial^2 P}{\partial x_2^2} - \epsilon_3 \frac{\partial^2 P}{\partial x_3^2} - \frac{\partial \epsilon_2}{\partial x_2}\frac{\partial P}{\partial x_2} + V_2 \frac{\partial P}{\partial x_2} - \frac{\partial \epsilon_3}{\partial x_3}\frac{\partial P}{\partial x_3} + (V_3 + V_p)\frac{\partial P}{\partial x_3} = 0 \qquad (2\text{-}20)$$

which is analogous to the equation of particle concentration

$$-\epsilon_2 \frac{\partial^2 C}{\partial x_2^2} - \epsilon_3 \frac{\partial^2 C}{\partial x_3^2} - \frac{\partial \epsilon_2}{\partial x_2}\frac{\partial C}{\partial x_2} - \frac{\partial \epsilon_3}{\partial x_3}\cdot\frac{\partial C}{\partial x_3} + V_2 \frac{\partial C}{\partial x_2} + (V_3 + V_p)\frac{\partial C}{\partial x_3} = 0 \qquad (2\text{-}21)$$

where

ϵ_2, ϵ_3 = the x_2 & x_3 -components of the diffusion coefficient for the transport of solid particles;

C = average concentration of solid particles at a point.;

V_p = settling velocity of the representative particle under the influence of gravity;

V_2, V_3 = the x_2 and x_3-components of the average secondary velocity at a point, which can be either positive or negative in the fluid carrying solid particles.

Above illustrations show that the transport of suspended solid particles can be represented by a random walk model. Since the equation (2-14) can not be solved analytically, the Monte Carlo method seems to be the only possible means for use.

C. Monte Carlo Method

The Monte Carlo method is one which applies the random sampling teachnique in the treatment of either deterministic or probabilistic problems. The random sampling includes: (1) modeling the probability process to be sampled, (2) deciding how to generate random variables from the given probability distribution in some efficient ways and (3) applying variance reducing techniques, that is, methods of increasing the accuracy of the estimates obtained from the sampling process.

When differential equations can not be solved analytically, the importance and value of a Monte Carlo method become apparent. Although equation (2-20) can be solved by a numerical method, such as the relaxation method, it requires boundary values which must be obtained from the experiments. Furthermore, the relaxation method is not suitable for machine computation.

III STOCHASTIC MODEL OF THE TRANSPORT OF SOLID PARTICLES.

In this study the transport or motion of a solid particle in a fluid is considered to arise as a result of the superposition of the following two independent phenomena: (1) random walk of the particle itself at the presence of the fluid turbulence, and (2) action of the gravity force and the mean convective flow on the particle which is considered to be a deterministic process. In brief the stochastic model of this study consists of random and deterministic components.

A. Random Walk of a Particle

Random walk can be used to simulate the normal diffusion process. The random process of this system is governed by the uniform or rectangular distribution probability law, that is, the particle diffuse with an isotropic diffusion coefficient when the fluid is macroscopically at rest. The basic step of random walk process of a particle consists of a constant length ℓ and a random direction. Therefore, the positions of a particle that undergoes random walk process can be described by the following model in Cartesian coordinates, as shown by Fig. 3-1

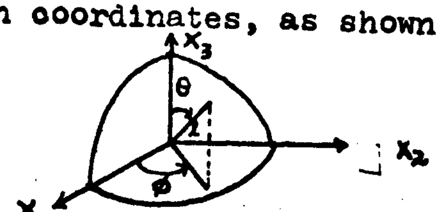


Fig. 3-1. Diagram of Random Walk of a Particle (Spherical coordinate system)

$$
\left.\begin{aligned}
(X_1)_{i+1} &= (X_1)_i + L_1\big|_i \\
(X_2)_{i+1} &= (X_2)_i + L_2\big|_i \\
(X_3)_{i+1} &= (X_3)_i + L_3\big|_i
\end{aligned}\right\} \text{ for } i = 0, 1, 2, \cdots \quad (3\text{-}1)
$$

where

$$
\begin{aligned}
L_1\big|_i &= \ell \sin\theta_i \cos\phi_i \\
L_2\big|_i &= \ell \sin\theta_i \sin\phi_i \\
L_3\big|_i &= \ell \cos\theta_i
\end{aligned}
$$

In which

ℓ is assumed to be a constant group mean value defined as

$$
\ell = \frac{1}{M}\sum_{k=1}^{M}\left(\frac{1}{N}\sum_{i=1}^{N}|\ell_{ki}|\right) = \frac{1}{MN}\sum_{k=1}^{M}\sum_{i=1}^{N}|\ell_{ki}| \qquad (3\text{-}2)
$$

It will be used as length unit in measuring quantities of length dimension in order to preserve the generality of the problem.

θ and ϕ are two independent random numbers which are governed by a certain probability distribution law. They can be generated easily by a digital computer. For an isotropic diffusion, they are governed by the uniform (or rectangular) probability distribution law. In other words, they vary uniformly from 0 to 360 (i, e, $0^\circ \leq \theta \leq 360^\circ$, $0^\circ \leq \phi \leq 360^\circ$)

B. Mean Convective Flow

The convective diffusion process in a corner of a straight channel is the transport due to the gravity force and primary and secondary flows. The suspended solid particles with densities greater than that of water have a settling velocity due to the gravity force. The primary flow is a translation of the fluid in the longitudinal direction of a channel. The secondary flow is a circulatory motion of the fluid in the plane perpendicular to the primary flow.

Liggett, Chiu and Miao[13] used an curvilinear orthogonal coordinate system, as shown in Fig. 3-2 in deriving equations for secondary velocities.

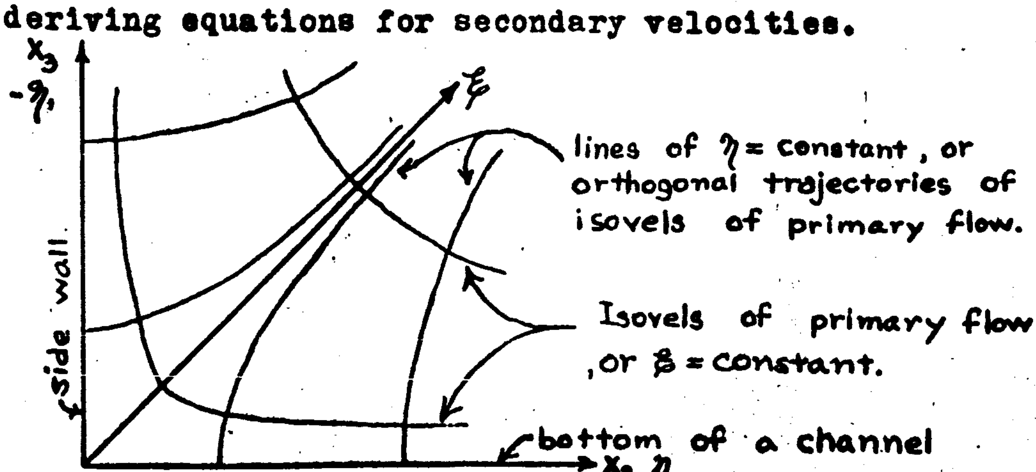


Fig. 3-2 Coordinate Systems

The ξ-curves are made to represent the isovels of the primary flow and the η-curves are orthogonal trajectories of the family of ξ-curves. In such a coordinate system, for a steady, uniform flow in the x_1-direction, the primary flow velocity is

$$V_{x_1} = V_{x_1}(\xi)$$

depending on ξ only, the equation of motion is

$$\rho \frac{1}{h_\xi} \cdot V_\xi \cdot \frac{\partial V_{x_1}}{\partial \xi} = -\frac{\partial}{\partial x_1}(P + \rho g h) + \frac{1}{h_\xi}\left(\frac{\partial \tau_{\xi x_1}}{\partial \xi} + \frac{1}{h_\eta}\frac{\partial h_\eta}{\partial \xi} \cdot \tau_{\xi x_1}\right) \qquad (3\text{-}3)$$

and the equation of continuity is

$$\frac{\partial}{\partial \xi}(h_\eta V_\xi) + \frac{\partial}{\partial \eta}(h_\xi V_\eta) = 0 \qquad (3\text{-}4)$$

where

V_ξ = the ξ-component of the average secondary velocity.

h_ξ, h_η = scale factors on the ξ and η coordinates, respectively

($h_\xi^2 = g_{\xi\xi}$, where $g_{\xi\xi}$ is the metric tensor of the coordinate transformation)

ρ = density of the fluid

Equation (3-3) gives

$$V_\xi = \left[-h_\xi \frac{\partial}{\partial x_1}(P + \rho g h) + \frac{\partial \tau_{\xi x_1}}{\partial \xi} + \frac{1}{h_\eta}\frac{\partial h_\eta}{\partial \xi} \cdot \tau_{\xi x_1}\right] \Big/ \left(\rho \frac{\partial V_{x_1}}{\partial \xi}\right) \qquad (3\text{-}5)$$

while equation (3-4) gives

$$V_\eta' = -\frac{1}{h_\xi}\frac{\partial}{\partial \xi}\int_0^\eta h_\eta V_\xi \, d\eta \qquad (3\text{-}6)$$

The numerical solution of equations (3-5) and (3-6) for secondary velocities can be accomplished once the primary velocity distribution and $\frac{\partial}{\partial x_1}(P+\rho g h)$ are determined empirically, since the shear distribution can be obtained from one primary velocity distribution. It was shown[13] that the vertical velocity profile of the primary flow can be adequately represented by a simple power law.

$$V_{x_1} = C\xi^{1/n}$$

Liggett, Chiu and Miao also used the following equation to represent a family of isovels of the primary flow

$$\xi = \frac{X_2 X_3}{(X_2^{\alpha} + X_3^{\alpha})^{1/\alpha}} \qquad (3\text{-}8)$$

which gives its orthogonal trajectories as

$$\eta = \frac{X_2^{\alpha+2} - X_3^{\alpha+2}}{\alpha+2} \qquad (3\text{-}9)$$

where α is a constant to be determined empirically. A greater value of α represents a greater curvature of the family of isovels. The scale factors can be derived from equations (3-8) and (3-9) as:

$$h_{\xi} = \frac{(X_2 X_3/\xi)^{\alpha+1}}{\sqrt{X_2^{2(\alpha+1)} + X_3^{2(\alpha+1)}}} \qquad (3\text{-}10)$$

$$h_{\eta} = \frac{1}{\sqrt{X_2^{2(\alpha+1)} + X_3^{2(\alpha+1)}}} \qquad (3\text{-}11)$$

Substituting equations (3-10) and (3-11) into equations (3-5) and (3-6), then

$$V_{\xi} = \left\{ \frac{\partial \tau_{\xi x_1}}{\partial \xi} - \frac{(\alpha+1)(X_2 X_3)^{3\alpha+2}}{\xi^{2(\alpha+1)}\left[X_2^{2(\alpha+1)} + X_3^{2(\alpha+1)}\right]^2} \tau_{\xi x_1} + \frac{(X_2 X_3/\xi)^{\alpha+1}}{\sqrt{X_2^{2(\alpha+1)} + X_3^{2(\alpha+1)}}} \frac{\partial}{\partial x_1}(p + \rho g h) \right\} \Bigg/ \left(\rho \frac{\partial V_{x_1}}{\partial \xi}\right) \qquad (3\text{-}12)$$

$$V_\eta = \frac{-\sqrt{X_2^{2(\alpha+1)} + X_3^{2(\alpha+1)}}}{(X_2 X_3/\xi)^{\alpha+1}} \frac{\partial}{\partial \xi} \int_0^\eta \frac{V_{\xi_0}}{\sqrt{X_2^{2(\alpha+1)} + X_3^{2(\alpha+1)}}} \, d\eta \qquad (3\text{-}13)$$

where the turbulent shear $\tau_{\xi X_1}$ can be obtained from von Karman's formula

$$\tau_{\xi X_1} = \rho K^2 \left(\frac{\partial V_{X_1}}{\partial \xi} \right)^4 \Big/ \left(\frac{\partial^2 V_{X_1}}{\partial \xi^2} \right)^2 \qquad (3\text{-}14)$$

where K is von Karman's constant (0.4 for clear water and less for sediment laden water).

Equations (3-7) and (3-14) give

$$\tau_{\xi X_1} = \rho K^2 \left(\frac{c}{n-1} \xi^{1/n} \right)^2 \qquad (3\text{-}15)$$

Secondary flow velocities can be calculated by numerical solution of equations (3-12) and (3-13).

C. Resultant Stochastic Model

Superposition of the deterministic and pure random components of the motion of a single solid particles, as described previously, forms the following resultant stochastic model. Let the position of a particle at the end of the i^th^ step be $((X_1)_i, \xi_i, \eta_i)$,

then

$$\left.\begin{aligned}
(X_1)_{i+1} &= (X_1)_i + L_1\big|_i + V_{X_1}\big|_i \cdot \tau \\
\xi_{i+1} &= \xi_i + \left(L_\xi\big|_i + V_\xi\big|_i \cdot \tau + (V_f)_\xi\big|_i \cdot \tau \right) \frac{1}{h_\xi} \\
\eta_{i+1} &= \eta_i + \left(L_\eta\big|_i + V_\eta\big|_i \cdot \tau + (V_f)_\eta\big|_i \cdot \tau \right) \cdot \frac{1}{h_\eta}
\end{aligned}\right\} \qquad (3\text{-}16)$$

where

$V_{x_1}\big|_i$ = average velocity of primary flow at the point

$V_\xi\big|_i\ ,V_\eta\big|_i$ = the ξ and η components of average secondary velocity at the point $((x_1)_i,\xi_i,\eta_i)$ respectively, which can be either positive or negative.

$(V_p)_\xi\big|_i\ ,(V_p)_\eta\big|_i$ = the components of the settling velocity of the particle in ξ and η direction respectively.

$L_1\big|_i,\ L_\xi\big|_i\ \&\ L_\eta\big|_i$ = the x_1, ξ and η -components of the pure random motion of the particle during the i^{th} step.

for a uniform flow in the x-direction,

$$\left.\begin{aligned}
V_{x_1}\big|_i &= V_{x_1}\big|_{i-1} + \frac{\partial V_{x_1}}{\partial \xi}\bigg|_{i-1}\cdot L_\xi\big|_{i-1}\\
V_\xi\big|_i &= V_\xi\big|_{i-1} + \frac{1}{h_\xi}\frac{\partial V_\xi}{\partial \xi}\bigg|_{i-1}\cdot L_\xi\big|_{i-1} + \frac{1}{h_\eta}\frac{\partial V_\xi}{\partial \eta}\bigg|_{i-1}\cdot L_\eta\big|_{i-1}\\
V_\eta\big|_i &= V_\eta\big|_{i-1} + \frac{1}{h_\xi}\frac{\partial V_\eta}{\partial \xi}\bigg|_{i-1}\cdot L_\xi\big|_{i-1} + \frac{1}{h_\eta}\frac{\partial V_\eta}{\partial \eta}\bigg|_{i-1}\cdot L_\eta\big|_{i-1}
\end{aligned}\right\}\qquad (3\text{-}17)$$

$$(V_p)_\xi\Big|_i = \left(\frac{1}{h_\xi}\cdot\frac{\partial X_3}{\partial \xi}\right)\Big|_i \cdot (V_p)_{x_3} = \left(h_\xi \frac{\partial \xi}{\partial X_3}\right)\Big|_i \cdot (V_p)_{x_3}$$

$$(V_p)_\eta\Big|_i = \left(\frac{1}{h_\eta}\cdot\frac{\partial X_3}{\partial \eta}\right)\Big|_i \cdot (V_p)_{x_3} = \left(h_\eta \cdot \frac{\partial \eta}{\partial X_3}\right)\Big|_i \cdot (V_p)_{x_3}$$

$$L_\xi\Big|_i = \left[\frac{\partial \xi}{\partial X_2}\Big|_i \cdot L_2\Big|_i + \frac{\partial \xi}{\partial X_3}\Big|_i \cdot L_3\Big|_i\right] \cdot h_\xi\Big|_i$$

$$L_\eta\Big|_i = \left[\frac{\partial \eta}{\partial X_2}\Big|_i \cdot L_2\Big|_i + \frac{\partial \eta}{\partial X_3}\Big|_i \cdot L_3\Big|_i\right] \cdot h_\eta\Big|_i .$$

where L_1, L_2, and L_3 are given by equation (3-2)

τ is a constant time interval between two consecutive steps. It can be determined ~~from the Lagrangian turbulence scale~~ as the upper measure of correlation.16 τ will be used as a time unit.

We can see from equation (3-16) that the distance travelled by a particle in each step can be expressed as:

$$\Delta(X_1)_{i+1} = (X_1)_{i+1} - (X_1)_i = L_1\Big|_i + V_{x_1}\Big|_i \cdot \tau$$

$$\Delta \xi_{i+1} = \xi_{i+1} - \xi_i = L_\xi\Big|_i + V_\xi\Big|_i \cdot \tau + (V_p)_\xi\Big|_i \cdot \tau$$

$$\Delta \eta_{i+1} = \eta_{i+1} - \eta_i = L_\eta\Big|_i + V_\eta\Big|_i \cdot \tau + (V_p)_\eta\Big|_i \cdot \tau$$

The positions of a particle in x_1, ξ and η ordinates can also be expressed in cartesian coordinates by a coordinate transformation.

D. Group Motion of Solid Particles

In the present study the motion of a group or cloud of solid particles emitted from a point source is studied as well as that of a single particle. The group motion of particles is complex. However, in order to simplify the problem, the chemical reaction and interaction among particles in the fluid are not considered in this study. Each particle is considered to behave independently.

IV DIGITAL COMPUTER SIMULATION

The simulation of the developed stochastic model was performed on the IBM 7090/1401 digital computer of Computing Center, University of Pittsburgh. The programs were written in MAD (Michigan Algorithm Decorder) language.

A. Computer Program

The computer program of the developed model is divided into two parts because of the limited computer storage. The first program is for computing primary and secondary velocities and their derivatives with respect to ξ and η at each ξ-η grid point. In other words, the output of the first program consists of values of V_x, V_ξ, V_η, $\frac{\partial V_x}{\partial \xi}$, $\frac{\partial V_\xi}{\partial \xi}$, $\frac{\partial V_\xi}{\partial \eta}$, $\frac{\partial V_\eta}{\partial \xi}$ & $\frac{\partial V_\eta}{\partial \eta}$ at each ξ-η grid point. The output of the first program is then stored in magnetic tapes and serve as the input for the second program. The second program is written for computing the positions of a particle after each time period. The flow charts of these programs are presented in Appendix I.

When the particle falls in the shaded area shown in Fig. 4-1 at the end of the i^{th} step, $V_x\big|_i$, $V_\xi\big|_i$, $V_\eta\big|_i$, $\frac{\partial V_x}{\partial \xi}\Big|_i$, $\frac{\partial V_\xi}{\partial \xi}\Big|_i$, $\frac{\partial V_\xi}{\partial \eta}\Big|_i$, $\frac{\partial V_\eta}{\partial \xi}\Big|_i$ and $\frac{\partial V_\eta}{\partial \eta}\Big|_i$ in equations (3-16) and (3-17) are considered equal to those at point O.

Fig. 4-1 Schematic Diagram of ξ-η Grid Points

Then the position of the particle at the end of the $(i+1)^{th}$ step can be determined from equation (3-16).

B. Generation of Random Numbers

Random numbers are a sequence of numbers which are characterized by the property that, knowing some of the numbers of the sequence, no other number in the sequence can be predicated. Such numbers can be easily generated by a digital computer. There are several random number generators available in "Michigan Execute System"[12]. Each random number generator is characterized by a particular probability distribution law. For example, there are uniformly distributed random numbers generator and normal distributed random numbers generator which are often used. The uniformly distributed random numbers generator was used in this study. It is a particular subroutine available in "Michigan Execute System". This subroutine provides the means of generating random numbers, uniformly distributed over the interval $0 \leq x \leq 1$.

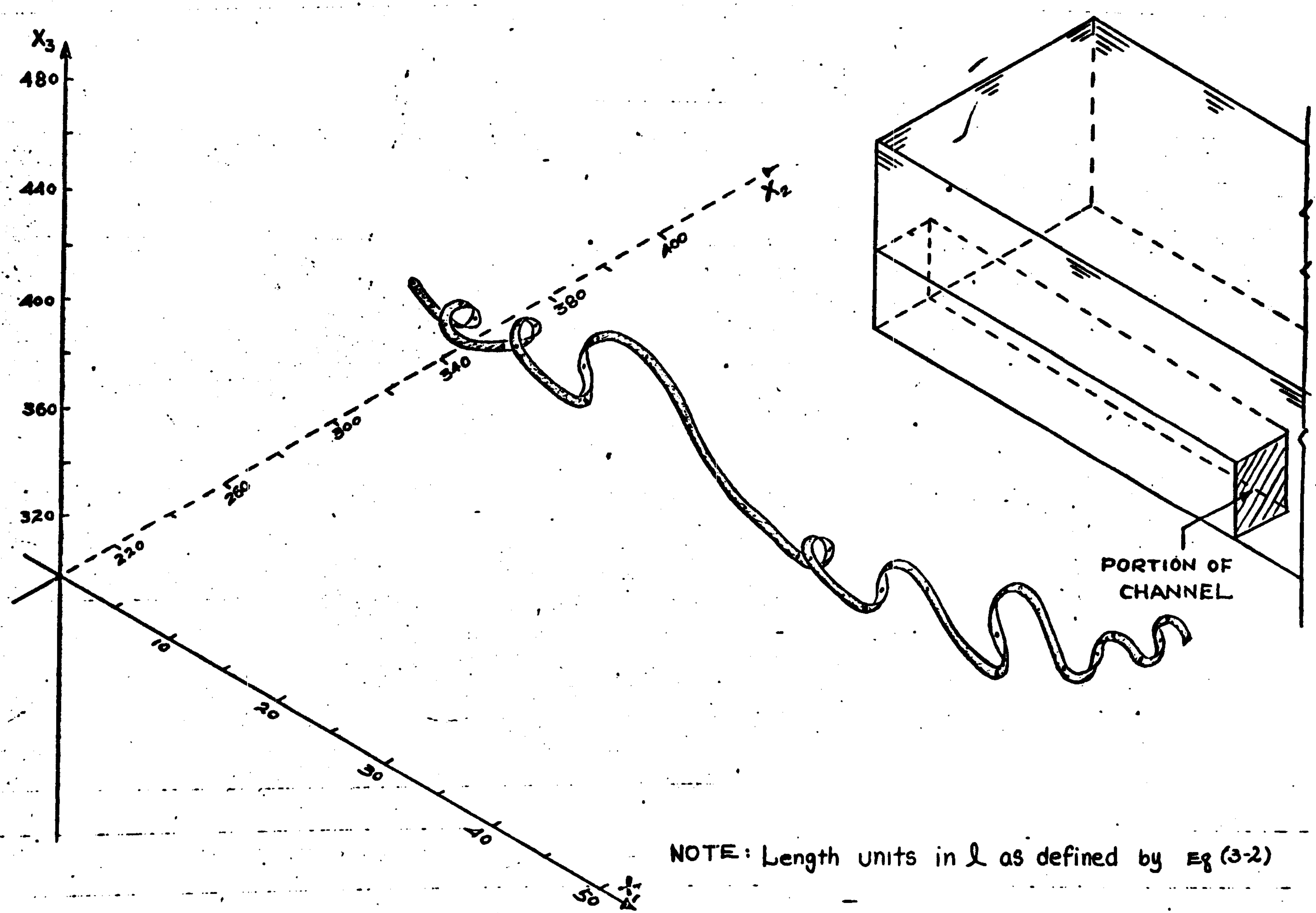
C. Flow Field

The same three dimensional spiral flow field in a corner of a straight rectangular channel as in McSparran's[10] experiment was considered in this study. In such a flow condition the the parameters α, c, n and k in equations (3-7), (3-8) and (3-15) were determined to be 2.5, 4.43, 5.59 and 0.277 respectively. These values were used in this study for calculating secondary velocities. The maximum primary flow was 4.35. It was also found that Von Karman's formula for turbulent shear was valid only for ξ values greater than 0.16 when α = 2.5 and that equation (3-8) describes the primary isovels very well only in the region bounded by ξ =0., ξ =0.36 and η =$\pm$.020. Therefore, this study was limitted in the region bounded by ξ = 0.16, ξ = 0.36, and η =$\pm$0.020.

D. Result of Computer Simulation

1. The path of a single particle

In order to understand in detail the transport process of suspended solid particles in a three dimensional spiral flow, it is desirable to investigate the path of a single solid particle. A calculated sample particle path is shown in Fig. 4-2, which describes a helical motion. Figs. 4-3, 4-4 and 4-5 show the projection of the particle path on the x_1-x_2, x_2-x_3 and x_1-x_3 planes respectively. The equations for the particle paths in the x_1-x_2, x_2-x_3 and x_1-x_3 planes were determined by the method of least squares.



NOTE: Length units in ℓ as defined by Eq (3-2)

Fig. 4-2 THE PATH OF A SINGLE PARTICLE

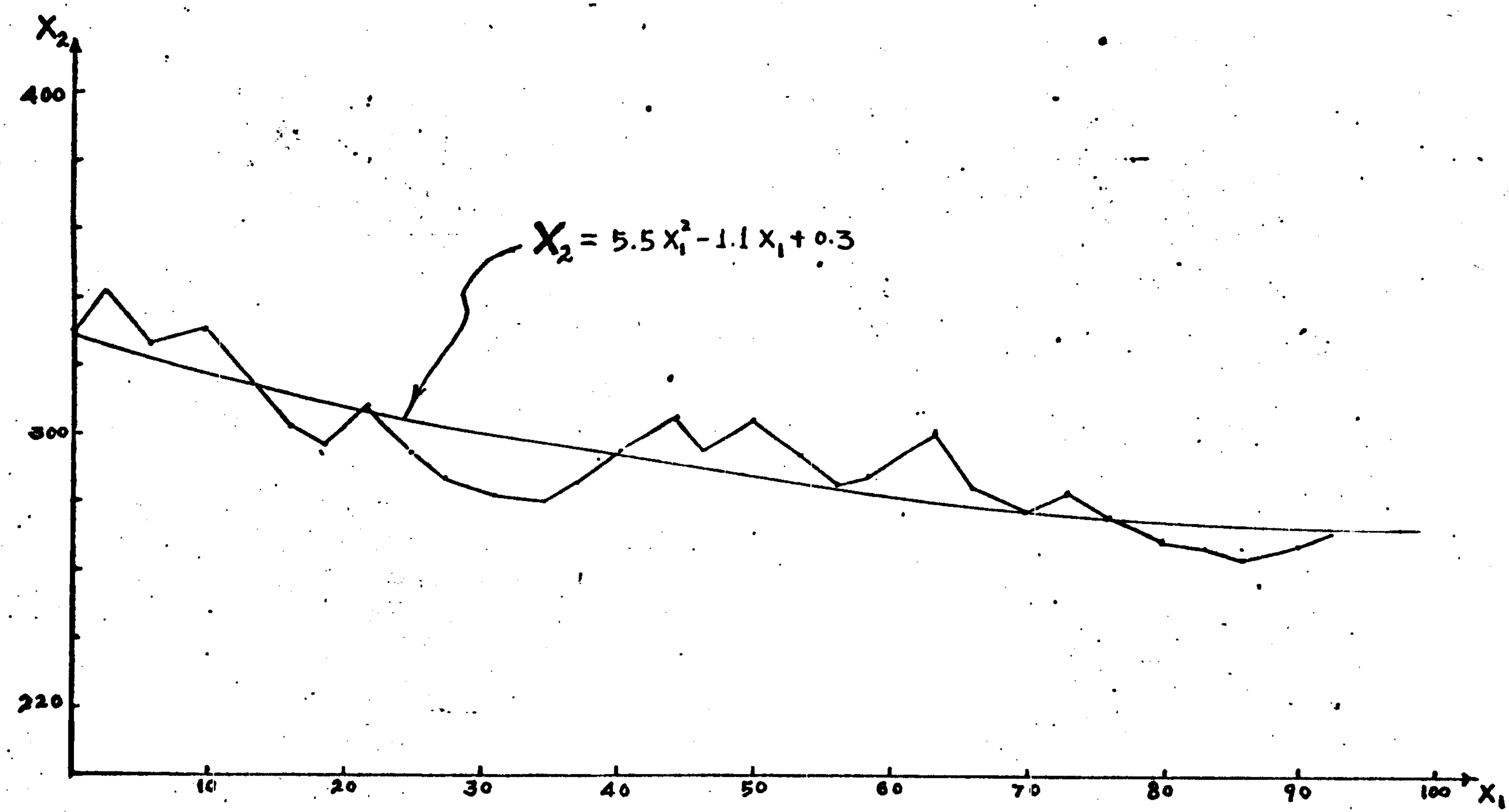


Fig. 4-3 THE PATH OF A SINGLE PARTICLE IN X_1–X_2 PLANE

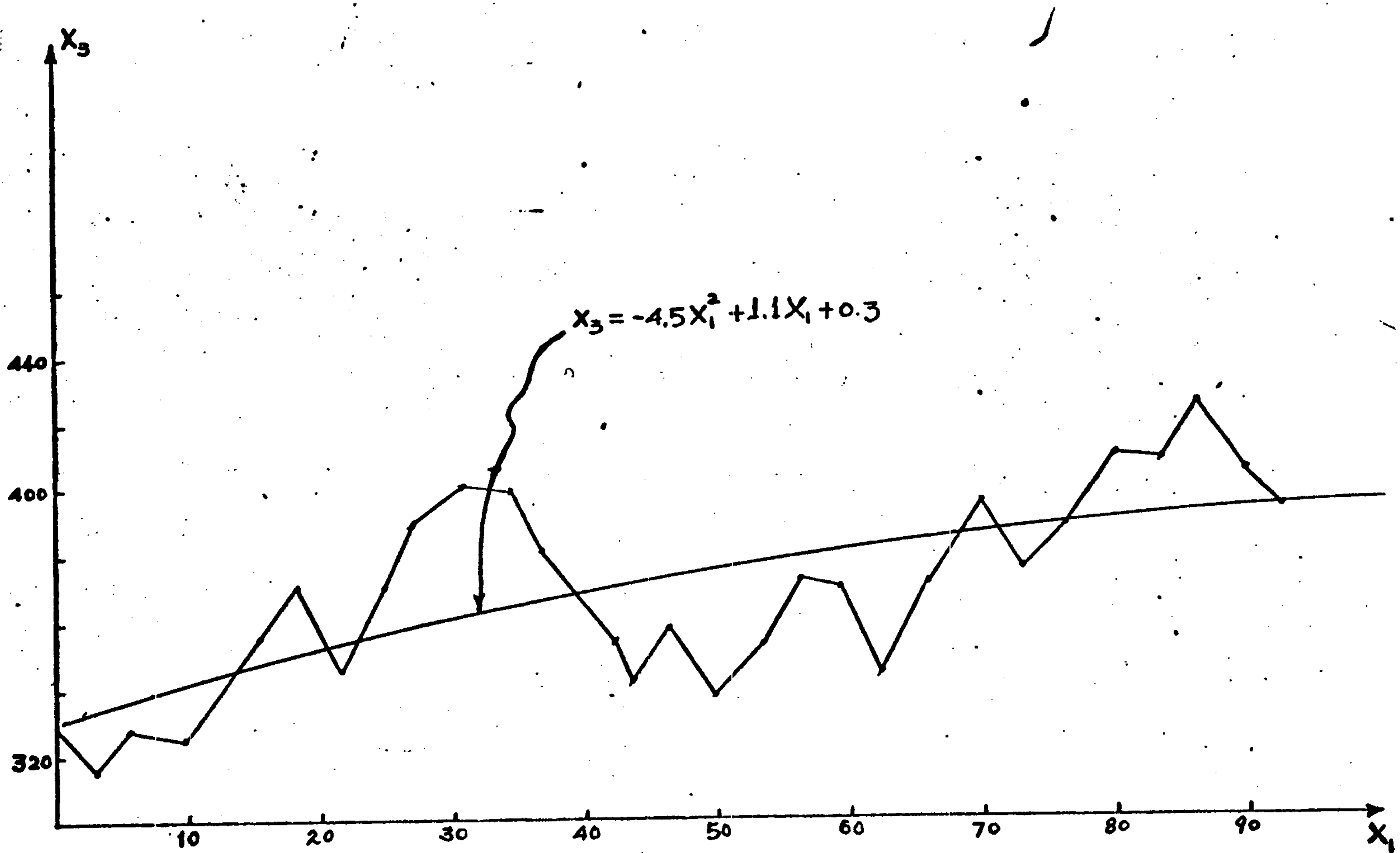


Fig. 4-4 THE PATH OF A SINGLE PARTICLE IN X_1-X_3 PLANE

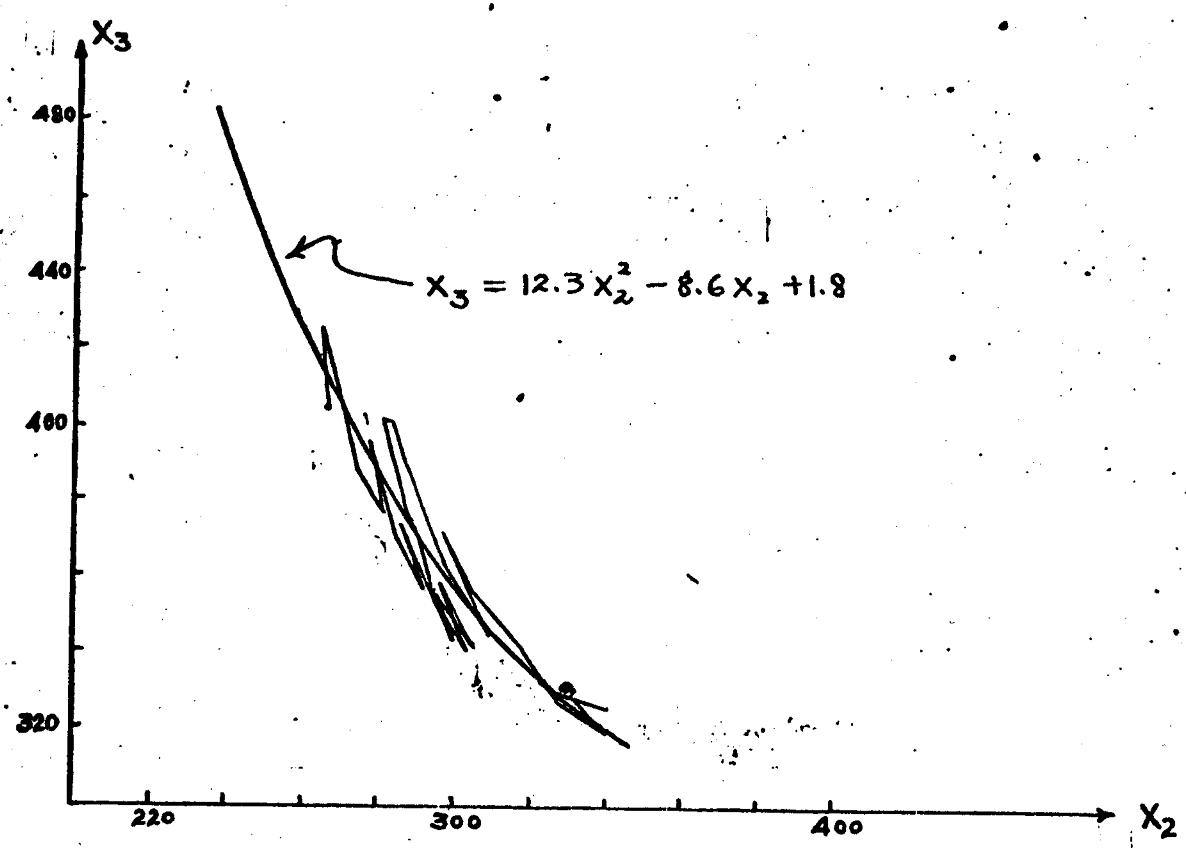


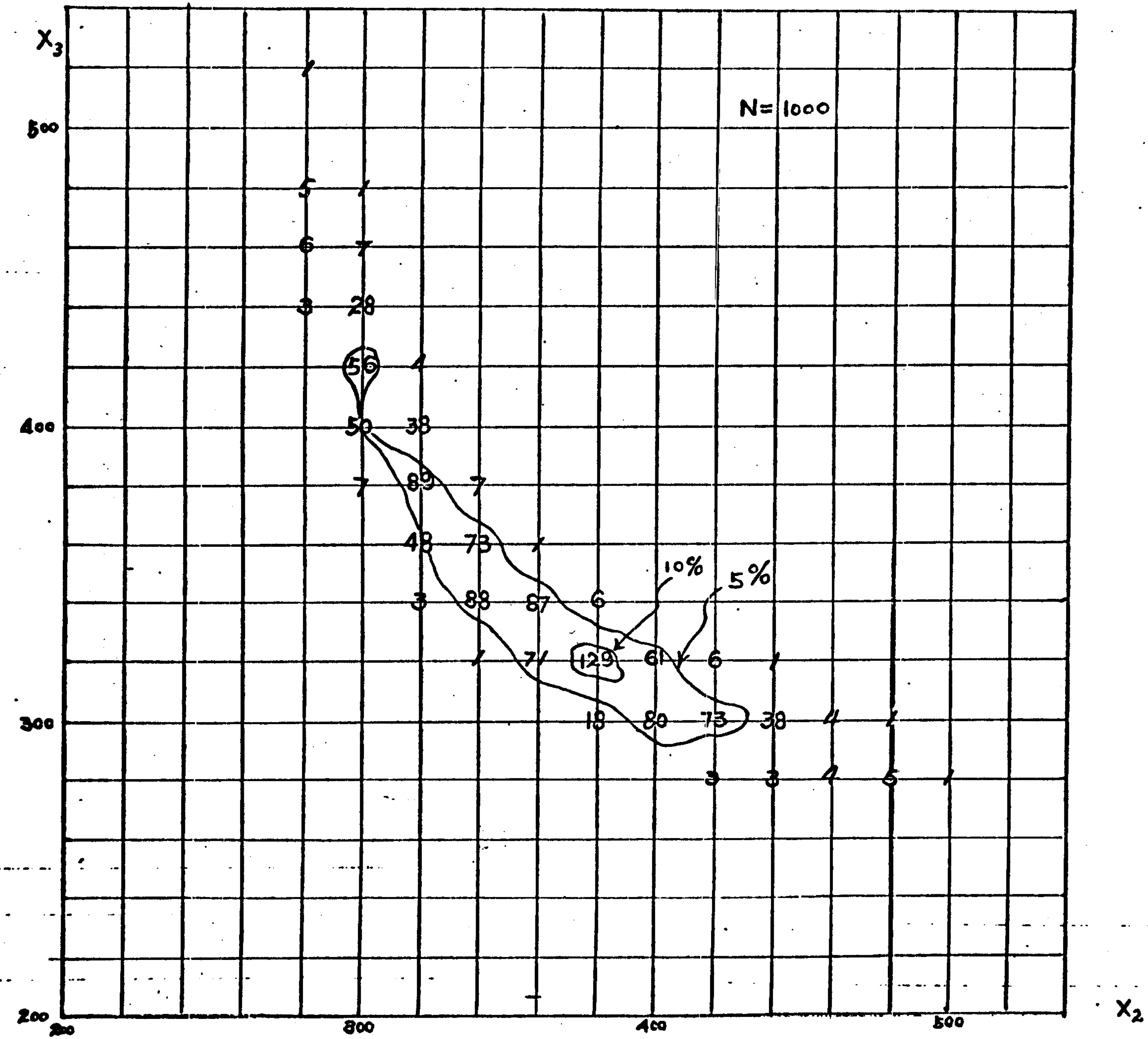
Fig. 4-5 THE PATH OF A SINGLE PARTICLE IN X_2-X_3 PLANE

2. Isopleth patterns

A typical set of results of computer simulation is presented in Figs. 4-6 through 4-13. This set of results is the Monte Carlo estimates of the solutions of the diffusion equation of solid particles (i, e, eq 2-14). Shown in the figures, for a selected time and a distance interval Δx_1, are the numbers of particles Ni (in thousandths of the source emission N) inside each 20 x 20 x 20 grid. In other words, Ni/N is the probability that a particle inside each grid at the instant t. Points of equal Ni/N were connected, for selected values of Ni/N, by isopleths. The local concentration c can be obtained by dividing Ni by the volume Vi (= 20 x 20 x 20) of each grid.

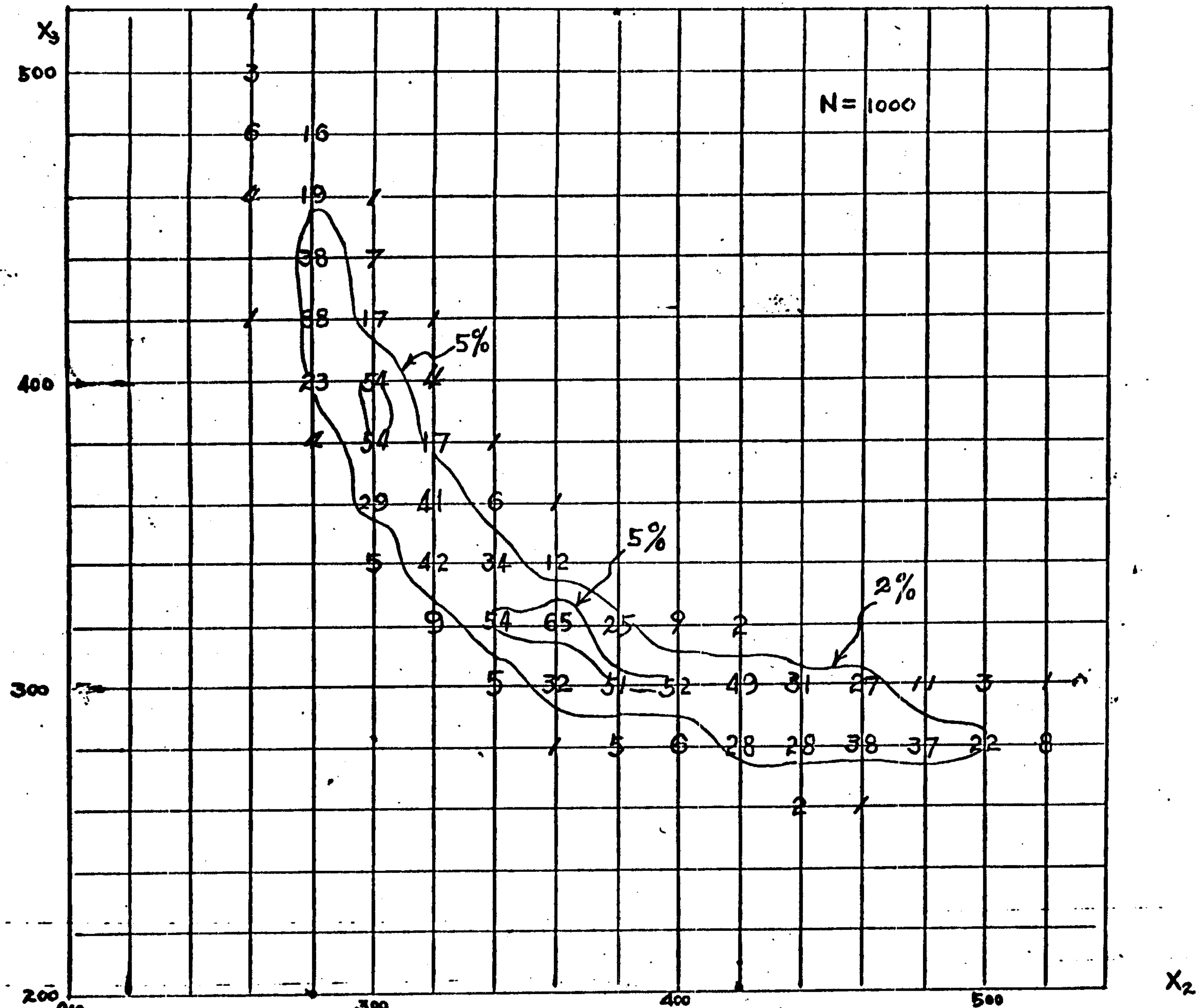
Figs.4-6 through 4-13 show isopleth patterns, which represent a solution to a diffusion problem. It can be seen that after t = 150 the isopleths are separated into two different systems, in a manner quite similar to that of secondary flow "cells". As time increases, the particle distribution tends to become uniform. In other words, the diffusion pattern tends to lose the memory of the source. This uniform state is the necessary condition for the application of equation (2-21).

In addition to an examination of isopleth patterns, several statistical parameters describing the diffusion process were analysed. The mass center of the cloud is



$t = 20 \quad 54 < x_1 < 74$

Fig. 4-6 ISOPLETH PATTERN OF THE CLOUD.



$t = 50$ $158 < x_1 < 178$

Fig. 4-7 ISOPLETH PATTERN OF THE CLOUD.

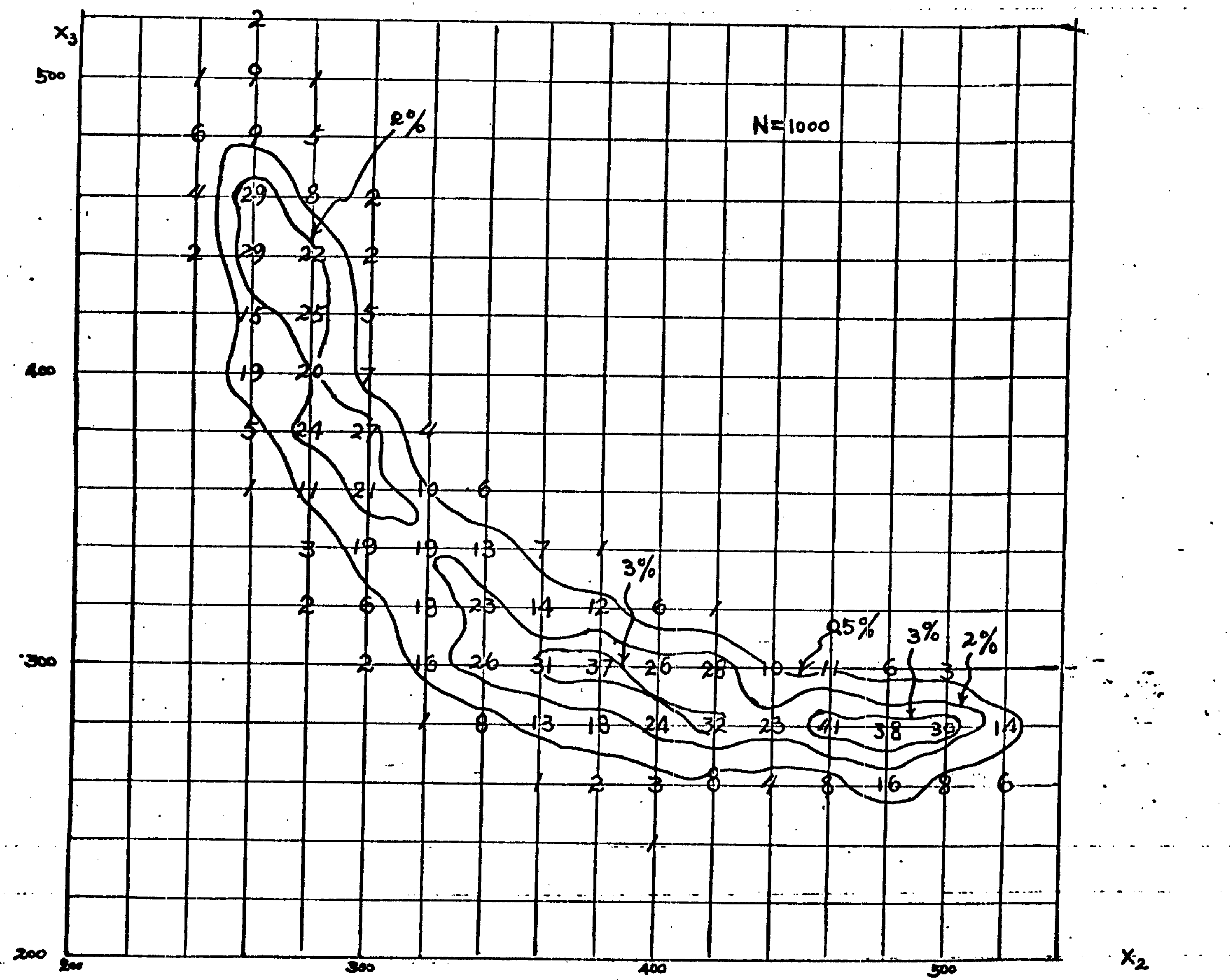


Fig. 4-8 ISOPLETH PATTERN OF THE CLOUD. $t = 80$ $268 < x_1 < 288$

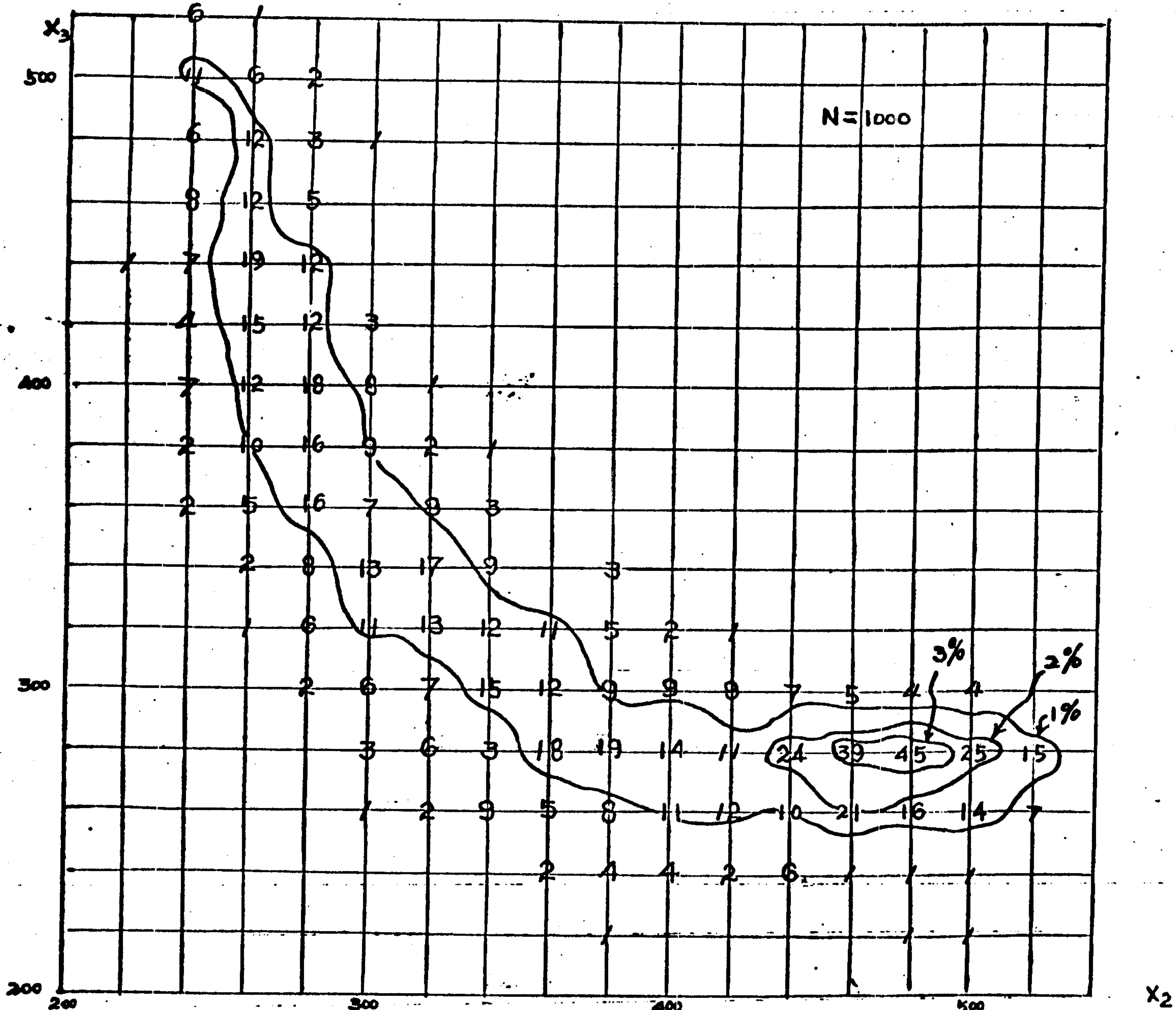


Fig. 4-9. ISOPLETH PATTERN OF THE CLOUD $t = 100$ $329 < x_1 < 349$

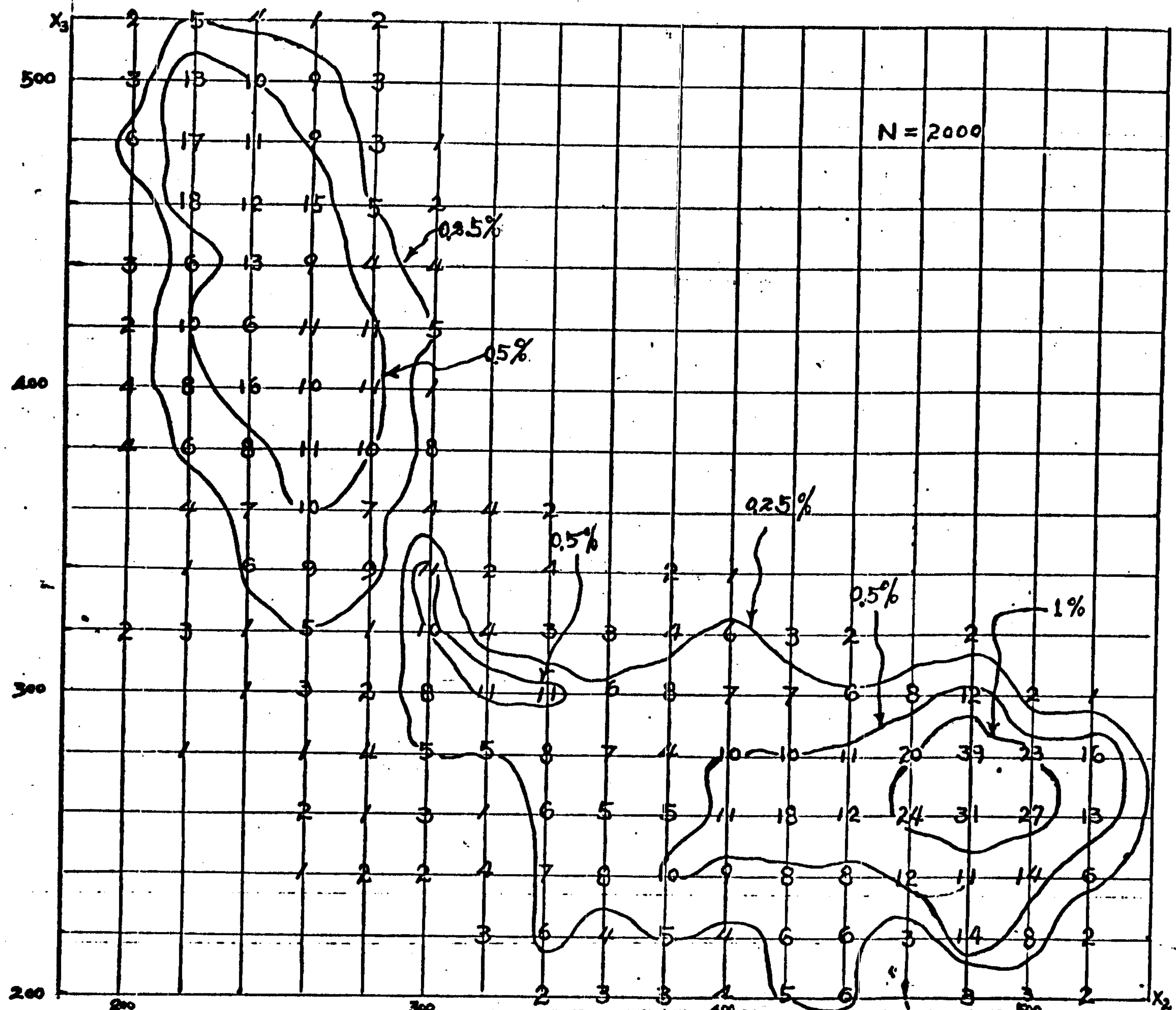


Fig 4-10 ISOPLETH PATTERN OF THE CLOUD $t = 150$ $513 < x_1 < 533$

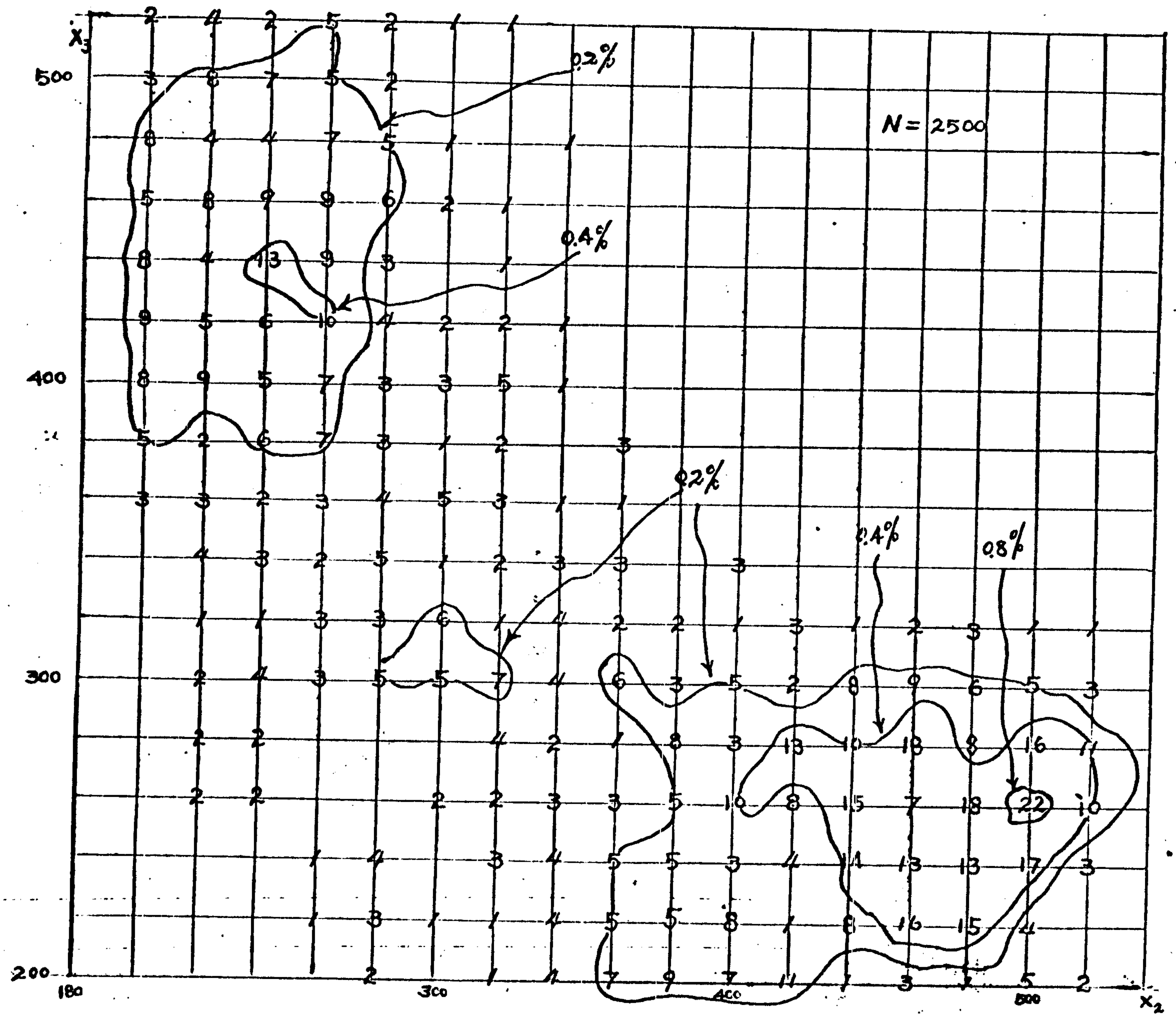


Fig 4-11 ISOPLETH PATTERN OF THE CLOUD

$t = 200$ $690 < X_1 < 710$

Fig 4-12 ISOPLETH PATTERN OF THE CLOUD $t = 250$ $860 < x_1 < 880$

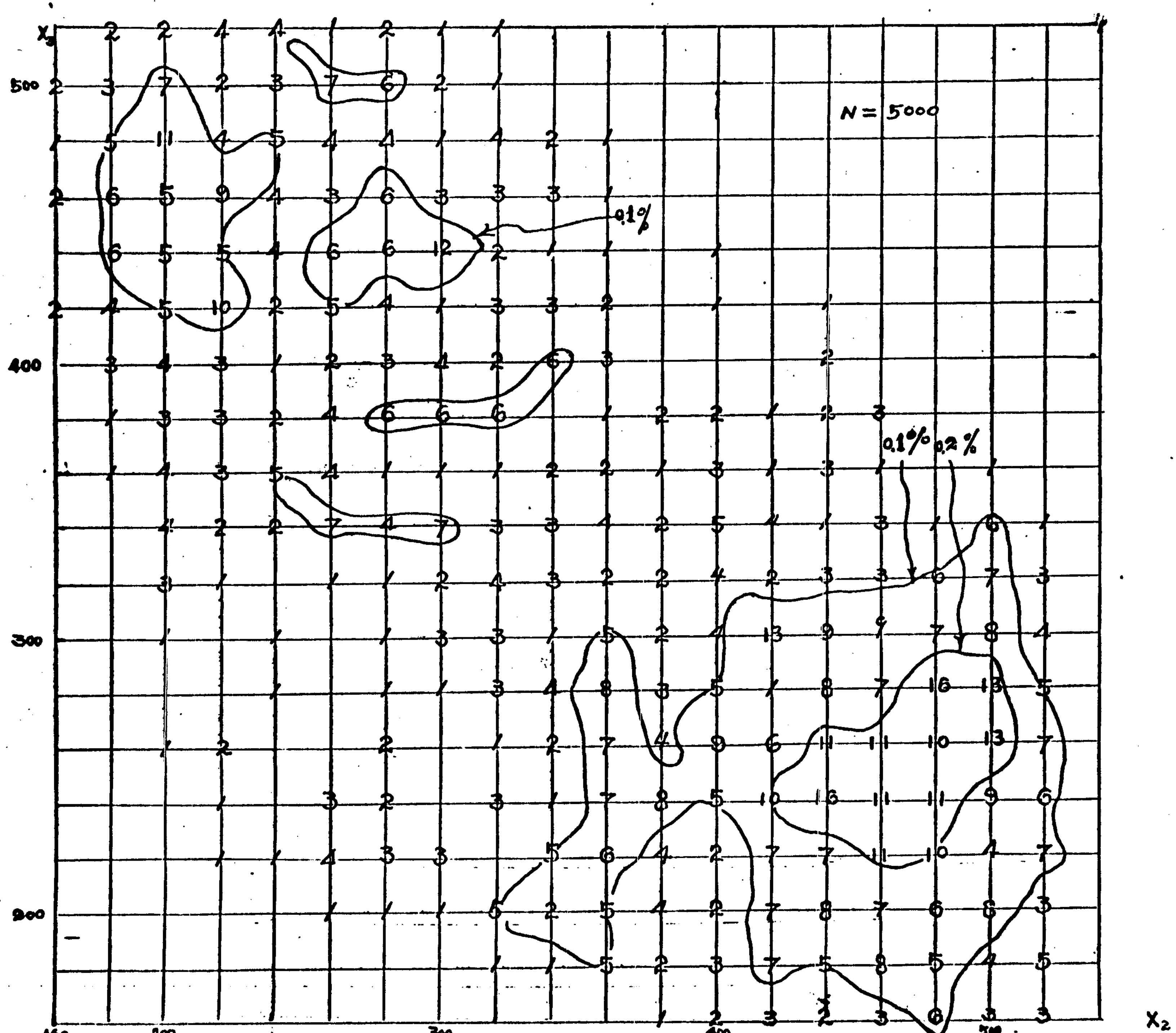


Fig. 4-13 ISOPLETH PATTERN OF THE CLOUD $t = 300$ $1023 < X_1 < 1043$

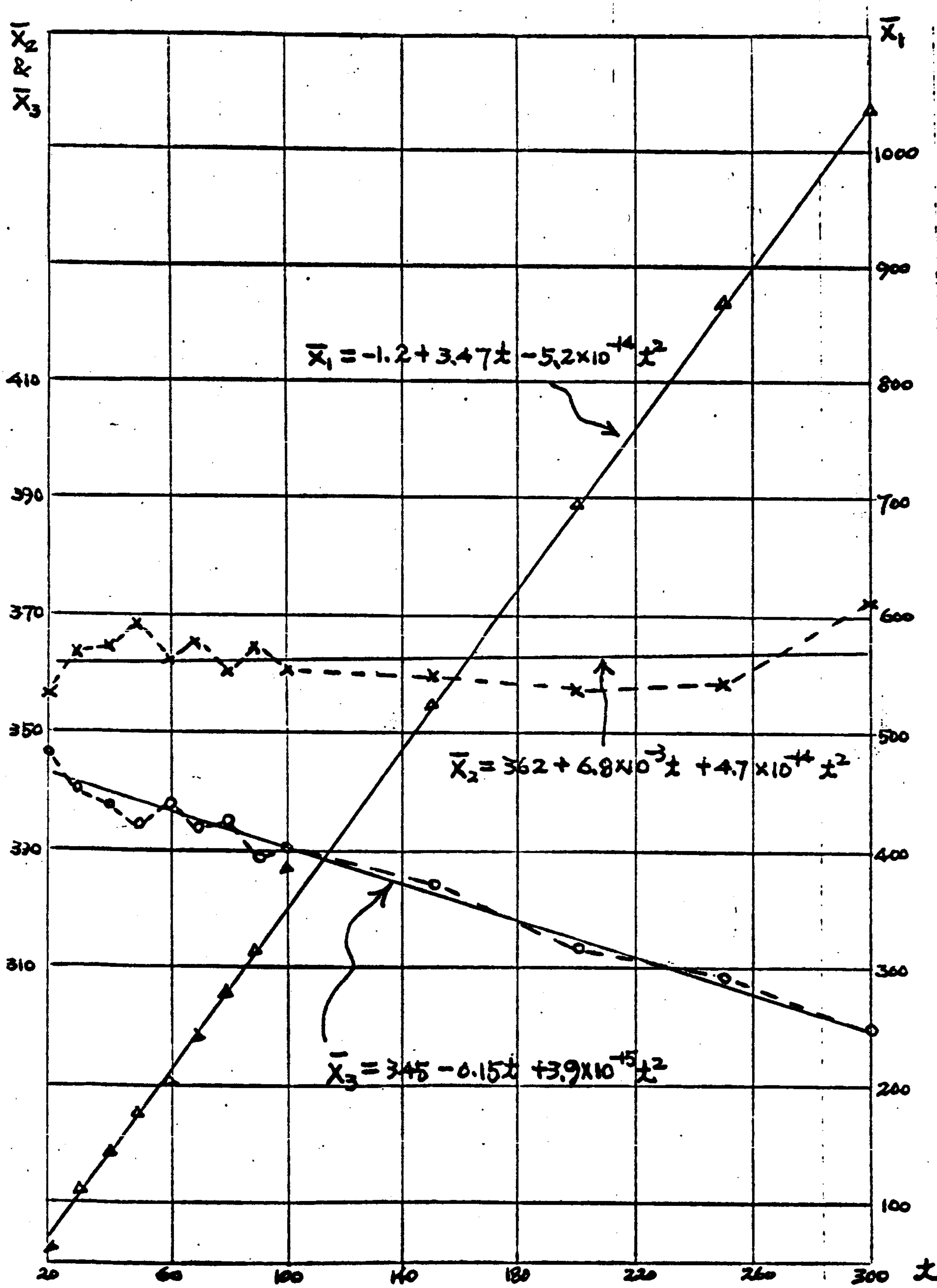


Fig. 4-14 THE MASS CENTER OF THE CLOUD

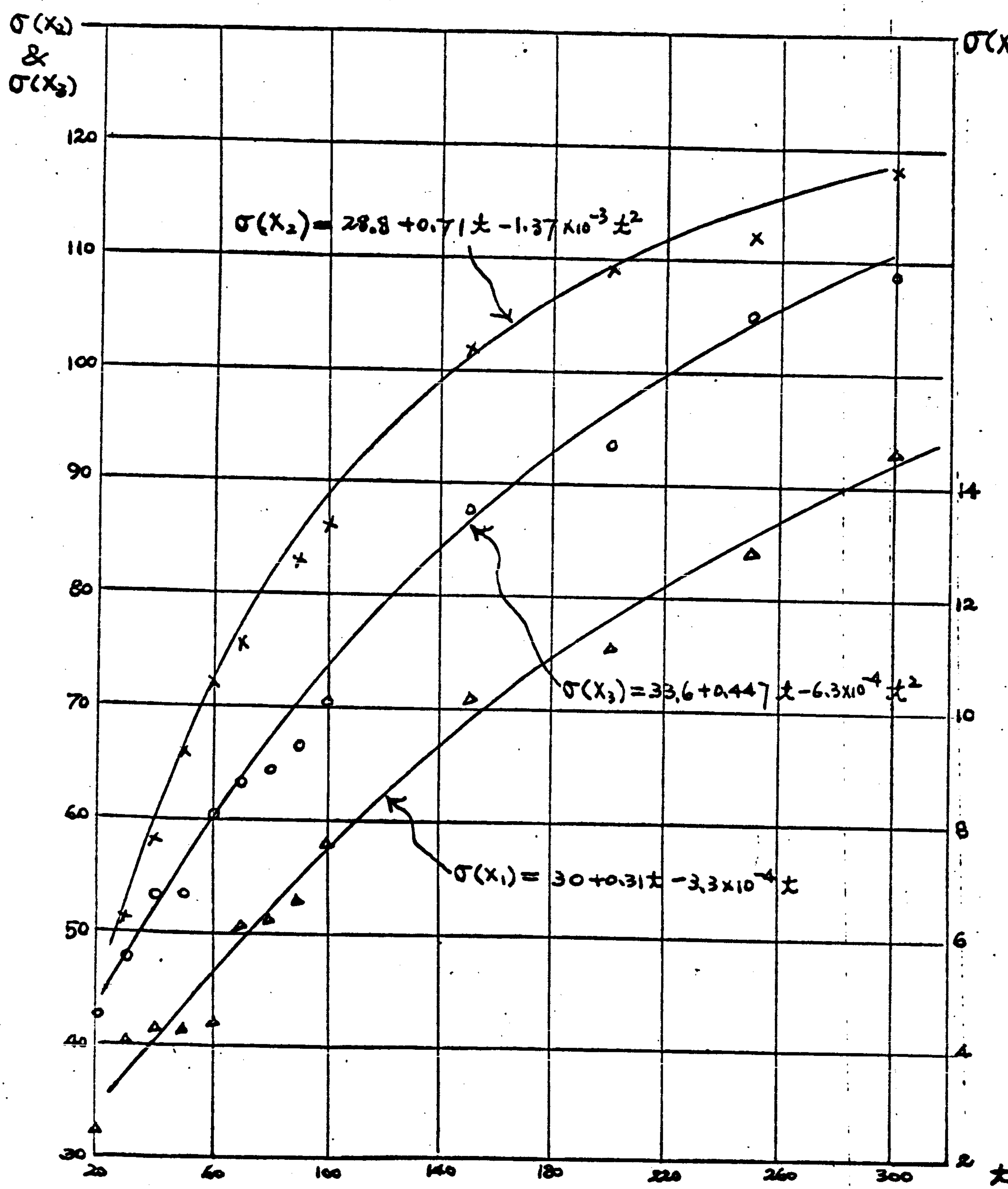


Fig. 4-15 STATISTICAL PARAMETERS DISCRIBING THE SPREAD OF THE CLOUD

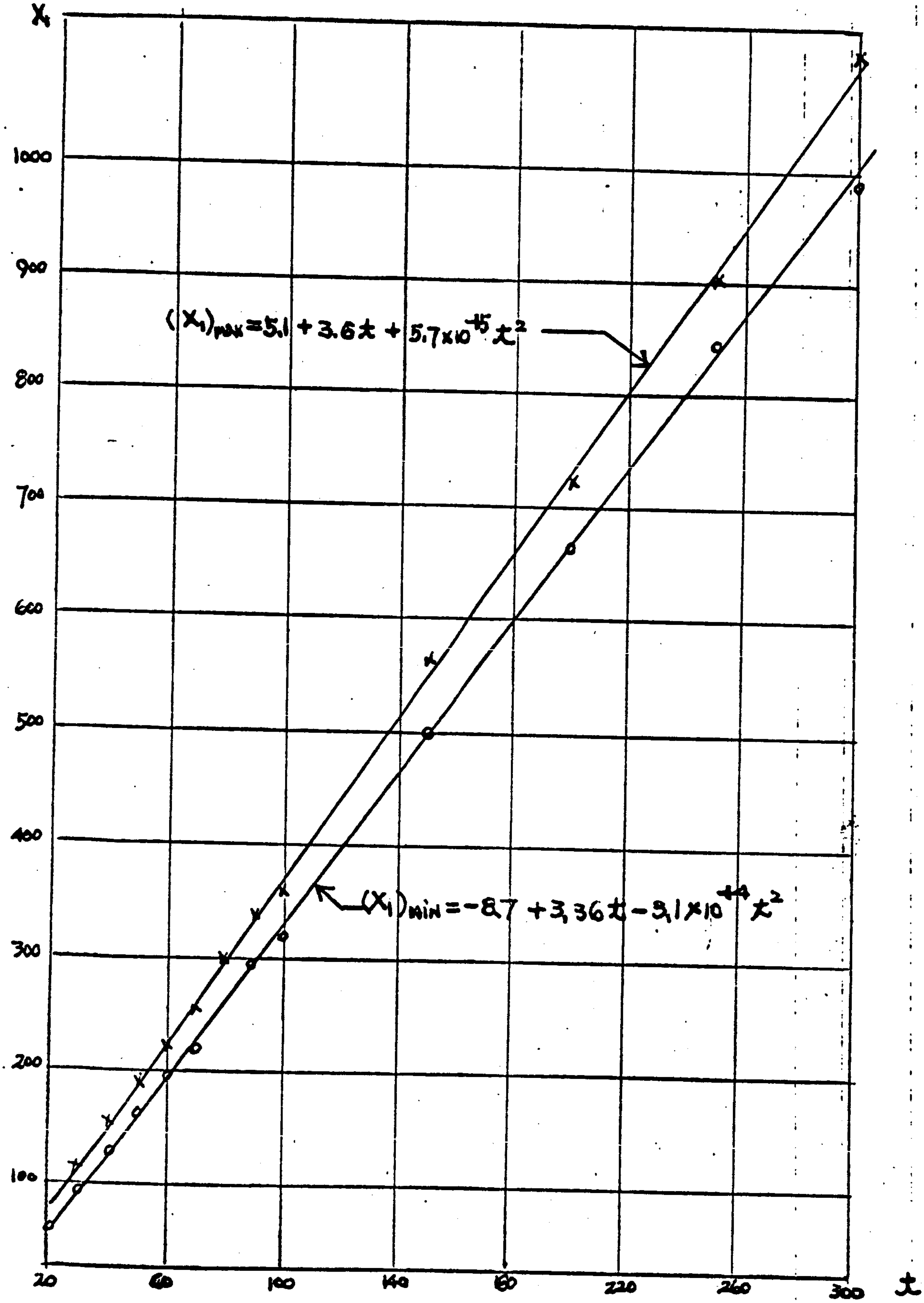


Fig. 4-16 THE MAXIMUM SPREADS OF THE CLOUD IN THE LONGITUDINAL DIRECTION

described in Fig. 4-14, by $\bar{x}_1, \bar{x}_2, \bar{x}_3$, at a time t. Three measures of the spread of the cloud are shown in Fig. 4-15. A measure of the longitudinal spread of the cloud is given by the standard deviation $\sigma(x_1)$ of the diffusing particles about the mass center. The measures of the transversal and vertical spreads of the cloud about the mass center are represented by $\sigma(x_2)$ and $\sigma(x_3)$, respectively. The best fitted line is determined by the least square method for each case. In Fig. 4-16 Xmax and Xmin indicate the positions of the most and least advanced particles of the cloud, contributing significant information concerning the diffusion process.

The computing time required to get the result for a plot of isopleth pattern for $t = 100$ and $N = 1000$ is about 160 minutes on IBM 7090 digital computer. The computing time increases as t or N increases. For example, for $t = 300$ and $N = 5000$ (as in Fig. 4-13), the computing time is about 1500 minutes.

V CONCLUSION

1. The stochastic model has given a solution to the problem of initial phase of the transport of solid particles in a corner of a straight rectangular channel. This has led to a belief that the mechanics of the transport of solid particles in a corner of a straight channel, as developed in this study by a stochastic process study, is promising. A summary of the theory established follows:

(a) The established stochastic model consists of pure random and deterministic processes. The pure random process represents the random walk of the particles at the presence of the fluid turbulence. The deterministic process is represented the transport of solid particles due to the gravity force and primary and secondary flows.

(b) A three dimensional diffusion equation of solid particles (i, e, eq (2-14)) has been developed by random walk method. It is a quite general diffusion equation. The one dimensional diffusion equation (eq 2-34) which can be found easily in the literature and the sediment diffusion equation (eq 2-37) are just two particular cases of it.

(c) The Monte Carlo method can be employed to solve the diffusion equation (eq 2-14). It appears that this is the only feasible method at present (1966) to solve (eq 2-14) without any experiential values.

(d) The motion of a single diffusing particle exhibits a spiral form. This indicates that the transport of a single particle is in-fluenced by secondary flow which makes its motion spiral.

(e) The diffusion of a cloud of solid particles emitted from a point source results in a particle distribution represented by isopleth pattern which is quite similar to secondary flow "cells".

2. It is believed that the diffusion coefficient as defined in equation (2-15) and the time required to reach uniform state, which are two important parameters of the diffusion process, can be determined by a further study. These investigations will be carried out in a subsequent research.

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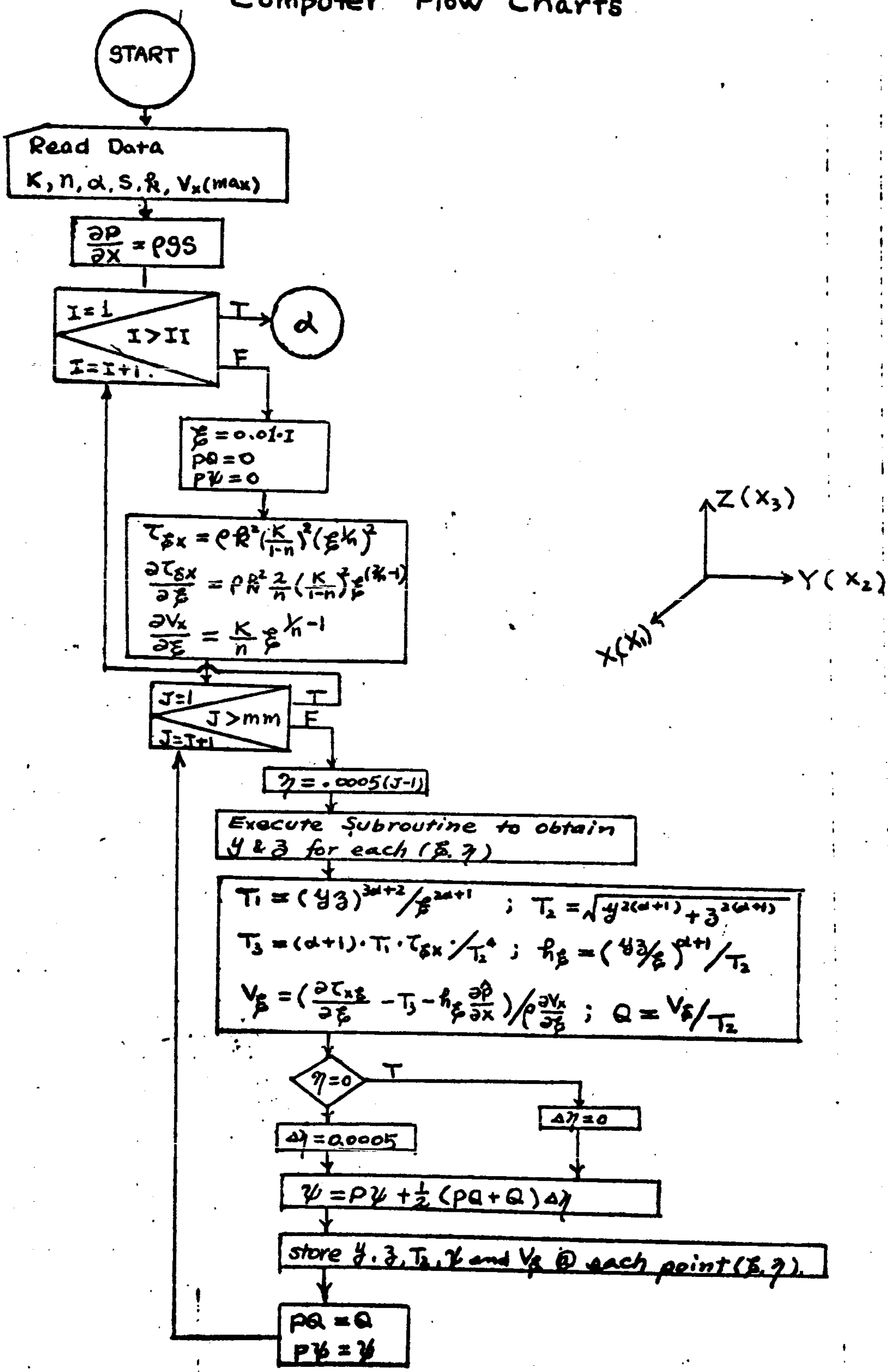
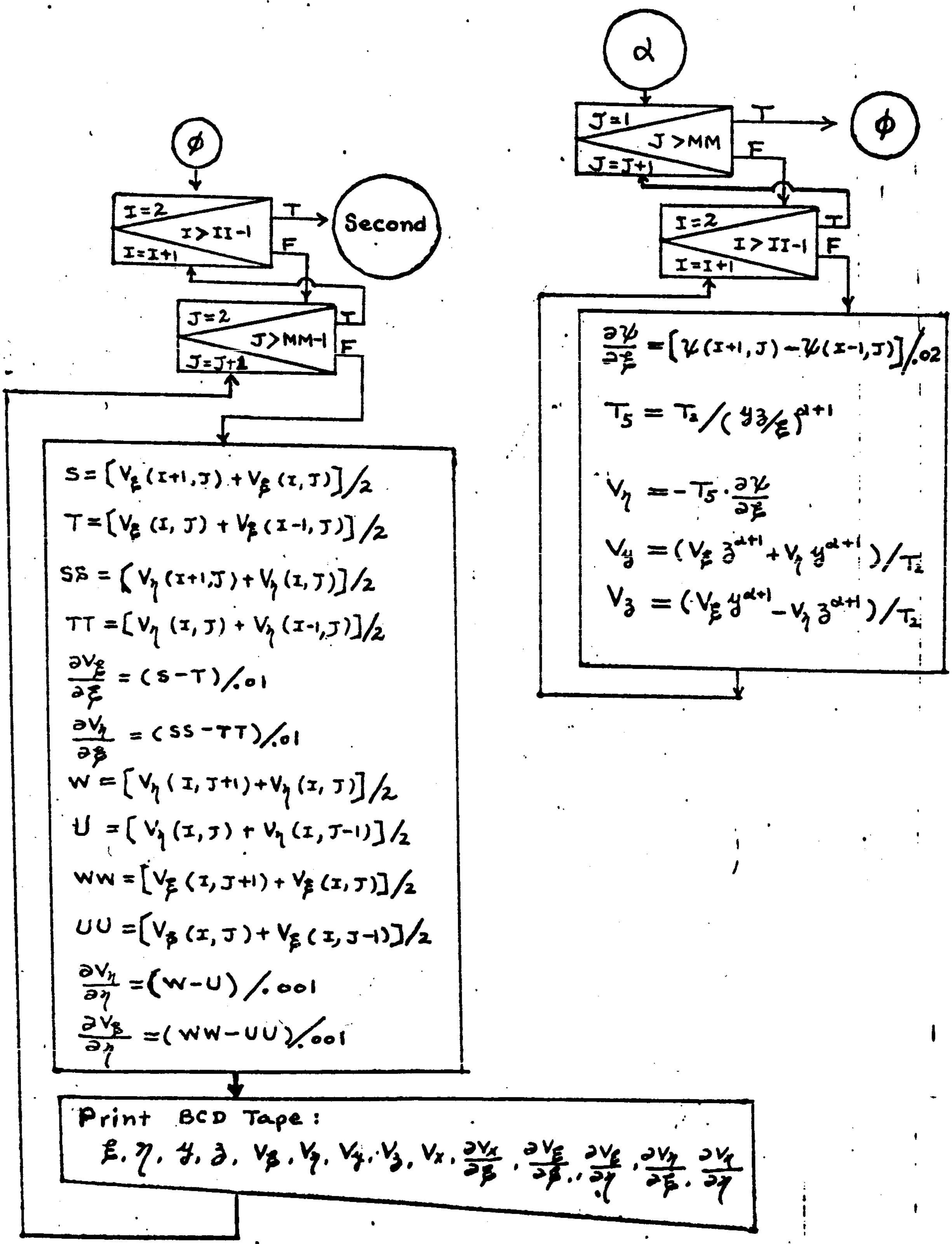
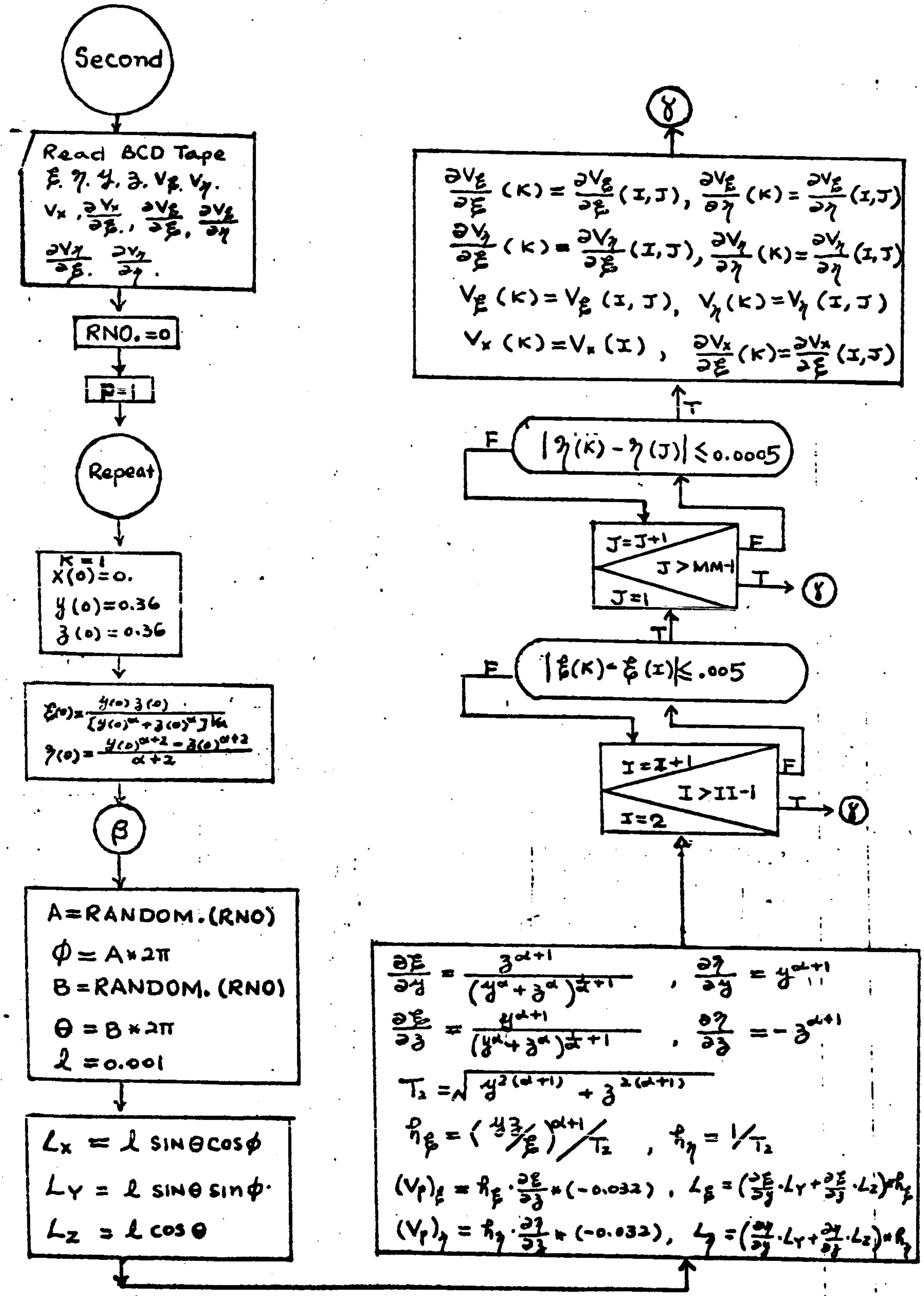
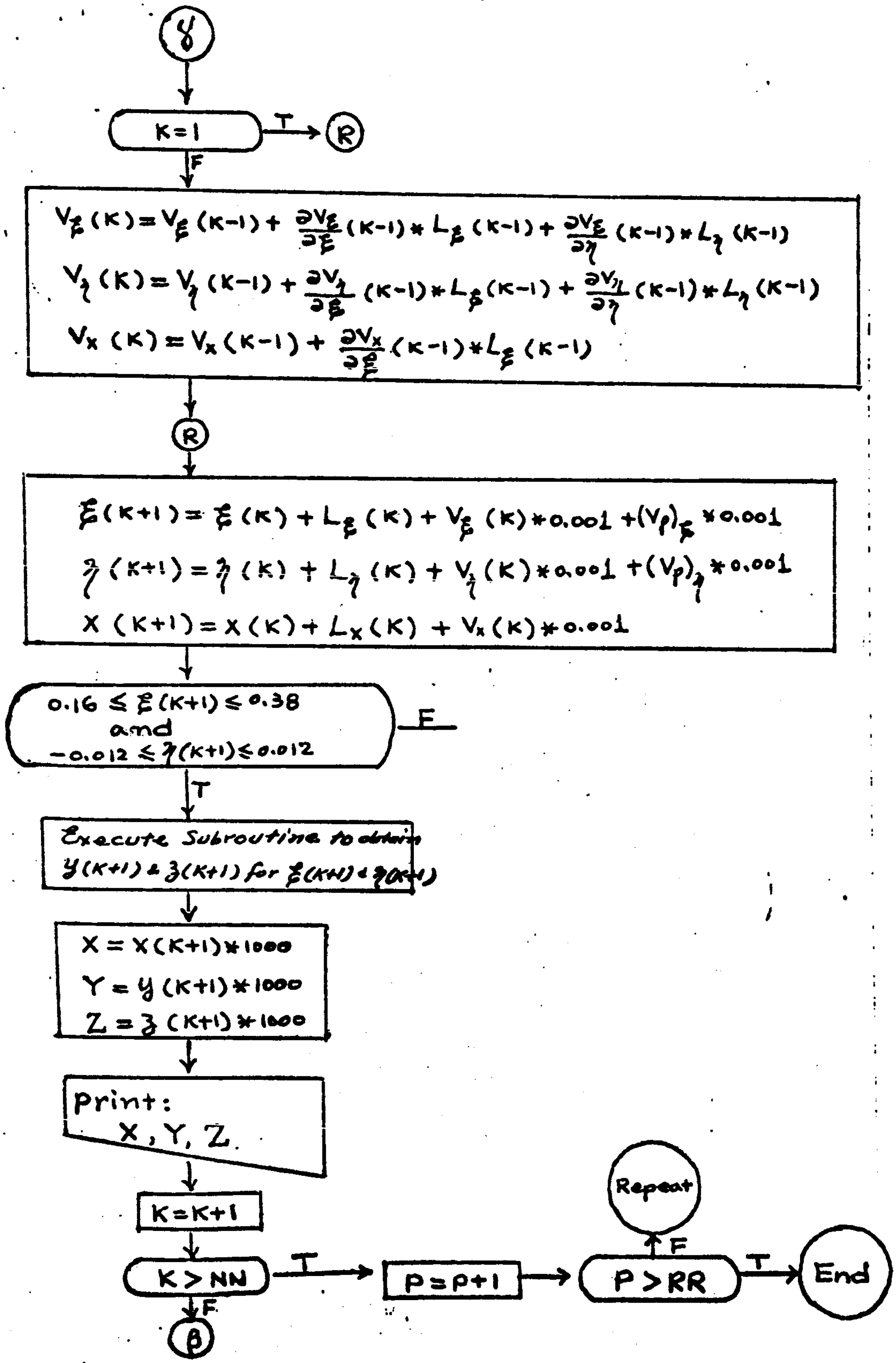
Appendix I

Computer Flow Charts



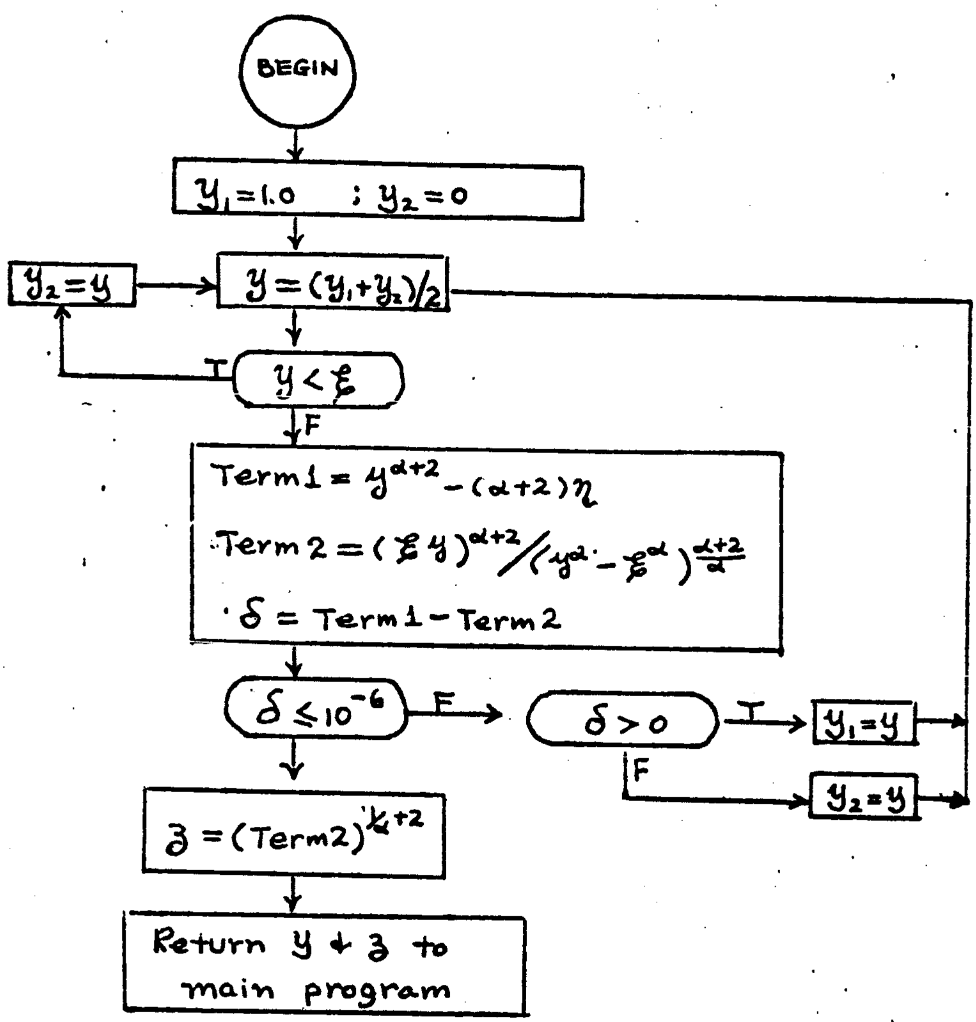

φ
I=2
I>II-1
I=I+1
T
Second
F
J=2
J>MM-1
J=J+1
T
F
S=[Vξ(I+1,J)+Vξ(I,J)]/2
T=[Vξ(I,J)+Vξ(I-1,J)]/2
SS=[Vη(I+1,J)+Vη(I,J)]/2
TT=[Vη(I,J)+Vη(I-1,J)]/2
∂Vξ/∂ξ=(S-T)/.01
∂Vη/∂ξ=(SS-TT)/.01
W=[Vη(I,J+1)+Vη(I,J)]/2
U=[Vη(I,J)+Vη(I,J-1)]/2
WW=[Vξ(I,J+1)+Vξ(I,J)]/2
UU=[Vξ(I,J)+Vξ(I,J-1)]/2
∂Vη/∂η=(W-U)/.001
∂Vξ/∂η=(WW-UU)/.001
Print BCD Tape:
ξ, η, y, z, Vξ, Vη, Vy, Vz, Vx, ∂Vx/∂ξ, ∂Vξ/∂ξ, ∂Vξ/∂η, ∂Vη/∂ξ, ∂Vx/∂η
α
J=1
J>MM
J=J+1
T
φ
F
I=2
I>II-1
I=I+1
T
F
∂ψ/∂ξ=[ψ(I+1,J)-ψ(I-1,J)]/.02
T5=T2/(yz/ξ)^(α+1)
Vη=-T5·∂ψ/∂ξ
Vy=(Vξ z^(α+1)+Vη y^(α+1))/T2
Vz=(Vξ y^(α+1)-Vη z^(α+1))/T2


Second
Read BCD Tape
ξ, η, y, z, Vξ, Vη,
Vx, ∂Vx/∂ξ, ∂Vξ/∂ξ, ∂Vξ/∂η
∂Vη/∂ξ, ∂Vη/∂η.
RNO.=0
P=1
Repeat
K=1
X(0)=0.
y(0)=0.36
z(0)=0.36
ξ(0)=y(0)z(0)/[y(0)^α+z(0)^α]^{1/α}
η(0)=(y(0)^{α+2}−z(0)^{α+2})/(α+2)
β
A=RANDOM.(RNO)
φ=A*2π
B=RANDOM.(RNO)
θ=B*2π
l=0.001
Lx = l SINθ COSφ
LY = l SINθ SINφ
Lz = l COSθ
∂ξ/∂y = z^{α+1}/(y^α+z^α)^{1/α+1}, ∂η/∂y = y^{α+1}
∂ξ/∂z = y^{α+1}/(y^α+z^α)^{1/α+1}, ∂η/∂z = −z^{α+1}
T2 = √(y^{2(α+1)} + z^{2(α+1)})
hξ = (yz/ξ)^{α+1}/T2, hη = 1/T2
(Vp)ξ = hξ·∂ξ/∂z*(−0.032), Lξ = (∂ξ/∂y·LY + ∂ξ/∂z·Lz)*hξ
(Vp)η = hη·∂η/∂z*(−0.032), Lη = (∂η/∂y·LY + ∂η/∂z·Lz)*hη
I=I+1
I>II-1
I=2
T
F
γ
|ξ(K)−ξ(I)| ≤ .005
J=J+1
J>MM-1
J=1
|η(K)−η(J)| ≤ 0.0005
∂Vξ/∂ξ(K) = ∂Vξ/∂ξ(I,J), ∂Vξ/∂η(K) = ∂Vξ/∂η(I,J)
∂Vη/∂ξ(K) = ∂Vη/∂ξ(I,J), ∂Vη/∂η(K) = ∂Vη/∂η(I,J)
Vξ(K) = Vξ(I,J), Vη(K) = Vη(I,J)
Vx(K) = Vx(I), ∂Vx/∂ξ(K) = ∂Vx/∂ξ(I,J)



γ
K=1
T
R
F
$V_\xi(K) = V_\xi(K-1) + \frac{\partial V_\xi}{\partial \xi}(K-1) * L_\xi(K-1) + \frac{\partial V_\xi}{\partial \eta}(K-1) * L_\eta(K-1)$
$V_\eta(K) = V_\eta(K-1) + \frac{\partial V_\eta}{\partial \xi}(K-1) * L_\xi(K-1) + \frac{\partial V_\eta}{\partial \eta}(K-1) * L_\eta(K-1)$
$V_x(K) = V_x(K-1) + \frac{\partial V_x}{\partial \xi}(K-1) * L_\xi(K-1)$
R
$\xi(K+1) = \xi(K) + L_\xi(K) + V_\xi(K) * 0.001 + (V_p)_\xi * 0.001$
$\eta(K+1) = \eta(K) + L_\eta(K) + V_\eta(K) * 0.001 + (V_p)_\eta * 0.001$
$X(K+1) = X(K) + L_x(K) + V_x(K) * 0.001$
$0.16 \leq \xi(K+1) \leq 0.38$
and
$-0.012 \leq \eta(K+1) \leq 0.012$
F
T
Execute Subroutine to obtain
$y(K+1)$ & $z(K+1)$ for $\xi(K+1)$ & $\eta(K+1)$
$X = X(K+1) * 1000$
$Y = y(K+1) * 1000$
$Z = z(K+1) * 1000$
Print:
X, Y, Z.
K=K+1
K > NN
T
F
β
P=P+1
P > RR
F
Repeat
T
End

Subroutine



Notes: 1. Assigned values of y_1 & y_2 depend on the boundary of the region in which the coordinate system is applicable.

2. Assigned value of δ depends on the accuracy required.