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A Precipitation Model and Experimental Correlation with Various Properties of Pentaerythritol Tetranitrate

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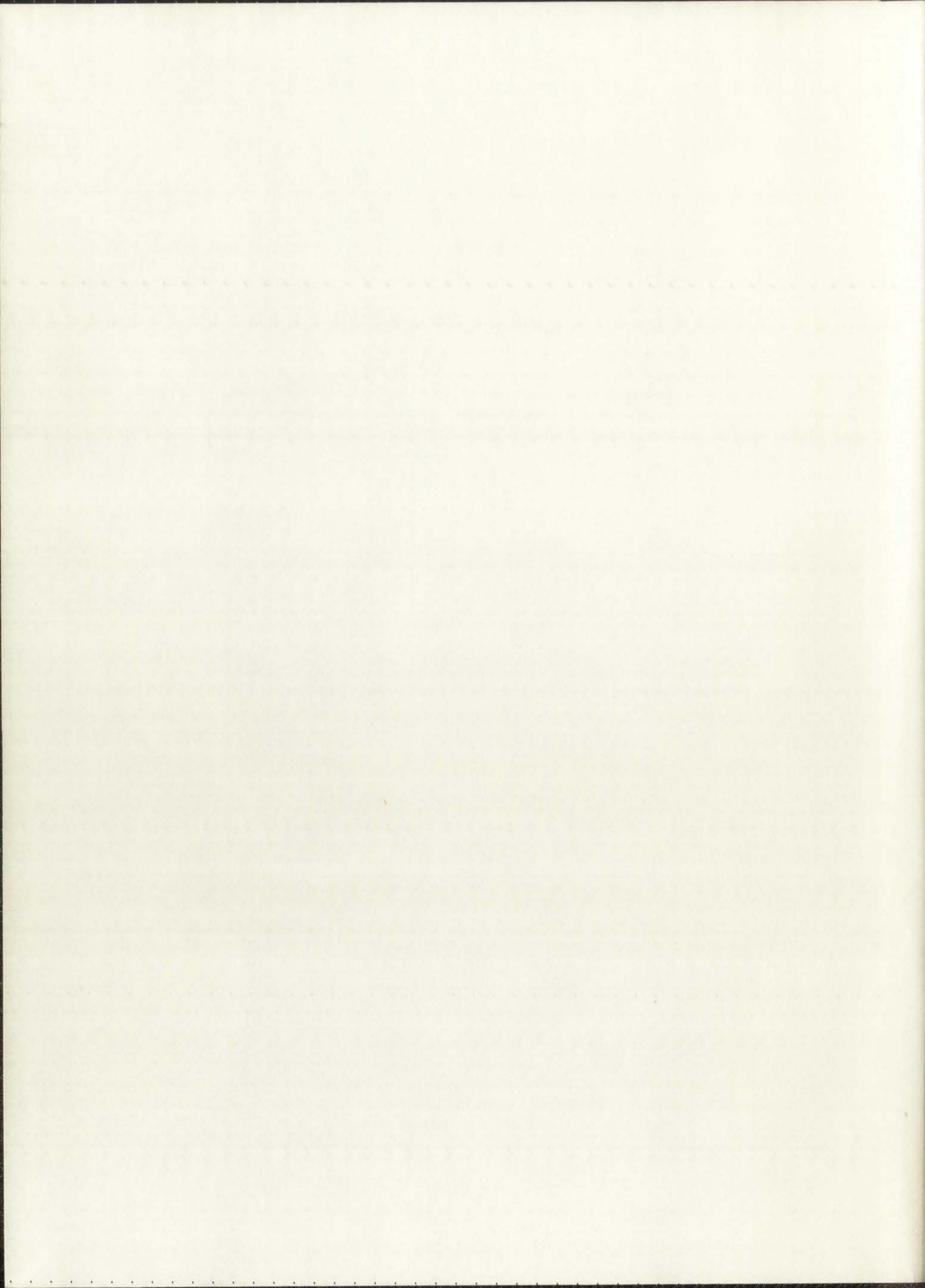
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A PRECIPITATION MODEL. — RIVERA



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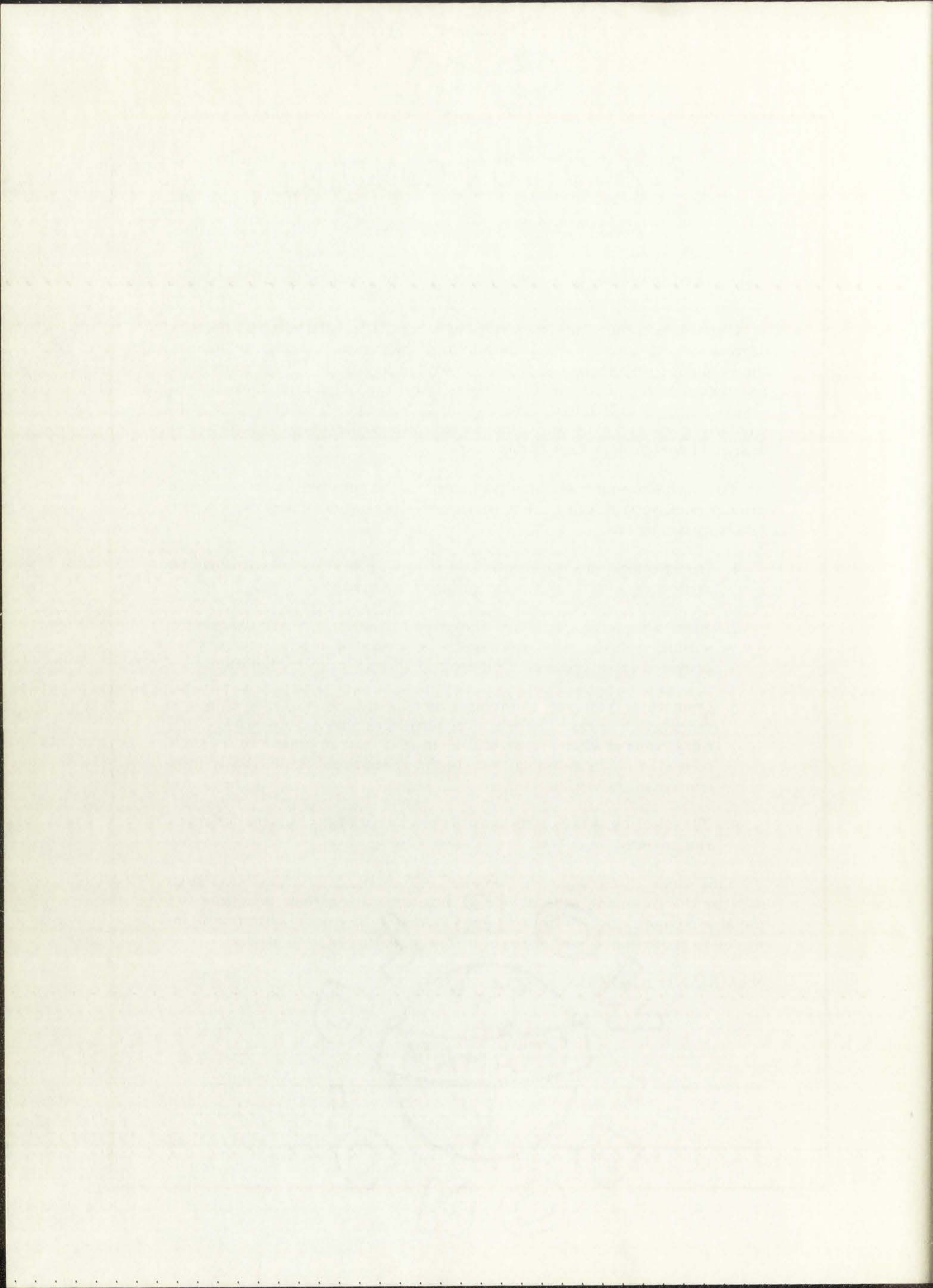
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This dissertation, directed and approved by the candidate's committee, has been accepted by the Graduate Committee of The University of New Mexico in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

A PRECIPITATION MODEL AND EXPERIMENTAL
CORRELATION WITH VARIOUS PROPERTIES OF
Title PENTAERYTHRITOL TETRANITRATE

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A PRECIPITATION MODEL AND EXPERIMENTAL
CORRELATION WITH VARIOUS PROPERTIES OF
PENTAERYTHRITOL TETRANITRATE

BY

THOMAS RIVERA

B.S., College of Santa Fe, 1962

M.S., University of New Mexico, 1971

DISSERTATION

Submitted in Partial Fulfillment of the
Requirements for the Degree of
Doctor of Philosophy in Chemistry

in the Graduate School of
The University of New Mexico
Albuquerque, New Mexico

December, 1975

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To my Mother



ACKNOWLEDGMENTS

A number of people have contributed to this effort. I wish to acknowledge the valuable counsel of Professor Alan D. Randolph who has offered many valuable and detailed suggestions throughout the whole project. My thanks to Dr. Peter G. Salgado for his helpful suggestions in the design of the apparatus, to Dr. William A. Cook for his kind assistance with the mathematics and programming, to Dr. Michael Steuerwalt for his assistance in providing the numerical analyses and programming, and to Robert E. Smith for providing the scanning electron micrographs of the products.

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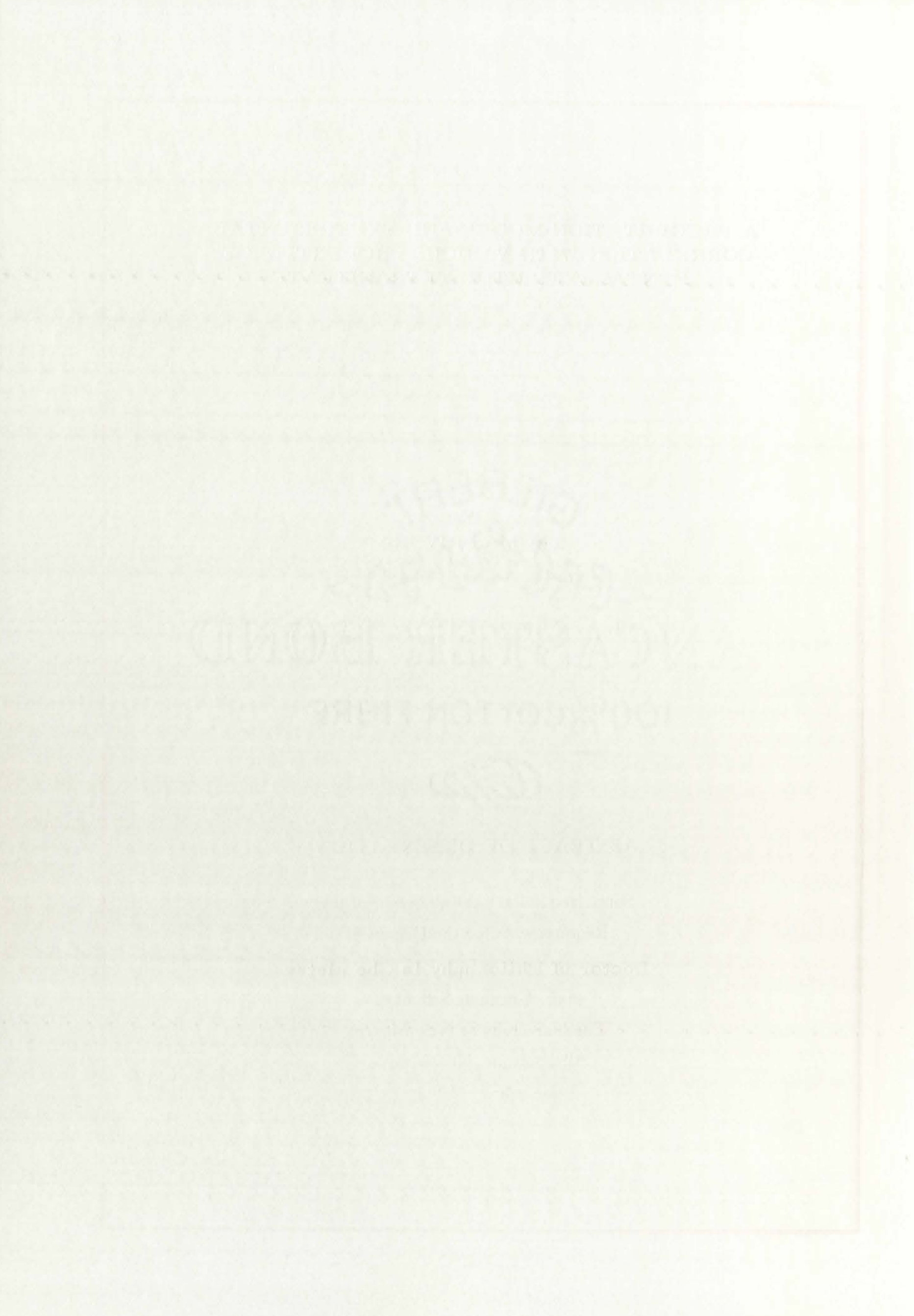
This work was performed at the Los Alamos Scientific Laboratory under the auspices of the Energy Research and Development Administration contract W-7405-ENG-36.

A PRECIPITATION MODEL AND EXPERIMENTAL
CORRELATION WITH VARIOUS PROPERTIES OF
PENTAERYTHRITOL TETRANITRATE

BY
THOMAS RIVERA

ABSTRACT OF DISSERTATION

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PENTAERYTHRITOL TETRANITRATE

Thomas Rivera, Ph. D.
Department of Chemistry
The University of New Mexico, 1975

ABSTRACT

A continuous precipitation method for the preparation of crystalline pentaerythritol tetranitrate (PETN) has been developed. The process involves the precipitation of PETN from an acetone solution by the addition of water in a static mixer. The principal independent variable is the ratio, R , of the acetone-PETN solution flow rate to the flow rate of water.

A mathematical model based on dispersed plug-flow equations adequately represents the physical process. The relationships developed can be used to predict particle size distributions, two explosion properties of PETN, and estimate the effective kinetics involved in the precipitation process. The mass-weighted mean particle size, \bar{L} , of the precipitated PETN is a linear function of R . The initial nucleation and growth rates are exponentially decaying functions of R . The nucleation exponent is 3.75 ± 0.05 ; the growth rate exponent is 1.56 ± 0.02 . The value of the diffusion parameter, Pe , is 51 ± 1 . Experimentally determined PETN initiation-threshold voltages can be expressed as a second degree polynomial in \bar{L} , with a minimum at about $50 \mu\text{m}$. Observed PETN explosion transit times follow a third degree polynomial in \bar{L} , increasing with increasing particle size.

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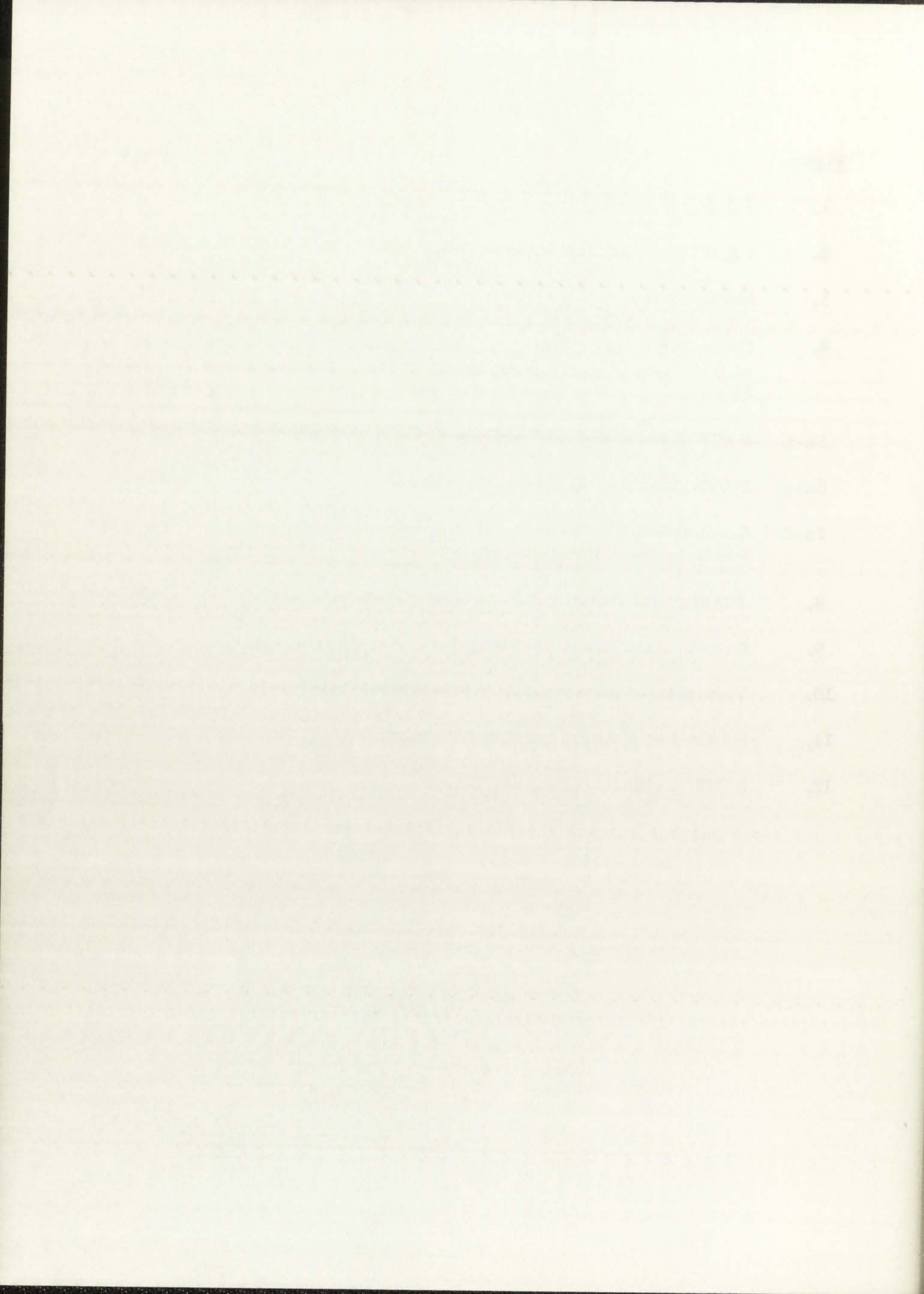
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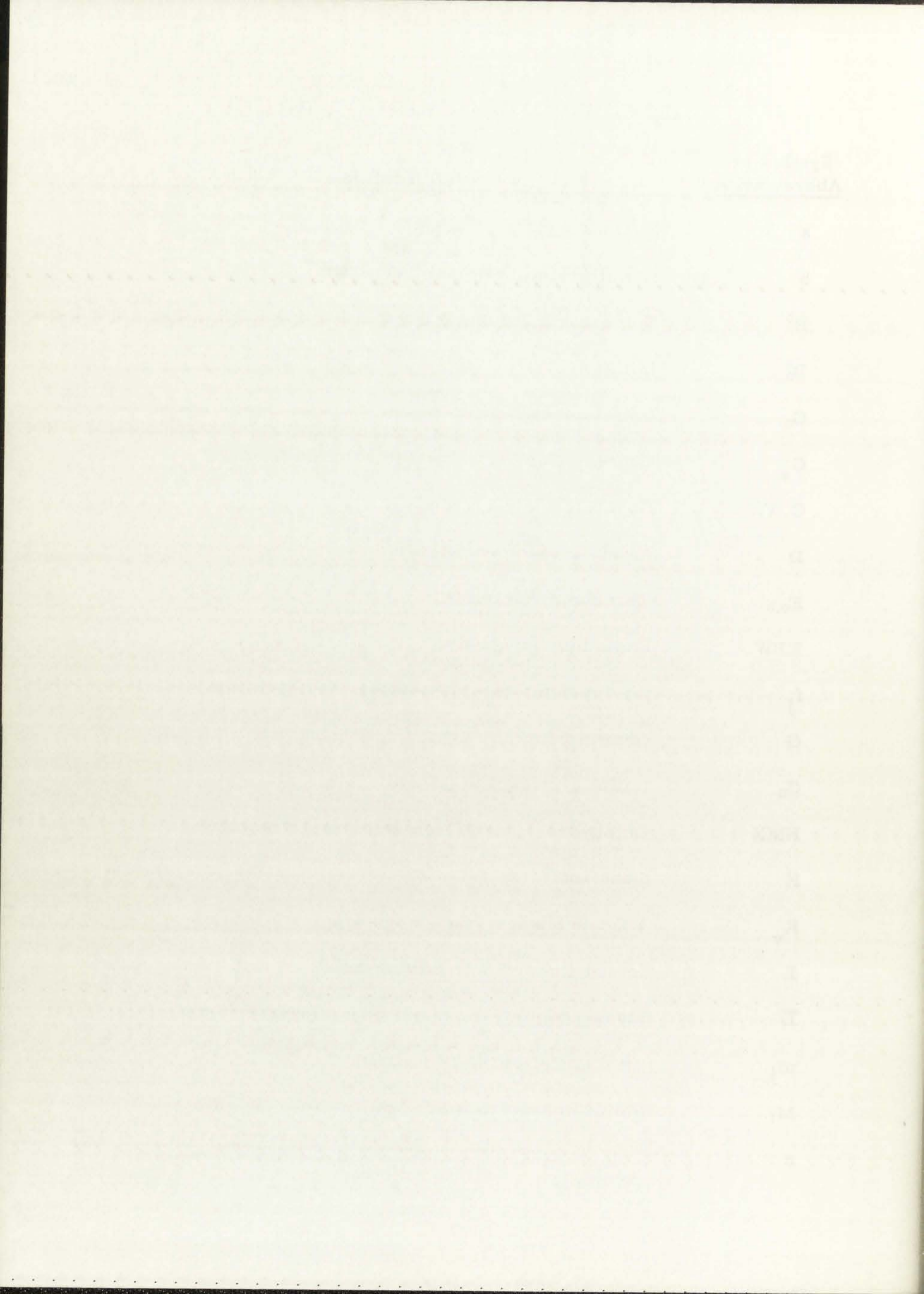
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LIST OF SYMBOLS AND ABBREVIATIONS

<u>Symbol or Abbreviation</u>	<u>Explanation</u>
a	Nucleation rate parameter, constant
b	Growth rate parameter, constant
B^0	Nucleation rate (nuclei/cm ³ · s)
B_0^0	Initial nucleation rate (nuclei/cm ³ · s)
C_0	Initial concentration (g/cm ³)
C_s	Concentration of saturated solution (g/cm ³)
C. V.	Coefficient of variation
D	Axial diffusion coefficient
$E_{0.5}$	Threshold voltage (V)
EBW	Exploding bridgewire
f_j	<u>j</u> th dimensionless moment of the population
G	Growth rate (μm/s)
G_0	Initial growth rate (μm/s)
HMX	Octahydro-1, 3, 5, 7-tetranitro-s-tetrazocine
K	Constant
K_v	Volume shape factor, constant
L	Internal coordinate (μm or cm)
\bar{L}	Mass-weighted mean particle size (μm or cm)
m_j	<u>j</u> th moment of the population
M_T	Solids concentration (g/cm ³), clear liquid basis
n	Population density [number/(unit length)(unit slurry volume)]

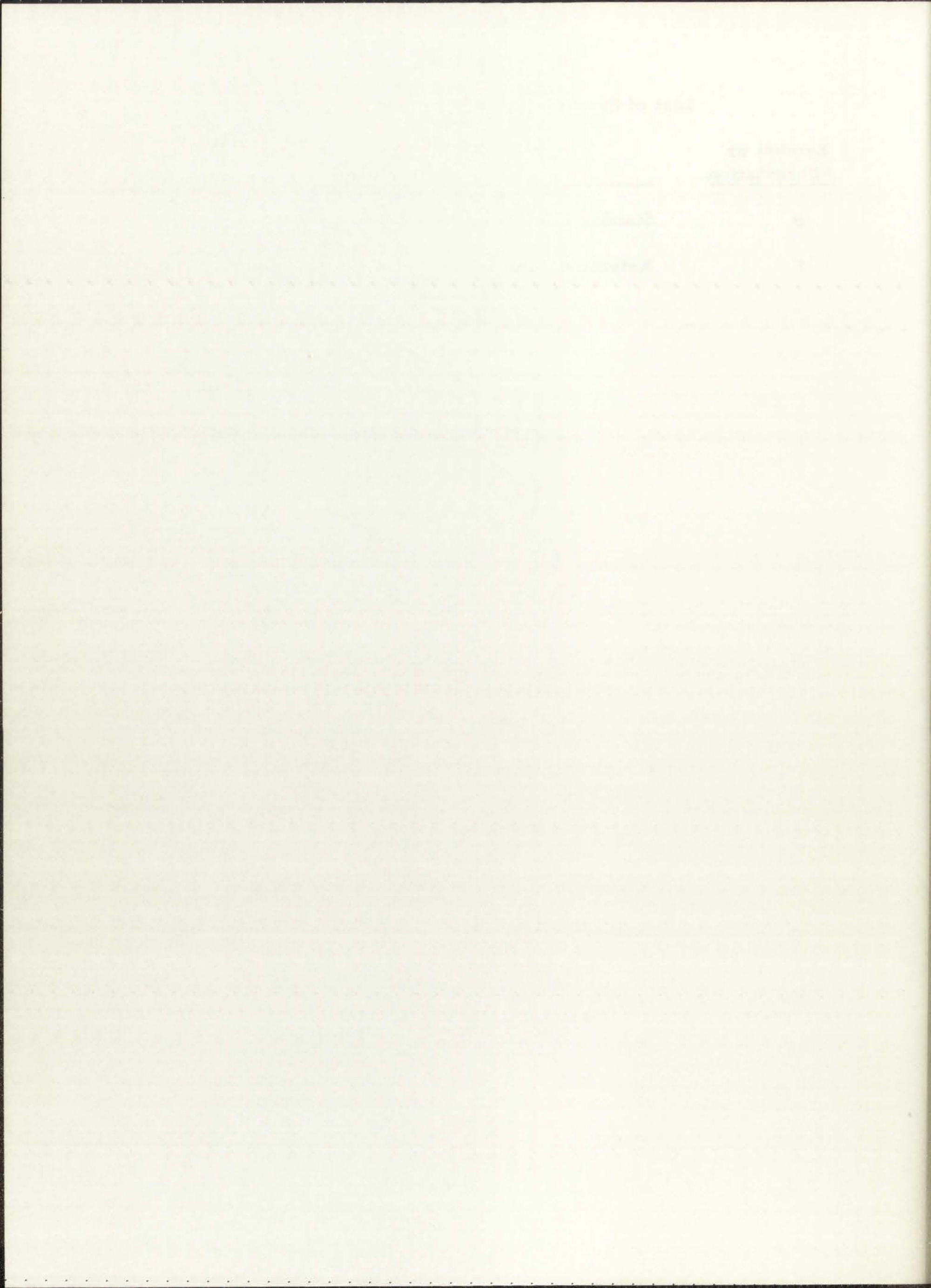


List of Symbols and Abbreviation--contd.

<u>Symbol or Abbreviation</u>	<u>Explanation</u>
n°	Nuclei population density [number/(unit length)(unit slurry volume)]
N	Number of crystals
Pe	Péclet number or diffusion parameter, constant
PETN	Pentaerythritol tetranitrate
R	Ratio of PETN-acetone solution flow rate to flow rate of water
RMC	Rotating mirror camera
t	Time (s)
t_m	Transit time (μ s)
u_x	Plug flow velocity (cm^3/s)
W	Weight distribution function
WW	Cumulative weight fraction distribution
x	External coordinate (cm)
\bar{x}	Effective reactor length (cm)
y	Dimensionless population density
z	Dimensionless external coordinate (reaction coordinate)
β	Dimensionless concentration
β_s	Dimensionless saturated concentration
ΔL	Width of crystal size range (μm or cm)
$\Delta \xi$	Dimensionless width of crystal size range
ρ	Particle density (g/cm^3)

List of Symbols and Abbreviations--contd.

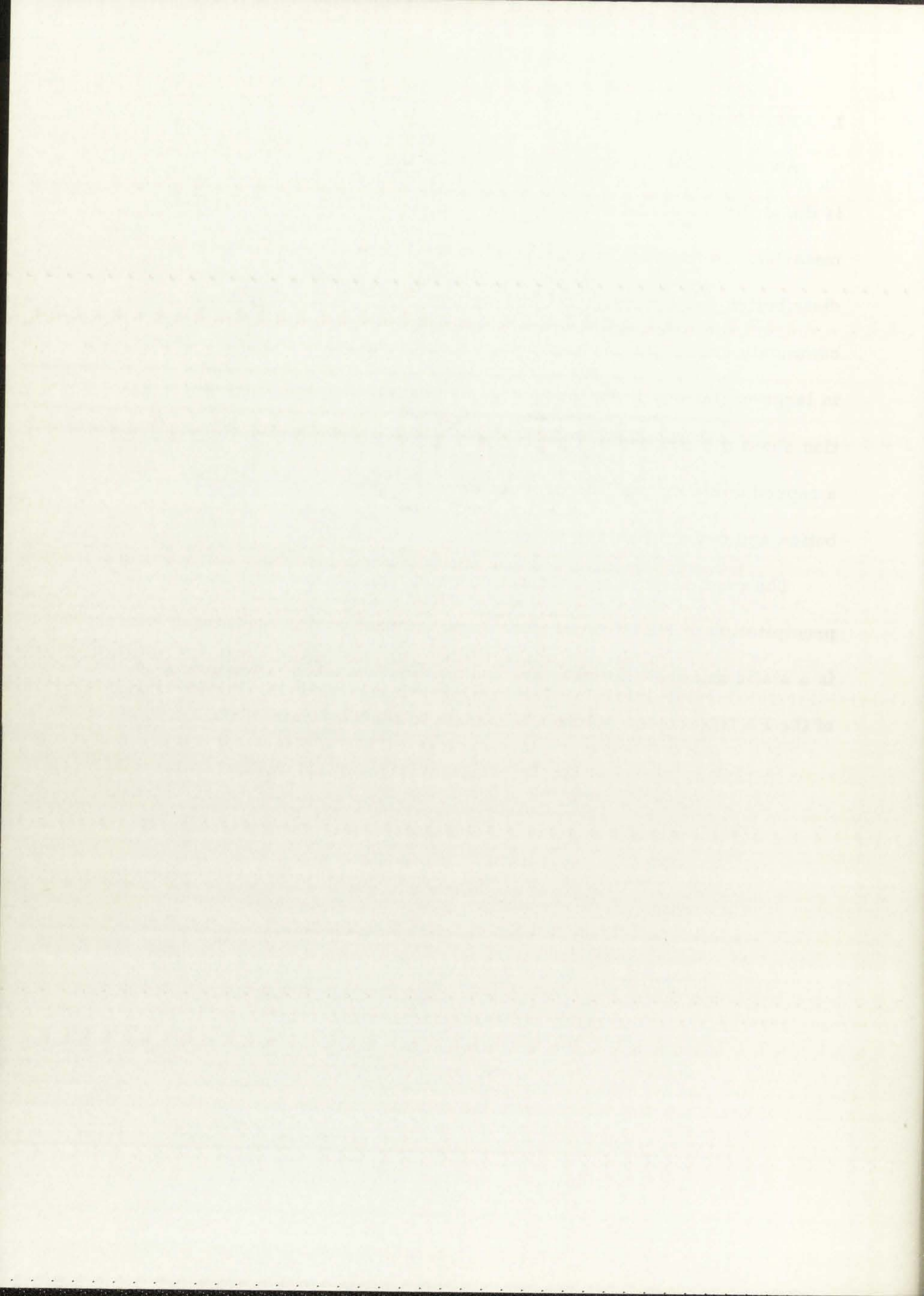
<u>Symbol or Abbreviation</u>	<u>Explanation</u>
σ	Standard deviation
τ	Retention time (s)



I. INTRODUCTION

An important consideration in the applications of high explosives is the ability to predict the physical and explosion properties of the material. In the case of a crystalline explosive, the particle size distribution and crystal habit are important.^{11,20} Batch processes commonly used in the preparation of high explosives frequently result in large variations in the products⁹ and usually provide little information about the kinetics of the process. A method for the preparation of a reproducible crystalline product having a known particle size distribution and crystal habit is desirable.

The method of recrystallization employed in this work involves the precipitation of PETN from an acetone solution by the addition of water in a static mixer. The primary independent variable is the ratio, R , of the PETN-acetone solution flow rate to the flow rate of water.



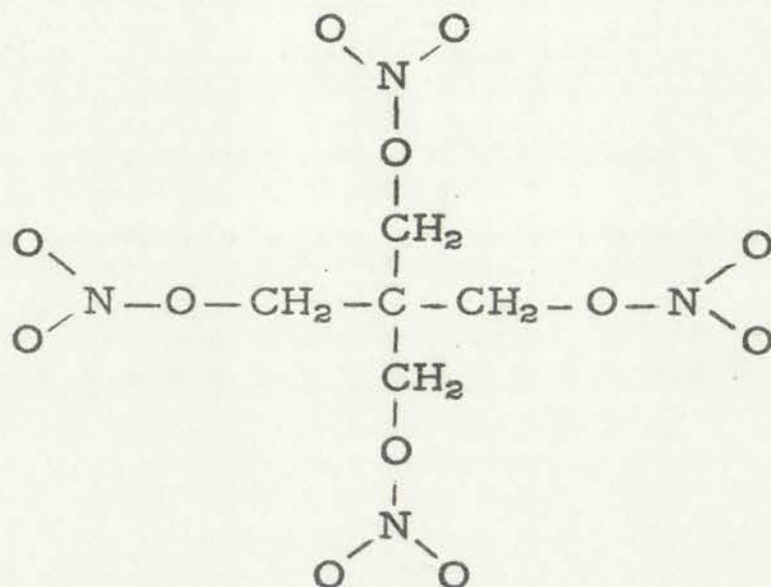
II. OBJECTIVES

The objectives of this study are to develop a continuous reproducible recrystallization technique for the preparation of the high explosive, pentaerythritol tetranitrate (PETN), which has definite crystalline properties, and to develop a model that provides some information on the kinetics and predicts the crystalline and explosion properties of the product.



III. PROPERTIES OF PETN

PETN is a symmetrical, nonpolar organic compound,
 $[C(CH_2ONO_2)_4]$, namely,



having a formula weight of 316.15. It forms colorless, nonhygroscopic crystals. PETN is readily compressible and has a maximum density of 1.77 g/cm³. It melts at 141°C and decomposes rapidly at temperatures above its melting point. PETN is insoluble in water, and soluble in acetone. Figure 1 gives the solubility of PETN in mixtures of acetone and water.¹⁹

Figure 1 shows the structure of the repeating unit of PETK.

Figure 1. Structure of the repeating unit of PETK.



having a formula weight of 216.12. It forms colorless, anhydrous crystals. PETK is readily compressible and has a maximum density of 1.17 (20°C). It melts at 141°C and decomposes rapidly at temperatures above its melting point. PETK is insoluble in water, but soluble in acetone. Figure 2 gives the solubility of PETK in various solvents and water.¹⁸

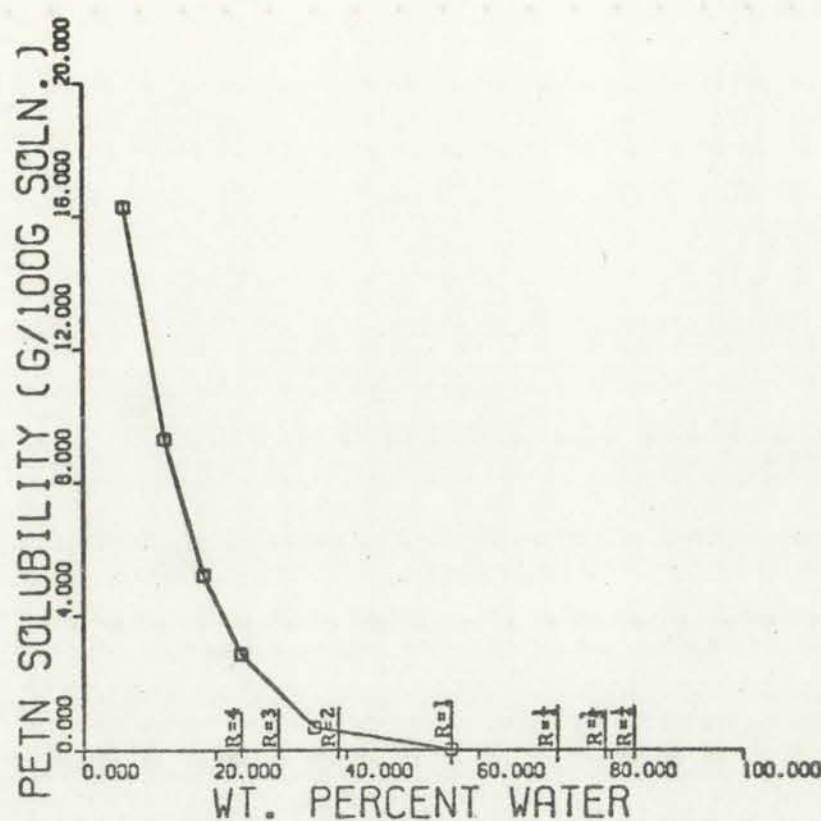
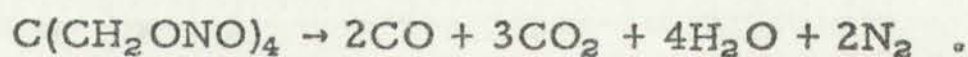


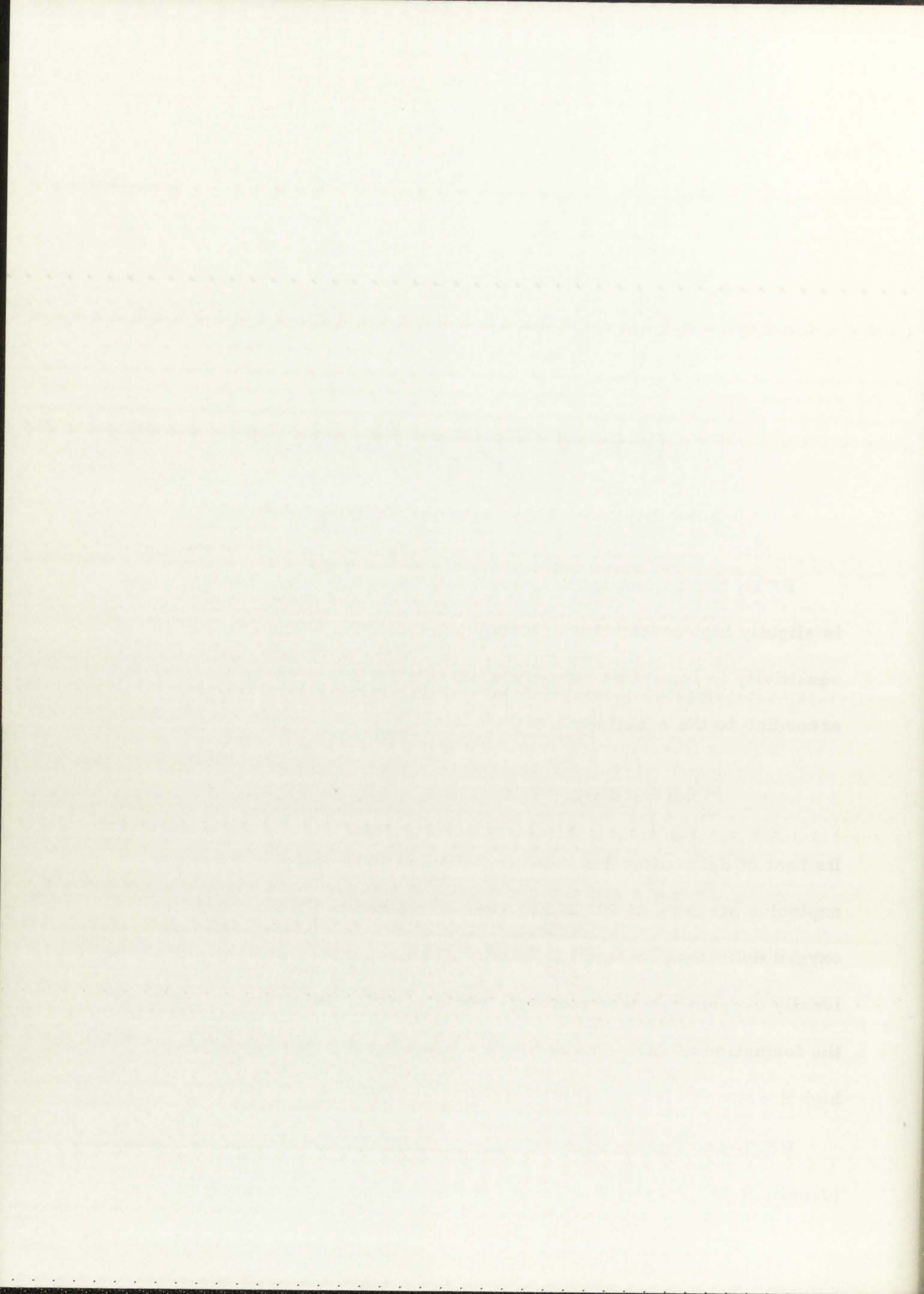
Figure 1.
Solubility of PETN in Aqueous Acetone Solutions.

PETN has an ignition temperature of approximately 215°C, which is slightly higher than that of nitroglycerin. It is of the same order of sensitivity to impact as nitroglycerin. PETN detonates or decomposes according to the equation



Its heat of detonation lies between 1466 and 1543 cal/g.¹ The high explosive strength of PETN has been attributed to the fact that its oxygen deficiency is small (10.1%). The decomposition products of the ideally oxygen-balanced material would be CO₂, H₂O, and N₂, without the formation of CO. The ability to compress PETN to a relatively high density is also a major contributing factor.

PETN has a detonation velocity of 5330 m/s for compacted material (density 0.85 g/cm³), 7600 m/s for material having a density of



1.5 g/cm³, and 8300 m/s for highly compressed material (density 1.70 g/cm³). The brisance or shattering power of PETN is much greater than that of nitroglycerin. Its explosive strength is at least 50% greater than TNT.⁵

Because of its great explosive power and brisance, PETN is widely used as a military and industrial explosive. Its ease of initiation and its high explosive power combine to make PETN exceptionally serviceable in detonators as the donor charge that initiates a less sensitive acceptor explosive. PETN has also been used in percussion caps and grenades and as a propellant in smokeless powders.^{1,5}

PETN can be used in the treatment of angina pectoris as a long-acting coronary vasodilator, which is capable of reducing the frequency and severity of the attack.¹

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IV. EBW DETONATORS

Chemical explosives comprise two main types: (1) detonating or "high" explosives, characterized by very high rates of reaction and high pressures and (2) deflagrating or "low" explosives, which burn more slowly and develop much lower pressures. Detonating explosives may be further subdivided into (a) primary and (b) secondary explosives. Primary explosives nearly always detonate by simple ignition such as by a spark, flame, impact, or other primary heat sources of appropriate magnitude. Secondary explosives require, in practical applications, the use of a detonator and frequently, a booster. A booster is a sensitive secondary high explosive that reinforces the detonation wave from the primary explosive or detonator and delivers a more powerful detonation wave to the main explosive charge.³

A problem encountered in explosive operations is that of initiating the detonation wave in the explosive. Often, this problem is complicated by the provisions of simplicity and safety, and the necessity of precisely controlled timing at widely separated points. A variety of devices, called detonators, have been developed to perform the function of initiation. The exploding bridgewire (EBW) detonator has an explosive train with a secondary explosive requiring an elaborate power source to vaporize or "explode" a wire by extremely rapid deposition of electrical energy to initiate detonation in the material.^{2a}

The basic circuit for exploding a wire consists of a power source to charge a capacitor, a capacitor for storage of electrical energy, a

Chemical explosives containing two kinds of ...

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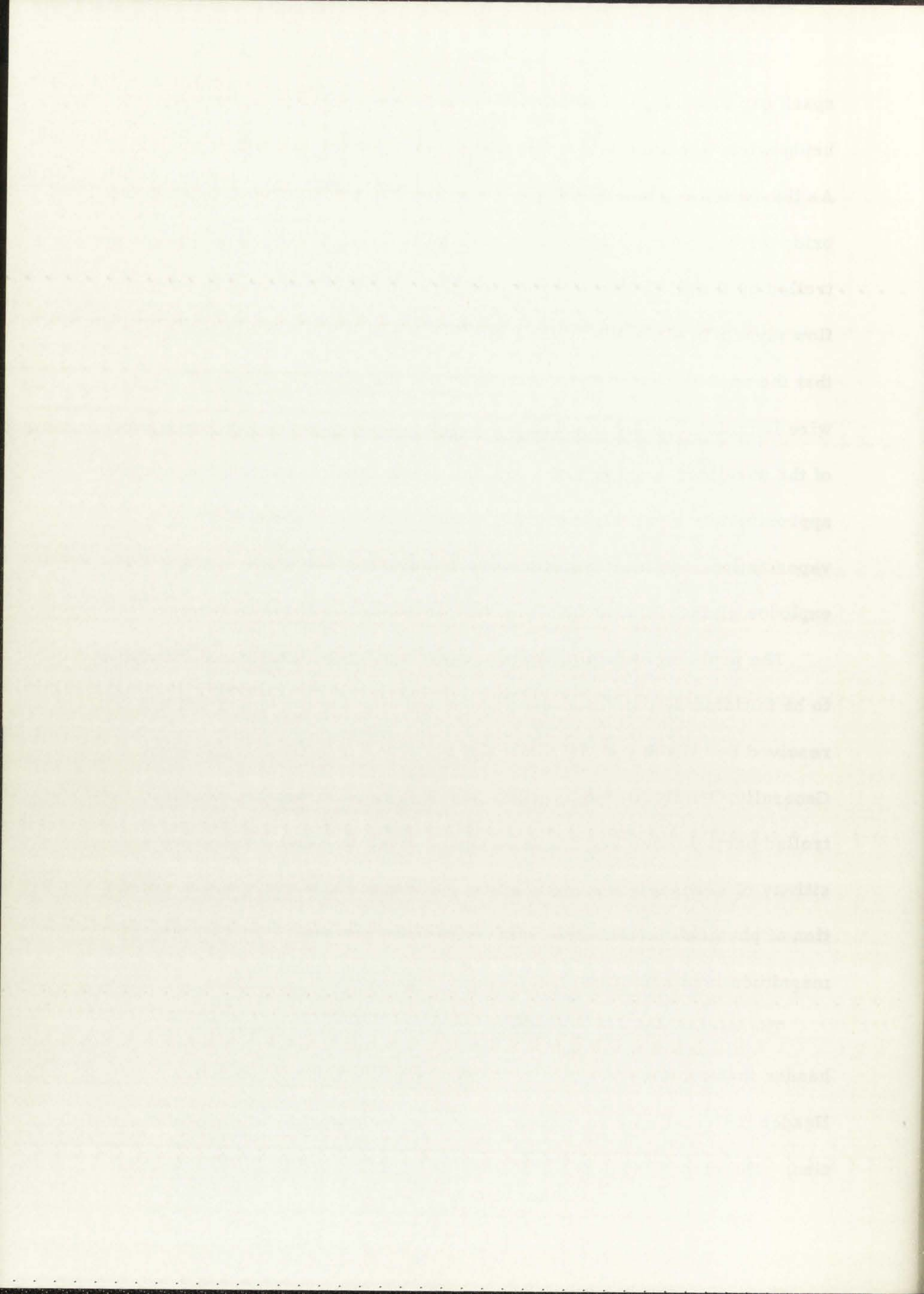
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spark gap and trigger switch to discharge the capacitor across the bridgewire, a transmission line to the bridgewire, and a bridgewire. As the switch is closed, voltage is applied to the transmission line and bridgewire circuit which causes current to begin to flow at a rate controlled by the RLC characteristics of the circuit. The rate of current flow (approximately $1000 \text{ A}/\mu\text{s}$) and the amount of energy are so great that the wire is heated to vaporization but the physical shape of the wire is maintained by inertia. As vaporization occurs, the resistance of the wire increases greatly. At this point, the current reduces within approximately one microsecond. Within a few nanoseconds after vaporization, the inertia of the wire material is overcome and the wire explodes giving off a shock wave and the contained thermal energy.¹⁸

The problem of finding a secondary explosive sufficiently sensitive to be initiated by the small shock developed by the exploding wire is resolved by utilizing an intrinsically sensitive secondary explosive. Generally, PETN loaded as a low density granular powder of controlled particle size and shape is used. Even though the effective sensitivity of secondary explosives may be increased by the proper selection of physical parameters, such materials are still 3 to 4 orders of magnitude less sensitive than primary explosives.²²

The basic inert components of an EBW detonator consist of a header that contains the electrical wire leads and the bridgewire. Header material may vary from plastic to a metal/ceramic combination. The electrical connection may be hookup wire leads or a coaxial



or multipin assembly into which the cable mates directly. The sleeve, which actually contains the explosive, may be a part of the header or a separate part that is threaded or crimped into place. End caps may be used. The explosive is generally pressed in two increments. The first increment, next to the bridgewire, is pressed into the header at a density of approximately 50% of that of the crystal density. The second increment, called the output charge, is pressed to approximately 90% of that of the crystal density.¹⁸

The shock wave and thermal energy released from the exploding bridgewire are transferred into the low density secondary explosive next to the bridgewire. In general, the shock wave from the wire travels at about 1500 m/s. As the wave travels into the explosive, a detonation of the explosive is initiated and builds up to the normal detonation velocity of the initial pressing explosive (approximately 5000 m/s). As the shock wave moves through the initial pressing and into the output pellet, the velocity of the wave again increases, because of the higher density pellet, to approximately 8000 m/s.¹⁸ The time from bridgewire burst to shock wave breakout is called the function or transit time of the detonator (t_m). This time is on the order of one to several microseconds, depending on the overall length of the detonator. Another quantity that is often used is the threshold voltage ($E_{0.5}$). The threshold voltage is the firing set capacitor voltage level at which one half of the detonators will fire.

on multiple assembly into which the whole system is divided. The whole
with already contains the explosive, and is a part of the holder or a
separate part that is threaded at certain places. And also they do

not. The explosive is generally pressed into the instrument. The

instrument is generally made of metal, is placed into the holder of a

device of approximately 50% of that of the crystal density. The second

instrument, called the output crystal, is pressed to approximately 70%

of that of the crystal density.

The shock wave and thermal energy released from the exploding

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due to the pyrodescent. In general, the shock wave from the wire

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detonation velocity of the initial pressure explosive (approximately

1000 m/s). As the shock wave moves through the initial pressure and

into the output pellet, the velocity of the wave again increases, because

of the higher density pellet, so approximately 8000 m/s. The time

from pyrotechnic burst to shock wave passage is called the detector or

transit time of the detector (t_d). This time is on the order of 100 to

several microseconds, depending on the overall length of the detector.

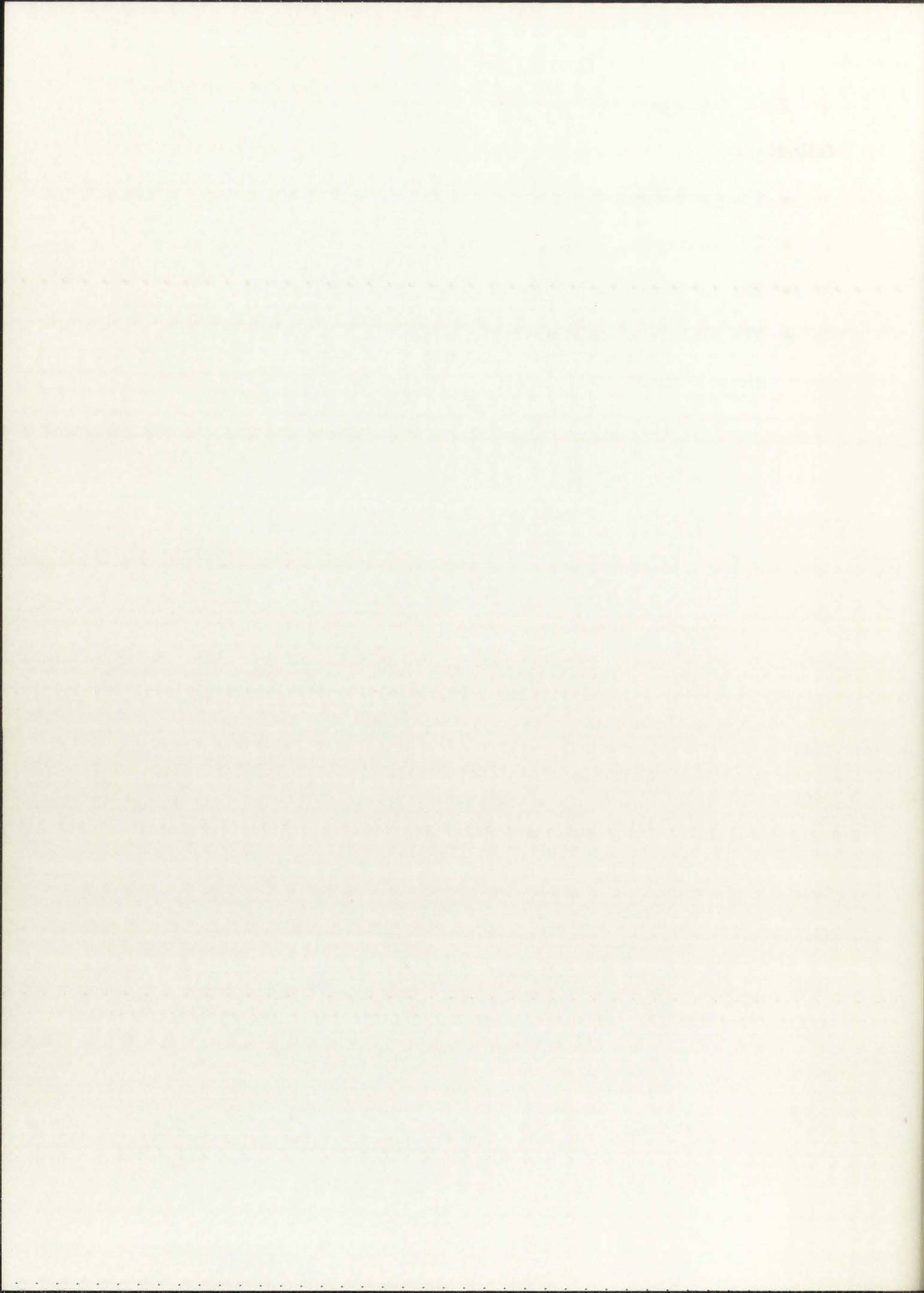
Another quantity that is often used is the threshold voltage (V_{th}). The

threshold voltage is the first cut capacitor voltage level at which one

fall of the detector will fire.

EBW detonators are used for many applications including the following:¹⁸

- The production of accurate and refined metal forming or welding
- The generation of shock waves for physics research studies
- The creation of small point energy or light sources
- The closure of an electrical switch in a very short and predictable time.



V. CRYSTALLIZATION THEORY

The techniques for interpreting crystal size distributions from crystallization processes to ascertain the nature of the controlling mechanism developed rapidly over the period from 1962 to 1964²⁴ (Randolph and Larson,¹⁶ Hulburt and Katz¹⁰). The work began with the first attempts to rationalize, model, and predict crystal size distributions from realistic mixed-magma crystallizers and is based on the concept of a population balance of crystal particles along the particle size axis.¹⁷ The detailed development of the particle-number continuity equations and the moment transformation of the population balance may be found in Ref. 17. A brief description of this work can be found in Appendix A.

A. Plug Flow Model

At steady state, with negligible breakage, the population balance is given by¹⁷

$$\nabla \cdot \vec{V}_e n + \frac{\partial}{\partial L} (Gn) = 0, \quad (1)$$

where n is the number population density of the system, and G is the linear growth rate, $\frac{dL}{dt}$. The internal coordinate is taken as the Stoke's diameter L , as determined by sedimentation techniques. The external coordinate system is represented by the single crystallizer length dimension, x . For small particles, and high velocities, V_x , the external linear velocity, may be taken as the plug flow velocity, u_x . Assuming that growth rate G remains independent of size, an

The population for crystallizing crystals is determined from

crystallization process to maintain the nature of the crystalline

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empirical observation known as McCabe's ΔL law, which often holds true, then Eq. (1) reduces to

$$u_x \frac{\partial n}{\partial x} + G \frac{\partial n}{\partial L} = 0 \quad (2)$$

Equation (2) is the plug flow equation that includes the following assumptions:

- Steady state is achieved
- Linear velocity = plug flow velocity = constant
- Negligible breakage is achieved
- Growth rate is independent of size.

Multiplying Eq. (2) by $L^j dL$, and integrating from zero to infinity, we have

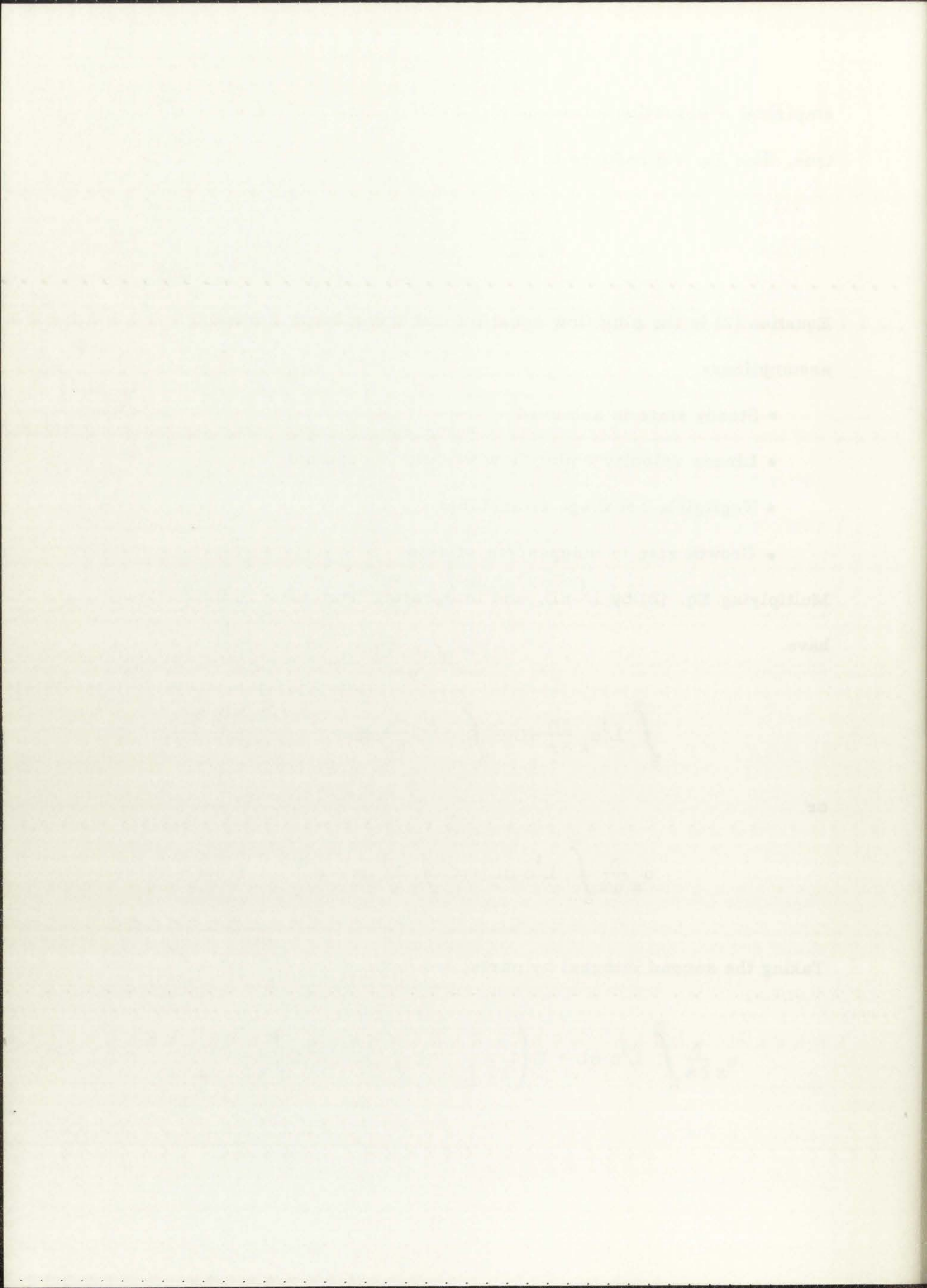
$$\int_0^{\infty} L^j u_x \frac{\partial n}{\partial x} dL + \int_0^{\infty} L^j G \frac{\partial n}{\partial L} dL = 0 \quad (3)$$

or

$$u_x \frac{\partial}{\partial x} \int_0^{\infty} L^j n dL + G \int_0^{\infty} L^j dn = 0 \quad (4)$$

Taking the second integral by parts, we have

$$u_x \frac{\partial}{\partial x} \int_0^{\infty} L^j n dL + G \left(L^j n \Big|_0^{\infty} - j \int_0^{\infty} L^{j-1} n dL \right) = 0 \quad (5)$$



Let us introduce the j th moment of the population defined by the integral, $m_j = \int_0^{\infty} L^j n \, dL$. If N is the total number of particles, the initial population density is $n_x^0 = (dN/dL)_{L \rightarrow 0}$ and the nucleation rate is $B_x^0 = (dN/dt)_{L \rightarrow 0}$. The boundary conditions are $n_x^0 = B_x^0 / G_x$ and $n_x^{\infty} = 0$. Here, the notation $r_x^L = r(x, L)$ is used. Equation (5) becomes

$$u_x \frac{dm_j}{dx} + (0)^j B^0 - j G m_{j-1} = 0 \quad (6)$$

where $j = 0, 1, 2, \dots$, and $(0)^j = 0$ when $j \neq 0$ and $(0)^j = 1$ when $j = 0$.

The equations given by Eq. (6) are the moment equations for the plug flow model.

We will now introduce the retention time, τ , defined by $\tau = \bar{x} / u_x$, where \bar{x} is the effective length of the plug flow reactor in cm, and u_x is the plug flow velocity in cm^3/s . For an ideal plug flow reactor, each infinitesimal reactant volume will have the same retention time.² The quantities C_0 , the initial concentration ($x = 0$), and C_s , the concentration of the saturated solution, will also be used.

It will be more convenient to use dimensionless quantities in the discussion. The new quantities will be normalized in terms of the initial conditions where $x = 0$. The dimensionless external coordinate becomes $z = x / \bar{x}$, the dimensionless internal coordinate becomes $\xi = L / G_0 \tau$, and the dimensionless population density becomes $y = n / n_0^0$ where $n_0^0 = B_0^0 / G_0$. The dimensionless concentration becomes $\beta = C / C_0$ and the dimensionless saturated concentration becomes $\beta_s = C_s / C_0$.

... the reaction rate is given by the equation ...
 ... the total number of particles, the ...
 ... and the reaction rate is ...
 ... the boundary conditions are ...
 ... the notation ... is used. Equation (5) becomes

$$(6) \quad \frac{d^2x}{dz^2} + \frac{1}{z} \frac{dx}{dz} - \frac{1}{2} x = 0$$

where $\lambda = 0, 1, 2, \dots$ and $\mu = 0$ and $(\lambda + \mu) = 0$.
 The equation given by (6) is the moment equation for the plug flow model.

We will now introduce the reaction time, τ , defined by $\tau = \frac{L}{v}$, where L is the effective length of the plug flow reactor in cm, and v is the plug flow velocity in cm³/sec. For an ideal plug flow reactor, each infinitesimal reaction volume will have the same retention time. The quantities C_0 , the initial concentration ($t = 0$), and C , the concentration of the extracted solution, will also be used.

It will be more convenient to use dimensionless quantities in this discussion. The new quantities will be normalized in terms of the initial conditions where $\lambda = 0$. The dimensionless spatial coordinate becomes $\lambda = x/L$, the dimensionless internal coordinate becomes $\lambda = \tau t$, and the dimensionless population density becomes $y = C/C_0$, where $C = C_0 y$. The dimensionless concentration becomes $y = C/C_0$ and the dimensionless extracted concentration becomes $\lambda = C_0 y$.

The dimensionless moments of the population, f , are

$$f_j = \int_0^{\infty} \xi^j y \, d\xi = \frac{m_j}{B_0^0 (G_0 \tau)^j \tau} \quad (7)$$

The dimensionless plug flow moment equations are

$$f_j' - (0)^j \frac{B_0^0}{B_0^0} - j \frac{G}{G_0} f_{j-1} = 0, \quad j=0, 1, 2, \dots \quad (8)$$

where $f_j' = df_j/dz$. The initial conditions are $f_j(0) = 0$, $j=0, 1, 2, \dots$.

The total solids concentration per unit volume of solids-free liquid is

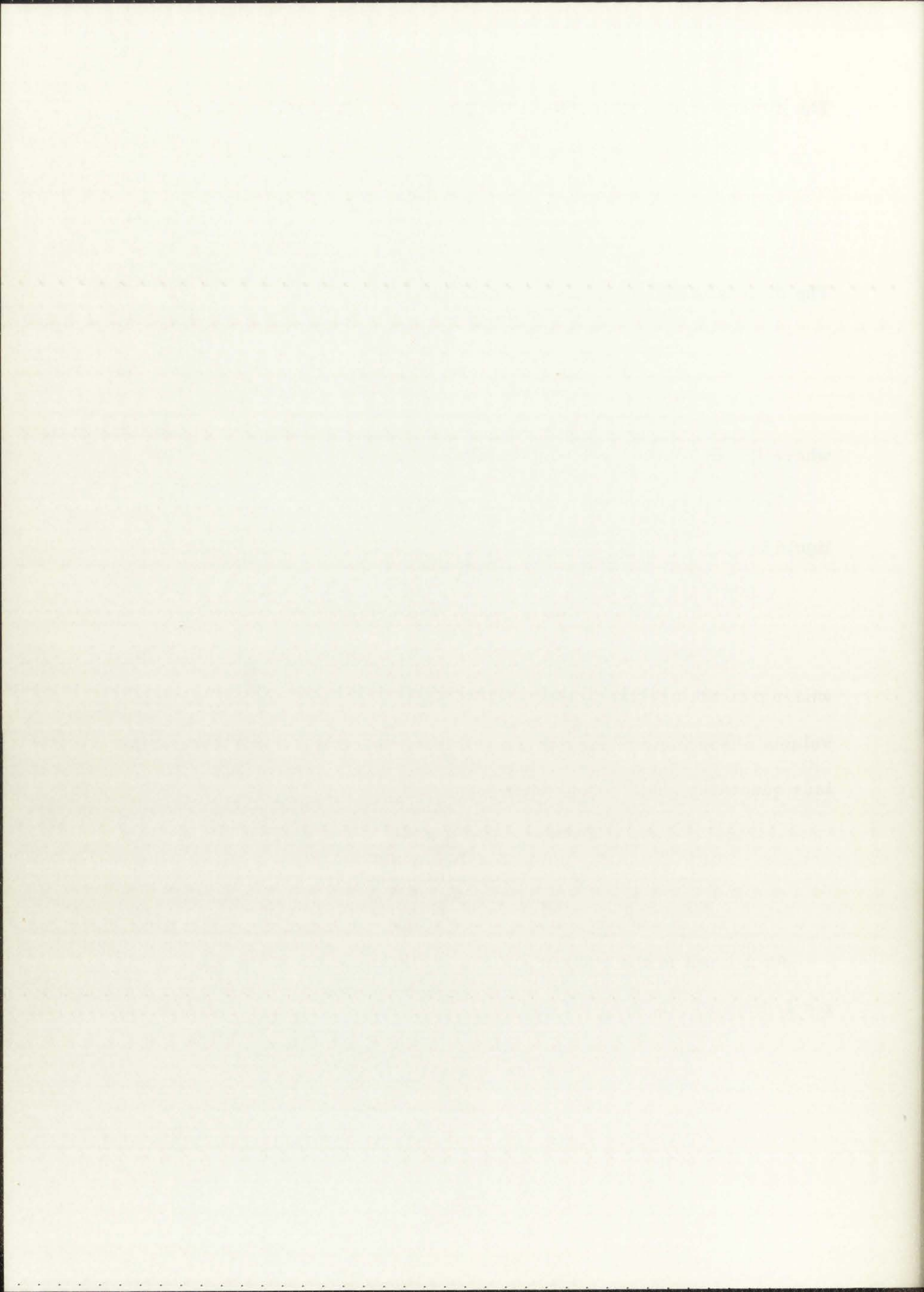
$$M_T = \rho K_V m_3(x) = [C_0 - C(x)] \quad (9)$$

where ρ is the crystal density of PETN, 1.77 g/cm^3 , and K_V is the volume shape factor based on Stokes' law. In terms of the dimensionless quantities, Eq. (9) becomes

$$[1 - \beta(z)] = \frac{\rho K_V B_0^0 (G_0 \tau)^3 \tau}{C_0} f_3(z) \quad (10)$$

At the exit of the reactor, $z = 1$. If the reaction is complete at $z = 1$, then $M_T/C_0 + \beta_s = 1$ and

$$\beta_s = \beta(1) \quad (11)$$



This relationship is verified experimentally by weighing the product for a given volume of solids-free liquid. The experimental M_T results are given in Table 1. The table is an experimental verification of the completeness of reaction at $z = 1$.

TABLE 1
EXPERIMENTAL M_T RESULTS

Sample	Measured M_T (g/cm ³)	C_0 (g/cm ³)	β_s	$M_T/C_0 + \beta_s$
3848	0.0008	0.0008	0.000	1.00
3849	0.0148	0.03	0.453	0.95
3851	0.0008	0.0008	0.000	1.00
3852	0.000775	0.0008	0.000	0.97
3853	0.00081	0.0008	0.000	1.01
3856	0.00144	0.00133	0.000	1.08
3857	0.00135	0.00133	0.000	1.01
3858	0.00134	0.00133	0.000	1.01
3861	0.00177	0.002	0.1125	0.99
3862	0.00171	0.002	0.1125	0.97
3863	0.00169	0.002	0.1125	0.96
3864	0.00161	0.002	0.1125	0.92
3866	0.00114	0.001	0.000	1.14
3867	0.00114	0.001	0.000	1.14
3868	0.00114	0.001	0.000	1.14
3871	0.00205	0.002	0.1125	1.14
3872	0.00182	0.002	0.1125	1.02
3873	0.00177	0.002	0.1125	1.00
3874	0.00195	0.002	0.1125	1.09
3876	0.0218	0.0267	0.162	0.98
3877	0.0213	0.0267	0.162	0.96
3878	0.0221	0.0267	0.162	0.99
3881	0.0128	0.03	0.453	0.88
3882	a	0.03	0.453	a
3883	0.0154	0.03	0.453	0.97

^a M_T not measured because of filtering difficulties.

The relationship between experimental frequency f and the theoretical frequency f_0 is given by the equation $f = f_0 \sqrt{1 - \frac{w}{w_0}}$. The experimental results are given in Table I. The table is an experimental verification of the relationship of equation (1).

TABLE I
EXPERIMENTAL RESULTS

Frequency f	Mass w	Mass w_0	Theoretical f_0	Calculated f
1.00	1.00	1.00	1.00	1.00
1.10	1.10	1.00	1.00	1.10
1.20	1.20	1.00	1.00	1.20
1.30	1.30	1.00	1.00	1.30
1.40	1.40	1.00	1.00	1.40
1.50	1.50	1.00	1.00	1.50
1.60	1.60	1.00	1.00	1.60
1.70	1.70	1.00	1.00	1.70
1.80	1.80	1.00	1.00	1.80
1.90	1.90	1.00	1.00	1.90
2.00	2.00	1.00	1.00	2.00
2.10	2.10	1.00	1.00	2.10
2.20	2.20	1.00	1.00	2.20
2.30	2.30	1.00	1.00	2.30
2.40	2.40	1.00	1.00	2.40
2.50	2.50	1.00	1.00	2.50
2.60	2.60	1.00	1.00	2.60
2.70	2.70	1.00	1.00	2.70
2.80	2.80	1.00	1.00	2.80
2.90	2.90	1.00	1.00	2.90
3.00	3.00	1.00	1.00	3.00
3.10	3.10	1.00	1.00	3.10
3.20	3.20	1.00	1.00	3.20
3.30	3.30	1.00	1.00	3.30
3.40	3.40	1.00	1.00	3.40
3.50	3.50	1.00	1.00	3.50
3.60	3.60	1.00	1.00	3.60
3.70	3.70	1.00	1.00	3.70
3.80	3.80	1.00	1.00	3.80
3.90	3.90	1.00	1.00	3.90
4.00	4.00	1.00	1.00	4.00

Using these results and substituting Eq. (11) into Eq. (10),

$$1 - \beta_s = \frac{\rho K_v B_0^0 (G_0 \tau)^3 \tau}{C_0} f_3(1) , \quad (12)$$

dividing Eq. (10) by Eq. (12) and rearranging,

$$\beta(z) = 1 + \frac{f_3(z)}{f_3(1)} \beta_s - \frac{f_3(z)}{f_3(1)} . \quad (13)$$

This is the relationship for the concentration as a function of the normalized external coordinate. The normalized external coordinate, z , will be referred to as the reaction coordinate.

For the case in which $\beta_s = 0$,

$$\beta(z) = 1 - \frac{f_3(z)}{f_3(1)} . \quad (14)$$

B. Dispersed Plug Flow Model

Consider the plug flow of a fluid, on top of which is superimposed some degree of intermixing, the magnitude of which is independent of position within the vessel. This is called the dispersed plug flow model.¹⁵

For molecular diffusion in the x -direction, the governing differential equation is given by Fick's law

$$u_x \frac{\partial n}{\partial x} + G \frac{\partial n}{\partial L} = D \frac{\partial^2 n}{\partial x^2} \quad (15)$$

where the parameter D , called the axial diffusion coefficient, uniquely characterizes the degree of backmixing between adjacent reactant

Using the boundary conditions $C(0) = C_0$ and $C(L) = C_1$, we find

$$C(x) = \frac{C_1 - C_0}{L} x + C_0 \quad (12)$$

Substituting Eq. (12) into Eq. (11) and integrating

$$J(x) = -D \frac{dC}{dx} = -D \frac{C_1 - C_0}{L} \quad (13)$$

This is the relationship for the concentration as a function of the normalized external coordinate. The normalized external coordinate

x , will be referred to as the reaction coordinate.

For the case in which $\lambda = 0$,

$$J(x) = -D \frac{dC}{dx} = -D \frac{C_1 - C_0}{L} \quad (14)$$

B. Dispersed Plug Flow Model

Consider the plug flow of a fluid, on top of which is superimposed some degree of turbulence, the magnitude of which is independent of

position within the vessel. This is called the dispersed plug flow

model.

For molecular diffusion in the x -direction, the governing differential equation is given by Fick's law

$$D \frac{d^2 C}{dx^2} = 0 \quad (15)$$

where the parameter D , called the axial diffusion coefficient, uniquely

characterizes the degree of backmixing between adjacent regions

volume elements during flow. The dimensionless group $(D/u_x \bar{x})$, called the vessel dispersion number, is the parameter that measured the extent of axial dispersions. Thus

$$\frac{D}{u_x \bar{x}} \rightarrow 0 \quad \text{negligible dispersion, hence, plug flow,}$$

$$\frac{D}{u_x \bar{x}} \rightarrow \infty \quad \text{large dispersion, hence, mixed flow.}$$

This model usually represents quite satisfactorily flow that deviates not too greatly from plug flow.¹⁵

Equation (15) may be rewritten as

$$-D \frac{\partial^2 n}{\partial x^2} + u_x \frac{\partial n}{\partial x} + G \frac{\partial n}{\partial L} = 0 \quad . \quad (16)$$

Multiplying by $L^j dL$ and integrating from zero to infinity gives

$$\int_0^{\infty} \left(-D \frac{\partial^2 n}{\partial x^2} \right) L^j dL + \int_0^{\infty} \left(u_x \frac{\partial n}{\partial x} \right) L^j dL + \int_0^{\infty} \left(G \frac{\partial n}{\partial L} \right) L^j dL = 0 \quad , \quad (17)$$

or

$$-D \frac{\partial^2}{\partial x^2} \left(\int_0^{\infty} n L^j dL \right) + u_x \frac{\partial}{\partial x} \left(\int_0^{\infty} n L^j dL \right) + G \int_0^{\infty} \frac{\partial n}{\partial L} L^j dL = 0 \quad . \quad (18)$$

Defining the j th moment as before, $m_j = \int_0^{\infty} n L^j dL$, we have

$$-D \frac{d^2 m_j}{dx^2} + u_x \frac{dm_j}{dx} + G \int_0^{\infty} L^j dn = 0 \quad . \quad (19)$$

velocity element dv in the direction θ is $v \sin \theta$. The velocity v is called the *axial velocity* and is the velocity of the fluid in the direction of the axis. The axial velocity is denoted by v_z .

$$v_z = v \sin \theta$$

$$v = \frac{v_z}{\sin \theta}$$

This model usually represents the flow in a pipe that is not too greatly from plug flow. Equation (1) may be written as

$$-\frac{D}{4\mu} \frac{dp}{dz} = \frac{1}{r} \frac{d}{dr} \left(r \frac{dv_r}{dr} \right) + \frac{d^2 v_z}{dr^2}$$

Multiplying by r^2 and integrating from $r=0$ to $r=R$

$$\int_0^R \left(-\frac{D}{4\mu} \frac{dp}{dz} \right) r^2 dr + \int_0^R \left(\frac{d}{dr} \left(r \frac{dv_r}{dr} \right) \right) r^2 dr + \int_0^R \left(\frac{d^2 v_z}{dr^2} \right) r^2 dr = 0$$

$$-\frac{D}{4\mu} \frac{dp}{dz} \left(\frac{r^3}{3} \right) \Big|_0^R + \left(\frac{1}{2} r^2 \frac{dv_r}{dr} \right) \Big|_0^R + \left(\frac{1}{2} r^2 \frac{dv_z}{dr} \right) \Big|_0^R = 0$$

Define the *jet moment* as $M_z = \int_0^R v_z r^2 dr$

$$-\frac{D}{4\mu} \frac{dp}{dz} \left(\frac{R^3}{3} \right) + \left(\frac{1}{2} R^2 \frac{dv_r}{dr} \right) \Big|_0^R + \left(\frac{1}{2} R^2 \frac{dv_z}{dr} \right) \Big|_0^R = 0$$

Integrating by parts and evaluating $n = 0$ as $L \rightarrow \infty$ and $n = B^0/G$ as $L \rightarrow 0$

$$-D \frac{d^2 m_j}{dx^2} + u_x \frac{dm_j}{dx} - (0)^j B^0 - j G m_{j-1} = 0 \quad (20)$$

Using the definitions given in Section C, namely,

$$\tau = \frac{\bar{x}}{u_x}, \quad z = \frac{x}{\bar{x}}, \quad \xi = \frac{L}{G_0 \tau}, \quad y = \frac{n G_0}{B_0^0}, \quad f_j = \frac{m_j}{B_0^0 (G_0 \tau)^j \tau}$$

we have

$$D \left(\frac{1}{\bar{x}^2} \right) \left(B_0^0 G_0^j \tau^{j+1} \right) \frac{d^2 f_j}{dz^2} - u_x \left(\frac{1}{\bar{x}} \right) \left(B_0^0 G_0^j \tau^{j+1} \right) \frac{df_j}{dz} + (0)^j B^0 + j G \left(B_0^0 G_0^{j-1} \tau^j \right) f_{j-1} = 0 \quad (21)$$

Simplifying:

$$\frac{D}{u_x \bar{x}} \frac{d^2 f_j}{dz^2} - \frac{df_j}{dz} + (0)^j \frac{B^0}{B_0^0} + j \frac{G}{G_0} f_{j-1} = 0 \quad (22)$$

Define the Péclet number, the reciprocal of the vessel dispersion number, $Pe = u_x \bar{x}/D$. The resulting dispersed plug flow moment equations are

$$\frac{1}{Pe} f_j'' - f_j' + (0)^j \frac{B^0}{B_0^0} + j \frac{G}{G_0} f_{j-1} = 0 \quad (23)$$

with the boundary conditions^{4,23} $f_j(0) - \frac{1}{Pe} f_j'(0) = 0$, and $f_j'(1) = 0$.

Equation 13 from Section A holds for the dispersed plug flow model,

namely, $\beta(z) = 1 + \frac{f_3(z)}{f_3(1)} \beta_s - \frac{f_3(z)}{f_3(1)}$ and for $\beta_s = 0$, $\beta(z) = 1 - \frac{f_3(z)}{f_3(1)}$.

Problem 1. Consider the boundary value problem for the Laplace equation in the upper half-plane $y > 0$:

$$\Delta u = 0, \quad y > 0, \quad u(x, 0) = f(x), \quad u(x, y) \rightarrow 0 \text{ as } y \rightarrow \infty. \quad (1)$$

Using the Poisson integral formula, find the solution $u(x, y)$ for the boundary value $f(x) = 1 - x^2$.

$$u(x, y) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{y \, f(\xi)}{(x - \xi)^2 + y^2} d\xi = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{y(1 - \xi^2)}{(x - \xi)^2 + y^2} d\xi.$$

Write the integral as a sum of two integrals:

$$\frac{y}{\pi} \int_{-\infty}^{\infty} \frac{1}{(x - \xi)^2 + y^2} d\xi - \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{\xi^2}{(x - \xi)^2 + y^2} d\xi.$$

$$\text{The first integral is } \frac{y}{\pi} \cdot \frac{\pi}{y} = 1. \quad \text{The second integral is } \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{\xi^2}{(x - \xi)^2 + y^2} d\xi.$$

Using the residue theorem, we find that the second integral is equal to $\frac{y}{\pi} \left(\frac{\pi}{y} - \frac{\pi x^2}{y^2} \right)$.

$$\text{Therefore, } u(x, y) = 1 - \frac{y^2}{\pi} \int_{-\infty}^{\infty} \frac{\xi^2}{(x - \xi)^2 + y^2} d\xi = 1 - \frac{y^2}{\pi} \left(\frac{\pi}{y} - \frac{\pi x^2}{y^2} \right) = 1 - y + x^2.$$

Thus the Poisson integral of the boundary value $f(x) = 1 - x^2$ is $u(x, y) = 1 - y + x^2$.

Check that $u(x, y)$ satisfies the Laplace equation and the boundary conditions.

Problem 2. Consider the boundary value problem for the Laplace equation in the upper half-plane $y > 0$:

$$\Delta u = 0, \quad y > 0, \quad u(x, 0) = f(x), \quad u(x, y) \rightarrow 0 \text{ as } y \rightarrow \infty. \quad (2)$$

Using the Poisson integral formula, find the solution $u(x, y)$ for the boundary value $f(x) = \frac{1}{1+x^2}$.

Problem 3. Consider the boundary value problem for the Laplace equation in the upper half-plane $y > 0$:

$$\Delta u = 0, \quad y > 0, \quad u(x, 0) = f(x), \quad u(x, y) \rightarrow 0 \text{ as } y \rightarrow \infty. \quad (3)$$

C. Kinetics

Equations (8) and (23) contain the quantities B° / B_0° and G/G_0 , which represent the normalized nucleation and growth rate functions, respectively. In order to solve these equations, some kinetic assumptions must be made.

1. Nucleation. The initial nucleation rate, B_0° , is the rate of formation of nuclei at $z = 0$, the entrance of the reactor. The assumption is made that the initial nucleation rate is a function of the ratio R .

Equation (12) may be written in the form

$$B_0^\circ = \left[\frac{1}{\rho K_v (G_0 \tau)^3 \tau f_3(1)} \right] C_0 (1 - \beta_s) = B_0^\circ(R) . \quad (24)$$

The total nucleation, B° , is assumed to be the product of the initial nucleation and a decay function of the form $(1 - z)^a$. The expression for B° is

$$B^\circ = B_0^\circ(R)(1 - z)^a \quad (25)$$

and the nucleation ratio B° / B_0° is

$$\frac{B^\circ}{B_0^\circ} = (1 - z)^a . \quad (26)$$

2. Growth. The initial growth rate at the entrance is G_0 . The initial growth rate is related to the mass-weighted mean particle size, \bar{L} , as follows:

5. Results

Equations (1) and (2) involve the quantities \bar{v}_1 and \bar{v}_2 , which represent the mean velocity and growth rate functions, respectively. In order to solve these equations, some kinetic assumptions must be made.

Assumption 1. The initial nucleation rate, \bar{v}_1 , is the rate of formation of nuclei at $t = 0$, the entrance of the reactor. The assumption is made that the initial nucleation rate is a function of the ratio \bar{v}_2 . Equation (1) may be written in the form

$$\bar{v}_1 = \frac{1}{A + B\bar{v}_2} \quad (2a)$$

The total nucleation, \bar{v}_1 , is assumed to be the product of the initial nucleation and a decay function of the form $(1 - \alpha)^t$. The expression for \bar{v}_1 is

$$\bar{v}_1 = \bar{v}_1(0)(1 - \alpha)^t \quad (2b)$$

and the nucleation rate \bar{v}_2 is

$$\bar{v}_2 = \frac{1}{1 - \alpha} \quad (2c)$$

Assumption 2. The initial growth rate at the entrance is \bar{v}_2 . The initial velocity rate is related to the mass-weighted mean particle size

\bar{v}_2 as follows:

\bar{L} , the mass-weighted mean particle size, is defined by the ratio of the 4th and 3rd moments ($L_{4,3}$ in Ref. 17)

$$\bar{L} = \frac{m_4(1)}{m_3(1)}, \quad (27)$$

and by Eq. (7),

$$\bar{L} = \frac{B_0^0 (G_0 \tau)^4 \tau f_4(1)}{B_0^0 (G_0 \tau)^3 \tau f_3(1)} = G_0 \tau \frac{f_4(1)}{f_3(1)}. \quad (28)$$

G_0 is assumed to be a function of the experimental parameter, R . The total growth rate, G , is assumed to be the product of the initial growth rate and decay function of the form $(1 - z)^b$, namely,

$$G = G_0(R)(1 - z)^b. \quad (29)$$

The growth ratio G/G_0 is

$$\frac{G}{G_0} = (1 - z)^b. \quad (30)$$

The moment equations, including the kinetic assumptions, are

$$\text{Plug Flow: } f_j' - (0)^j (1 - z)^a - j(1 - z)^b f_{j-1} = 0 \quad (31)$$

$$\text{Dispersed Plug Flow: } \frac{1}{Pe} f_j'' - f_j' + (0)^j (1 - z)^a + j(1 - z)^b f_{j-1} = 0. \quad (32)$$

Equations (31) and (32), together with the appropriate boundary conditions, can be solved numerically to obtain the j th moments of the

the boundary conditions are satisfied, is defined by the ratio of the
 the total growth rate, Ω , is assumed to be the product of the initial growth

$$(57) \quad \frac{\partial \Omega}{\partial t} = \dots$$

$$(58) \quad \frac{\partial \Omega}{\partial t} = \dots$$

is assumed to be a function of the exponential growth rate, Ω . The
 total growth rate, Ω , is assumed to be the product of the initial growth
 rate and decay constant of the form $(1 - \alpha)^t$, namely,

$$(59) \quad \Omega = \Omega_0 (1 - \alpha)^t$$

The growth rate Ω_0 is

$$(60) \quad \frac{\partial \Omega}{\partial t} = \dots$$

The moment equations, including the kinetic equations, are

$$(61) \quad \dots$$

$$(62) \quad \dots$$

Equations (61) and (62), together with the appropriate boundary

conditions, can be used to obtain the full moments of the

of the distribution. A discussion of the numerical methods can be found in Appendix B.

D. Inversion of the Moments

The solution of either the plug flow or dispersed plug flow moment equations by methods given in the Appendixes, gives a set of $\{f_j\}$ dimensionless moments. The number of moments used in this study is ten, that is, $j = 0, 1, \dots, 9$.

The set of moments can be approximated by the equation

$$f_j \cong \sum_{k=0}^9 \xi_k^j y_k \Delta \xi_k, \quad (33)$$

from which the dimensionless population distribution function, y_k , may be calculated for a given ξ_k and $\Delta \xi_k$ using matrix inversion techniques.

The cumulative weight fraction distribution is¹⁷

$$WW(L) = \frac{\rho k_v \int_0^L p^3 n(p) dp}{M_T}, \quad (34)$$

where $n(p)$ is the population density of particles having size less than L . Substituting the value for M_T from Eq. (9), and cancelling ρk_v ,

$$WW(L) = \frac{\int_0^L p^3 n(p) dp}{\int_0^L L^3 n(L) dL}. \quad (35)$$

The relation ...

equation ...

dimensional ...

is seen that ...

The set of ...

from which the ...

may be calculated ...

technique ...

The ...

where $\epsilon(\rho)$ is the ...

1. ...

Substituting the dimensionless quantities given in Section V. A, namely,

$n = n_0^0 y$ and $L = G_0 \tau \xi$, we have

$$WW(L) = \frac{\int_0^{\xi} p^3 y(p) dp}{f_3(1)} \quad (36)$$

where $y(p)$ is the dimensionless population density of particles having dimensionless size less than ξ .

Equation (36) may be approximated by the sum

$$WW(L) = \frac{1}{f_3(1)} \sum_{i=0}^{\xi} p_i^3 y_i(p) \Delta p_i, \quad (37)$$

that is, $WW(L_0) = \frac{1}{f_3(1)} (\xi_0^3 y_0 \Delta \xi_0)$, $WW(L_1) = \frac{1}{f_3(1)} (\xi_0^3 y_0 \Delta \xi_0 + \xi_1^3 y_1 \Delta \xi_1)$, $WW(L_2) = \frac{1}{f_3(1)} (\xi_0^3 y_0 \Delta \xi_0 + \xi_1^3 y_1 \Delta \xi_1 + \xi_2^3 y_2 \Delta \xi_2)$, etc.

E. Comparison of Theory with Experiment

The differential equations representing the dispersed plug flow model are solved for a given set of parameters a , b , and Pe . The resulting dimensionless moments are inverted to obtain the population distribution functions and finally, the cumulative weight fraction distribution is calculated by means of Eq. (37). This cumulative weight fraction distribution can be directly compared with experimentally determined distributions.

The moments of the population may be compared directly without inversion by converting cumulative weight fraction distribution data to

where μ is the mean and σ^2 is the variance of the population being sampled. The sample mean \bar{y} is given by

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$$

where y_i is the value of the variable being sampled in the i th sample. The variance of the sample mean is given by

$$\text{var}(\bar{y}) = \frac{\sigma^2}{n}$$

where σ^2 is the variance of the population being sampled. The standard error of the sample mean is given by

$$\text{se}(\bar{y}) = \frac{\sigma}{\sqrt{n}}$$

The distribution of the sample mean is approximately normal for large samples. The central limit theorem states that if the population is normally distributed, then the sample mean is also normally distributed. If the population is not normally distributed, then the sample mean will be approximately normally distributed for large samples. The normal distribution is characterized by its mean and variance. The probability density function of the normal distribution is given by

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$

moments based on weight distribution, and then converting to moments based on a population distribution.

The weight distribution function is defined by¹⁷

$$W(L) = \frac{dWW(L)}{dL} \quad (38)$$

and the j th moment of the weight distribution function is

$$m_j(\text{wt}) = \int_0^{\infty} L^j W(L) dL \quad (39)$$

or, approximately,

$$m_j(\text{wt}) \cong \sum_i L_i^j \Delta[WW(L_i)] \quad (40)$$

The weight distribution may be converted to population distribution by the equation¹⁷

$$W(L) = \frac{1}{m_3(\text{popl.})} L^3 n(L) \quad , \quad (41)$$

from which the following relationships are derived:

$$m_j(\text{wt}) = \frac{m_{j+3}(\text{popl.})}{m_3(\text{popl.})} \quad (42)$$

and

$$m_j(\text{wt}) = (G_0 \tau)^j \frac{f_{j+3}}{f_3} \quad (43)$$

... and the weight function is defined by ...

$$w(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$$

... and the moment of the weight distribution function is

$$\int_{-\infty}^{\infty} x^n w(x) dx = \begin{cases} 0 & n \text{ odd} \\ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} x^n e^{-x^2/2} dx & n \text{ even} \end{cases}$$

... or approximately

$$\int_{-\infty}^{\infty} x^n w(x) dx \approx \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} x^n e^{-x^2/2} dx$$

The weight distribution may be converted to population distribution by the relation

$$W(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$$

From which the following relationships are derived:

$$m_1 = \int_{-\infty}^{\infty} x W(x) dx = 0$$

$$m_2 = \int_{-\infty}^{\infty} x^2 W(x) dx = 1$$

Equation (43) allows the comparison of experimental data with calculated quantities derived from the theoretical model directly, without moment inversion. An alternate method, which utilizes three of the moments, is the calculation of the coefficient of variation (C. V.) of the distribution. The coefficient of variation, or relative dispersion, is the measure of dispersion stated as a function of its average, that is,

$$\text{C. V.} = \frac{\sigma}{\bar{L}}, \quad (44)$$

where σ is the standard deviation from the mean for the distribution.

The coefficient of variation may be calculated from the moments by

$$\text{C. V.} = \left(\frac{m_2(\text{wt})}{m_1^2(\text{wt})} - 1 \right)^{\frac{1}{2}} \quad (45)$$

and by

$$\text{C. V.} = \left(\frac{f_5 f_3}{f_4^2} - 1 \right)^{\frac{1}{2}}. \quad (46)$$

(Note that $m_0(\text{wt}) \equiv 1.$)

... (1) ... of experimental data ...
 ... (2) ... the theoretical model ...
 ... (3) ... which differs from the ...
 ... (4) ... the coefficient of variation ...
 ... (5) ... the distribution ...
 ... (6) ... the measure of dispersion ...

$$C.V. = \frac{s}{\bar{x}} \quad (44)$$

where s is the standard deviation from the mean for the distribution.
 The coefficient of variation may be calculated from the moments

$$C.V. = \frac{\sqrt{\frac{\mu_2}{n} - \left(\frac{\mu_1}{n}\right)^2}}{\frac{\mu_1}{n}} \quad (45)$$

$$C.V. = \frac{\sqrt{\frac{\mu_2}{n} - \left(\frac{\mu_1}{n}\right)^2}}{\frac{\mu_1}{n}} \quad (46)$$

(Note that $\mu_1 = \bar{x}$)

VI. EXPERIMENTAL

A. Apparatus

The crystallization apparatus consists of three sections: (1) the constant flow feed system, (2) the static mixer, and (3) the filtering system. A diagram of the apparatus is shown in Fig. 2.

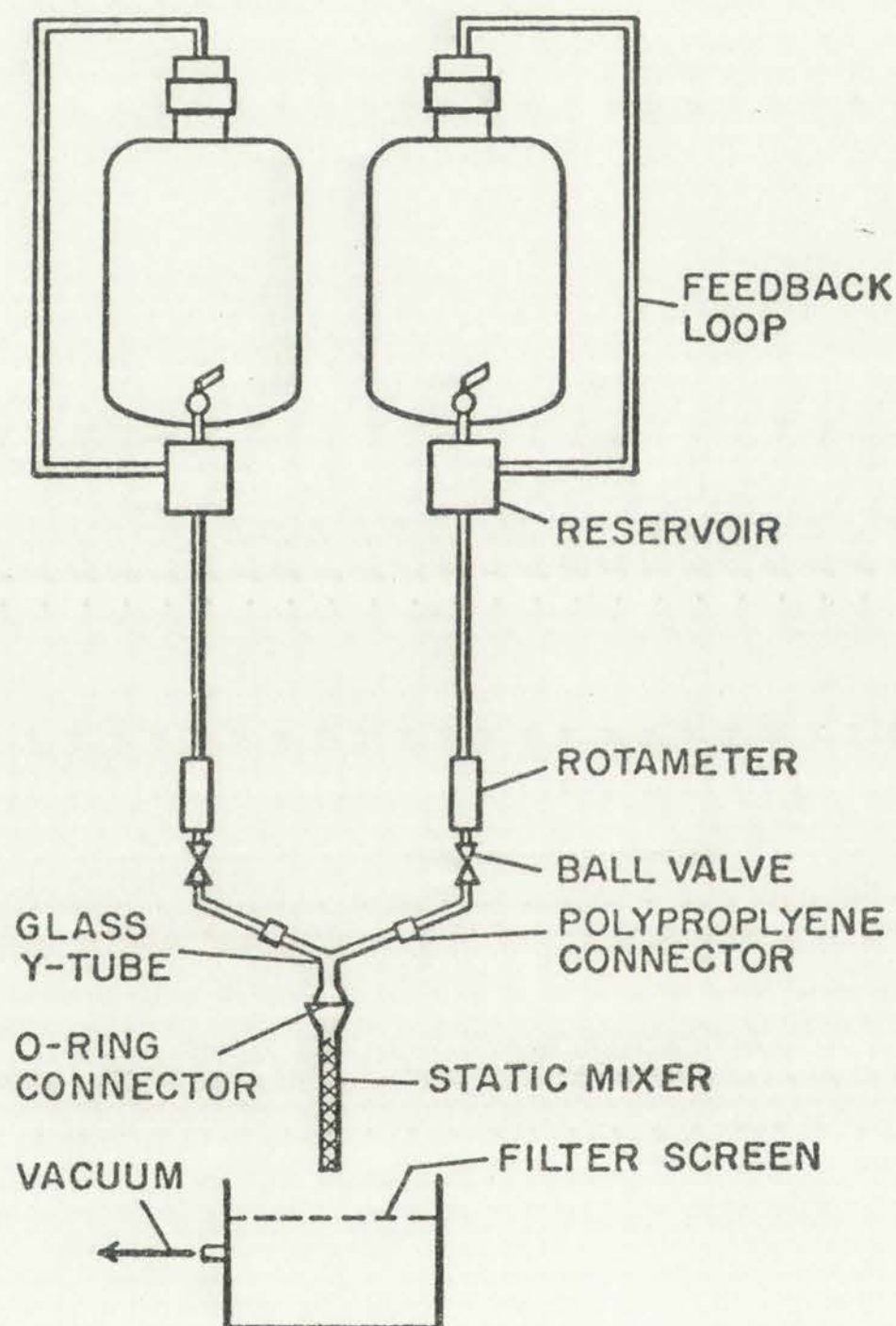
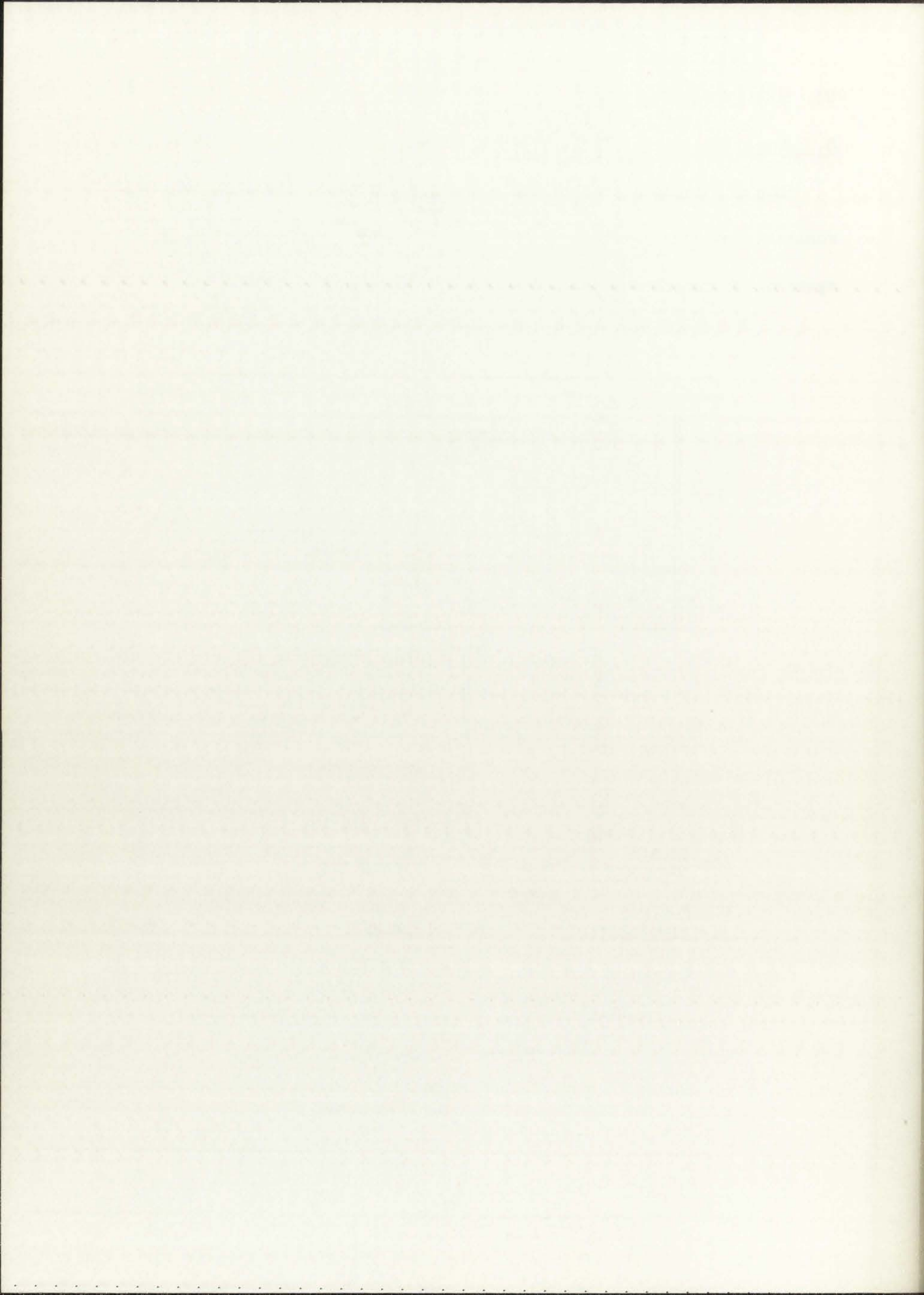


Figure 2.
PETN Crystallization Apparatus.



1. Constant Flow Feed System. There are two identical feed systems, one for the acetone-PETN solution, and one for the water. Each solution is held in a 24-liter capacity polyethylene bottle equipped with a polyethylene stopcock located through the sidewall at the bottom of the bottle. The solution is allowed to flow into a polyethylene reservoir (about 1 liter) situated just below the bottle and about 2 m above the static mixer. The polyethylene stopcock outlet extends into the reservoir. The liquid level is controlled in the reservoir by an airtight, 1.27-cm-o.d. polyethylene tube (feedback loop) that connects the top sidewall of the reservoir to the top of the bottle. If the liquid level in the reservoir drops below the tube inlet, the pressure above the liquid in the bottle increases to atmospheric allowing more liquid to pour into the reservoir. If the tube inlet is full of liquid, the feed solution will not flow into the reservoir. The solution is fed through a 1.27-cm-o.d. polyethylene tube to a rotameter ahead of the static mixer. The rotameters were calibrated using either pure acetone or water. Each solution is fed to the static mixer through a 0.635-cm-o.d. polyethylene tube.

The flow limitations of the system, including the rotameters, are:

Minimum acetone flow rate	1.3 cm ³ /s
Maximum acetone flow rate	15.0 cm ³ /s
Minimum water flow rate	1.0 cm ³ /s
Maximum water flow rate	15.0 g/cm ³

The flow rate of the solution is controlled by a reservoir of the solution. The liquid level is controlled in the reservoir by an air-tight 1.57-cm-od polyethylene tube (Mason's type) that connects the top of the reservoir to the top of the bottle. If the liquid level in the reservoir drops below the tube inlet, the pressure above the liquid in the bottle increases so atmospheric pressure forces more liquid to pass into the reservoir. If the tube inlet is full of liquid, the flow solution will not flow into the reservoir. The solution is fed through a 1.57-cm-od polyethylene tube to a reservoir above the static mixer. The reservoir was calibrated using either pure acetone or water. Each solution is fed to the static mixer through a 0.635-cm-od polyethylene tube.

The flow instabilities of the system, including the rotameters, are discussed in terms of flow rate. The flow rate of the solution is 1.0 cm³/s. The flow rate of the water is 1.0 cm³/s. The flow rate of the water is 1.0 cm³/s.

2. Static Mixer. The effluent from the rotameters mix together at the first element of the static mixer by means of a glass Y-tube with a glass divider. The Y-tube is connected to the static mixer by means of an O-ring connector. Figure 3 is a schematic of the static mixer and Y-tube connector.

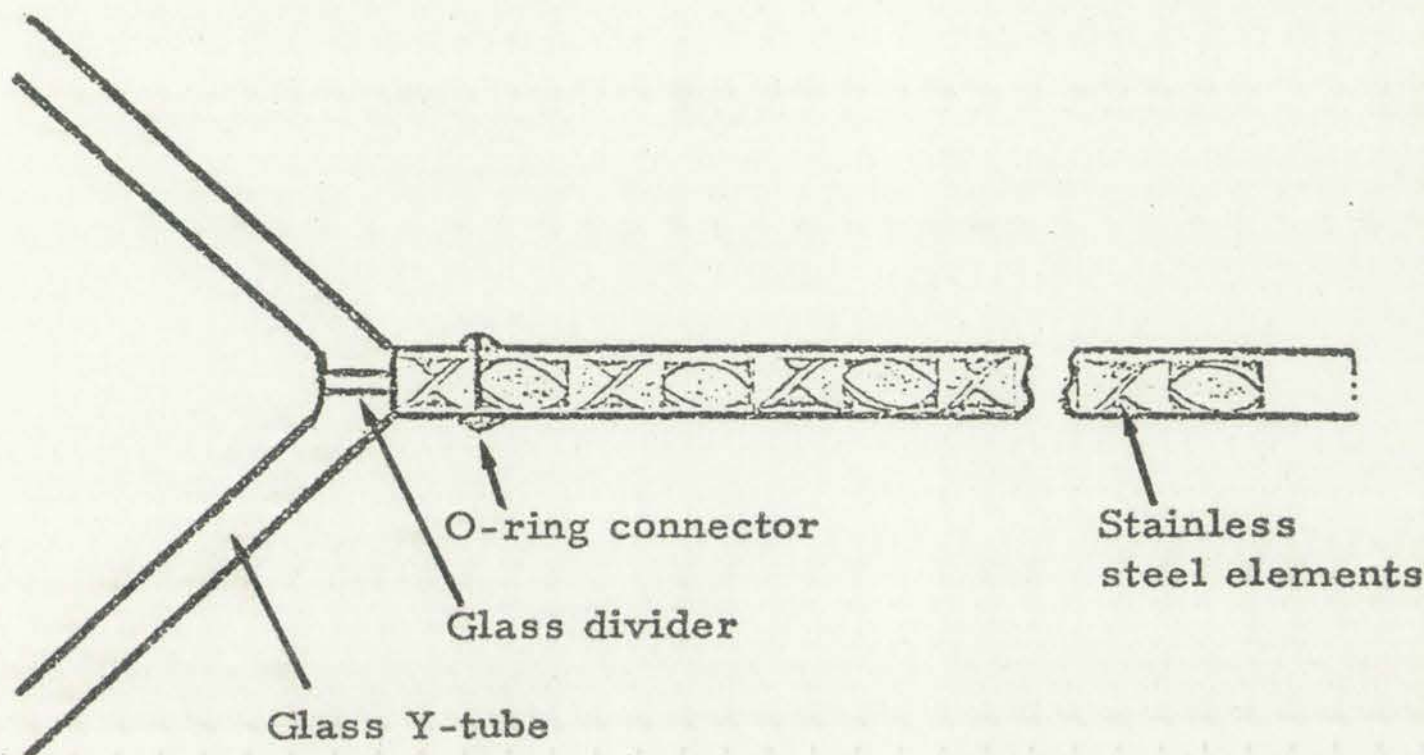


Figure 3.
Static Mixer.

The static mixer contains no moving parts. The mixing is achieved by the bow tie-shaped blades or elements. Their configuration imparts four basic motions to the flowing material:¹²

- Flow division--Each element divides material received from the preceding element.
- Flow reversal--The opposite twist of each succeeding element constantly reverses the circular direction of flow.

The static mixer is a device which is used to mix two or more fluids together. It is a type of mixer which is used in a wide variety of applications. The static mixer is a device which is used to mix two or more fluids together. It is a type of mixer which is used in a wide variety of applications. The static mixer is a device which is used to mix two or more fluids together. It is a type of mixer which is used in a wide variety of applications.



The static mixer is a device which is used to mix two or more fluids together. It is a type of mixer which is used in a wide variety of applications. The static mixer is a device which is used to mix two or more fluids together. It is a type of mixer which is used in a wide variety of applications. The static mixer is a device which is used to mix two or more fluids together. It is a type of mixer which is used in a wide variety of applications. The static mixer is a device which is used to mix two or more fluids together. It is a type of mixer which is used in a wide variety of applications.

- Flow inversion--The material migrates from the center of the pipe to the outside walls and back.
- Backmixing--There is a constant change in flow profile.

Velocity, pressure, and time have no influence upon the degree of mix. Pressure drop is low, and radial temperature differences are effectively eliminated.

Because of the continuous flow division reversal and flow inversion at every element of the mixer, ideal plug flow conditions are approached.²

The static mixer is a 0.635-cm-i.d. glass tube, 30.5 cm long, containing 24 stainless steel bow tie elements. The volume, as measured by water delivery at 20°C, is 9.0 cm³.

The holding time of the static mixer is calculated by the equation

$$\text{Holding time(s)} = \frac{\text{Volume of mixer (cm}^3\text{)}}{\text{Total volume flow rate (cm}^3\text{/s)}} \cdot \quad (47)$$

Table 2 gives the scheme for holding times and flow rates used in the experiments.

The following table shows the results of the experiments conducted on the effect of temperature on the rate of reaction between hydrogen peroxide and potassium iodide. The rate of reaction was measured by the volume of oxygen gas evolved in a given time.

Temperature (°C)	Volume of oxygen (ml)
10	10
20	20
30	40
40	80
50	160

From the above table, it is clear that the rate of reaction increases with an increase in temperature. This is because the molecules of the reactants have more energy at higher temperatures and hence they collide more frequently and with more force, leading to a faster reaction.

Table 2

EXPERIMENT HOLDING TIMES AND FLOW RATES

Holding Time = 0.5 s
Total Flow Rate = 18.0 cm³/s

<u>Acetone Solution Flow Rate (cm³/s)</u>	<u>Water Flow Rate (cm³/s)</u>	<u>R</u>
3.6	14.4	$\frac{1}{4}$
6.0	12.0	$\frac{1}{2}$
9.0	9.0	1

Holding Time - 2.0 s
Total Flow Rate - 4.5 cm³/s

1.13 ^a	3.38	$\frac{1}{3}$
2.25	2.25	1
3.0	1.5	2
3.38	1.13	3

^aThis is below the rotameter measurement limit. The flow rate was measured with a graduate and stopwatch.

3. Filtering System. Small samples (about 2 g) were collected on a 350-cm³ tared Buchner funnel with a fritted glass disc (medium porosity) mounted on a 2-liter suction flask. The volume of the solids-free liquid collected in the flask was measured. The PETN sample was washed with distilled water and dried under vacuum for 18 h at 65°C. The dried sample was weighed on a single-pan analytical balance. The data were used to calculate the M_T value for the run.

TABLE I
RESULTS OF THE ANALYSES

Flow rate = 0.5 cm³/min
Temperature = 100°C

Retention Time (min)	Flow Rate (cm ³ /min)	Temperature (°C)
1.0	0.5	100
1.5	0.5	100
2.0	0.5	100
2.5	0.5	100
3.0	0.5	100
3.5	0.5	100
4.0	0.5	100
4.5	0.5	100
5.0	0.5	100
5.5	0.5	100
6.0	0.5	100
6.5	0.5	100
7.0	0.5	100
7.5	0.5	100
8.0	0.5	100
8.5	0.5	100
9.0	0.5	100
9.5	0.5	100
10.0	0.5	100

This is below the standard measurement limit. The flow rate was measured with a graduated and stop watch.

2. Retention System. Small samples (about 5 g) were collected

on a 500-ml. tapered bottom funnel with a fitted glass disc (medium

porosity) mounted on a 2-liter suction flask. The volume of the solids

was held in the flask was measured. The 100 ml sample

was washed with distilled water and dried under vacuum for 18 hr

at 60°C. The dried sample was weighed on a single-pan analytical

balance. The data were used to calculate the R_c values for the run

Large samples (30 to 50 g) were collected on a 29-cm-diam stainless steel screen nominally rated at 5 μm . The screen was mounted on a holder that was on a stainless steel can (about 10-liter capacity) equipped with a vacuum connection.

B. Materials

- PETN--The PETN used was recrystallized Cap Grade (Lot 4-28-32) purchased from Du Pont. The material was analyzed for Group WX-3 use. The result of the nitrogen analysis is 17.26% N. The theoretical value is 17.72% N.
- Acetone--The acetone used was Analytical Reagent Grade.
- Water--Distilled water was used.
- Static Mixer--A Kenics Static Mixer, * purchased from Kenic's Corporation, Danvers, MA, was used.
- Metal Filter Screen--A furnace-sintered woven wire mesh filter screen nominally rated at 5 μm was purchased from Pall Trinity Micro Corporation, Cortland, NY. A type 304 stainless steel filter screen, nominally rated at 5 μm , was purchased from The Bendix Corporation, Filter Division, Madison Heights, MI.
- Plastic Fittings--All connections exposed to the acetone-PETN solution were made from polypropylene tube fittings purchased from United States Plastic Corporation, Lima, OH.

*Registered trademark.

Larger amounts of the material were collected on a 150-mesh sieve... The residue was retained... on a 100-mesh sieve... equipped with a vacuum connection.

ANALYSIS

ANALYSIS - The PERM analysis was performed on the material... 4-28-52 purchased from Du Pont. The material was analyzed for Group IX-3 acid. The result of the nitrogen analysis is 17.5% N. The theoretical value is 17.5% N.

ANALYSIS - The analysis was performed on the material... Water - Distilled water was used.

ANALYSIS - A Keweenaw Brand Filter, purchased from Keweenaw Corporation, Lansing, MI, was used.

ANALYSIS - A furnace-stained woven wire mesh filter screen nominally rated at 5 microns was purchased from

Full Textile Filter Corporation, Cortland, NY. A type 504 stainless steel filter screen, nominally rated at 5 microns, was

purchased from The Borden Corporation, Filter Division, Madison Heights, MI.

ANALYSIS - All connections exposed to the atmosphere were made from polyethylene and were thoroughly cleaned

from United States Filter Corporation, Lansing, MI.

ANALYSIS -

C. Procedure

The acetone-PETN solution (about 10 liters) was adjusted to $20 \pm 3^\circ\text{C}$ and placed into the polyethylene bottle. The PETN concentration was 0.5 wt% for $R \leq 1$, and 5.0 wt% for $R > 1$. The distilled water (about 20 liters) was adjusted to $20 \pm 3^\circ\text{C}$ and placed in the second polyethylene bottle. The solutions were allowed to flow into their respective reservoirs and the bottles and feedback loops were checked for air leaks. The control valves were adjusted for the proper R-value to be used. The total flow rate was checked with a stopwatch and graduate. After allowing at least 30 s for equilibration, the metal screen was placed into position for collection of the sample. During the run, the rotameters were monitored for proper flow. Usually no further adjustment was necessary unless precipitated PETN began plugging the mixer. Precipitate buildup was significant for $R > 1$ runs. If precipitate buildup did occur, the sample collection was stopped and the mixer was "cleared" by opening the acetone solution to maximum flow until the precipitate redissolved in the acetone. After clearing the mixer, the flow was readjusted and the sample collection began again. During the run, the small sample was collected in a Buchner funnel with a fritted glass disc for M_T measurements. The procedures for each R value are summarized below:

The reaction of the polymer with the monomer was carried out in a 250 ml. flask equipped with a mechanical stirrer. The reaction mixture was stirred at 50°C and allowed to react for 24 hours. The reaction mixture was then poured into a large volume of methanol to precipitate the polymer. The precipitate was filtered and dried in a vacuum oven at 50°C for 24 hours. The yield of the polymer was 0.8 g. The inherent viscosity of the polymer in benzene at 30°C was 0.12 dl/g. The reaction was carried out with 0.1 mole of monomer and 0.1 mole of polymer. The reaction was carried out in a 250 ml. flask equipped with a mechanical stirrer. The reaction mixture was stirred at 50°C and allowed to react for 24 hours. The reaction mixture was then poured into a large volume of methanol to precipitate the polymer. The precipitate was filtered and dried in a vacuum oven at 50°C for 24 hours. The yield of the polymer was 0.8 g. The inherent viscosity of the polymer in benzene at 30°C was 0.12 dl/g.

$R = \frac{1}{4}$ (Batches 3848, 3851, * 3852, and 3853)

The acetone-PETN feed solution consisted of 39.75 g of PETN in 10 liters of acetone (0.5 wt%). The acetone-PETN flow rate was $3.6 \text{ cm}^3/\text{s}$, and that of the water was $14.4 \text{ cm}^3/\text{s}$. The holding time for the reactor was 0.5 s. Some difficulties were encountered in filtering the product. There was a tendency for a slight buildup of liquid on the filter. This problem was circumvented by supplementing the metal filter with three additional 600-cm^3 Buchner funnels with fritted glass discs that were used in rotation so that little or no fluid accumulation occurred. The precipitated PETN collected on the filters was combined to form a single batch.

 $R = \frac{1}{3}$ (Batches 3866, 3867, and 3868)

The acetone-PETN flow rate was $1.13 \text{ cm}^3/\text{s}$ and that of the water was $3.37 \text{ cm}^3/\text{s}$. The reactor holding time was 2.0 s. The feed solutions were similar to the $R = \frac{1}{4}$ runs. The same filtering procedure was used.

 $R = \frac{1}{2}$ (Batches 3856, 3857, and 3858)

The acetone-PETN flow rate was $6.0 \text{ cm}^3/\text{s}$ and that of the water was $12.0 \text{ cm}^3/\text{s}$. The reactor holding time was 0.5 s. The feed solutions were similar to the $R = \frac{1}{4}$ and $R = \frac{1}{3}$ runs. The filtering procedure was the same.

*Batch 3851 was found to be contaminated with a fibrous material originating from the acetone stock. The batch was not included in the study.

The reaction of ethyl acrylate with nitrogen was studied at 100°C and 1 atm.

The rate of reaction was measured by the decrease in the volume of the gas.

The reaction was first order with respect to the ethyl acrylate.

The rate constant was found to be $k = 1.5 \times 10^{-4} \text{ min}^{-1}$.

The activation energy was determined to be 15.5 kcal/mole.

The reaction was studied in the presence of various inhibitors.

The reaction was found to be inhibited by benzoyl peroxide.

The reaction was also studied in the presence of a radical scavenger.

The reaction was found to be inhibited by hydroquinone.

The reaction was also studied in the presence of a chain transfer agent.

Reaction of Ethyl Acrylate with Nitrogen

The reaction of ethyl acrylate with nitrogen was studied at 100°C and 1 atm.

The rate of reaction was measured by the decrease in the volume of the gas.

The reaction was first order with respect to the ethyl acrylate.

Further work is needed.

Reaction of Ethyl Acrylate with Nitrogen

The reaction of ethyl acrylate with nitrogen was studied at 100°C and 1 atm.

The rate of reaction was measured by the decrease in the volume of the gas.

The reaction was first order with respect to the ethyl acrylate.

Further work is needed.

The reaction was also studied in the presence of a radical scavenger.

The reaction was found to be inhibited by hydroquinone.

R = 1 (Batches 3861, 3862, 3863, 3864, 3871, 3872, 3873, and 3874)

Two reactor holding times were used. Batches 3861 through 3864 were made with an acetone-PETN solution flow rate of $9.0 \text{ cm}^3/\text{s}$ and water flow rate of $9.0 \text{ cm}^3/\text{s}$, giving a holding time of 0.5 s. Batches 3871 through 3874 were made with an acetone-PETN solution flow rate of $2.25 \text{ cm}^3/\text{s}$ and water flow rate of $2.25 \text{ cm}^3/\text{s}$, giving a holding time of 2.0 s. The feed solutions were similar to the $R = \frac{1}{4}$, $R = \frac{1}{3}$, and $R = \frac{1}{2}$ runs. No filtering difficulties were encountered, and there was no need to supplement the metal filter.

R = 2 (Batches 3876, 3877, and 3878)

The acetone-PETN feed solution consisted of 416.3 g of PETN in 10 liters of acetone (5.0 wt%). The PETN concentration was increased because of its large solubility in the combined acetone-water solvent. The acetone-PETN solution flow rate was $3.0 \text{ cm}^3/\text{s}$ and that of the water was $1.5 \text{ cm}^3/\text{s}$. The reactor holding time was 2.0 s. A 0.5-s holding time was not used because of a rapid irreversible plugging that occurred at the higher flow rates. No filtering problems were encountered.

R = 3 (Batches 3881, 3882, and 3883)

The acetone-PETN feed concentration was 5.0 wt%. The acetone-PETN flow rate was $3.33 \text{ cm}^3/\text{s}$ and that of the water was $1.11 \text{ cm}^3/\text{s}$. The reactor holding was 2.0 s. Higher flow rates were not used because of irreversible plugging in the mixer. Difficulties

The reaction between the polymer and the solvent was studied at various temperatures and water flow rates of 1.0 and 2.0 cm³/min.

It was found that the reaction rate increased with increasing temperature and decreasing water flow rate. The reaction rate was also found to be dependent on the initial concentration of the reactants.

The reaction rate was found to be first order with respect to the concentration of the reactants. The reaction rate was also found to be independent of the initial concentration of the reactants.

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Received

The reaction between the polymer and the solvent was studied at various temperatures and water flow rates of 1.0 and 2.0 cm³/min.

It was found that the reaction rate increased with increasing temperature and decreasing water flow rate. The reaction rate was also found to be dependent on the initial concentration of the reactants.

with product filtering were encountered. It was necessary to supplement the 29-cm-diam metal filter with the three fritted glass filters and with an additional 29-cm-diam metal filter.

D. Particle Measurement

1. Photelometer Technique.^{7,13} The estimation of particle size distribution for subsieve particles below the 45- μm sieve size was made possible by a particle sedimentation-in-liquid method. In this method, a representative PETN sample is dispersed homogeneously in a 50-vol% mixture of n-octane and 1, 1, 2, 2-tetrachloroethane in a sedimentation tube. The intensity of a collimated beam of light passed through the suspension is measured after varying sedimentation times, and at varying levels. The particle size distribution is calculated by means of Stoke's law.

About one gram of each PETN sample was placed in about 300 cm^3 of the dispersing medium. The slurry was stirred for about 30 min by means of an air-driven rotary stirrer. The suspension was examined microscopically at 60X magnification to ensure total deagglomeration. Duplicate photelometer runs were made.

The samples were wet sieved using PETN-saturated ethanol as the transfer fluid. The following sieve sizes were used: 250, 177, 125, 88, 62, and 45 μm . Photelometer results were used for sub 45- μm particles. Sieve analyses were used for the large particle size. The correlation of photelometer results with sieve analyses for HMX (octahydro-1, 3, 5, 7-tetranitro-s-tetrazocine) is shown in Fig. 4.⁷

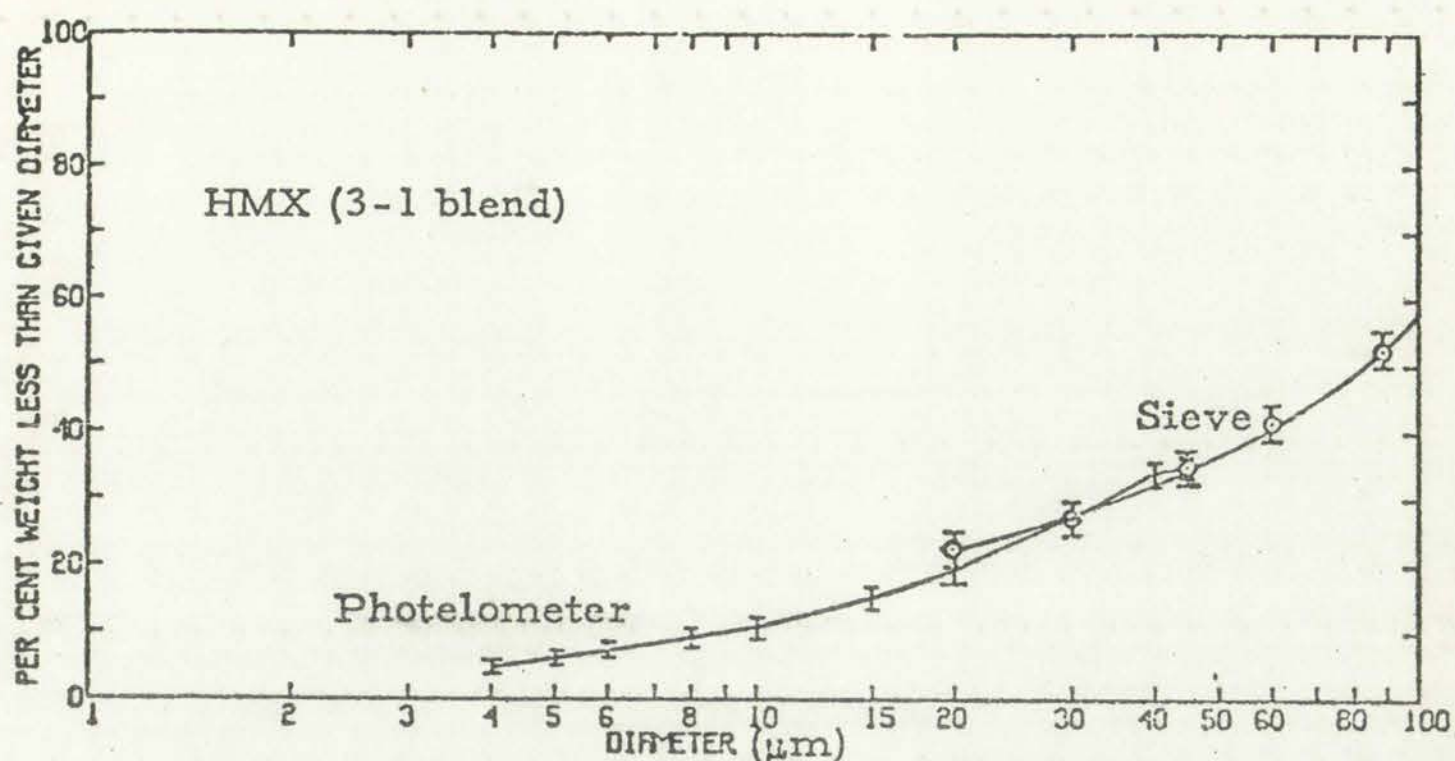


Figure 4.

Cumulative logarithmic plot of photometer analysis of HMX and of sieve analysis of coarse fraction above 45 μm . Curve is average of four runs \pm one standard deviation.

2. Scanning Electron Microscopy. Each sample was photographed at 100, 300, and 1000X. The samples were gold shadowed to avoid any thermal effects on the heat-sensitive particles.

E. Detonator Test Firing

The PETN samples that were used in the detonators had the following pressed characteristics:

PETN pressed density	0.88 g/cm ³
PETN pressed diameter	4.064 mm
PETN pressed length	2.540 mm
PETN pressed mass	29 mg

1. Threshold Voltage Tests. Ten PETN pressings per sample were used. The PETN samples were initiated by a bursting gold



Figure 4
 Cumulative logarithmic plot of photoluminescence analysis of PETN
 and of stave analysis of coarse fraction showed in Curve
 is average of four runs - one standard deviation.

A. Scanning Electron Microscopy - Both single and double

at 100, 500, and 1000X. The samples were gold sputtered to avoid
 thermal effects on the heat-sensitive particles.

B. Laser Raman Test

The PETN samples that were used in the dispersion test for
 following pressed characteristics:

- PETN pressed density: 0.88 g/cm³
- PETN pressed diameter: 2.021 mm
- PETN pressed length: 2.540 mm
- PETN pressed mass: 1.29 mg

C. Threshold Voltage Tests - For PETN pressed for 20 min

were used. The PETN samples were initiated by a constant 200

bridgewire 0.0381 mm diam and 1.016 mm long. The firing capacitance was $1 \mu\text{F}$ per detonator. The firing cables consisted of a 4.41-m-long cable (21-C-31) connected to a 0.457-m-long cable (31-L-121) by means of a double-ended connector. The inductance of the cables plus bridgewire was $1.0413 \mu\text{H}$ and the resistance was 0.266Ω . The Brucceton "up and down" method⁶ of determining the 50% values of the firing voltages ($E_{0.5}$) was used.

2. Transit Time Tests. Two detonators per sample were fired. A high density (1.65 g/cm^3) PETN pressing 7.62 mm diam by 1.143 mm long was added to the PETN sample to increase the output light intensity. The transit time contribution of the high density PETN is a known constant for the tests. Any resulting variations in t_m are due to the PETN samples. The measured t_m value is the difference in time of the appearance of light between the bursting bridgewire and the shock wave breakout. The light appearances are observed with a rotating mirror camera (RMC).

The bridgewire used in the t_m tests is the same type as that used in the $E_{0.5}$ measurements. The firing capacitance was $1 \mu\text{F}$ with a firing voltage of 2500 V per detonator. The firing cables used consisted of a 1.524-m-long cable (21-C-31) connected to a 0.762-m-long cable (31-L-121) by means of a double-ended connector. The

inductance of the cables plus bridgewire was $0.5389 \mu\text{H}$ and the resistance was 0.191Ω .

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VII. RESULTS

A. Experimental Particle Size Distributions

The cumulative weight distribution curves for all R-values are shown in Figs. 5a through 5f. The error bars represent standard deviations. Photometer runs were sufficient for $R < 1$; for $R \geq 1$, the photometer method was supplemented by sieves. Table 3 summarizes the particle size characteristics of the products.

Table 3

PARTICLE SIZE CHARACTERISTICS

<u>R-Value</u>	<u>Average \bar{L} (μm)</u>	<u>Average Coefficient of Variation</u>
$\frac{1}{4}$	12.2	0.34
$\frac{1}{3}$	12.7	0.35
$\frac{1}{2}$	13.3	0.40
1	30.2	0.49
2	41.0	0.47
3	63.5	0.52

Representative product scanning electron micrographs are shown in Figs. 6a through 6g.

EXPERIMENTAL PROCEDURE

The reaction mixture was prepared by... The reaction was carried out at 100°C... The product was purified by... The yield was 85%.

CHARACTERIZATION DATA

Sample	Yield (%)	mp (°C)	IR (cm ⁻¹)	¹ H NMR (ppm)	ANAL. Calcd (%)
1	85	120	1715	7.2, 6.8, 6.4	C 72.1, H 5.8
2	82	118	1710	7.1, 6.7, 6.3	C 71.8, H 5.7
3	80	115	1705	7.0, 6.6, 6.2	C 71.5, H 5.6
4	78	112	1700	6.9, 6.5, 6.1	C 71.2, H 5.5
5	75	110	1695	6.8, 6.4, 6.0	C 70.9, H 5.4
6	72	108	1690	6.7, 6.3, 5.9	C 70.6, H 5.3
7	70	105	1685	6.6, 6.2, 5.8	C 70.3, H 5.2
8	68	102	1680	6.5, 6.1, 5.7	C 70.0, H 5.1
9	65	100	1675	6.4, 6.0, 5.6	C 69.7, H 5.0
10	62	98	1670	6.3, 5.9, 5.5	C 69.4, H 4.9

Representative product showing... The IR spectrum shows a strong absorption at 1715 cm⁻¹... The ¹H NMR spectrum shows peaks at 7.2, 6.8, and 6.4 ppm.

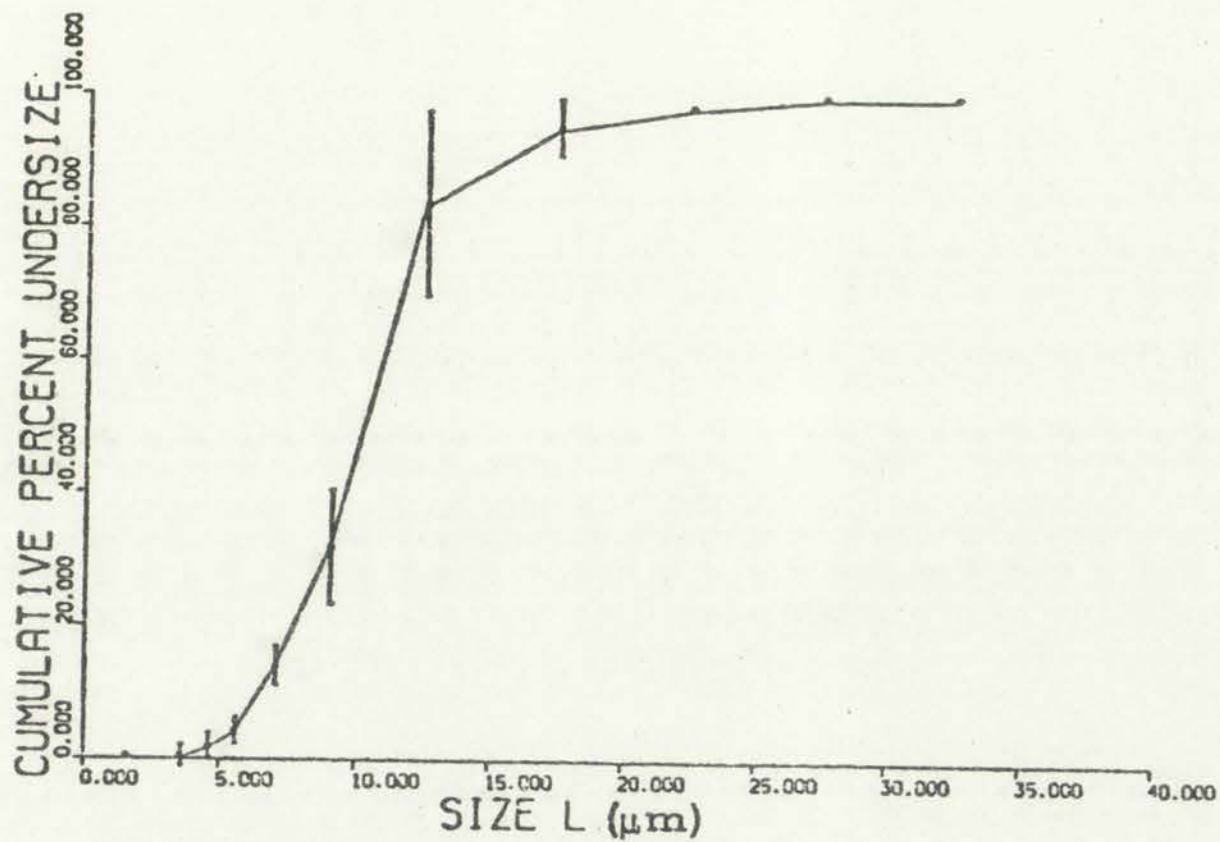


Figure 5a.
 $R = \frac{1}{4}$.

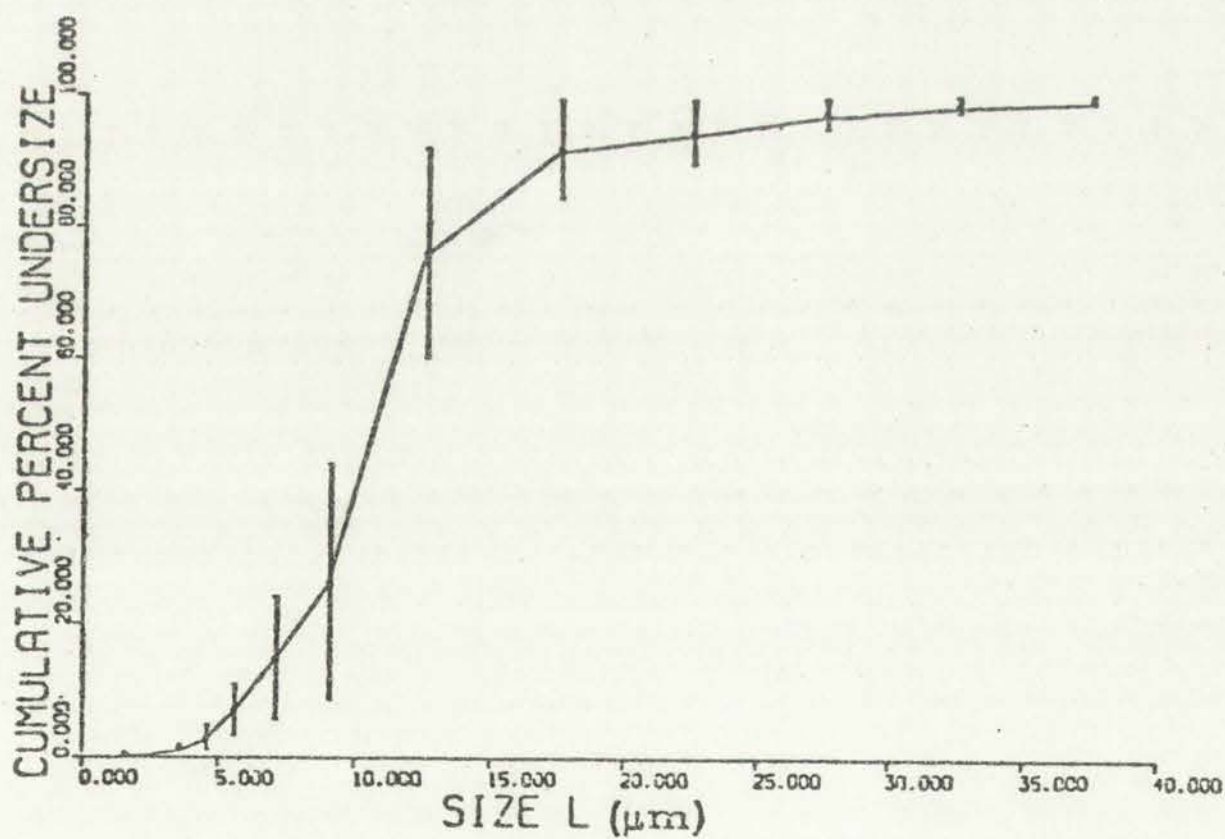


Figure 5b.
 $R = \frac{1}{3}$.

PETN Experimental Particle Size Distribution.

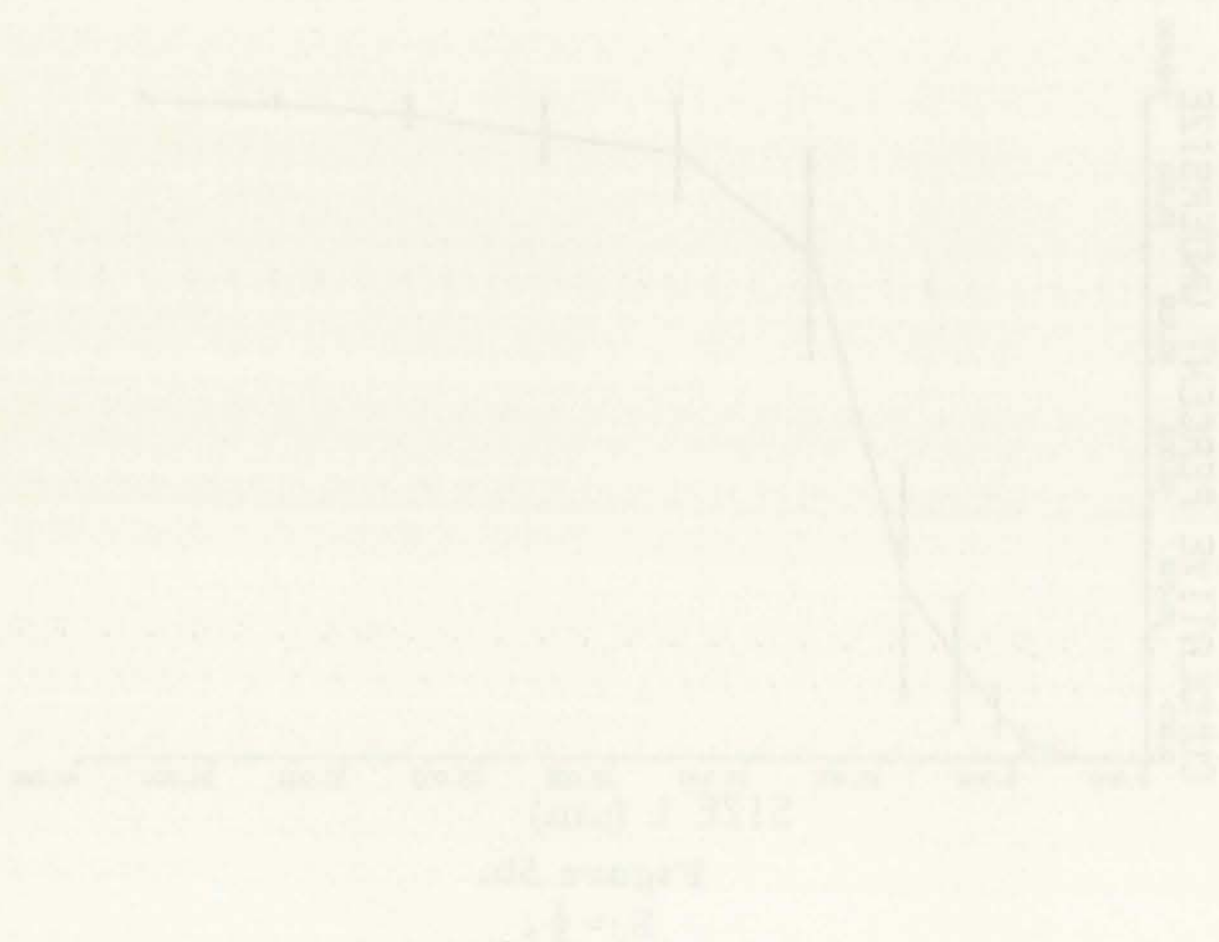


Fig. 1. Experimental results for Vignos 04.

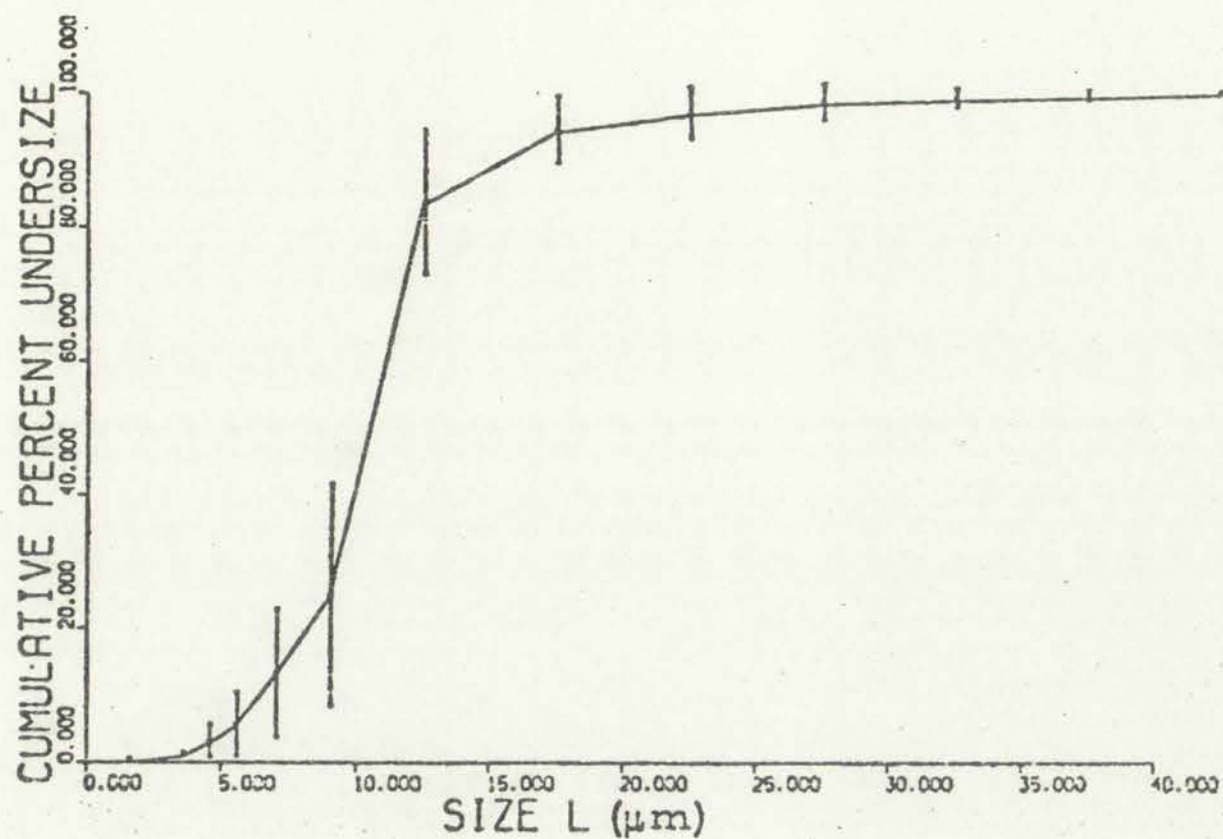


Figure 5c.
 $R = \frac{1}{2}$.

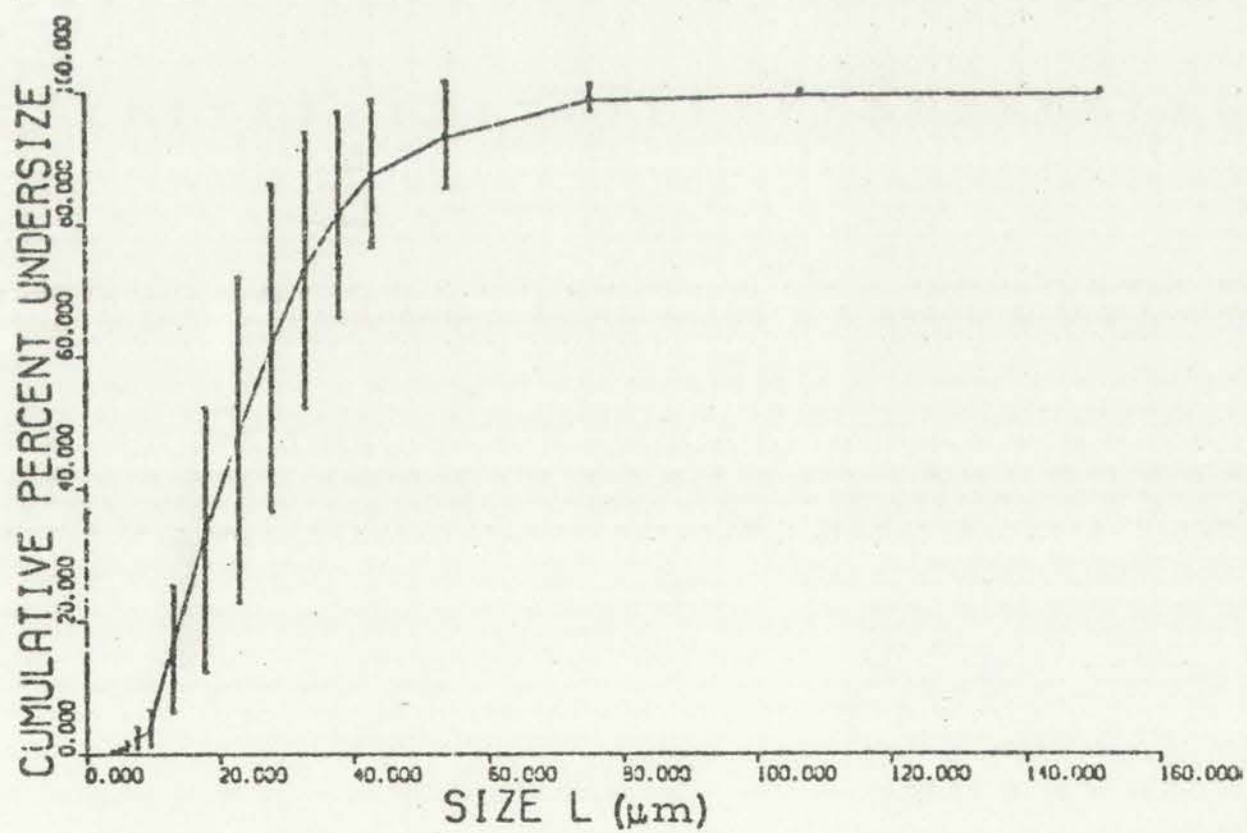


Figure 5d.
 $R = 1$.

PETN Experimental Particle Size Distribution.



NOTE: Experimental Parameters are Identical

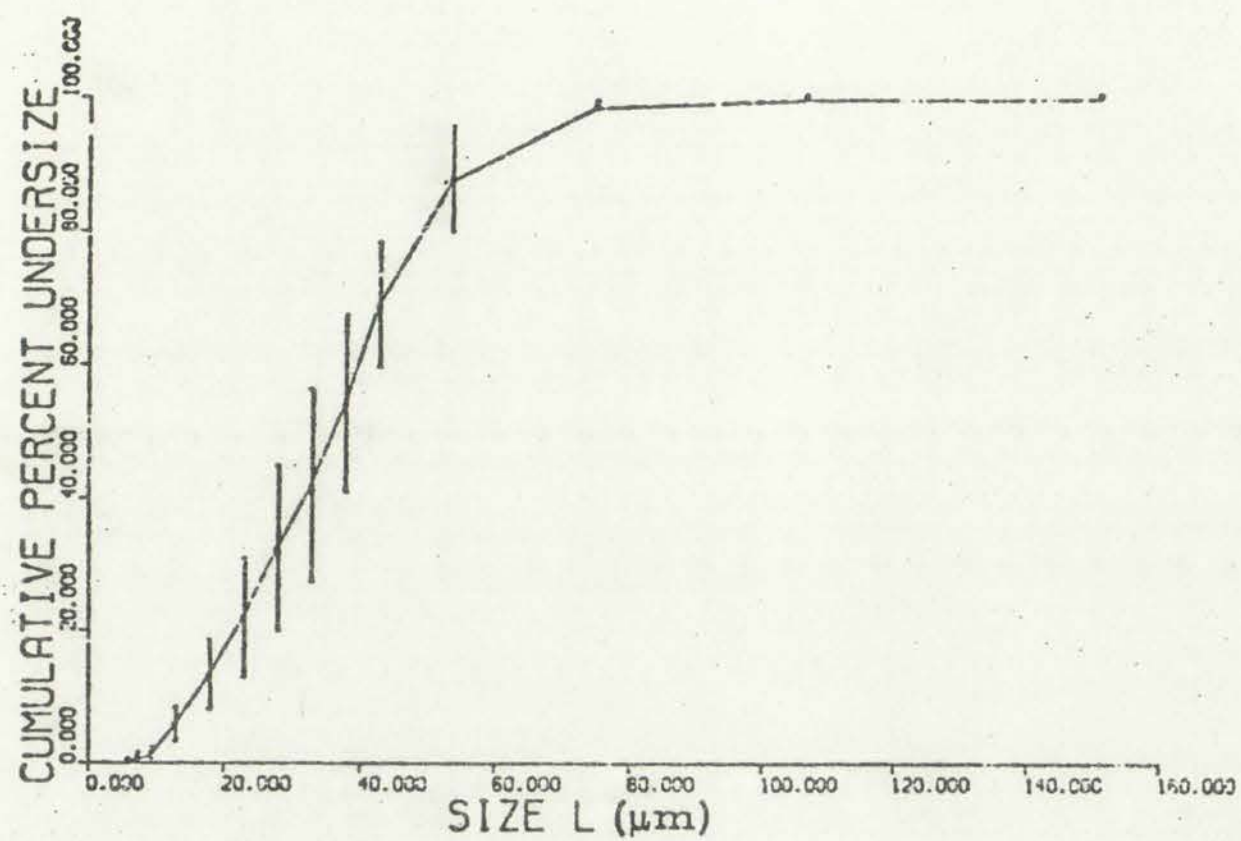


Figure 5e.
R = 2.

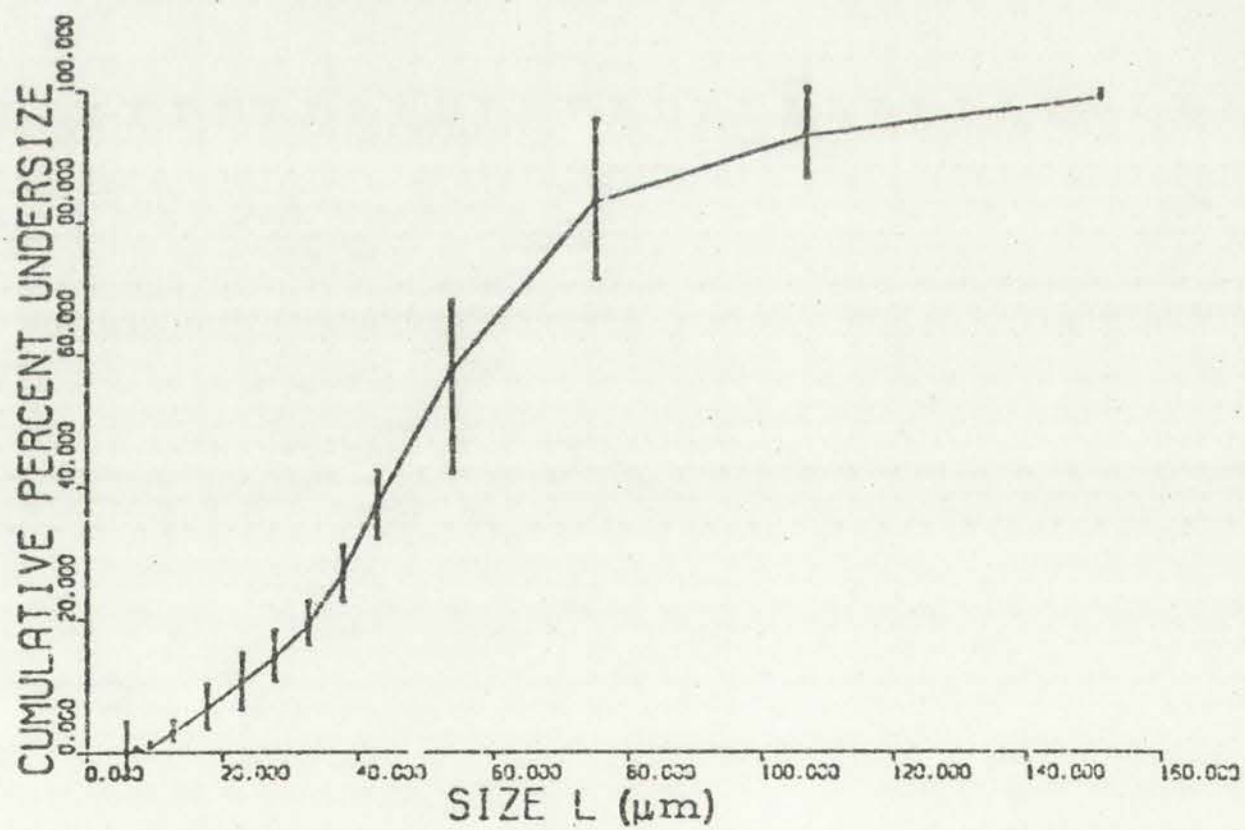
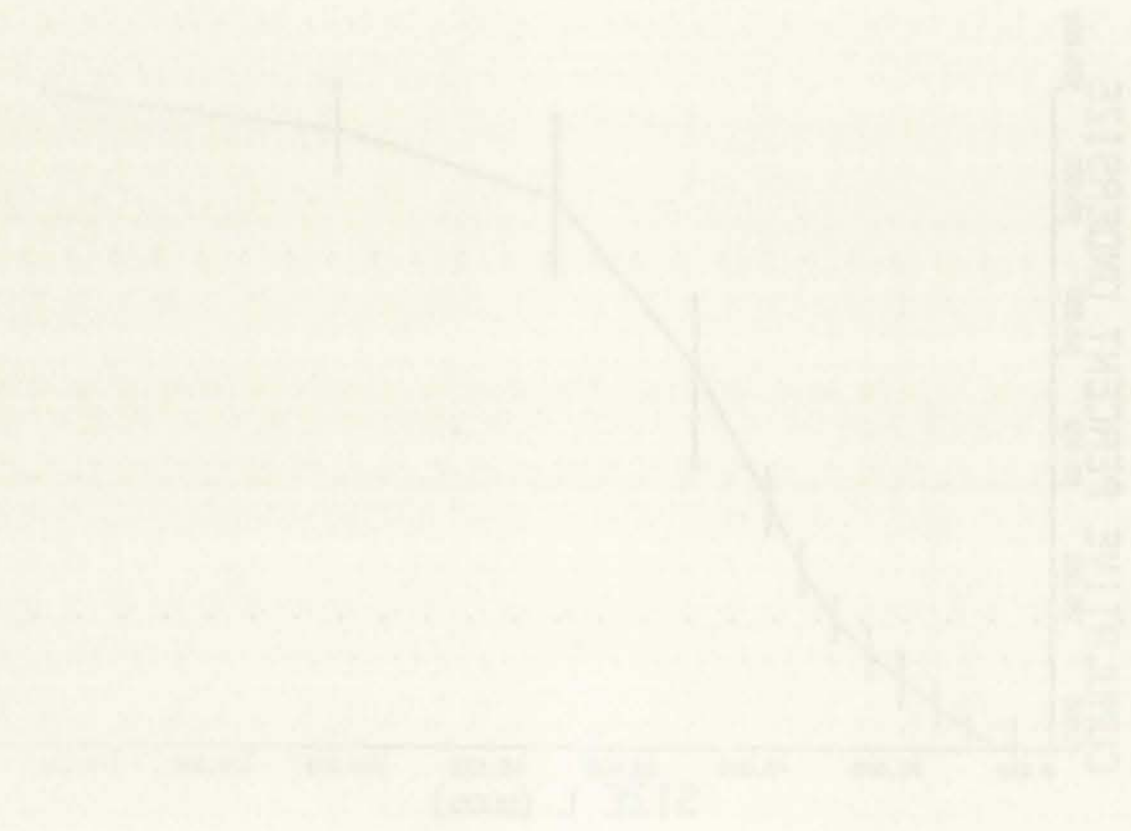
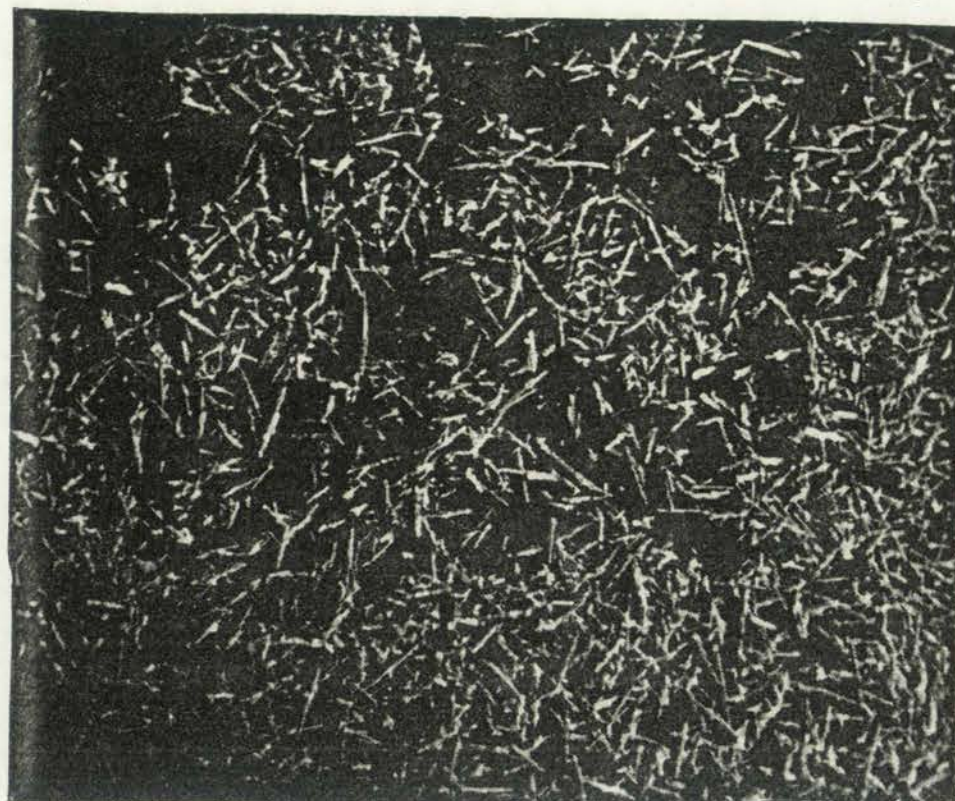


Figure 5f.
R = 3.

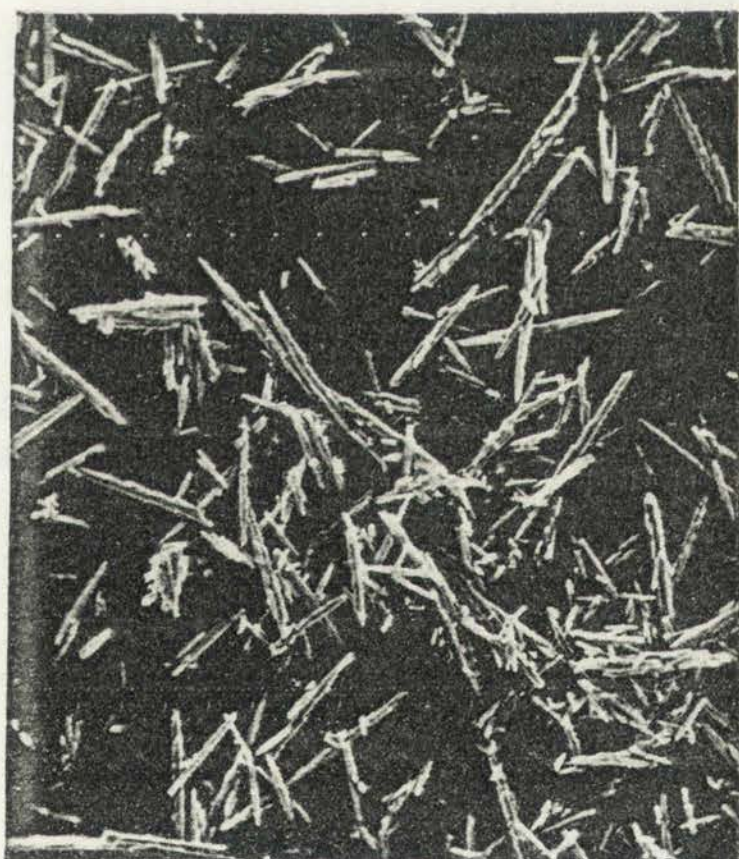
PETN Experimental Particle Size Distribution.



The Experimental Particle Size Distributions



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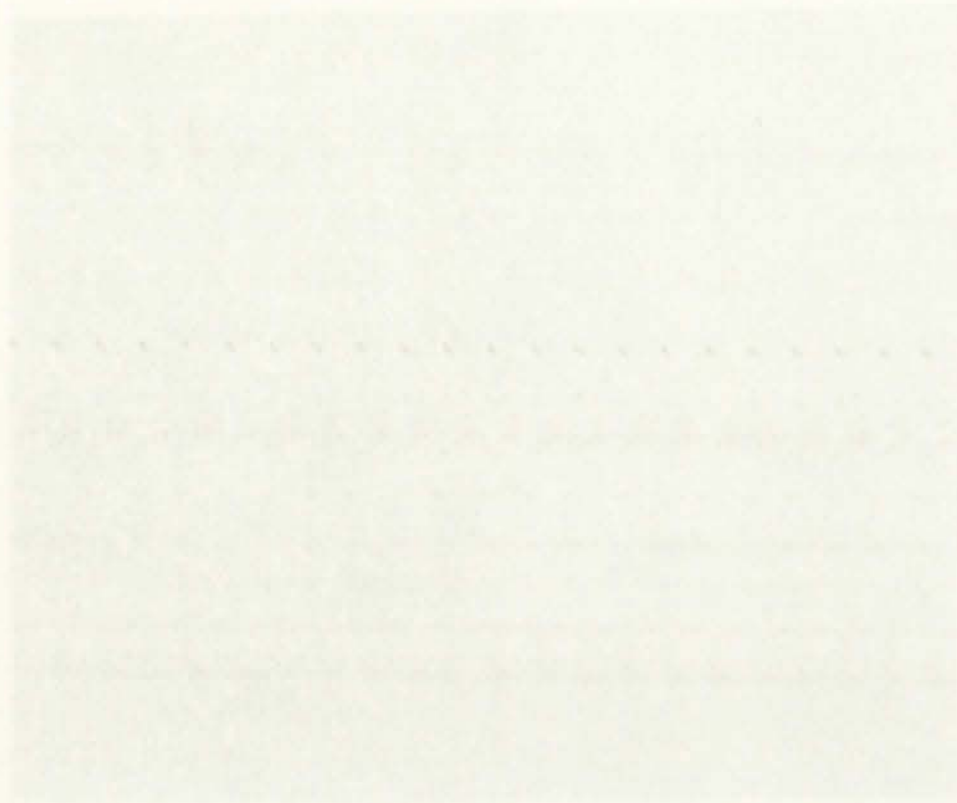


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Figure 6a.
Scanning Electron Micrographs, PETN-3848 ($R = \frac{1}{4}$).



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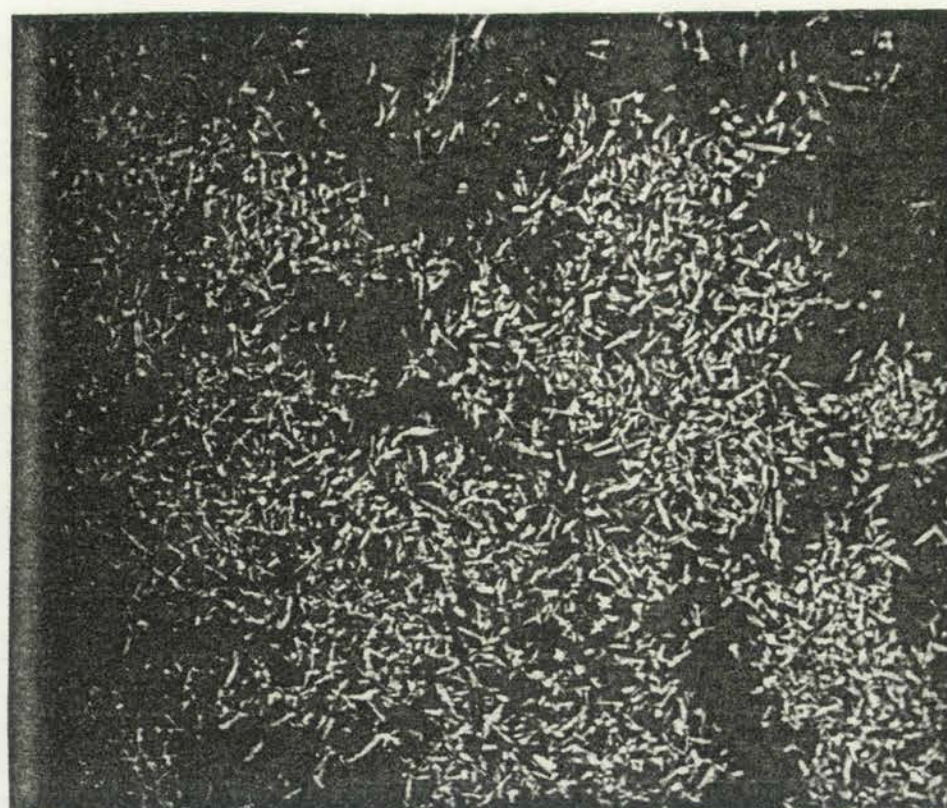


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Scanning Electron Micrographs of Polyethylene Glycol (PEG) Sponges



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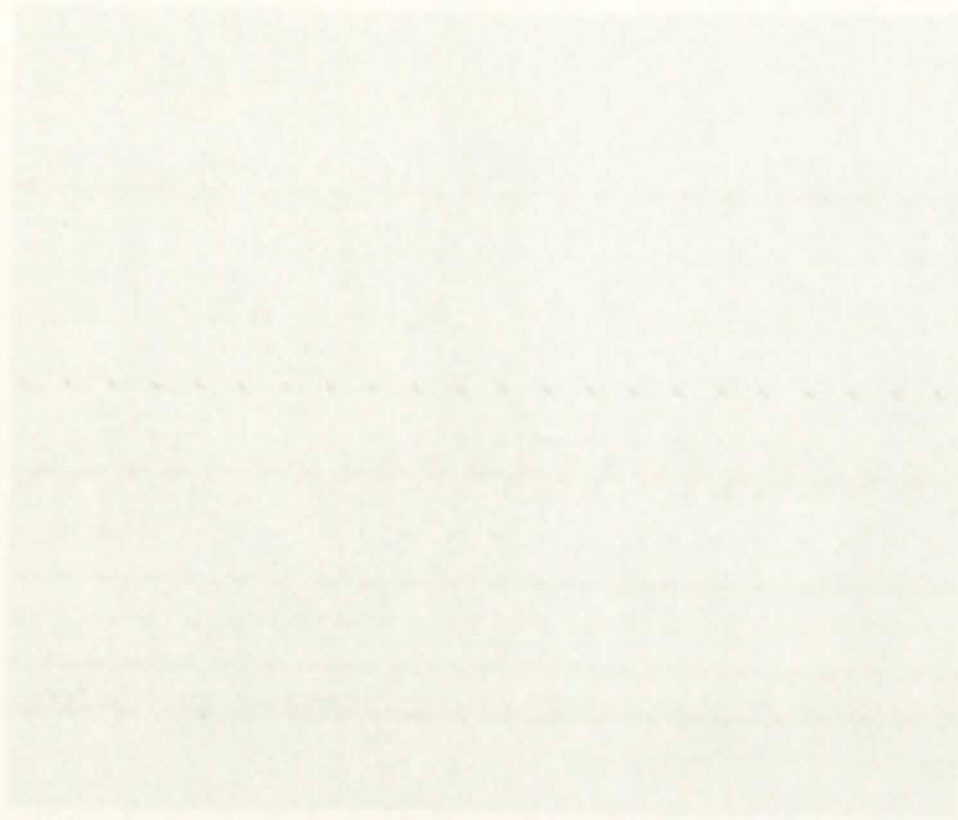


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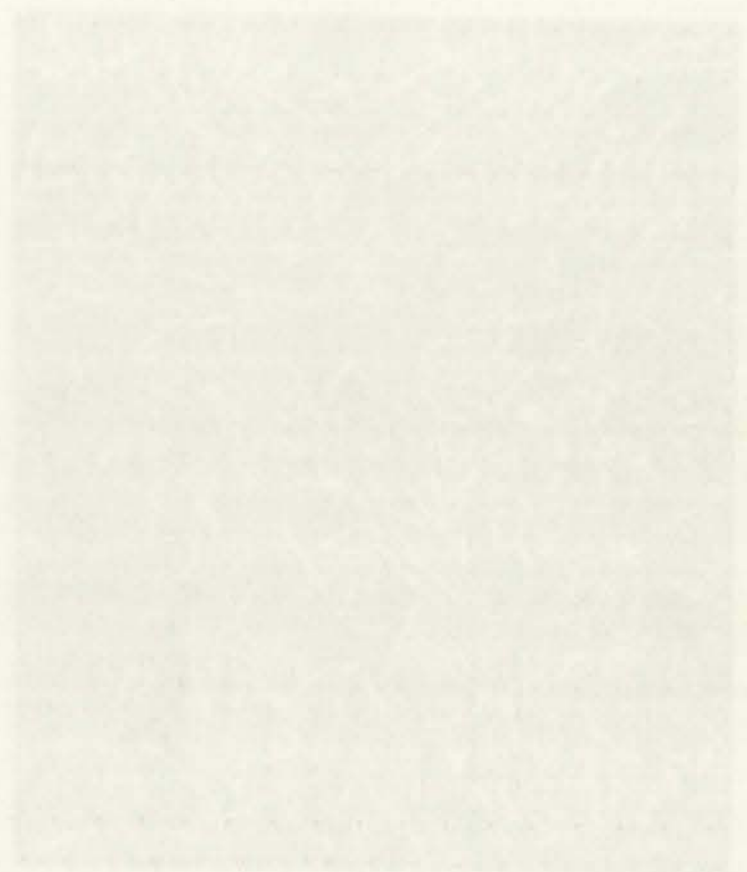
Figure 6b.
Scanning Electron Micrographs, PETN-3866 ($R = \frac{1}{3}$).



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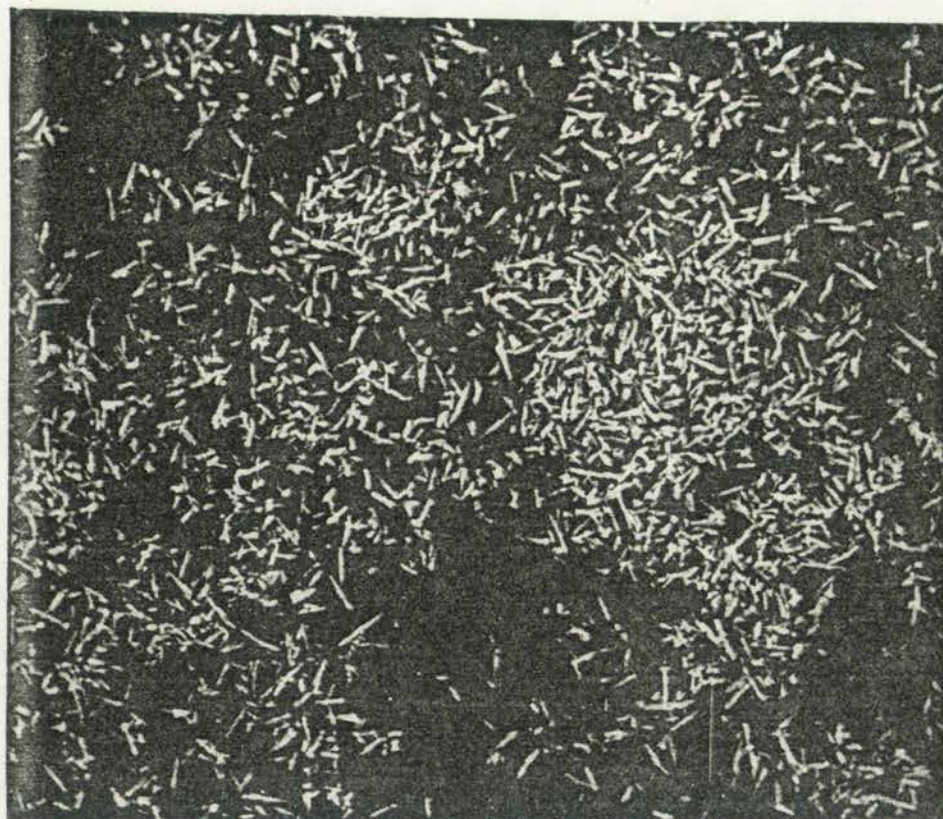


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PLATE 10
GENERAL VIEW OF THE INTERIOR OF THE TEMPLE



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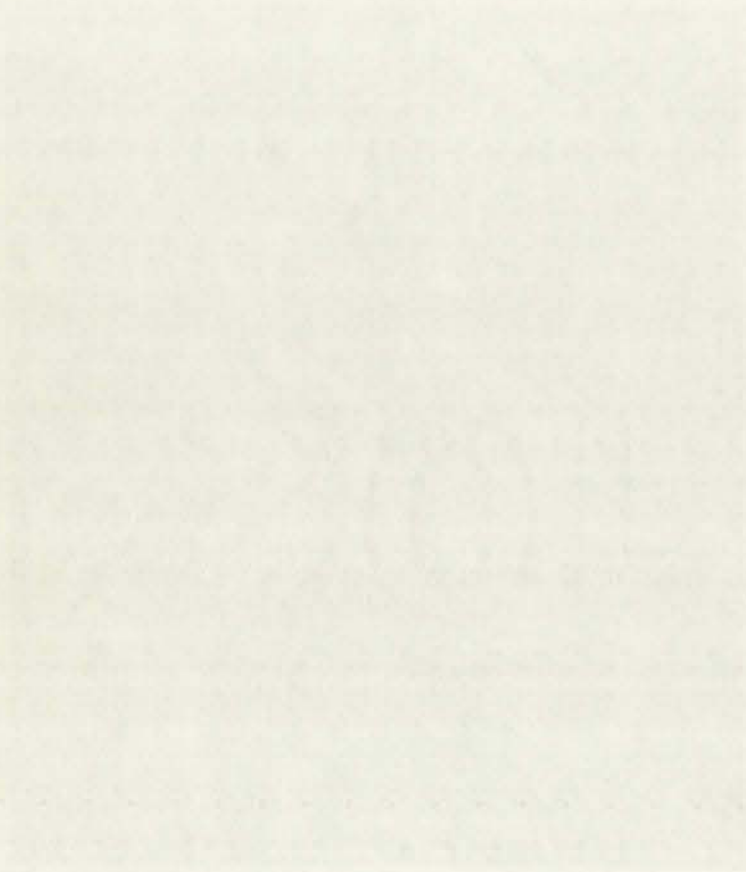
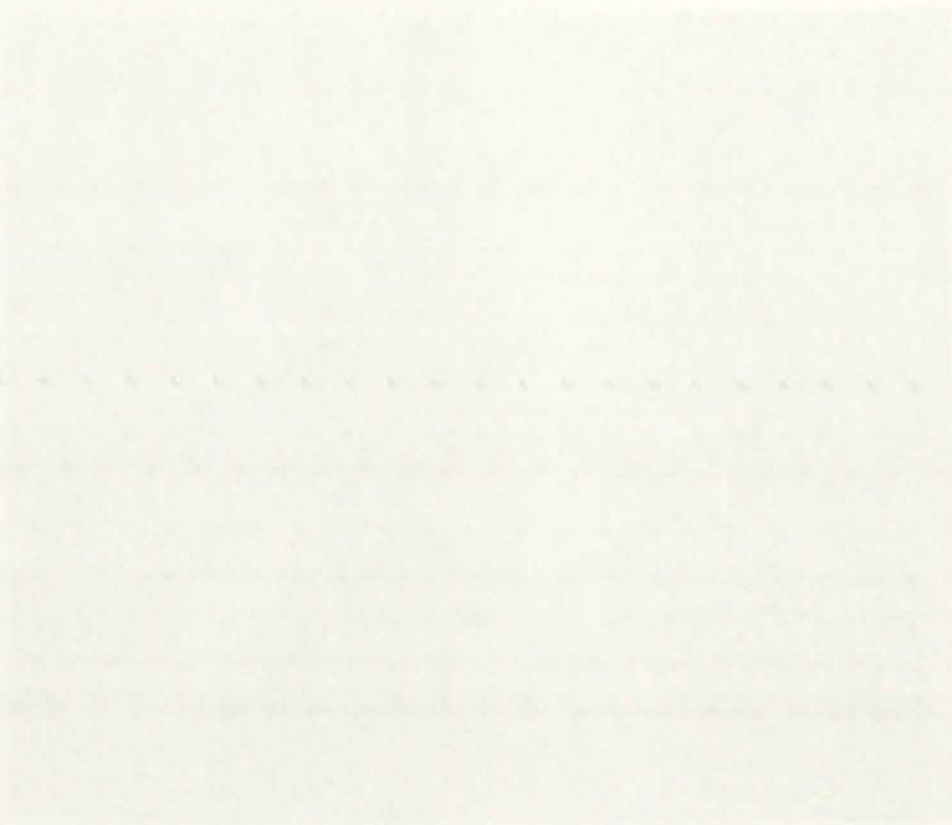


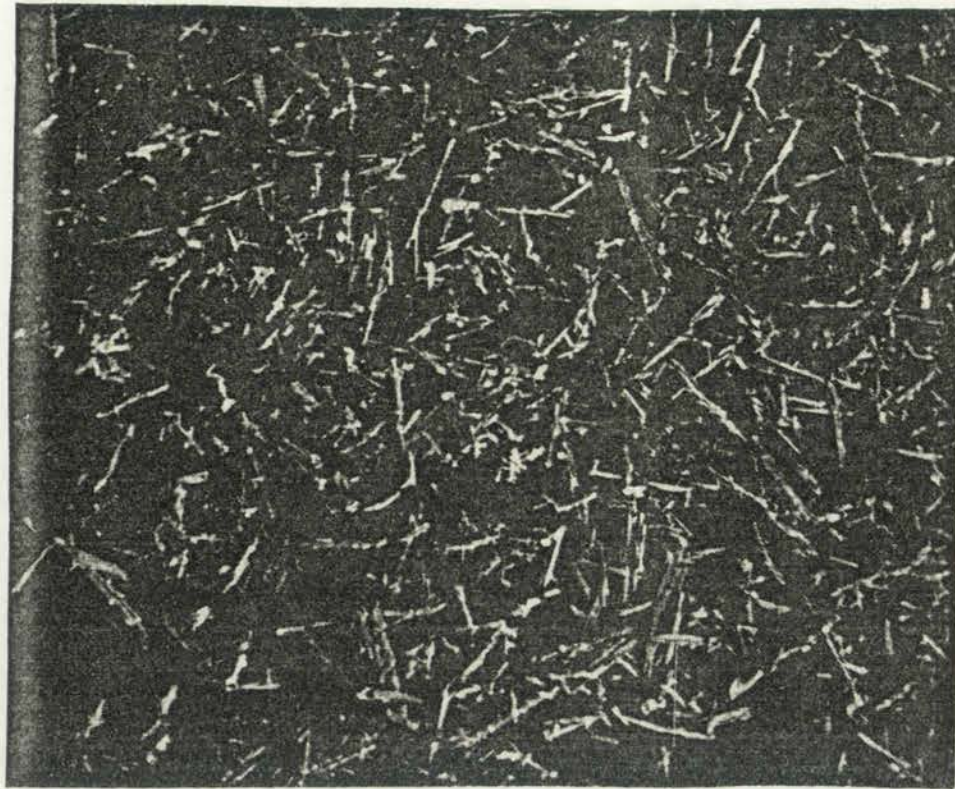
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Figure 6c.
Scanning Electron Micrographs, PETN-3856 ($R = \frac{1}{2}$).

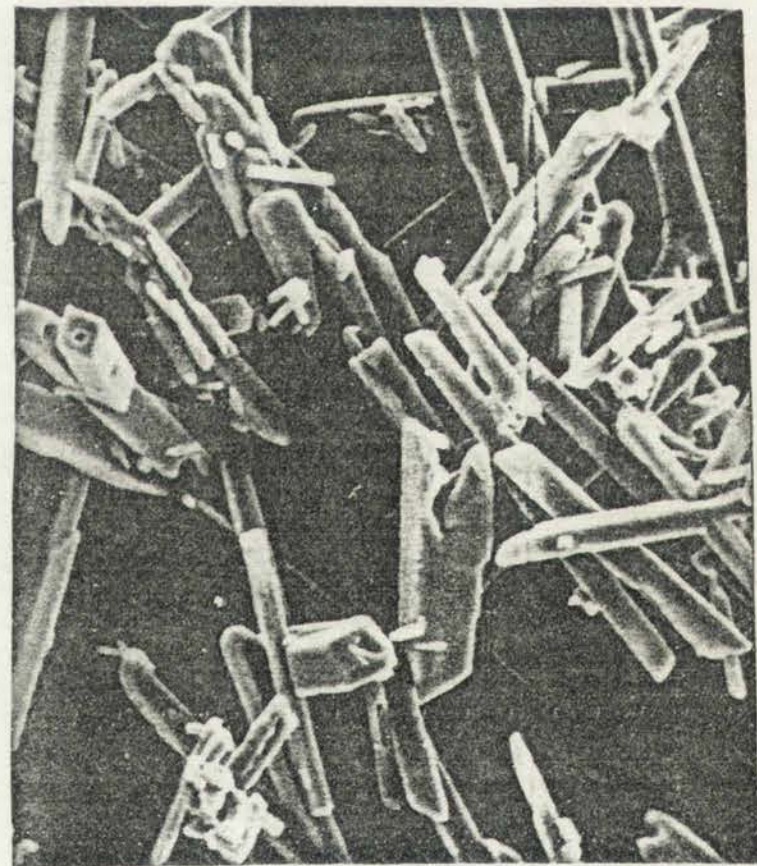




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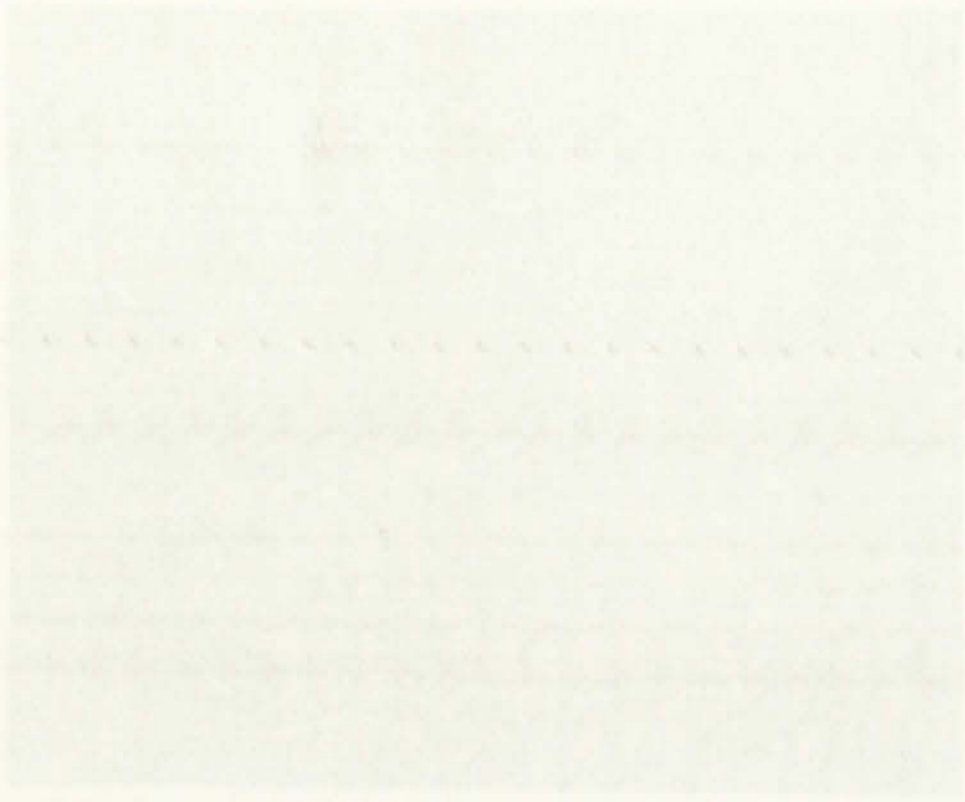


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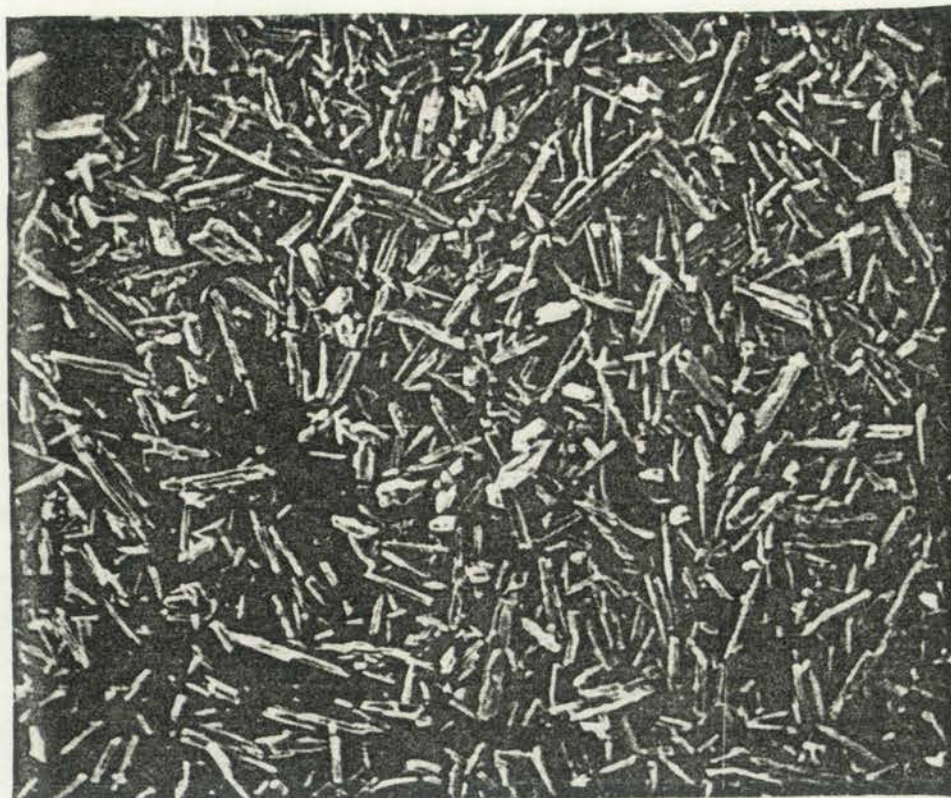


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Figure 6d.
Scanning Electron Micrographs, PETN-3861 ($R = 1$, $\tau = 0.5$ s).



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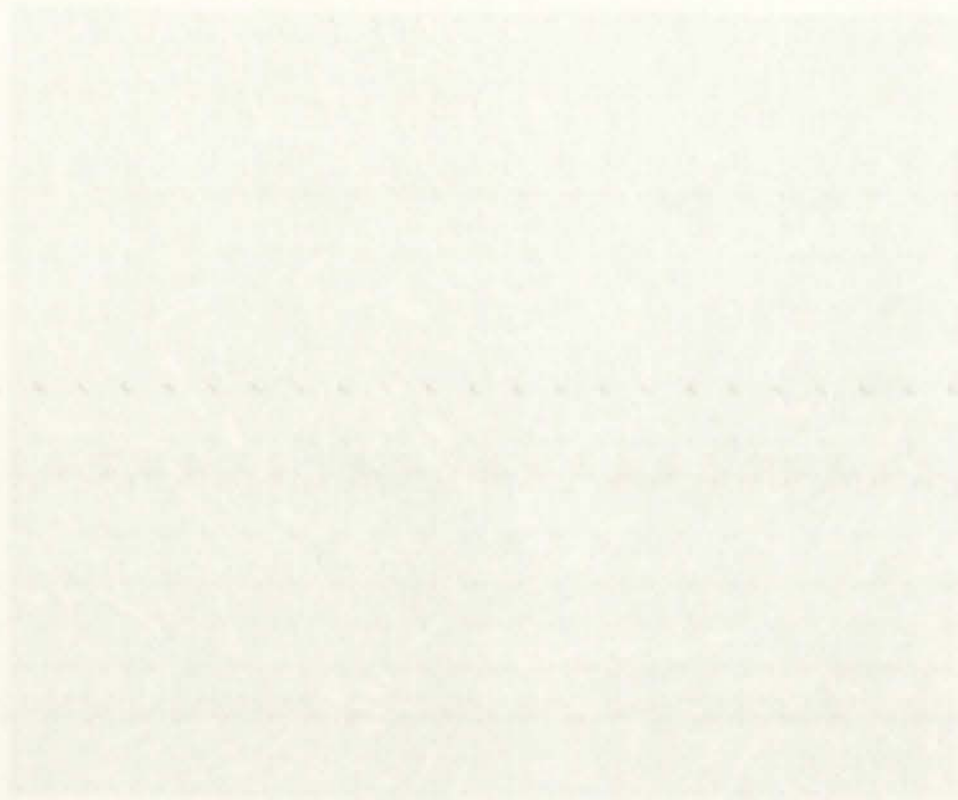


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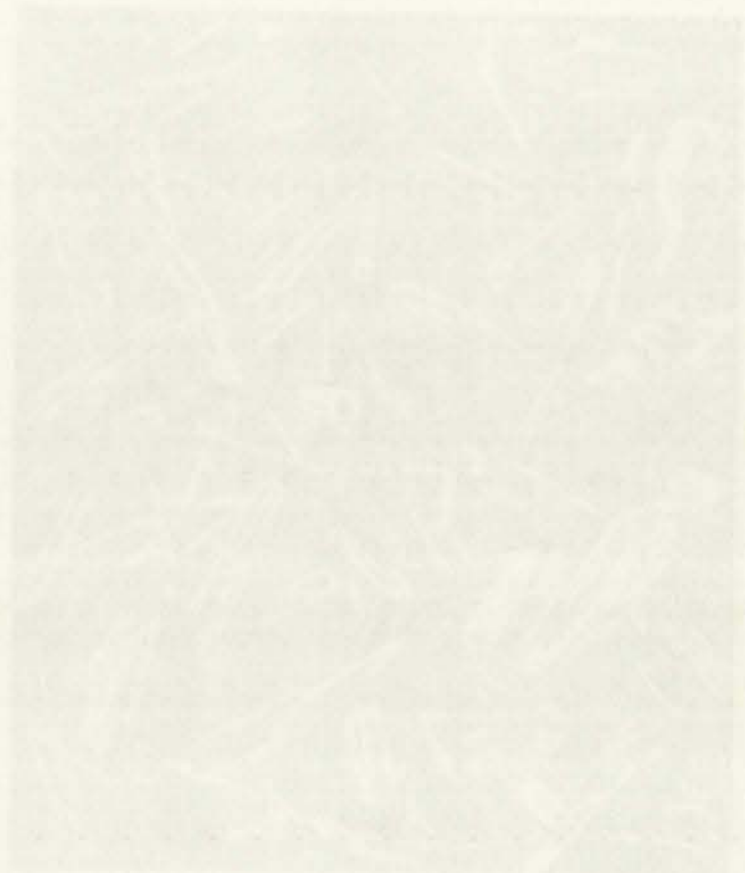
Figure 6e.
Scanning Electron Micrographs, PETN-3871 ($R = 1$, $\tau = 2.0$ s).



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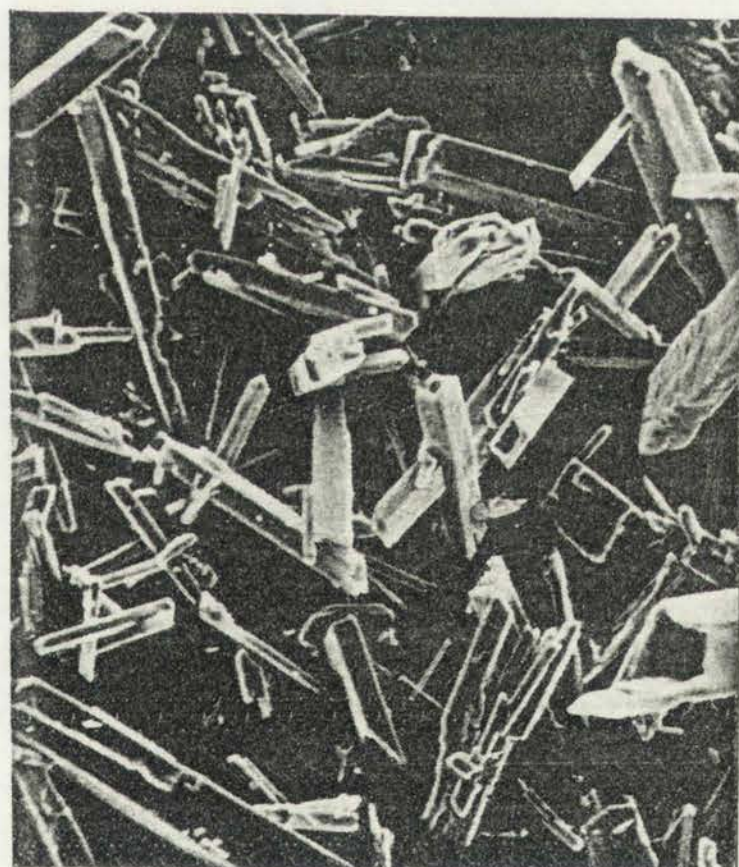
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Figure 6

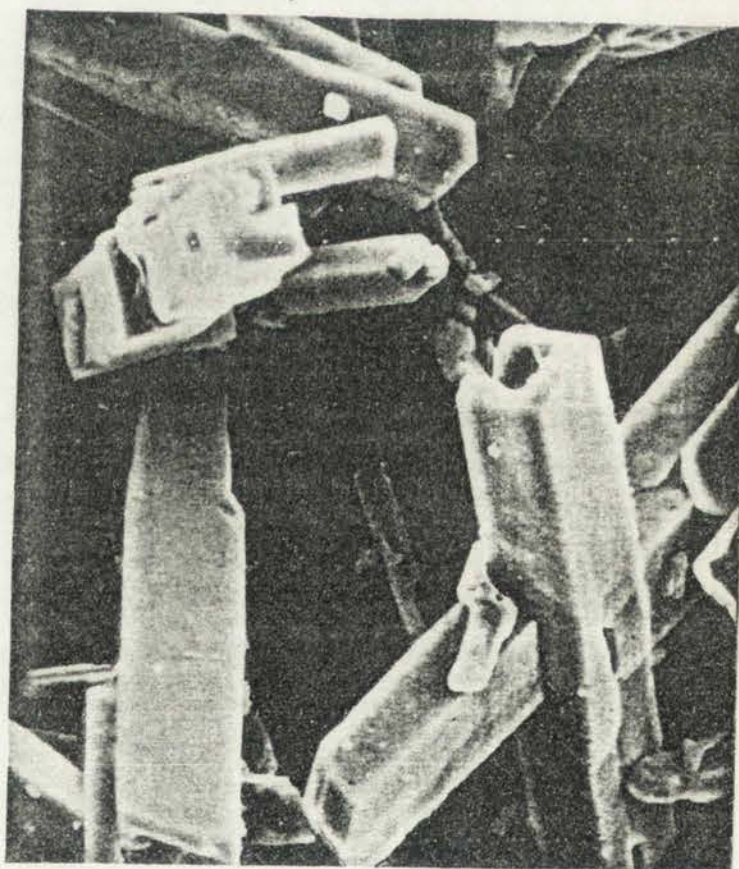
Scanning Electron Micrographs of the surface of the polymer film after 100X magnification.



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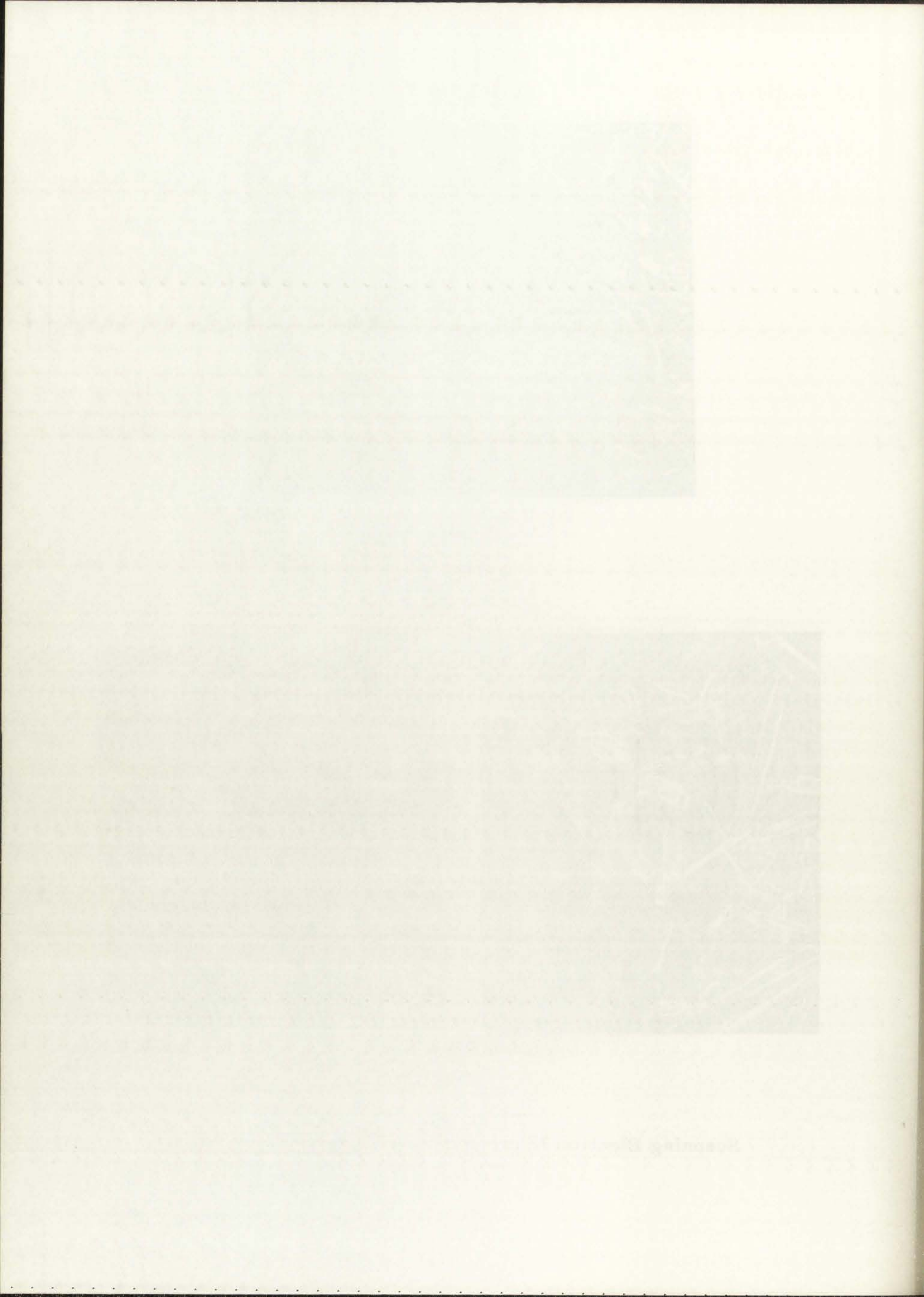


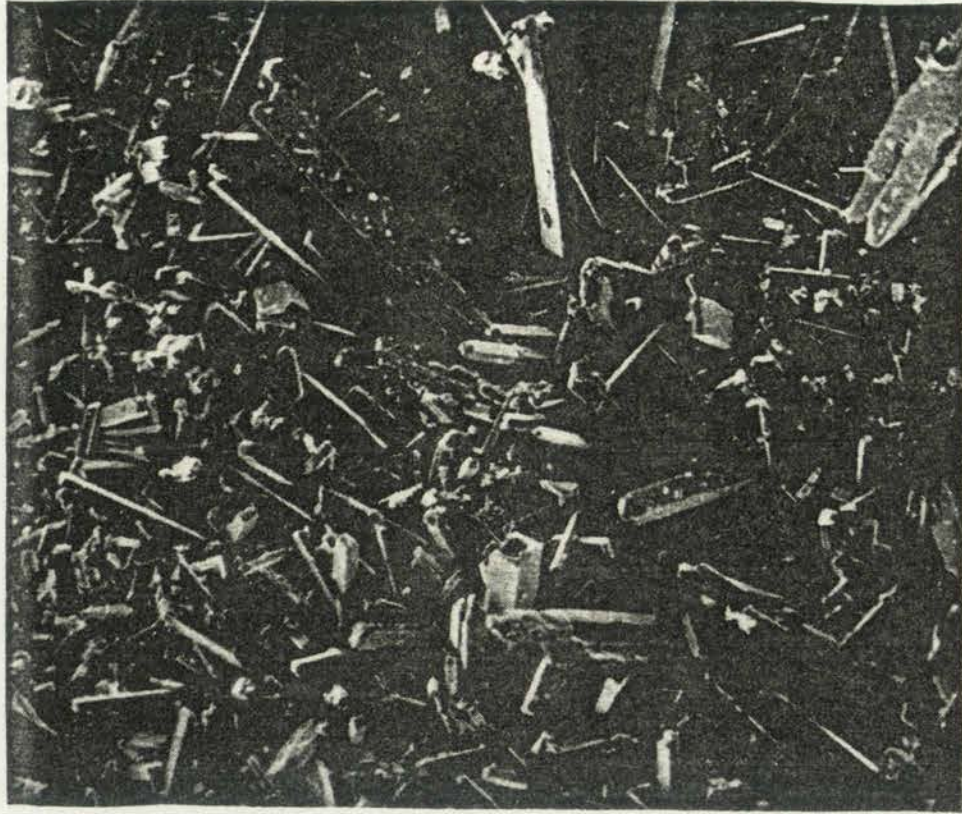
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Figure 6f.
Scanning Electron Micrographs, PETN-3877 (R = 2).

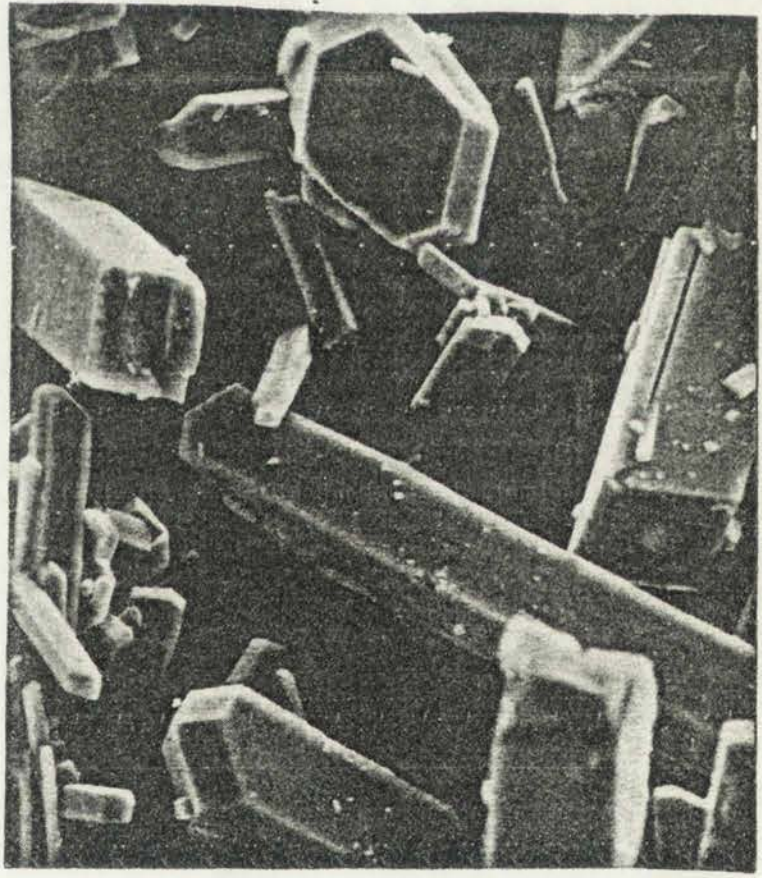




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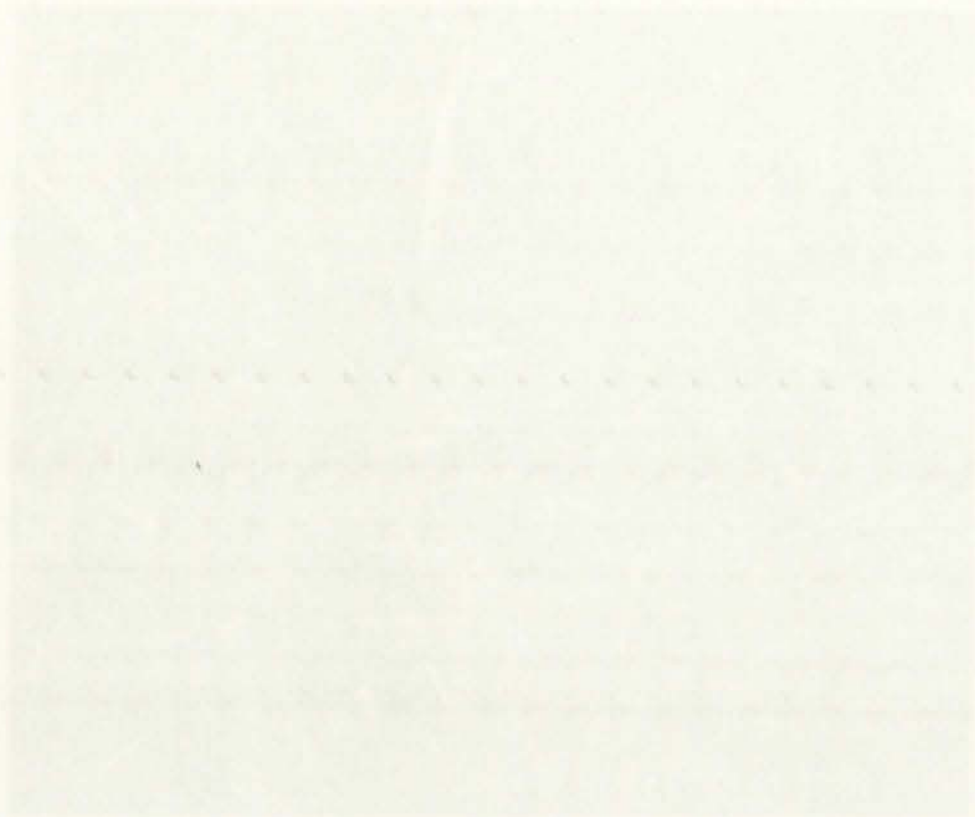


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Figure 6g.
Scanning Electron Micrographs, PETN-3883 (R = 3).



10001



10002



10003

Figure 10

Primary Electron Micrographs, 7.21K-200V (A - 1000x)

B. Theoretical Model Predictions

1. Particle Size Distribution. The plug flow model calculations predict distributions that are significantly narrower than the experimentally determined ones. The coefficients of variation predicted by the plug flow model range from 0.11 to 0.21. The inclusion of the Péclet number causes the predicted distributions to broaden as Pe is lowered. The Péclet value of 250 gives results very nearly approaching plug flow values. The results described were obtained from the calculations based on the dispersed plug flow model.

A series of about 500 computer runs was made with combinations of the nucleation parameter, \underline{a} , ranging from 1.0 to 4.0; the growth parameter, \underline{b} , ranging from 0.5 to 1.7; and the diffusion parameter, Pe, ranging from 25 to 250. Additional runs were made to refine the calculations.

2. Effect of Varying Parameters. The effect of decreasing \underline{a} (longer nucleation period) is primarily to increase the coefficient of variation. It also tends to decrease the mean particle size. It predicts a wider distribution of slightly smaller particles. The primary effect of increasing \underline{b} (shorter growth period) is to decrease the mean particle size. It also increases the coefficient of variation. It predicts smaller particles having a wider distribution. The primary effect of decreasing Pe (increasing diffusion) is to increase the coefficient of variation with a small increase of particle size. The resulting best fit parameters are $a = 3.75 \pm 0.05$, $b = 1.56 \pm 0.02$, and $Pe = 51 \pm 1$. The resulting

5. Theoretical Model

5.1. Particle Size Distribution

The particle size distribution is defined as the number of particles per unit volume in a given size range. The distribution is usually represented by a log-normal function. The mean diameter \bar{D} and the standard deviation σ are the two parameters that define the distribution. The mean diameter is the diameter at which the number of particles is maximum. The standard deviation is a measure of the spread of the distribution. The distribution is usually assumed to be log-normal because of the multiplicative nature of the growth and coagulation processes. The distribution is usually assumed to be log-normal because of the multiplicative nature of the growth and coagulation processes.

A series of about 100 experiments was made with variations of the nucleation parameter, α , ranging from 1.5 to 4.0; the growth parameter, β , ranging from 0.5 to 1.5; and the diffusion parameter, γ , ranging from 0.5 to 1.5. Additional runs were made to verify the calculations.

5.2. Effect of Varying Parameters

The effect of increasing α is to increase the number of particles per unit volume. It also tends to decrease the mean particle size. In general, a wider distribution of particle sizes is obtained. The primary effect of increasing β is to increase the mean particle size. It also tends to decrease the number of particles per unit volume. The primary effect of increasing γ is to increase the number of particles per unit volume. It also tends to decrease the mean particle size. The primary effect of increasing α is to increase the number of particles per unit volume. It also tends to decrease the mean particle size. In general, a wider distribution of particle sizes is obtained. The primary effect of increasing β is to increase the mean particle size. It also tends to decrease the number of particles per unit volume. The primary effect of increasing γ is to increase the number of particles per unit volume. It also tends to decrease the mean particle size.

predicted particle size distributions, compared with experimental results, are shown in Figs. 7a through 7f. Any further attempts to obtain a closer fit or to increase the coefficient of variation without deviation from a best fit gave unstable results. The resulting particle size distribution curves were not smooth, but rather the points were scattered in an oscillatory pattern.

3. Kinetics. A least-squares linear fit for \bar{L} vs R gives the equation, for \bar{L} in μm :

$$\bar{L} = (6.90 + 18.56R) \quad (48)$$

with a linear correlation factor of 0.99. From Eq. (28), we have

$$G_0\tau = \frac{f_3(1)}{f_4(1)} \bar{L} \quad (49)$$

For $a = 3.75$, $b = 1.56$, and $Pe = 51$, the ratio $[f_3(1)/f_4(1)]$ is 2.44.

For $G_0\tau$ in μm , $G_0\tau = 2.44(6.90 + 18.56R)$ or

$$G_0\tau = 16.84 + 45.29R \quad (50)$$

Four experimental runs were made with $R = 1$ and a 0.5-s holding time. Four more runs were made with $R = 1$ and a 2.0-s holding time. The resulting particle size distributions, using the two holding times, were essentially the same. This information suggests that the true holding time of the system is either equal to, or less than 0.5 s.

$$\tau \leq 0.5 \text{ s} \quad (51)$$

predicted particle size distribution, the results of the
analysis, are shown in Figure 1. The distribution of
particles from a pure 100% water-soluble polymer

obtains a sharp peak at the position of the
distribution curves were not analyzed. The polymer
scattered in an oscillatory pattern.

Figure 2. A least-squares fit for a two-parameter
equation for L in terms of Q and T .

$$L = 0.95 + 15.0Q$$

with a linear correlation factor of 0.99. From Eq. (1) we have

$$Q = \frac{L - 0.95}{15.0}$$

For $a = 1.75$, $b = 1.25$, and $T = 21$, the ratio $L(T)/L(21)$ is 2.51.

For $Q = 0$ in Eq. (1), $L = 0.95$ and $T = 21$.

$$Q = 16.04 + 15.0T$$

Four experimental runs were made with $L = 0.95$ and $T = 21$.

Three of the runs were made with $L = 0.95$ and $T = 21$.

The resulting particle size distribution, shown in Figure 3, was

essentially the same. The information regarding the particle

holding time of the system is shown in Figure 4. The

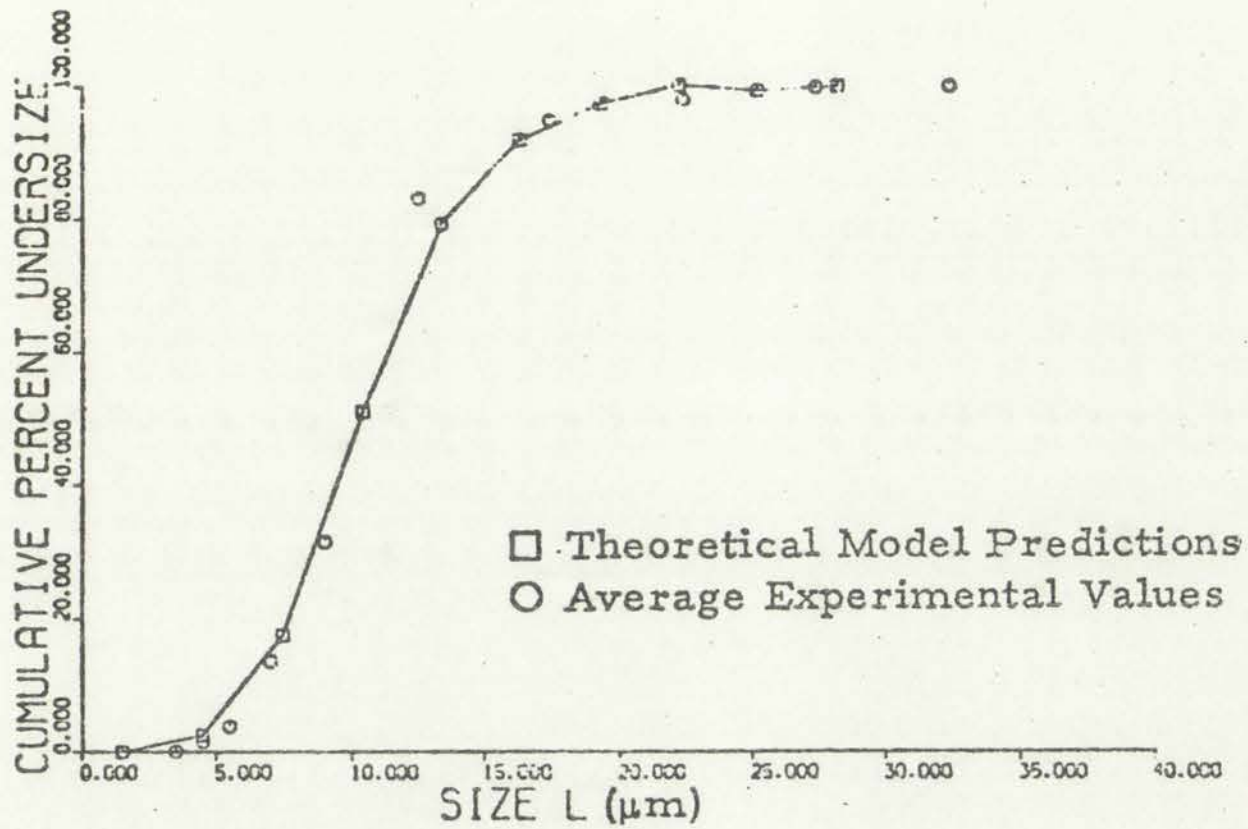


Figure 7a.
 $R = \frac{1}{4}$.

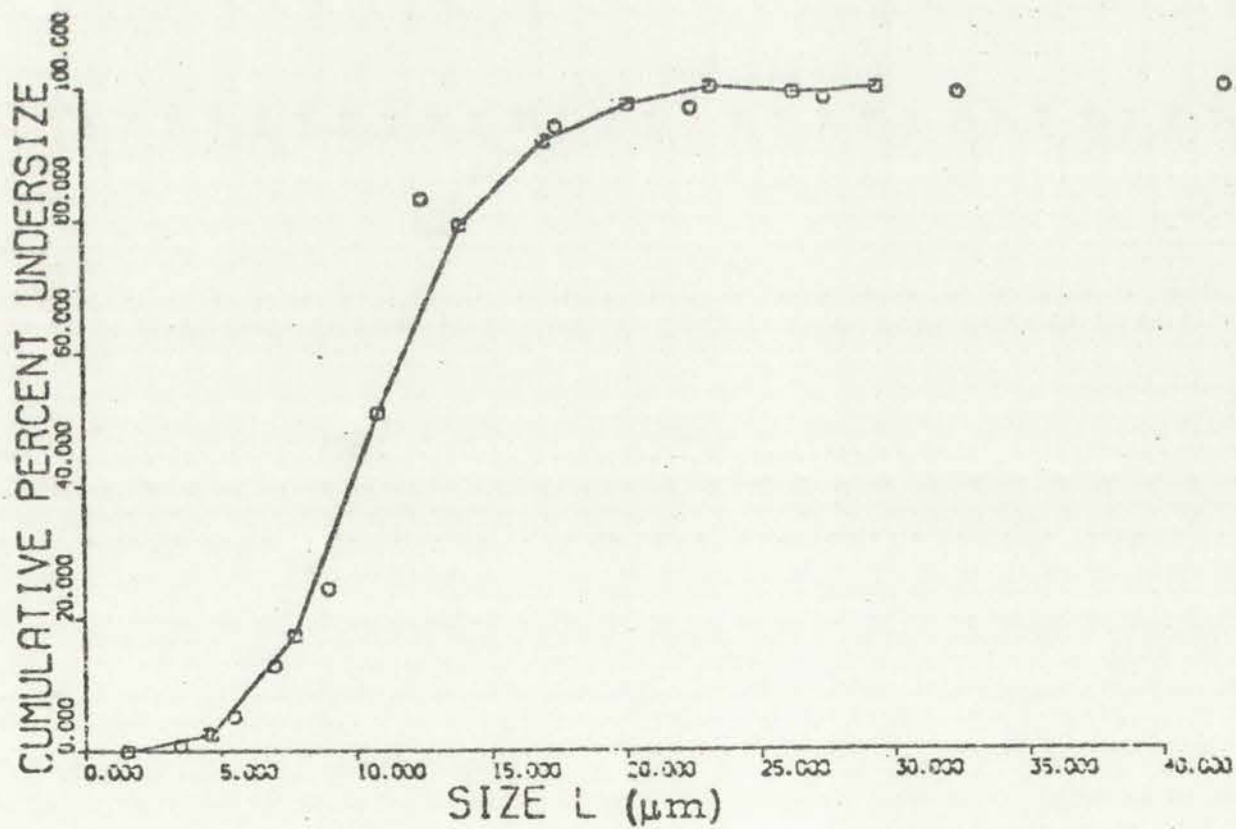
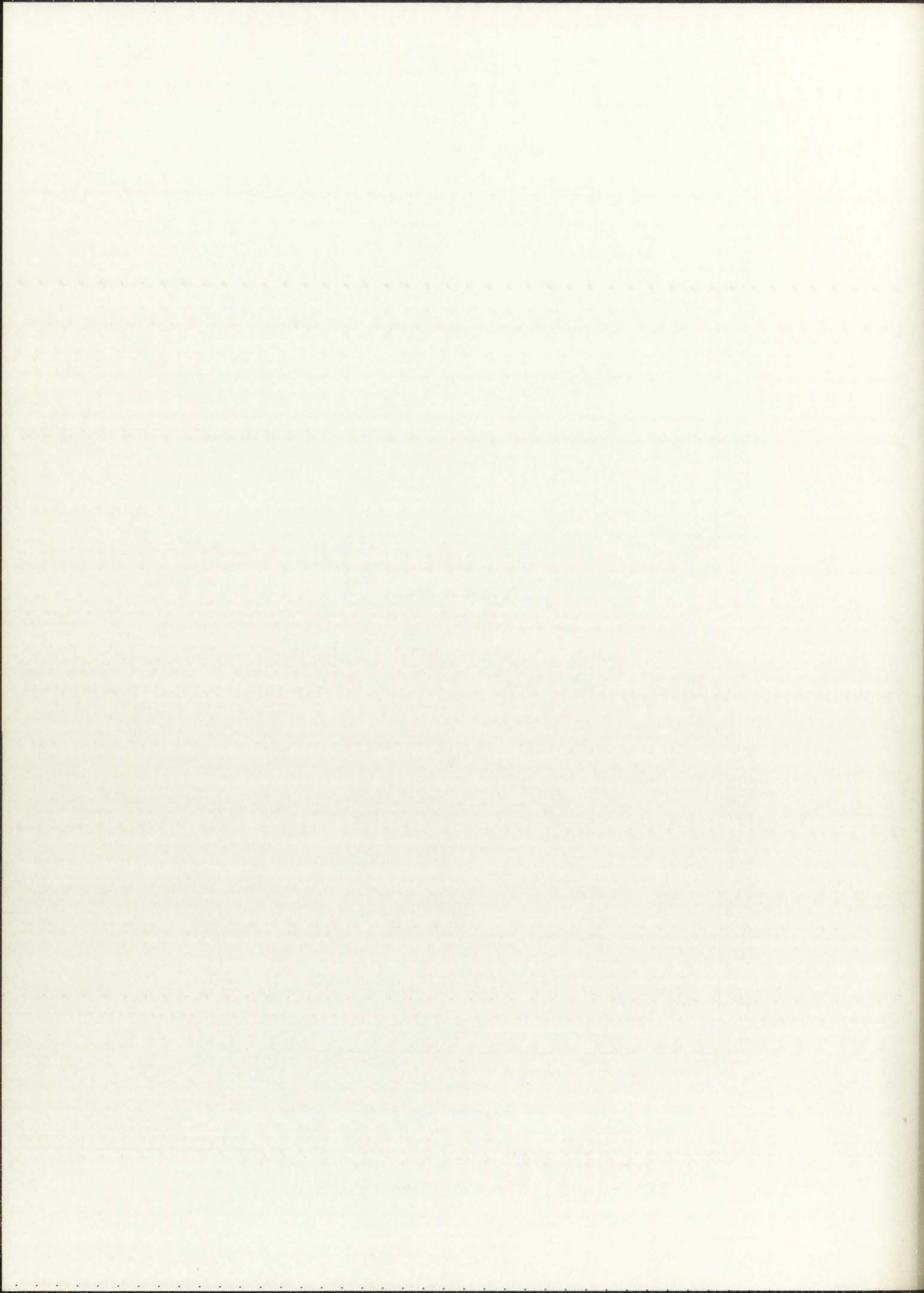


Figure 7b.
 $R = \frac{1}{3}$.

Comparison of Theoretical Values with
 Experimental Particle Size Distributions.



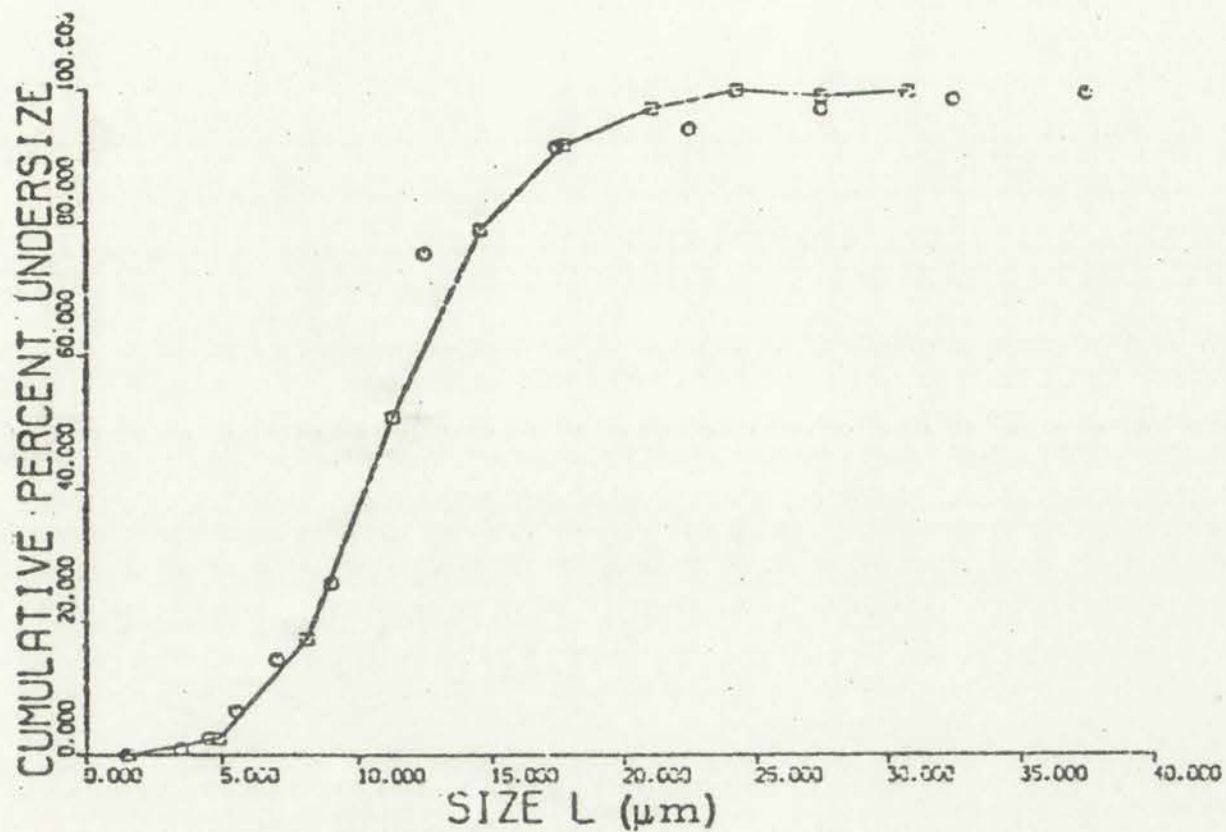


Figure 7c.
 $R = \frac{1}{2}$.

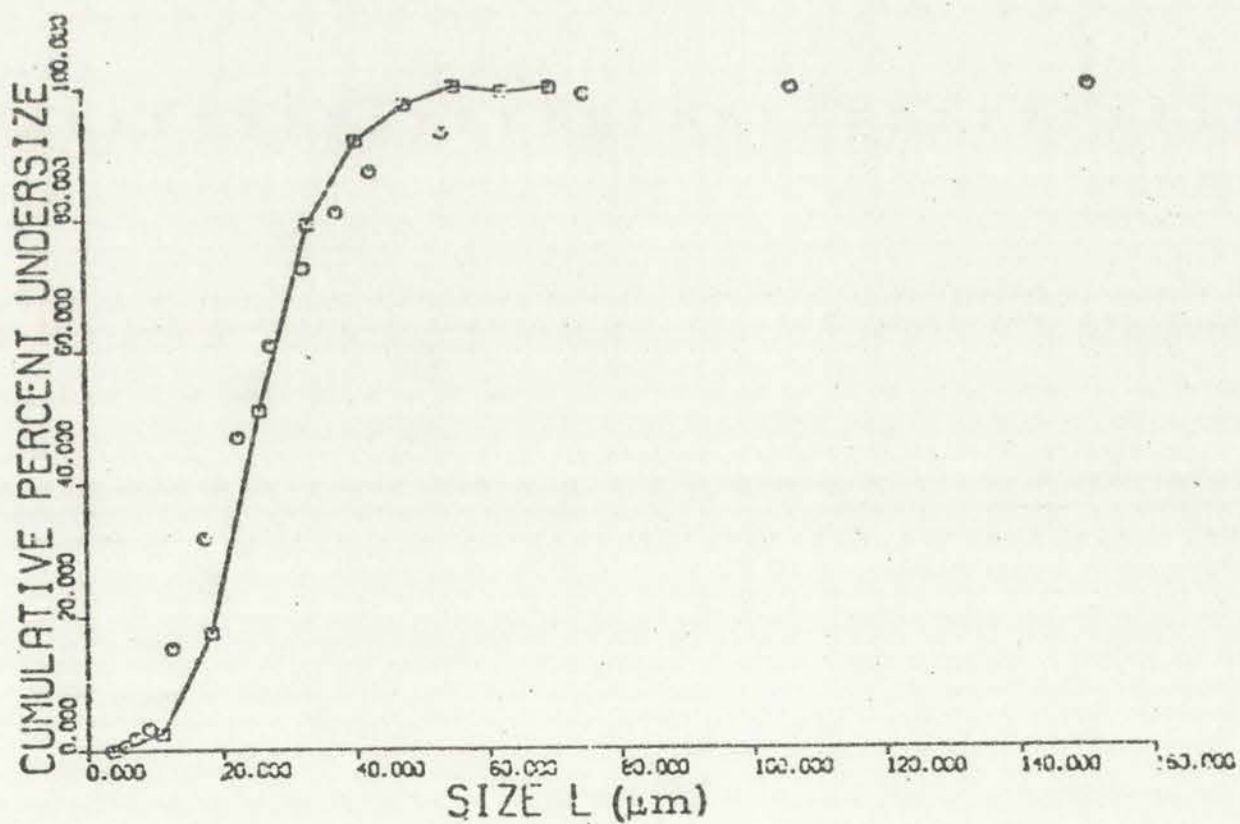


Figure 7d.
 $R = 1$.

Comparison of Theoretical Values with
Experimental Particle Size Distributions.

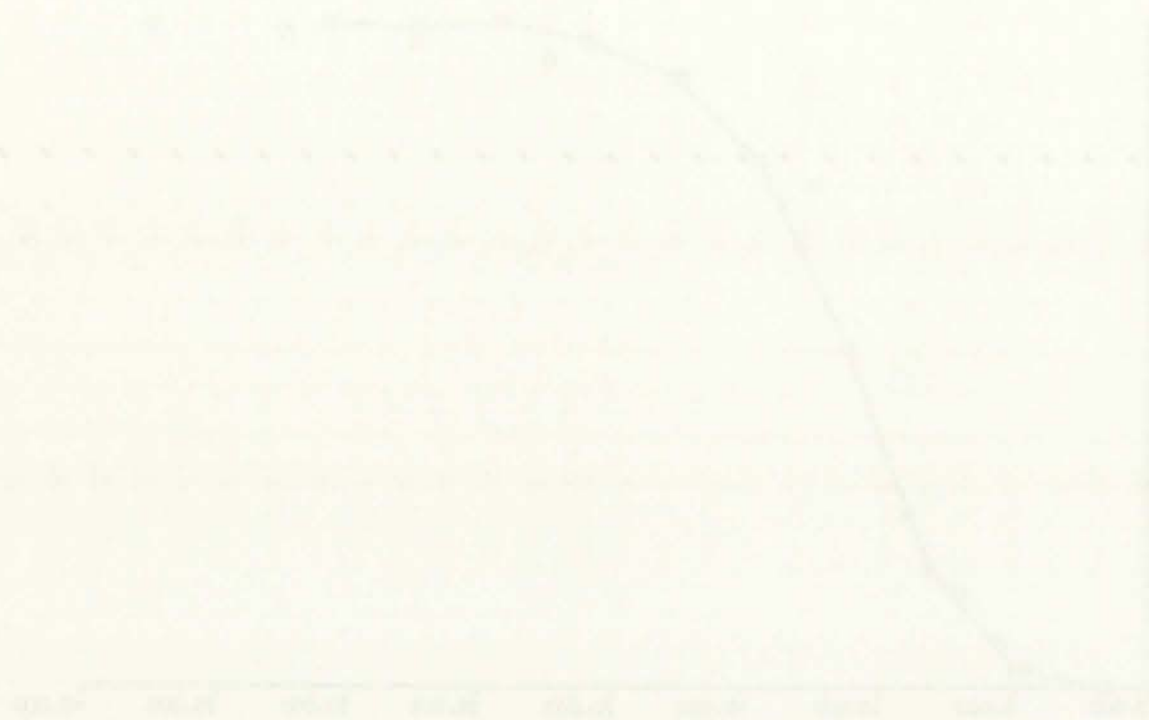


Figure 1a
 $n = 5$



Figure 1b
 $n = 5$

Comparison of Theoretical Values with Experimental Results

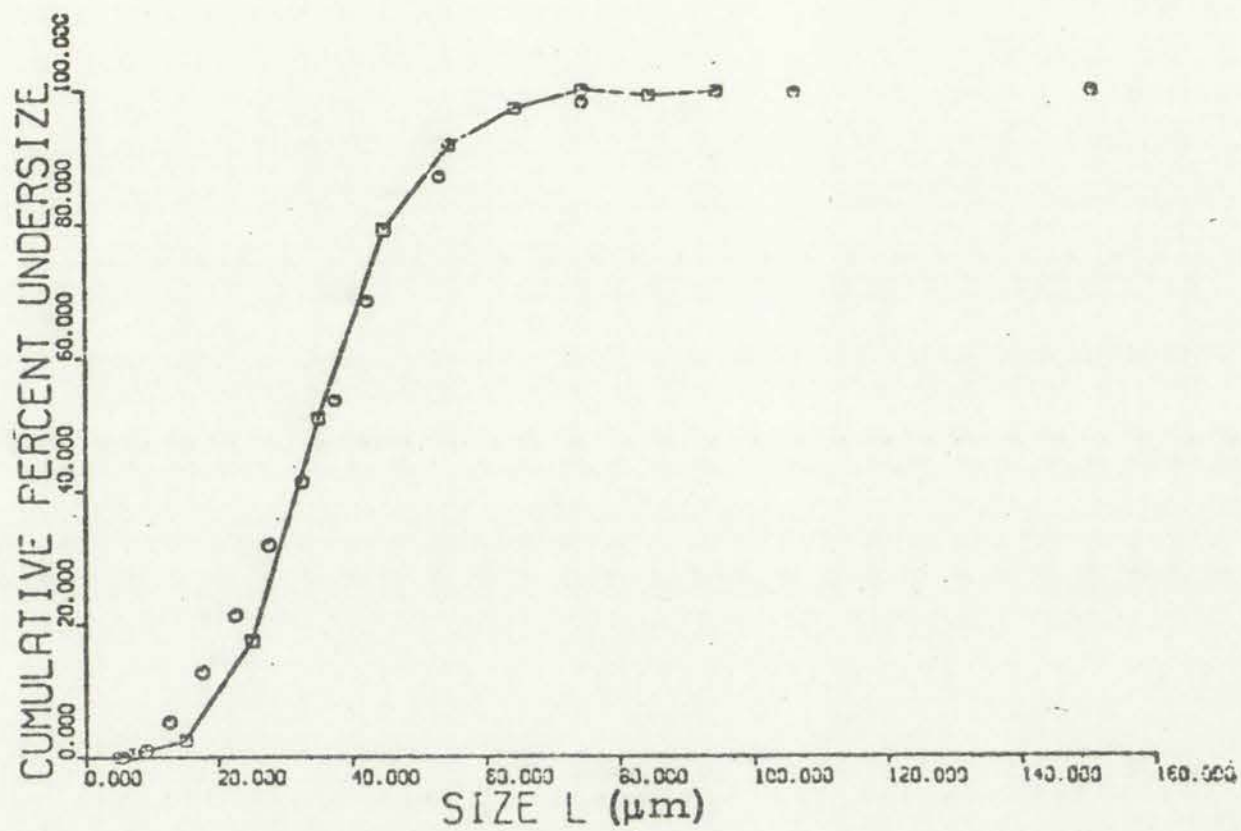


Figure 7e.
R = 2.

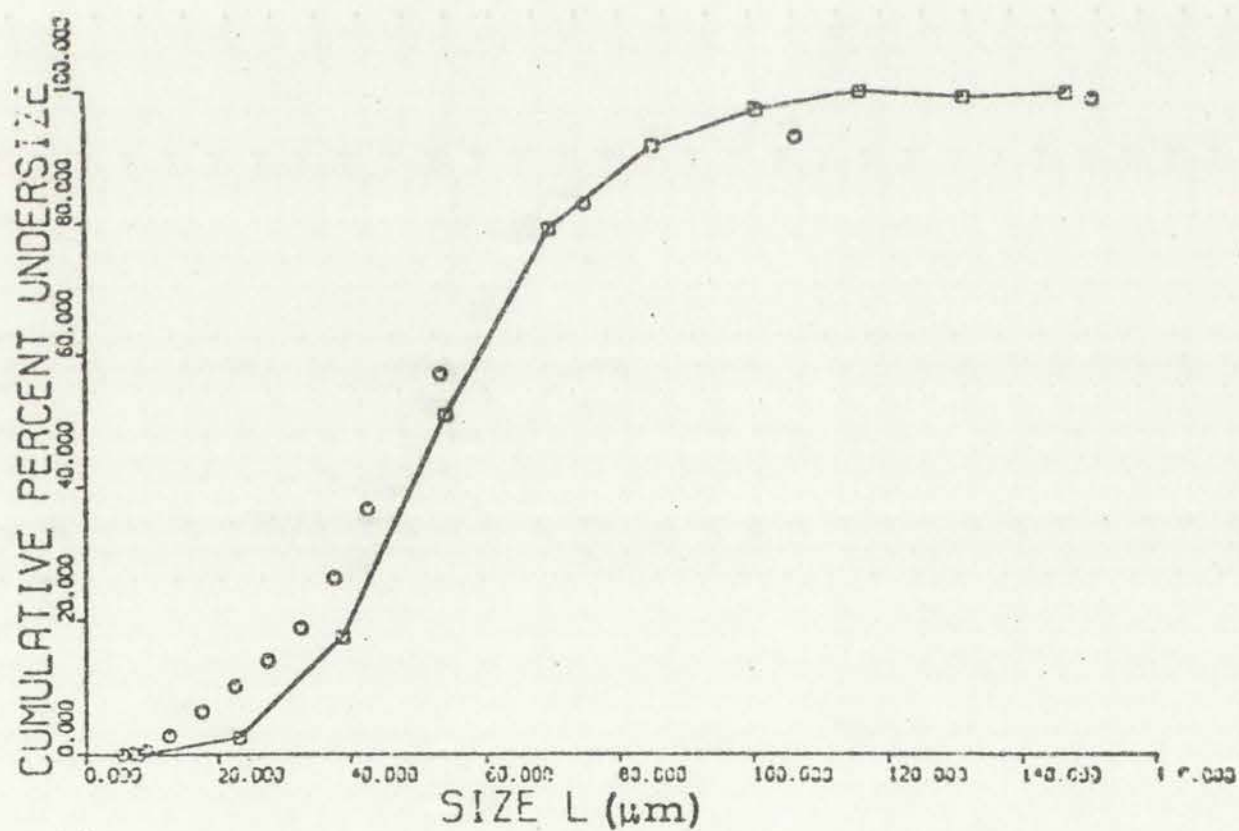
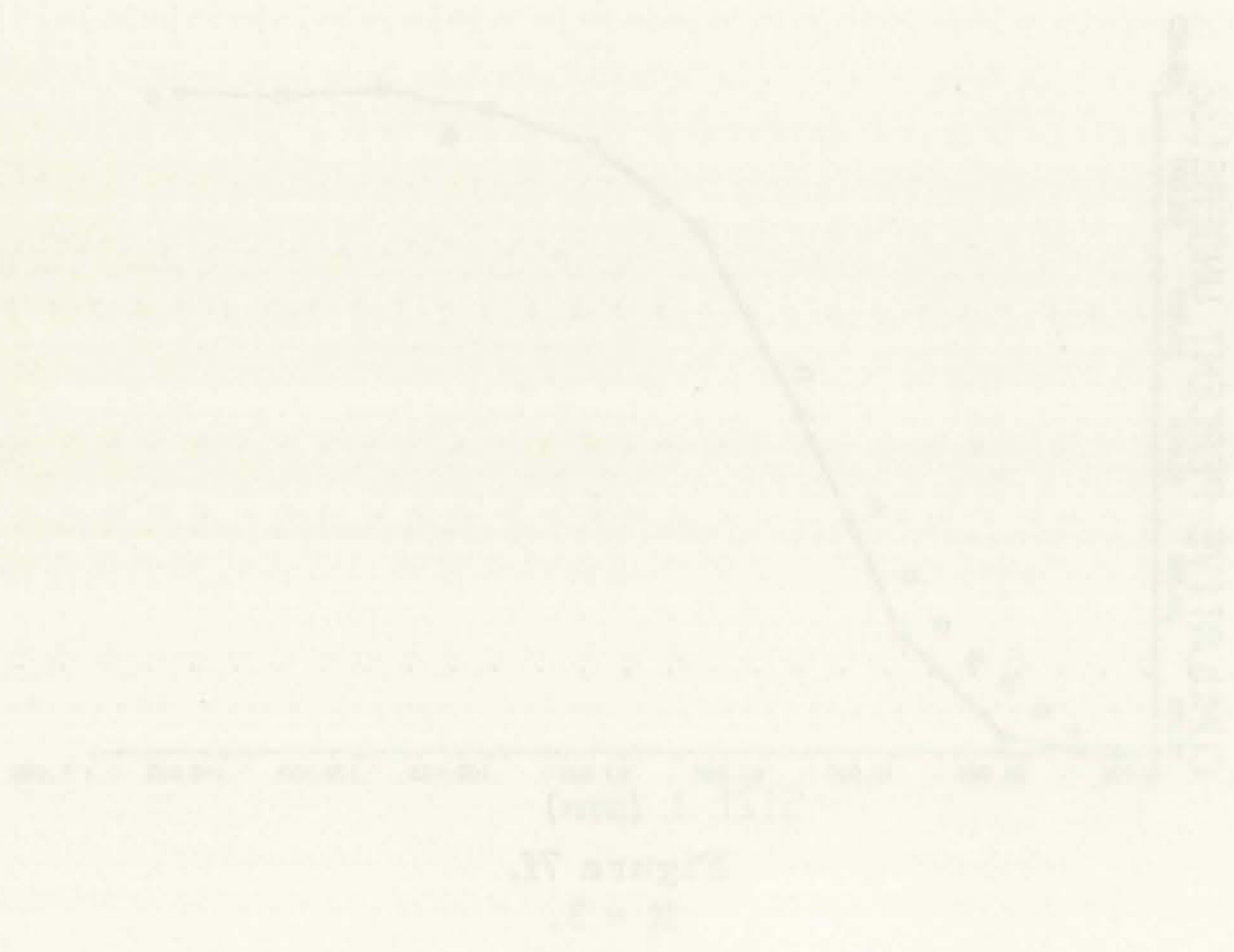


Figure 7f.
R = 3.

Comparison of Theoretical Values with
Experimental Particle Size Distributions.



Comparison of Theoretical Values with
Experimental Values for Experiments

If τ is taken equal to 0.5 s, the resulting calculations result in limiting quantities, subject to the flow rate range of the system used. The resulting kinetic quantities are limiting, or effective, kinetic quantities. These effective kinetics are valid for this system, but may not be valid if significantly higher flow rates are used, either by increasing the height of the column of solution above the static mixer, or by using a mechanical pump.

The effective initial growth rate in $\mu\text{m/s}$ is

$$G_0 = 33.68 + 90.58R \quad (52)$$

or

$$G_0 = 4.88L \quad (53)$$

The total effective growth rate kinetics are

$$G = (33.68 + 90.58R)(1 - z)^{1.56} \quad (54)$$

with G in $\mu\text{m/s}$. For purposes of simplicity, the quantity $B_0^0 / C_0 (1 - \beta_s)$ will be used in the discussion so that Eq. (24) becomes

$$\frac{B_0^0}{C_0 (1 - \beta_s)} = \frac{1}{\rho K_V (G_0 \tau)^3 \tau f_3(1)} \quad (55)$$

where $\rho = 1.77 \text{ g/cm}^3$, $K_V = \pi/6$, $f_3(1) = 0.006745$ (using best fit parameters), $\tau = 0.5 \text{ s}$, and

$$\frac{B_0^0}{C_0 (1 - \beta_s)} = \frac{K}{(G_0 \tau)^3} \quad (56)$$

It is taken from the ... the ...
quantities ... the law ...
resulting electric ...

These electric ...
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the ... of ...
a mechanical pump.

The electric ...

$$P = 0.1 \text{ watt}$$

10

$$P = 0.1 \text{ watt}$$

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$$C(0.1) = \dots$$

where $P = 0.1$ watt, $R = \dots$
parameters, $\tau = 0.1 \text{ sec}$

where $K = [\rho K_v \tau f_3(1)]^{-1} = 320 \text{ cm}^3/\text{g}\cdot\text{s}$. Also,

$$\frac{B_0^\circ}{C_0(1 - \beta_s)} = \frac{K}{(16.84 + 45.29R)^3} \cdot$$

The total effective nucleation rate kinetics are

$$B^\circ = 320 (16.84 + 45.29R)^{-3} C_0(1 - \beta_s)(1 - z)^{3.75} \quad (58)$$

with B° in nuclei/cm³·s.

Experimental values for G and B° are those in which the kinetic quantities were calculated from experimentally measured \bar{L} using Eqs. (49) and (56). These data, compared with those calculated directly from R by Eqs. (48), (50), and (57), are presented in Table 4.

Figure 8 is a plot of the normalized concentration of PETN in the acetone-water solvent, $\beta(z)$; the normalized growth rate, $G(z)$; and the normalized nucleation rate, $B^\circ(z)$; as functions of the reaction coordinate z . The early part of the reaction appears to be due to the combination of a rapidly decaying nucleation with a nearly linearly decaying growth. In the later part of the reaction, there is practically no nucleation, the growth rate being the primary mechanism at this stage.

The change of the growth rate as a function of concentration is shown in Fig. 9. The reaction proceeds from right to left along the concentration axis. The relationship is nearly linear, except for the initial and final stages of the reaction.

$$\frac{dM_w}{dM_n} = 1 + \frac{M_n}{M_w} \left(\frac{dM_n}{dM_n} - \frac{dM_w}{dM_n} \right)$$

THEORY OF POLYMERIZATION

It is well known that the rate of polymerization is given by

Experimentally, values for α and β are those in which the kinetic quantities were obtained, and the theoretical values are calculated from eq. (1) and (2).

Figure 2 is a plot of the normalized concentration of PDI in the polymer solution against $\ln(1 - \alpha + \beta x)$, and the

normalized polymerization rate, R_p , is shown as a function of the reaction time.

The early part of the reaction appears to be due to the

formation of a rapidly decaying reaction with a nearly linear decrease in the later part of the reaction, there is practically no

inclusion, the growth rate being the primary mechanism at this stage. The change of the growth rate as a function of concentration is

shown in fig. 3. The reaction proceeds from right to left along the concentration axis. The relationship is nearly linear, except for the

initial and final stages of the reaction.

TABLE 4
CALCULATED KINETIC^a QUANTITIES

R	\bar{L}^b (experimental)	Standard Deviation (μm)	\bar{L} (calculated)	Residual	Deviation (%)	Average Deviation (%)
$\frac{1}{4}$	12.2	± 1.1	11.5	-0.7	6.1	
$\frac{1}{3}$	12.7	± 1.8	13.1	0.4	3.0	
$\frac{1}{2}$	13.3	± 2.3	16.2	2.9	17.9	8.9
1	30.2	± 9.0	25.5	-4.7	18.4	
2	41.0	± 5.2	44.0	3.0	6.8	
3	63.5	± 10.4	62.6	-0.9	1.4	

R	G_0^c (experimental)	G_0 (calculated)	Residual	Deviation (%)	Average Deviation (%)
$\frac{1}{4}$	59.54	56.33	-3.21	5.7	
$\frac{1}{3}$	61.98	63.87	1.89	3.0	
$\frac{1}{2}$	64.90	78.97	14.07	17.8	8.9
1	147.38	124.26	-23.12	18.6	
2	200.08	214.84	14.76	6.9	
3	309.88	305.42	-4.46	1.5	

R	B_0^d (experimental)	B_0^c (calculated)	Residual	Deviation (%)	Average Deviation (%)
$\frac{1}{4}$	0.97×10^7	1.14×10^7	0.17×10^7	14.9	
$\frac{1}{3}$	1.07×10^7	0.98×10^7	-0.09×10^7	9.2	
$\frac{1}{2}$	1.24×10^7	0.69×10^7	-0.55×10^7	79.7	28.6
1	1.42×10^8	2.36×10^8	0.94×10^8	39.8	
2	7.16×10^8	5.77×10^8	-1.39×10^8	24.1	
3	1.41×10^8	1.47×10^8	0.06×10^8	4.1	

^aEffective kinetic quantities.

^b \bar{L} in μm .

^c G_0 in $\mu\text{m}/\text{s}$.

^d B_0^c in nuclei/ $\text{cm}^3 \cdot \text{s}$.

TABLE 2
 MEAN AND STANDARD DEVIATION OF THE MEAN

Age	Mean	Standard Deviation	Age	Mean	Standard Deviation
1.0	1.3	0.41	1.1	1.5	0.5
1.2	1.4	0.41	1.3	1.7	0.5
1.4	1.5	0.41	1.5	1.9	0.5
1.6	1.6	0.41	1.7	2.1	0.5
1.8	1.7	0.41	1.9	2.3	0.5

Age	Mean	Standard Deviation	Age	Mean	Standard Deviation
2.0	18.0	15.0	2.1	19.0	16.0
2.2	19.0	16.0	2.3	20.0	17.0
2.4	20.0	17.0	2.5	21.0	18.0
2.6	21.0	18.0	2.7	22.0	19.0
2.8	22.0	19.0	2.9	23.0	20.0

Age	Mean	Standard Deviation	Age	Mean	Standard Deviation
3.0	23.0	20.0	3.1	24.0	21.0
3.2	24.0	21.0	3.3	25.0	22.0
3.4	25.0	22.0	3.5	26.0	23.0
3.6	26.0	23.0	3.7	27.0	24.0
3.8	27.0	24.0	3.9	28.0	25.0

Source: Author's calculations.
 N = 100
 a - Sample size of 10

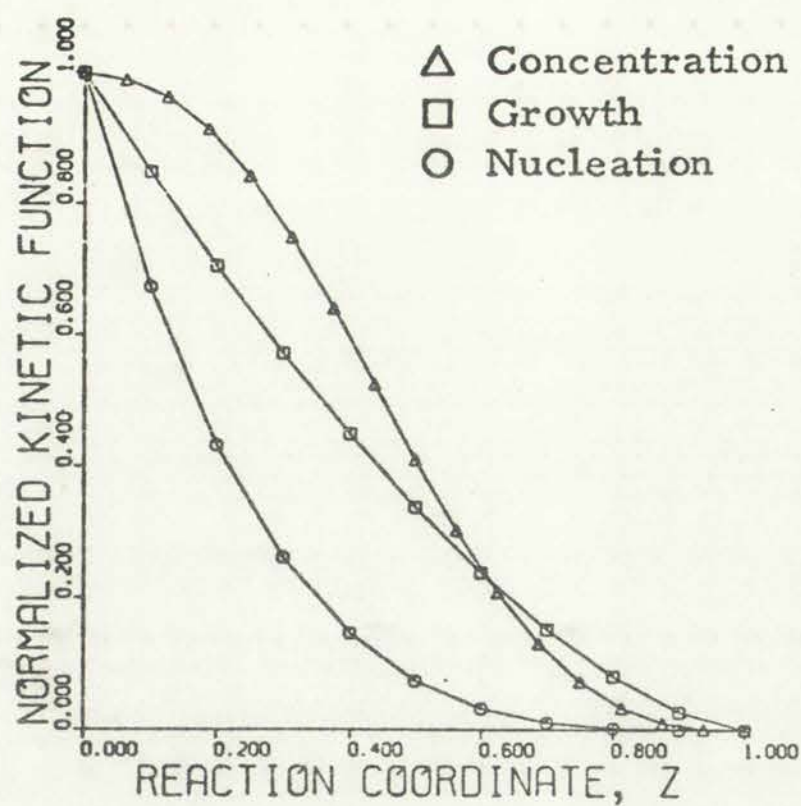


Figure 8.
Theoretical Kinetics Along Reaction Coordinate.

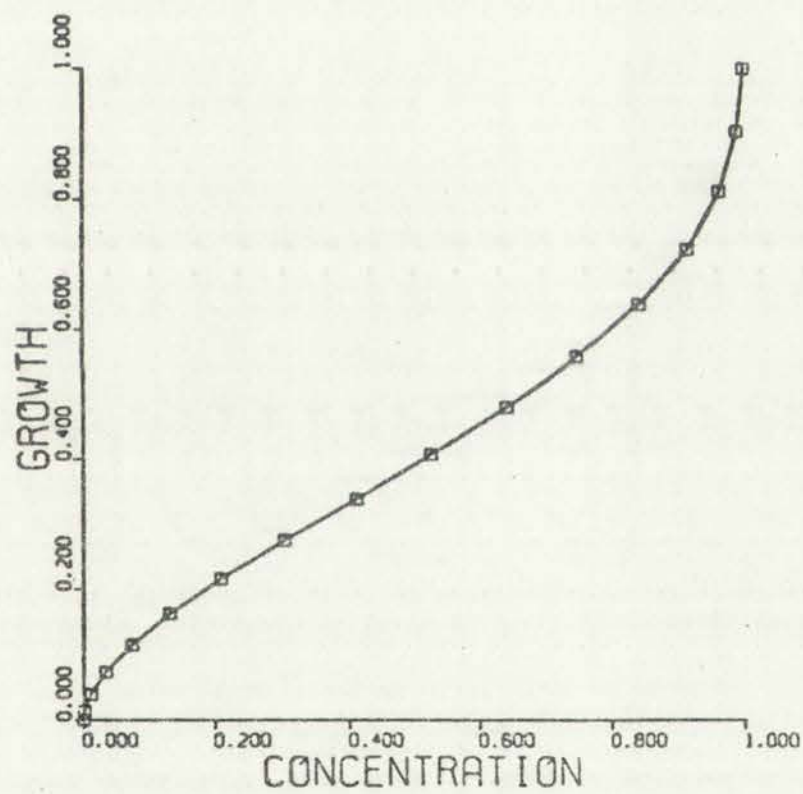
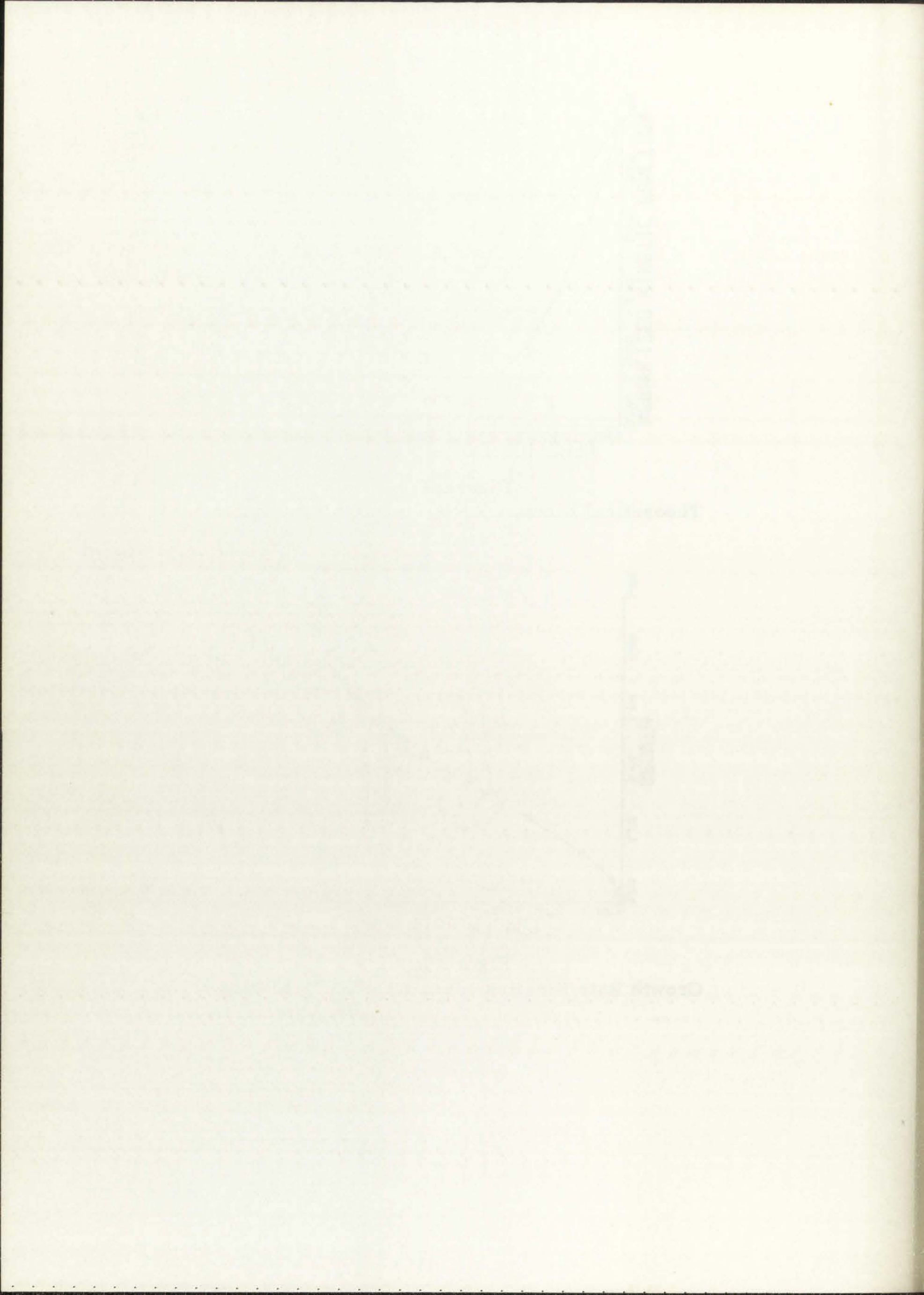


Figure 9.
Growth Rate Kinetics Along Reaction Coordinate.



The variation of the first four moments along the reaction coordinate is shown in Fig. 10. The 0th moment may be thought of as the total number of crystals in the volume under consideration. The rather large slope at the early part of the reaction may be due to the large nucleation occurring at this stage. The first moment represents the sum of the lengths of all the crystals in the distribution. This moment is controlled principally by growth. There appears to be an increase in the slope of the curve after the initial "surge" of nucleation. The second moment is related to the specific surface area and the third moment is related to the specific mass of crystals in the distribution.

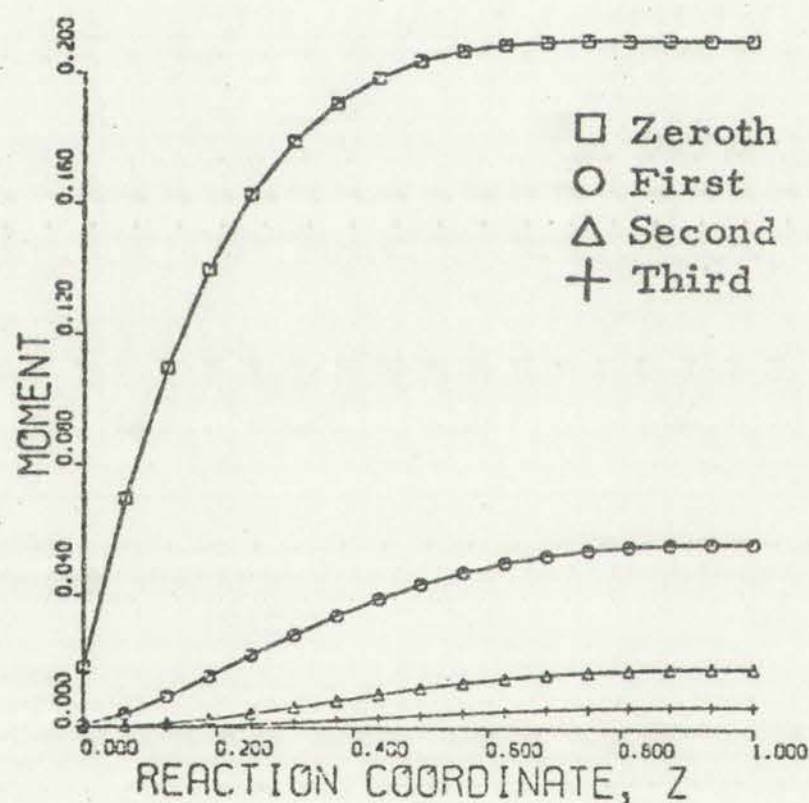


Figure 10.
Variation of Moments Along Reaction Coordinate.

The variation of the reaction rate with the reaction coordinate is shown in Figure 10. The reaction rate is plotted against the total number of crystals in the volume under consideration. The large change in the reaction rate at the origin may be due to the large induction period at this stage. The first maximum represents the growth of the nuclei of all the crystals in the distribution. This maximum is controlled principally by growth. The second maximum is due to the growth in the crystal size when the nuclei are formed. The second maximum is related to the specific surface area and the third maximum is related to the specific mass of crystals in the distribution.

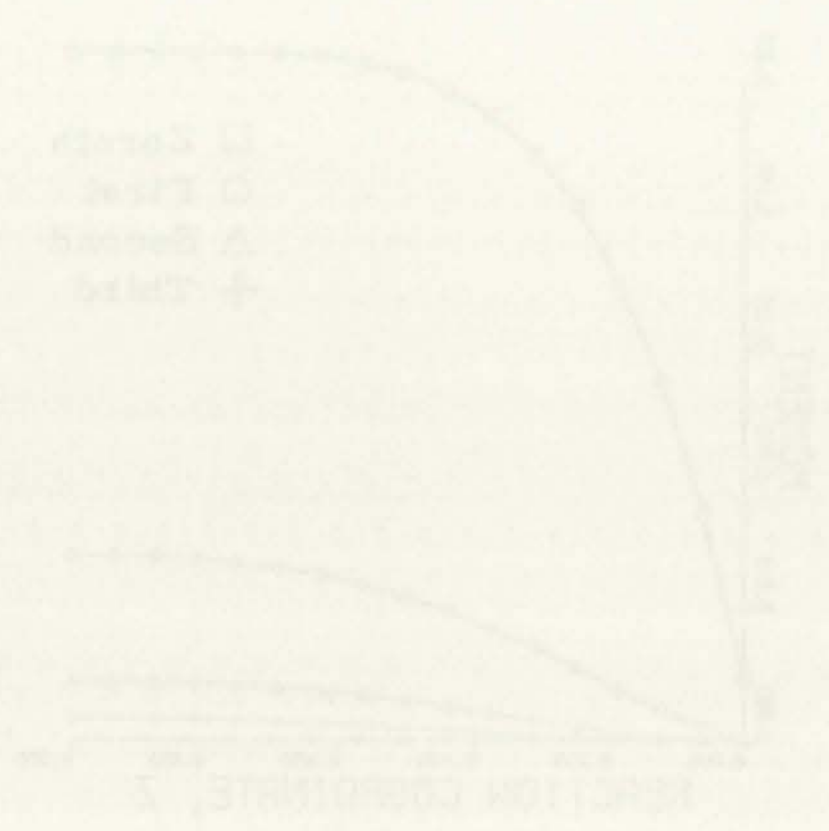


Figure 10. Variation of Reaction Rate with Reaction Coordinate.

C. Detonation Characteristics

The results of the threshold voltage measurements for the PETN samples are shown in Fig. 11. A polynomial regression was performed on the experimental data. The resulting second-degree polynomial curve is represented by the solid line in Fig. 11, and is referred to as the theoretical curve. The average percent deviation of the experimental data from the theoretical curve is 4.1. The experimental points are indicated in Fig. 11 by circles. Since the value for \bar{L} may be calculated from an R-value using Eq. (48), a correlation was made between $E_{0.5}$ and \bar{L} . The data are presented in Table 5. The equation for the calculation of $E_{0.5}$ from \bar{L} is

$$E_{0.5} = 1029.977 - 18.56256 \bar{L} + 0.19019 \bar{L}^2 \quad (59)$$

with \bar{L} in μm and $E_{0.5}$ in V.

The results of the transit time measurements for the PETN samples are shown in Fig. 12. The curve represented by the solid line resulted from a polynomial regression performed on the experimental data. The third-degree polynomial curve is referred to as the theoretical curve. The average percent deviation of the experimental data from the theoretical curve is 4.4. The correlation between t_m and \bar{L} is presented in Table 6. The equation for the calculation of t_m from \bar{L} is

$$t_m = 0.5562 + 0.03913 \bar{L} - 0.001227 \bar{L}^2 + 0.00001726 \bar{L}^3 \quad (60)$$

with \bar{L} in μm and t_m in μs .

Experimental Results

The results of the above-mentioned measurements for the 1950-51 season are shown in Fig. 11. A polynomial regression was formed on the experimental data. The resulting theoretical curve is represented by the solid line in Fig. 11, and is related to the experimental curve. The average percent deviation of the experimental data from the theoretical curve is 2.1%. The values of \bar{I}_m and \bar{I}_s are calculated from the \bar{I} values using Eq. (48). A correlation was made between \bar{I}_m and \bar{I}_s . The data are presented in Table 5. The equation for the calculation of \bar{I}_m from \bar{I}_s is

$$\bar{I}_m = 0.971 \bar{I}_s + 0.029 \bar{I}_s^2 \quad (49)$$

with \bar{I} in cm and \bar{I}_m in cm. The results of the present time measurements for the 1951-52 season are shown in Fig. 12. The curve represented by the solid line resulted from a polynomial regression performed on the experimental data. The third-degree polynomial curve is related to the theoretical curve. The average percent deviation of the experimental data from the theoretical curve is 2.4%. The correlation between \bar{I}_m and \bar{I}_s is presented in Table 6. The equation for the calculation of \bar{I}_m from \bar{I}_s is

$$\bar{I}_m = 0.985 \bar{I}_s + 0.015 \bar{I}_s^2 + 0.00015 \bar{I}_s^3 \quad (50)$$

with \bar{I} in cm and \bar{I}_m in cm.

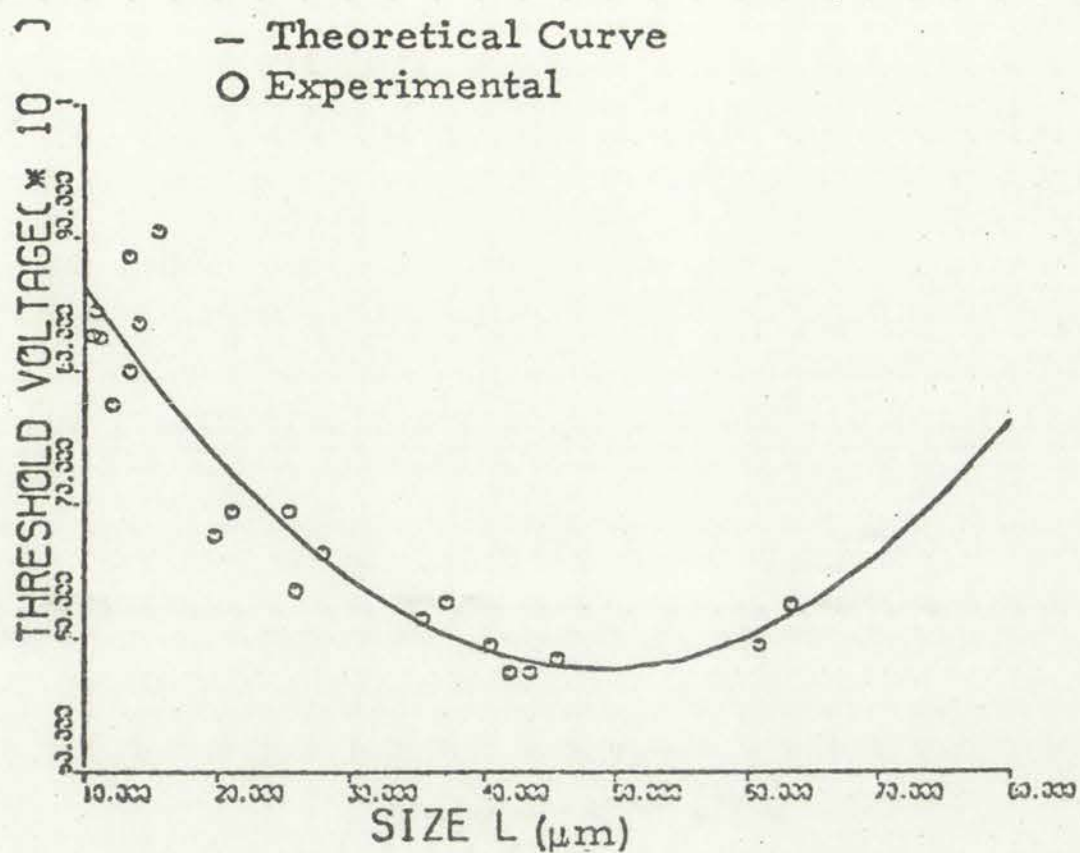


Figure 11.
PETN Detonator Threshold Voltages.

TABLE 5

CORRELATION OF THRESHOLD VOLTAGE WITH \bar{L}

\bar{L} (μm)	Average $E_{0.5}$ (V)	Standard Deviation (%)	Theoretical $E_{0.5}$ (V)	Deviation (%)
12.2	800	4.4	832	3.8
12.7	825	1.3	825	0.5
13.3	875	3.5	817	7.6
30.2	650	7.0	432	0.3
41.0	600	3.5	589	0.5
63.5	625	2.8	618	0.5



Figure 11
Plot of $\log k$ vs $1/T$

TABLE 2

CORRELATION OF TEMPERATURES FOR FACTORIAL

Temp (°C)	Average Rate (V)	Standard Deviation	Temp (°C)
15.5	800	4.4	15.5
15.7	825	1.3	15.7
16.3	875	2.2	16.3
20.5	900	7.0	20.5
21.0	900	2.2	21.0
22.7	950	2.8	22.7

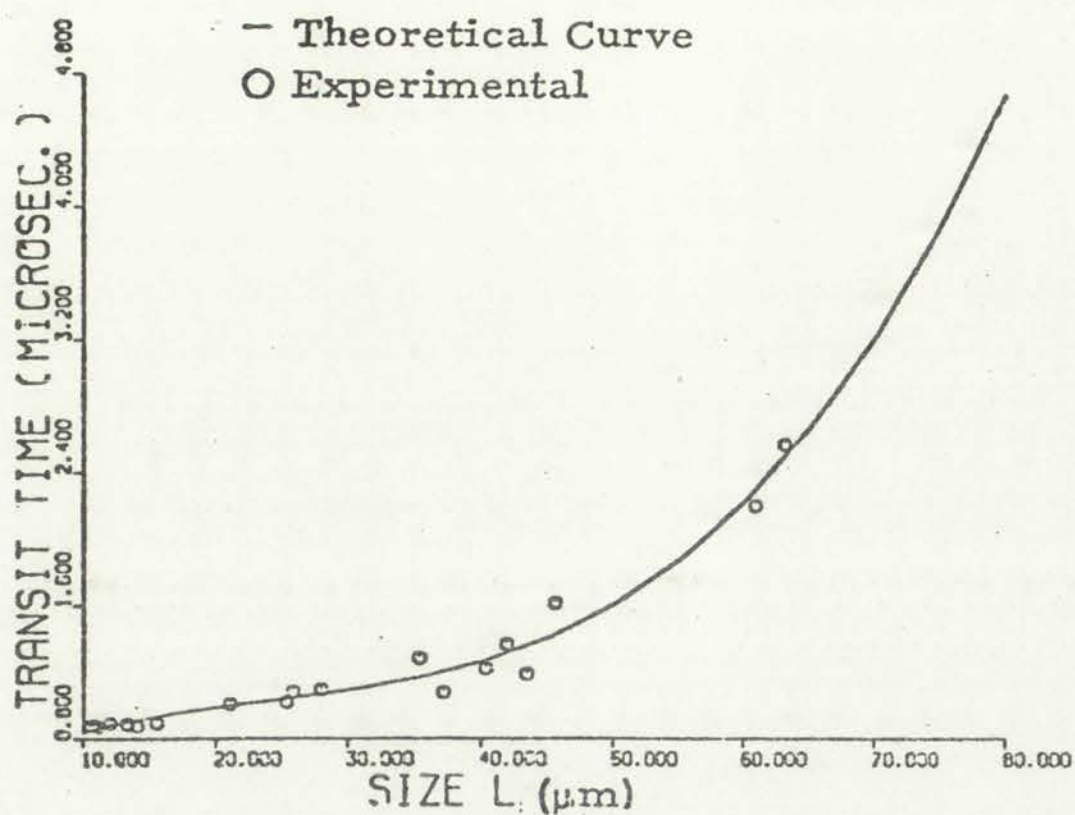


Figure 12.
PETN Detonator Transit Times.

TABLE 6

CORRELATION OF TRANSIT TIME WITH \bar{L}

\bar{L} (μm)	Average t_m (μs)	Standard Deviation (%)	Theoretical t_m (μs)	Deviation (%)
12.2	0.882	1.6	0.882	0.0
12.7	0.878	0.5	0.891	1.5
13.3	0.890	0.7	0.900	1.1
30.2	1.099	7.3	1.094	0.5
41.0	1.422	12.1	1.287	10.5
63.5	2.385	10.9	2.513	5.1

Figure 1
 O.K. (K)



Figure 1
 PETI (K)

TABLE I

CORRELATION OF ...

...	Average
...	0.982	1.4	...
...	0.878	0.8	...
...	0.890	0.7	...
...	1.059	1.1	...
...	1.622	1.1	...
...	2.362	1.6	...

VIII. CONCLUSIONS

For a given R-value, the various quantities, including effective nucleation and growth rates, mass-weighted mean particle size, concentration function, transit time, and threshold voltage may be calculated using the equations summarized in Table 7.

The crystals obtained from the continuous plug flow crystallizer have narrow distributions and are fairly uniform in crystal habit. The dispersed plug flow model calculations provide a reasonably good prediction of these properties.

The objectives for developing a continuous reproducible recrystallization technique and a predictive model for the preparation of PETN have been achieved.

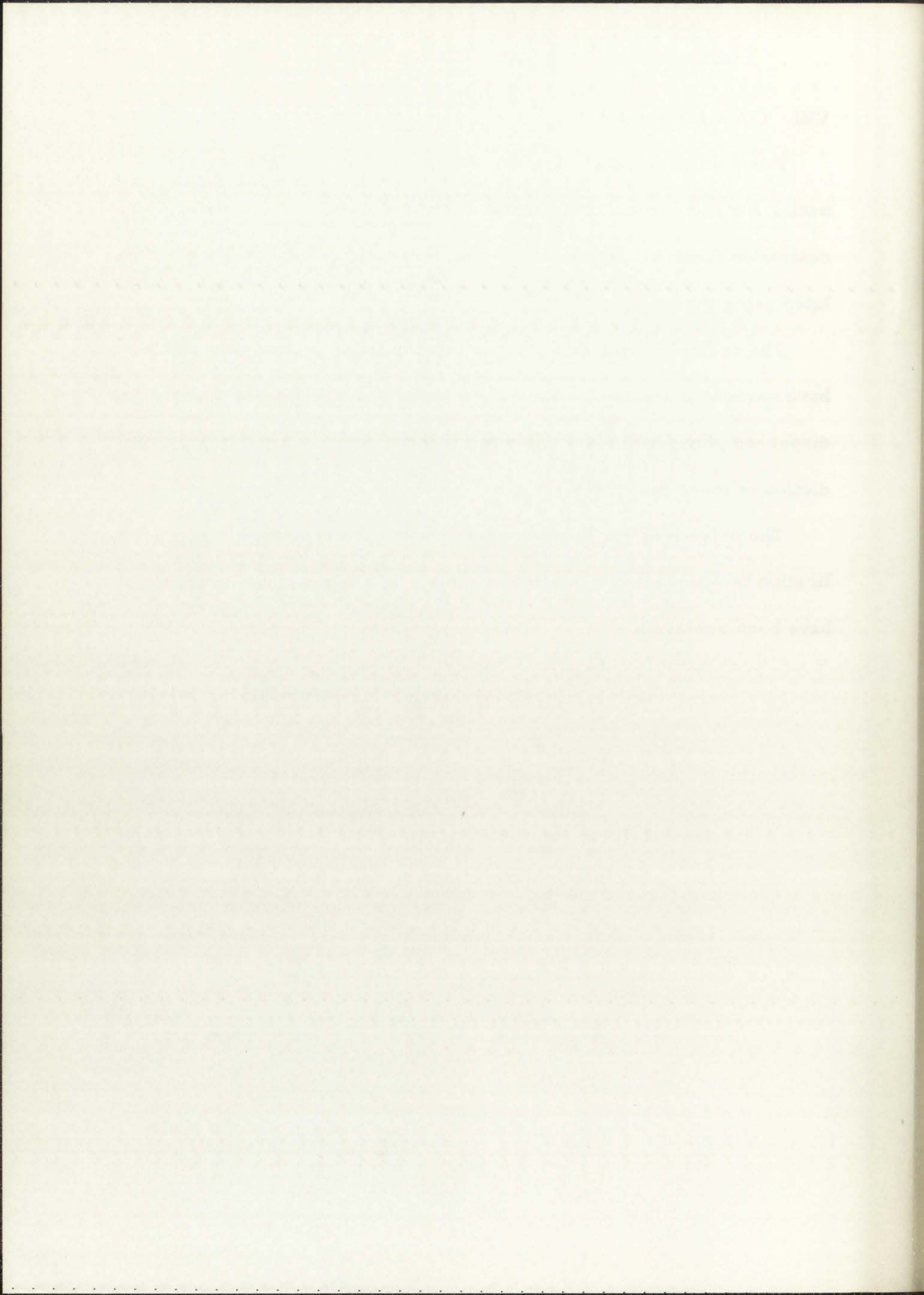


TABLE 7

SUMMARY OF THEORETICAL EQUATIONS

Quantity	Equation	Average Deviation from Experimental Results (%)
Mass-weighted mean particle size (μm)	$\bar{L} = 6.90 + 18.56 R$	8.9
Effective growth rate ($\mu\text{m}/\text{s}$)	$G(R, z) = (33.68 + 90.58 R)(1 - z)^{1.56}$	8.9
Effective nucleation rate (nuclei/ $\text{cm}^3 \cdot \text{s}$)	$B^0(R, z) = 320(16.84 + 45.29 R)^{-3} C_0 (1 - \beta_s)(1 - z)^{3.75}$	28.7
Concentration	$\beta(z) = 1 + \frac{f_3(z)}{f_3(1)} \beta_s - \frac{f_3(z)}{f_3(1)}$	a
Threshold voltage (V)	$E_{0.5} = 1029.977 - 18.56256 \bar{L} + 0.19019 \bar{L}^2$	4.1
Transit time (μs)	$t_m = 0.5562 + 0.03913 \bar{L} - 0.001227 \bar{L}^2 + 0.00001726 \bar{L}^3$	4.4

^a Not determined.

Experiment 1

Date: _____

Page: _____

Objectives:

To determine the rate of reaction between hydrogen peroxide and potassium iodide.

To determine the order of reaction with respect to hydrogen peroxide.

Theory:

Hydrogen peroxide decomposes to form water and oxygen gas.

$$2H_2O_2(aq) \rightarrow 2H_2O(l) + O_2(g)$$

The rate of reaction is measured by the volume of oxygen gas evolved over a given period of time.

Procedure

1. Preparation of standard solutions of hydrogen peroxide and potassium iodide.

2. Measurement of the rate of reaction by the volume of oxygen gas evolved.

3. Determination of the order of reaction with respect to hydrogen peroxide.

4. Calculation of the rate constant and the half-life of hydrogen peroxide.

5. Discussion of the results and comparison with the theoretical values.

6. Conclusion and summary of the experiment.

7. References.

$$C_1 = 0.005 + 0.005 = 0.010 \text{ mol dm}^{-3}$$

$$C_2 = 0.005 + 0.005 = 0.010 \text{ mol dm}^{-3}$$

$$C_3 = \frac{C_1 + C_2}{2} = \frac{0.010 + 0.010}{2} = 0.010 \text{ mol dm}^{-3}$$

Rate of reaction = $\frac{d[O_2]}{dt} = \frac{d[O_2]}{V \cdot dt}$

Order of reaction with respect to hydrogen peroxide = n

$$\log k = \log \frac{d[O_2]}{dt} - n \log [H_2O_2]$$

Results

Table 1: Rate of reaction between hydrogen peroxide and potassium iodide.

Table 2: Order of reaction with respect to hydrogen peroxide.

Table 3: Rate constant and half-life of hydrogen peroxide.

Conclusion:

APPENDIX A

CRYSTALLIZATION THEORY*

Particle Phase Space

Particle phase space consists of the least number of independent coordinates of a particle distribution that gives a complete description of the properties of the distribution. Particle phase space is divided into two subregions given by internal and external particle coordinates. External coordinates refer to the spacial distribution of these particles. The prime example of an internal coordinate property is particle size. The definition of the linear size, L , of a particle is often a difficult choice and depends on how particle size is measured.

The linear growth rate is the rate of change of L . Thus, $G = dL/dt$, where G is the convective velocity of a particle along the L -axis. An important restriction to be made is that each particle behaves identically at a given point in particle phase space.

Particle Number Continuity Equation

A population balance for particles in some fixed subregion of particle phase space is stated as

$$\text{Accumulation} = \text{Input} + \text{Output} + \text{Net Generation} .$$

The resulting population balance equation is

$$\frac{\partial n}{\partial t} + \nabla \cdot (\vec{V}n) - B + D = 0 , \quad (61)$$

*This material has been abstracted from Ref. 17 (Randolph and Larson).

CRYSTALLIZATION

Particle Size Distribution

Particle size distribution is a function of time and temperature.

Characteristics of a particle distribution are: number, size, and shape.

of the properties of the distribution. The distribution is defined

into two subdistributions given by $N(r, t) = N_1(r, t) + N_2(r, t)$

where N_1 and N_2 are the number of particles per unit volume.

The general example of an isothermal crystallization process is

The definition of the linear rate G is $G = \frac{dr}{dt}$ where r is the radius

choice and depends on how particles grow in a given medium.

The linear growth rate is the rate of change of the radius

of a particle where G is the constant of proportionality.

is also an important restriction for the growth of particles

above initially in a given medium. Particle growth is

Particle Number Conservation Equation

A population balance for particles is given by

particle phase space is stated as

Accumulation = Input - Output + Birth - Death

The resulting population balance equation is

$$\frac{\partial N}{\partial t} + \frac{\partial}{\partial r} (GN) = \int_0^{\infty} \beta(N, r) N dr - \int_0^{\infty} \delta(N, r) N dr$$

* This material has been adapted from "Introduction to Chemical Engineering Kinetics" by H. S. Fogel, McGraw-Hill, 1968.

in which B and D represent birth and death functions, respectively, of the particle distribution where particles suddenly appear or disappear at a point in the internal phase space, and n is the number population distribution function. \vec{V} is the velocity vector of the particle in phase space.

Moment Transformation of the Population Balance

The solution of the partial differential equation in conjunction with side conditions and auxiliary equations would, in principle, uniquely define the particle-size distribution at each point in particle phase space. However, there is often an incompatibility of dimension with regard to the various equations involved. The resulting incompatibility of dimension results in a difficult-to-solve integro-partial-differential form of equations. In many systems of interest, some average or total quantities are sufficient to represent the particle distribution.

Often, in such cases, a type of transformation may be employed in order to simplify the calculations. One such transformation is the moment transformation of the population balance equation. Such a transformation results in a tradeoff in which the dimensionality of the system is reduced by one at the expense of obtaining average, rather than distributed, information concerning the particle size distribution.

Recovery of the Particle-Size Distribution Function From the Moments

Although a continuous distribution function containing an infinite amount of information cannot be exactly specified with the finite information contained in the finite set of numbers, $\{m_j\}$, we might hope to

in which ρ and \mathbf{v} are the density and velocity of the particles, \mathbf{r} is the position vector, \mathbf{v} is the velocity vector, and $\mathbf{v} \cdot \nabla$ is the convective derivative. The continuity equation is written as

$$\frac{d\rho}{dt} + \nabla \cdot (\rho \mathbf{v}) = 0$$

The solution of the partial differential equations is subject to the initial conditions and auxiliary equations which are prescribed at each point in space. However, these are often an inconveniently complicated

regard to the various equations involved. The method of characteristics of Lagrange results in a different set of equations which are often of the form of ordinary differential equations. In many systems of interest, auxiliary equations are sufficient to represent the particle distribution

Often, in each case, a type of transformation may be employed in order to simplify the calculations. One such transformation is the moment transformation of the position balance equations, which transformation results in a reduced set of equations

system is reduced by one at the expense of additional equations. This distributed information concerning the particle distribution is the subject of the Recovery of the Particle-Density Distribution from the Moment

Although a continuous distribution function is often used, a moment of information cannot be readily specified with the same accuracy as is contained in the finite set of moments $\{ \rho \langle v^n \rangle \}$

recover n to an accuracy adequate for a simulation of a particulate process. A useful technique for the approximate recovery of the distribution function is outlined below.

The transformation that will be used is the moment transformation where m_j is given by the definition

$$m_j = \int_0^{\infty} nL^j dL \quad (62)$$

This integral, to a first-order approximation, is given as

$$m_j = \sum_{k=1}^N n_k L_k^j \Delta L_k \quad (63)$$

where n_k is the value of n at the midpoint, L_k , of a size range ΔL_k .

The equation can be rewritten as a linear combination of the N ordinate values of the distribution, $\{n_k\}$, thus,

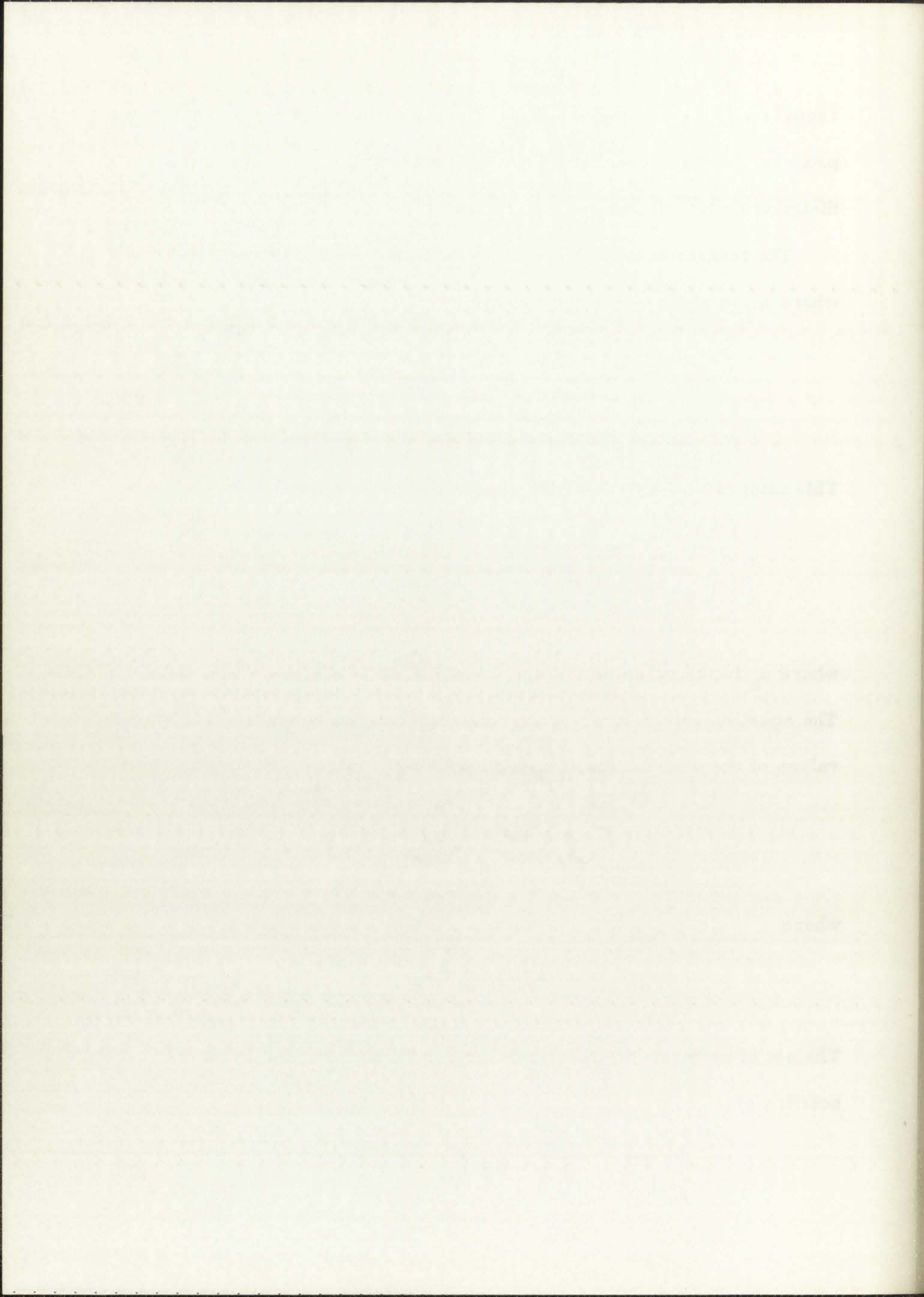
$$m_j = \sum_{k=1}^N a_k^{(j)} n_k \quad (64)$$

where

$$a_k^{(j)} = L_k^j \Delta L_k \quad (65)$$

The set of moments to (N-1)th order can then be written in matrix notation as

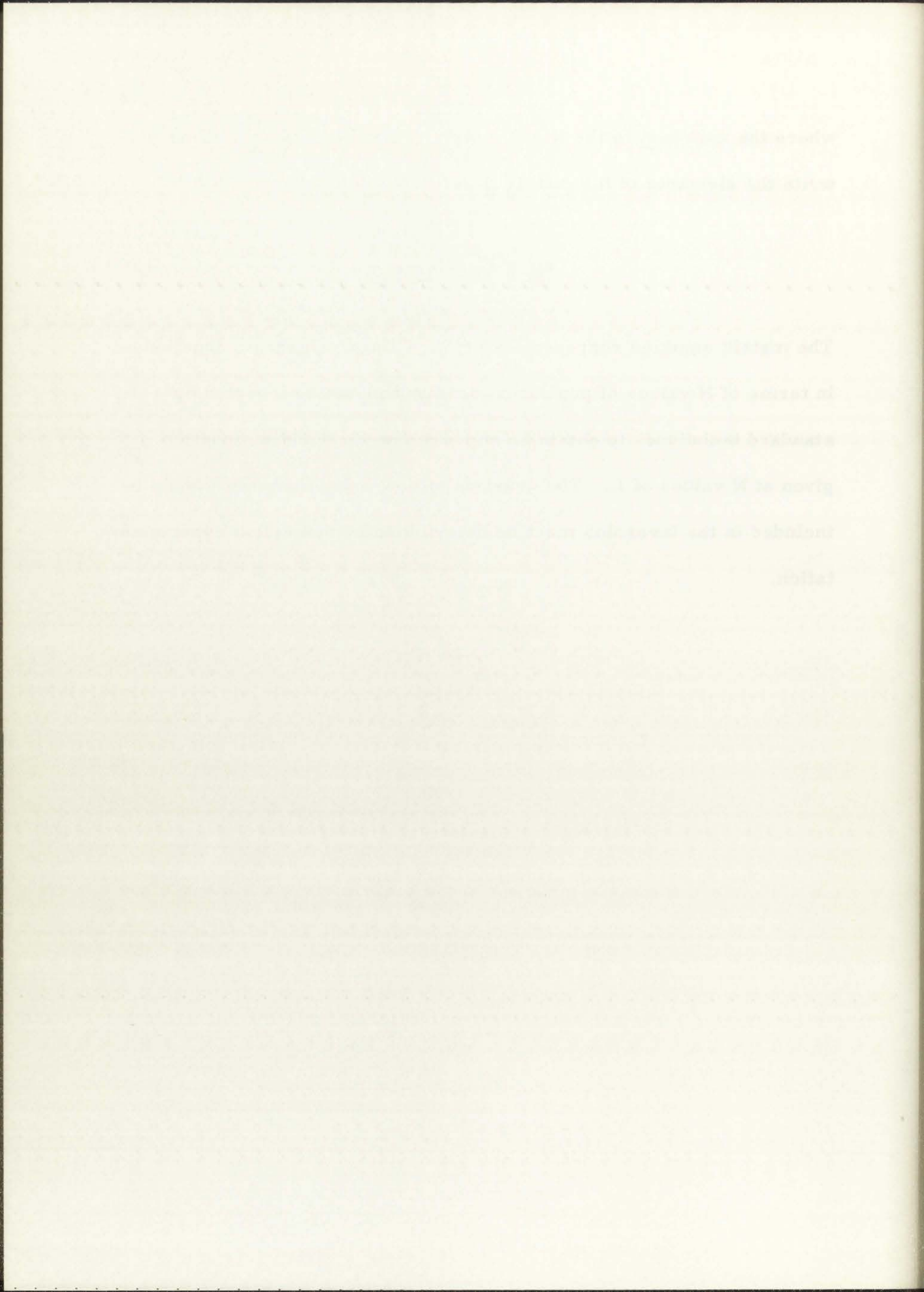
$$\underline{M} = \underline{A}n \quad (66)$$



where the matrix \underline{A} is the $N \times N$ matrix of coefficients $a_k^{(j)}$. Thus we write the elements of the matrix \underline{A} as

$$a_{jk} = L_k^j \Delta L_k . \quad (67)$$

The matrix equation represents a set of N linear algebraic equations in terms of N values of population density and can be inverted by standard techniques to obtain an approximate distribution function given at N values of L . The question of how many moments should be included in the inversion must be determined by numerical experimentation.



APPENDIX B

NUMERICAL METHODS

The plug flow differential equation solutions were obtained by means of a Runge Kutta method. The IBM System/360 Scientific Subroutine Package, DRKG, was used. The IBM System/360 Scientific Subroutine Package, SIMQ, was used to obtain the solutions of the simultaneous linear equations. The runs were made on an IBM-360 Model 50 computer. Brief descriptions of DRKG and SIMQ are given below.

DRKG FROM THE SCIENTIFIC SUBROUTINE PACKAGE

SUBROUTINE DRKGS

PURPOSE

TO SOLVE A SYSTEM OF FIRST ORDER ORDINARY DIFFERENTIAL EQUATIONS WITH GIVEN INITIAL VALUES.

USAGE

CALL DRKGS (PRMT, Y, DERY, NDIM, IHLF, FCT, OUTP, AUX)
PARAMETERS FCT AND OUTP REQUIRE AN EXTERNAL STATEMENT.

DESCRIPTION OF PARAMETERS

PRMT - DOUBLE PRECISION INPUT AND OUTPUT VECTOR WITH DIMENSION GREATER THAN OR EQUAL TO 5, WHICH SPECIFIES THE PARAMETERS OF THE INTERVAL AND OF ACCURACY AND WHICH SERVES FOR COMMUNICATION BETWEEN OUTPUT SUBROUTINE (FURNISHED BY THE USER) AND SUBROUTINE DRKGS. EXCEPT PRMT(5) THE COMPONENTS ARE NOT DESTROYED BY SUBROUTINE DRKGS AND THEY ARE

PRMT(1) - LOWER BOUND OF THE INTERVAL (INPUT),

PRMT(2) - UPPER BOUND OF THE INTERVAL (INPUT),

PRMT(3) - INITIAL INCREMENT OF THE INDEPENDENT VARIABLE (INPUT),

PRMT(4) - UPPER ERROR BOUND (INPUT). IF ABSOLUTE ERROR IS GREATER THAN PRMT(4), INCREMENT GETS HALVED. IF INCREMENT IS LESS THAN PRMT(3) AND ABSOLUTE ERROR LESS THAN PRMT(4)/50, INCREMENT GETS DOUBLED. THE USER MAY CHANGE PRMT(4) BY MEANS OF HIS OUTPUT SUBROUTINE.

PRMT(5) - NO INPUT PARAMETER. SUBROUTINE DRKGS INITIALIZES PRMT(5)=0. IF THE USER WANTS TO TERMINATE SUBROUTINE DRKGS AT ANY OUTPUT POINT, HE HAS TO CHANGE PRMT(5) TO NON-ZERO BY MEANS OF SUBROUTINE OUTP. FURTHER COMPONENTS OF VECTOR PRMT ARE FEASIBLE IF ITS DIMENSION IS DEFINED GREATER THAN 5. HOWEVER SUBROUTINE DRKGS DOES NOT REQUIRE AND CHANGE THEM. NEVERTHELESS THEY MAY BE USEFUL FOR HANDLING RESULT VALUES TO THE MAIN PROGRAM (CALLING DRKGS) WHICH ARE OBTAINED BY SPECIAL MANIPULATIONS WITH OUTPUT DATA IN SUBROUTINE OUTP.

Y - DOUBLE PRECISION INPUT VECTOR OF INITIAL VALUES (DESTROYED). LATER ON Y IS THE RESULTING VECTOR OF DEPENDENT VARIABLES COMPUTED AT INTERMEDIATE POINTS X.

APPENDIX B

OF MATHEMATICAL METHODS

The first part of this appendix is devoted to the derivation of the

fundamental equations of the theory of the motion of a rigid body

under the action of external forces and moments. The second part

is devoted to the derivation of the fundamental equations of the

theory of the motion of a rigid body under the action of

internal forces and moments. The third part is devoted to the

DERIVATION OF THE

FUNDAMENTAL

EQUATIONS OF THE THEORY OF THE MOTION OF A RIGID BODY

UNDER THE ACTION OF EXTERNAL FORCES AND MOMENTS

1.1

Let us consider a rigid body B of mass m and center of mass C .

Let O be an arbitrary point of the body. Let r be the vector

OF THE CENTER OF MASS

OF THE BODY RELATIVE TO THE POINT O . Let r_1, r_2, \dots, r_n be the

vectors of the particles P_1, P_2, \dots, P_n of the body relative to

the point O . Let m_1, m_2, \dots, m_n be the masses of the

particles P_1, P_2, \dots, P_n . Let F_1, F_2, \dots, F_n be the

external forces acting on the particles P_1, P_2, \dots, P_n .

Let M_1, M_2, \dots, M_n be the external moments acting on the

particles P_1, P_2, \dots, P_n . Let $r_1 \times F_1, r_2 \times F_2, \dots, r_n \times F_n$ be the

external moments acting on the particles P_1, P_2, \dots, P_n .

Let M_1, M_2, \dots, M_n be the external moments acting on the

particles P_1, P_2, \dots, P_n . Let $r_1 \times F_1, r_2 \times F_2, \dots, r_n \times F_n$ be the

external moments acting on the particles P_1, P_2, \dots, P_n .

Let M_1, M_2, \dots, M_n be the external moments acting on the

particles P_1, P_2, \dots, P_n . Let $r_1 \times F_1, r_2 \times F_2, \dots, r_n \times F_n$ be the

external moments acting on the particles P_1, P_2, \dots, P_n .

Let M_1, M_2, \dots, M_n be the external moments acting on the

particles P_1, P_2, \dots, P_n . Let $r_1 \times F_1, r_2 \times F_2, \dots, r_n \times F_n$ be the

external moments acting on the particles P_1, P_2, \dots, P_n .

Let M_1, M_2, \dots, M_n be the external moments acting on the

particles P_1, P_2, \dots, P_n . Let $r_1 \times F_1, r_2 \times F_2, \dots, r_n \times F_n$ be the

external moments acting on the particles P_1, P_2, \dots, P_n .

Let M_1, M_2, \dots, M_n be the external moments acting on the

particles P_1, P_2, \dots, P_n . Let $r_1 \times F_1, r_2 \times F_2, \dots, r_n \times F_n$ be the

external moments acting on the particles P_1, P_2, \dots, P_n .

Let M_1, M_2, \dots, M_n be the external moments acting on the

particles P_1, P_2, \dots, P_n . Let $r_1 \times F_1, r_2 \times F_2, \dots, r_n \times F_n$ be the

external moments acting on the particles P_1, P_2, \dots, P_n .

Let M_1, M_2, \dots, M_n be the external moments acting on the

particles P_1, P_2, \dots, P_n . Let $r_1 \times F_1, r_2 \times F_2, \dots, r_n \times F_n$ be the

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particles P_1, P_2, \dots, P_n . Let $r_1 \times F_1, r_2 \times F_2, \dots, r_n \times F_n$ be the

external moments acting on the particles P_1, P_2, \dots, P_n .

Let M_1, M_2, \dots, M_n be the external moments acting on the

particles P_1, P_2, \dots, P_n . Let $r_1 \times F_1, r_2 \times F_2, \dots, r_n \times F_n$ be the

external moments acting on the particles P_1, P_2, \dots, P_n .

- DERY** - DOUBLE PRECISION INPUT VECTOR OF ERROR WEIGHTS (DESTROYED). THE SUM OF ITS COMPONENTS MUST BE EQUAL TO 1. LATER ON DERY IS THE VECTOR OF DERIVATIVES, WHICH BELONG TO FUNCTION VALUES Y AT INTERMEDIATE POINTS X.
- NDIM** - AN INPUT VALUE, WHICH SPECIFIED THE NUMBER OF EQUATIONS IN THE SYSTEM.
- IHLF** - AN OUTPUT VALUE, WHICH SPECIFIED THE NUMBER OF BISECTIONS OF THE INITIAL INCREMENT. IF IHLF GETS GREATER THAN 10, SUBROUTINE DRKGS RETURNS WITH ERROR MESSAGE IHLF-11 INTO MAIN PROGRAM, ERROR PRMT(3)=0 OR IN CASE SIGN(PRMT(3)).NE.SI GN(PRMT(2))-MESSAGE IHLF=12 OR IHLF=13 APPEARS IN CASE PRMT(1)) RESPECTIVELY.
- FCT** - THE NAME OF AN EXTERNAL SUBROUTINE USED. THIS SUBROUTINE COMPUTES THE RIGHT HAND SIDES DERY OF THE SYSTEM TO GIVEN VALUES X AND Y. ITS PARAMETER LIST MUST BE X, Y, DERY. SUBROUTINE FCT SHOULD NOT DESTROY X AND Y.
- OUTP** - THE NAME OF AN EXTERNAL OUTPUT SUBROUTINE USED. ITS PARAMETER LIST MUST BE X, Y, DERY, IHLF, NDIM, PRMT. NONE OF THESE PARAMETERS (EXCEPT, IF NECESSARY, PRMT(4), PRMT(5),...) SHOULD BE CHANGED BY SUBROUTINE OUTP. IF PRMT(5) IS CHANGED TO NON-ZERO, SUBROUTINE DRKGS IS TERMINATED.
- AUX** DOUBLE PRECISION AUXILIARY STORAGE ARRAY WITH 8 ROWS AND NDIM COLUMNS.

REMARKS

THE PROCEDURE TERMINATES AND RETURNS TO CALLING PROGRAM, IF

- (1) MORE THAN 10 BISECTIONS OF THE INITIAL INCREMENT ARE NECESSARY TO GET SATISFACTORY ACCURACY (ERROR MESSAGE IHLF= 11),
- (2) INITIAL INCREMENT IS EQUAL TO 0 OR HAS WRONG SIGN (ERROR MESSAGES IHLF=12 OR IHLF=13,
- (3) THE WHOLE INTEGRATION INTERVAL IS WORKED THROUGH,
- (4) THE SUBROUTINE OUTP HAS CHANGED PRMT(5) TO NON-ZERO.

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED THE EXTERNAL SUBROUTINES FCT(X, Y, DERY) AND OUTP(X, Y, DERY, IHLF, NDIM, PRMT) MUST BE FURNISHED BY THE USER.

METHOD

EVALUATION IS DONE BY MEANS OF FOURTH ORDER RUNGE-KUTTA FORMULAE IN THE MODIFICATION DUE TO GILL. ACCURACY IS TESTED COMPARING THE RESULTS OF THE PROCEDURE WITH SINGLE AND DOUBLE INCREMENT.

SUBROUTINE DRKGS AUTOMATICALLY ADJUSTS THE INCREMENT DURING THE WHOLE COMPUTATION BY HALVING OR DOUBLING. IF MORE THAN 10 BISECTIONS OF THE INCREMENT ARE NECESSARY TO GET SATISFACTORY ACCURACY, THE SUBROUTINE RETURNS WITH ERROR MESSAGE IHLF=11 INTO MAIN PROGRAM.

TO GET FULL FLEXIBILITY IN OUTPUT, AN OUTPUT SUBROUTINE MUST BE FURNISHED BY THE USER.

FOR REFERENCE, SEE

RALSTON/WILF, MATHEMATICAL METHODS FOR DIGITAL COMPUTERS, WILEY, NEW YORK/LONDON, 1960, PP. 110-120.

DOUBLE PRECISION ARITHMETIC WITH
MESSAGE DE-7-II ON DEPENDENT VALUES
REMAINING SEPARATELY.

DATA

THE NAME OF AN EXTERNAL FUNCTION
IS REQUIRED TO COMPUTE THE VALUE OF
THE STATE TO GIVE VALUES OF THE
THE LIST MUST BE X, Y, OR Z, OR
NOT DEPENDENT X AND Y.

NAME

THE NAME OF AN EXTERNAL FUNCTION
IS REQUIRED TO COMPUTE THE VALUE OF
THE STATE TO GIVE VALUES OF THE
THE LIST MUST BE X, Y, OR Z, OR
NOT DEPENDENT X AND Y.

TEXT

THE NAME OF AN EXTERNAL FUNCTION
IS REQUIRED TO COMPUTE THE VALUE OF
THE STATE TO GIVE VALUES OF THE
THE LIST MUST BE X, Y, OR Z, OR
NOT DEPENDENT X AND Y.

DATA

DOUBLE PRECISION ARITHMETIC WITH
MESSAGE DE-7-II ON DEPENDENT VALUES
REMAINING SEPARATELY.

DATA

THE NAME OF AN EXTERNAL FUNCTION
IS REQUIRED TO COMPUTE THE VALUE OF
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DOUBLE PRECISION ARITHMETIC WITH
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DOUBLE PRECISION ARITHMETIC WITH
MESSAGE DE-7-II ON DEPENDENT VALUES
REMAINING SEPARATELY.

DATA

THE NAME OF AN EXTERNAL FUNCTION
IS REQUIRED TO COMPUTE THE VALUE OF
THE STATE TO GIVE VALUES OF THE
THE LIST MUST BE X, Y, OR Z, OR
NOT DEPENDENT X AND Y.

DATA

SIMQ FROM THE SCIENTIFIC SUBROUTINE PACKAGE

SUBROUTINE SIMQ

PURPOSE

OBTAIN SOLUTION OF A SET OF SIMULTANEOUS LINEAR EQUATIONS,
 $AX = B$

USAGE

CALL SIMQ(A, B, N, KS)

DESCRIPTION OF PARAMETERS

A - MATRIX OF COEFFICIENTS STORED COLUMNWISE. THESE ARE DESTROYED IN THE COMPUTATION. THE SIZE OF MATRIX A IS N BY N.
 B - VECTOR OF ORIGINAL CONSTANTS (LENGTH N). THESE ARE REPLACED BY FINAL SOLUTION VALUES, VECTOR X.
 N - NUMBER OF EQUATIONS AND VARIABLES. N MUST BE .GT. ONE.
 KS - OUTPUT DIGIT
 0 FOR A NORMAL SOLUTION
 1 FOR A SINGULAR SET OF EQUATIONS

REMARKS

MATRIX A MUST BE GENERAL.
 IF MATRIX IS SINGULAR, SOLUTION VALUES ARE MEANINGLESS.
 AN ALTERNATIVE SOLUTION MAY BE OBTAINED BY USING MATRIX INVERSION (MINV) AND MATRIX PRODUCT (GMPRD).

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED

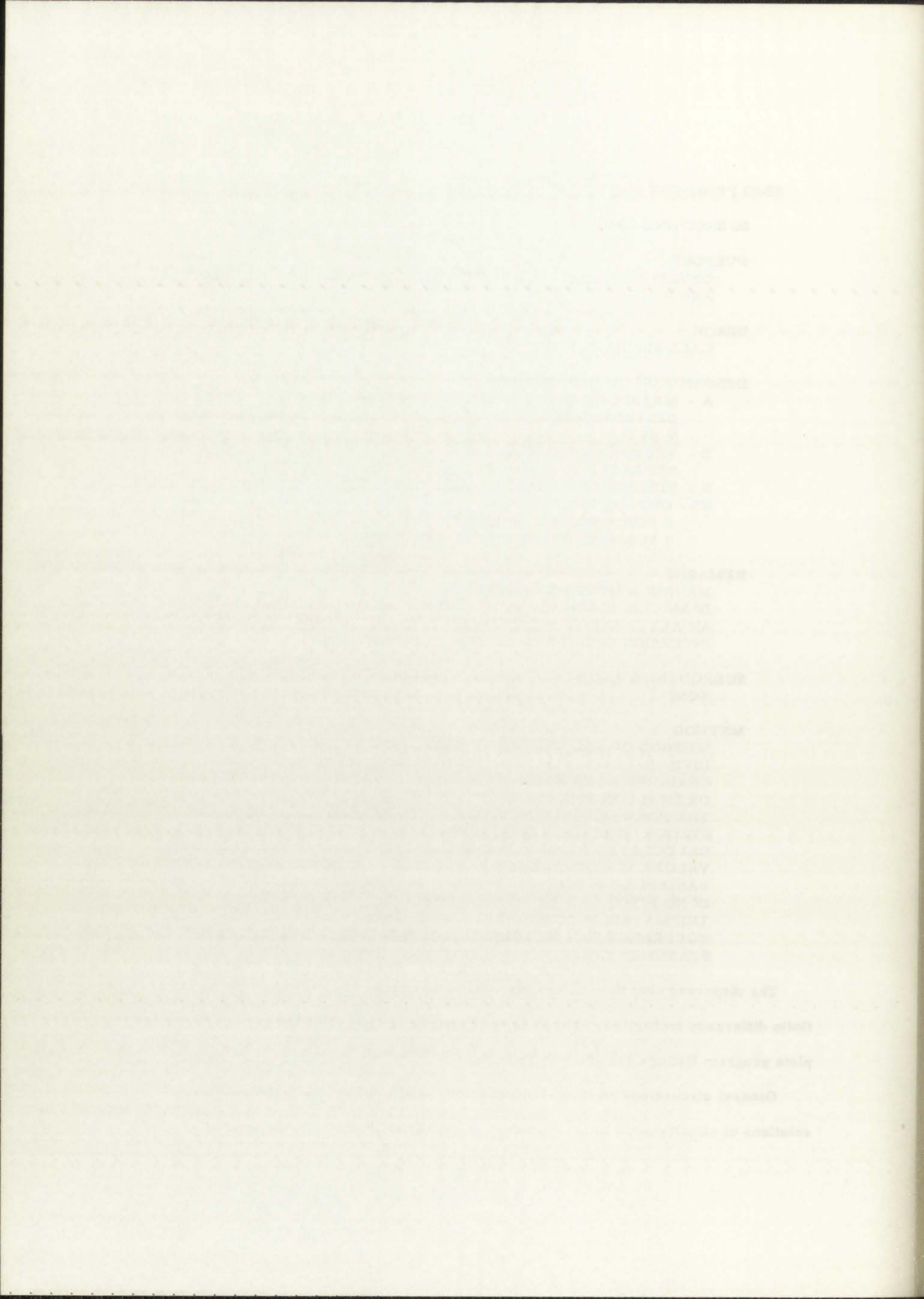
NONE

METHOD

METHOD OF SOLUTION IS BY ELIMINATION USING LARGEST PIVOTAL DIVISOR. EACH STAGE OF ELIMINATION CONSISTS OF INTERCHANGING ROWS WHEN NECESSARY TO AVOID DIVISION BY ZERO OR SMALL ELEMENTS.
 THE FORWARD SOLUTION TO OBTAIN VARIABLE N IS DONE IN N STAGES. THE BACK SOLUTION FOR THE OTHER VARIABLES IS CALCULATED BY SUCCESSIVE SUBSTITUTIONS. FINAL SOLUTION VALUES ARE DEVELOPED IN VECTOR B, WITH VARIABLE 1 IN B(1), VARIABLE 2 IN B(2),, VARIABLE N IN B(N).
 IF NO PIVOT CAN BE FOUND EXCEEDING A TOLERANCE OF 0.0, THE MATRIX IS CONSIDERED SINGULAR AND KS IS SET TO 1. THIS TOLERANCE CAN BE MODIFIED BY REPLACING THE FIRST STATEMENT.

The dispersed plug flow differential equation solutions were obtained by means of finite difference techniques. The runs were made on a CDC-7600 computer. The complete program listings are given in Appendix C.

General discussions on Rung-Kutta methods, finite difference techniques, and solutions of simultaneous linear equations may be found in Refs. 8, 14, and 21.



APPENDIX C
DISPERSED PLUG FLOW MODEL LISTINGS

```

PROGRAM DRVR(OUT,FSET6=OUT)
DIMENSION B(100)
COMMON/EPSILON/EPS, EPS2
COMMON/VARY/NA, NB, NP
EPS=2.0**(-47)
EPS2=(2.0**(-48))*(1.0-2.0**(-48))
DO 100 NA=2,2
A=3.7+FLOAT(NA-1)*.05
DO 100 NB=2,2
D=1.54+FLOAT(NB-1)*.02
DO 100 NP=2,2
P=46.+FLOAT(NP-1)*5.
WRITE(6,2000)A,D,P
CALL PROG1 (B,N)
CALL PROG2 (B,N)
100 CONTINUE
2000 FORMAT(5X,4HA = ,F6.2,6H, B = ,F6.2,6H, P = ,F6.2)
STOP
END

SUBROUTINE PROG1(B,N0)
C ** FINITE DIFFERENCE SOLUTION OF THE SECOND ORDER ODE
C   L(U) = -U**/P + U* = F ON (ALEFT,ARIGHT)
C   B(U) = 0 DIRICHLET/NEUMANN/MIXED BC
DIMENSION Q(16400), IT(4097), B(100)
COMMON /DIFEQU/ ISIDEC, XSIDEC(10), P, NMOM, JDE
COMMON /FDMESH/ ALEFT, ARIGHT, H, N
COMMON /APPROX/ U(10250), NH
COMMON /OTHER/ MODE, MXITER, MXMESH
PRINT 500
500 FORMAT(/* PROBLEM*,15X,*BY FINITE DIFFERENCES*//)
C ** WRITE THE TITLE

MODE = 1
CALL SOLU(I,X,V)
C ** SET VARIOUS PARAMETERS FOR THE ODE
10 MODE = 2
CALL SOLU(I,X,V)
C ** SOLVE THE JDE-TH EQUATION, FOR 0 .LE. JDE .LE. NMOM
JDE = 0
IJDE = 1
20 CONTINUE
C ** FROM THE FD EQUATIONS AND SIDE CONDITIONS,
C   GENERATE THE BANDED SYSTEM MATRIX IN Q AND THE RHS IN U
MODE = 3
CALL FDEQU(Q,U(IJDE))
C ** COMPUTE THE APPROXIMATE SOLUTION U BY BAND/BANS1
CALL BAND(N,1,1,Q,N,IT,DET)
IF(ABS(DET) .LE. 1.E-7) PRINT 601,JDE,DET
601 FORMAT(2X,*** FOR MOMENT EQUATION*,14,* DET **,E14.7,* ***)
CALL BANS1(N,1,1,Q,N,IT,U(IJDE))
IF(JDE .EQ. NMOM) GO TO 30
JDE = JDE + 1
IJDE = IJDE + N
GO TO 20

C ** THE SYSTEM IS SOLVED
C   OUTPUT THE MOMENTS U
30 CONTINUE
IST = NMOM + 1
IP = NMOM*N + 1
IST0=0
IST1=IST-1
PRINT 501, (I,I=IST0,IST1)
501 FORMAT (* IX *,10(* U*,12,6X))
IST=16
DO 31 I=1,N,IST

```

APPENDIX 2

EXHIBIT 1 - LIST OF DOCUMENTS

Doc No.	Description	Date
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100

```

      IQT=I-1
      PRINT 502, (IQT,(U(K),K=I,IP,N))
31   IP = IP + IST
502  FORMAT(I5,10E12.4)
      NQ = NMOM + 1
      DO 40 IFB = 1,NQ
      IFU = IFB*N
      B(IFB) = U(IFU)
40   CONTINUE
      END FD

```

```

C   ** SUBROUTINE FDFQU(Q,U)
C   ** FILL SYSTEM MATRIX Q AND RHS U
      COMMON /DIFEGU/ ISIDEC,XSIDEC(10),P,NMOM,JDE
      COMMON /FDMESH/ ALEFT,ARIGHT,H,N
      DIMENSION Q(1),U(1)
C   ** FIRST ZERO Q AND U, THEN FILL BY ROWS
      I2 = N
      I3 = I2 + N
      DO 1 I=1,N
        I2 = I2 + 1
        I3 = I3 + 1
        U(I) = 0.
        Q(I) = 0.
        Q(I2) = 0.
        Q(I3) = 0.
      1
      HH = H*H
      ISIDEC = 1
      I = 1
      I2 = I + N
      I3 = I2 + N
      X = ALEFT
C   ** DO THE I-TH ROW
C   FIRST CHECK FOR SIDE CONDITIONS
      2 IF(X .EQ. XSIDEC(ISIDEC)) GO TO 3
C   ** THIS IS NOT A SIDE CONDITION ROW
      Q(I) = -1. - 0.5*P*H
      Q(I2) = 2.
      Q(I3) = -1. + 0.5*P*H
      CALL SOLU(I,X,V)
      U(I) = HH*V
      GO TO 4
C   ** THIS IS A SIDE CONDITION ROW
      3 J = I + (2 - ISIDEC)*N
      CALL FDSID(I,Q(J),U(I))
C   ** RETURN IF ALL ROWS FILLED
      4 IF(I .EQ. N) RETURN
C   ** UPDATE FOR NEXT ROW
      X = ALEFT + FLOAT(I)*H
      I = I + 1
      I2 = I2 + 1
      I3 = I3 + 1
      GO TO 2
      END FDEQU

```

1074-1
PAINT 200, 4101, 1074, 1075, 1076
1077, 1078, 1079, 1080, 1081, 1082
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1125, 1126, 1127, 1128, 1129, 1130
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3123, 3124, 3125, 3126, 3127, 3128

```

SUBROUTINE FDSID(I,Q,U)
C ** FILL Q AND U AT THE SIDE CONDITION ROWS
COMMON /DIFFQU/ ISIDEC,XSIDEC(10),P,NMOM,JDE
COMMON /FDMESH/ ALEFT,ARIGHT,H,N
DIMENSION Q(1)
HH = H*H
GO TO (10,20,99),ISIDEC
C ** MIXED BC P*U(ALEFT) = U*(ALEFT) = U*(ARIGHT) = 0
10 X = XSIDEC(ISIDEC)
Q(1) = 1. + P*H
Q(N+1) = -1.
U = 0.
GO TO 90
20 X = XSIDEC(ISIDEC)
Q(1) = -2.
Q(N+1) = 2.
CALL SOLU(I,X,V)
U = HH*V
90 ISIDEC = ISIDEC + 1
99 RETURN.
END FDSID

SUBROUTINE SOLU(I,X,V)
COMMON/VARY/NA,NB,NC
COMMON /DIFEQU/ ISIDEC,XSIDEC(10),P,NMOM,JDE
COMMON /FDMESH/ ALEFT,ARIGHT,H,N
COMMON /APPROX/ U(10250),NH
COMMON /OTHER/ MODE,MXITER,MXMESH
GO TO (10,20,30,40),MODE
C ** WRITE OUTPUT HEADING
10 CONTINUE
P=46,+FLOAT(NP-1)*5.
NMOM = 9
NH = 64
DO 11 I=1,5
IF(FLOAT(NH) .GE. P) GO TO 12
11 NH = NH + NH
12 CONTINUE
NH = NH + NH + NH + NH
PRINT 100, NMOM,P,NH
RETURN
100 FORMAT(40H -UJ**/P + UJ# = F1 + F2*UM , 0 .LE. J .LE. 13,
. /* UJ(ALEFT) = UJ*(ALEFT)/P = 0 , UJ*(ARIGHT) = 0*,
. /** P =*,E14.8,5X,*NH =*,IS//)
C ** INITIALIZE EVERYTHING
20 CONTINUE
ALEFT = 0.
ARIGHT = 1.
XSIDEC(1) = ALEFT
XSIDEC(2) = ARIGHT
H = (ARIGHT - ALEFT)/FLOAT(NH).
N = NH + 1
RETURN
C ** PROVIDE VALUE AT X OF RHS F1 + F2*U(J-1)
30 CONTINUE
V = F1(IX,X)
IF(JDE .EQ. P) RETURN
I = (JDE - 1)*N + IX
V = V + F2(IX,X)*U(I)
RETURN
C ** PROVIDE VALUE AT X OF THE EXACT SOLUTION IF KNOWN
40 CONTINUE
V = VALUE
RETURN
END SOLU

```



```

FUNCTION F1(IX,X)
COMMON/VARY/NA,NB,NP
COMMON /DIFEQU/ ISIDEC,XSIDEC(10),P,NMOM,JDE
F1 = 0.
IF(JDE .NE. 0) RETURN
A=3.7+FLOAT(NA-1)*.05
F1 = P*(1. - X)**A
RETURN
END F1

```

```

FUNCTION F2(IX,X)
COMMON/VARY/NA,NB,NP

COMMON /DIFEQU/ ISIDEC,XSIDEC(10),P,NMOM,JDE
F2 = 0.
IF(JDE .EQ. 0) RETURN
D=1.54+FLOAT(NB-1)*.02
F2=P*FLOAT(JDE)*(1,-X)**D
RETURN
END F2

```

```

SUBROUTINE BAND(N,ML,MU,A,IA,INT,DET)
DIMENSION A(IA,1),INT(1)
DATA XND/0377777777777777/
IF(N.LT.1.OR.IA.LT.N.OR.ML.LT.0.OR.MU.LT.0) GO TO 12
IF(N.EQ.1.OR.ML.EQ.0) GO TO 9
MA = IA
LL = ML + MU + 1
NM = N - 1
DET = 1.
C ** SHIFT THE FIRST *ML* ROWS OF *A* TO THE LEFT
K = MU + 1
KJ = ML*MA
DO 3 I=1,ML
  IJ = I
  IL = I + KJ
  DO 1 J=1,K
    A(IJ) = -A(IL)
    IJ = IJ + MA
  1 IL = IL + MA
  K = K + 1
  DO 2 J=K,LL
    A(IJ) = 0.
  2 IJ = IJ + MA
  3 KJ = KJ - MA
C ** BEGIN GAUSS ELIMINATION LOOP
L = ML
KK = LL - 1
IL = KK*MA
DO 8 K=1,NM
  KP = K + 1
  IF(L.LT.N) L = L + 1

```

1. The first part of the report is devoted to a description of the experimental apparatus and the method of measurement. The results of the measurements are given in Table I.

TABLE I
 Results of the measurements

The second part of the report is devoted to a discussion of the results of the measurements. It is shown that the results are in good agreement with the theoretical predictions.

The third part of the report is devoted to a discussion of the errors in the measurements. It is shown that the errors are small and that the results are reliable.

In conclusion, it is shown that the results of the measurements are in good agreement with the theoretical predictions.

REFERENCES
 1. J. D. Jackson, "Classical Electrodynamics", Wiley, New York, 1975.

APPENDIX
 A. Theoretical predictions

B. Experimental data

```

      IF(KK.GT.N-K) KK = N - K
C  ** SEARCH FOR PIVOT ELEMENT IN COLUMN **
      I = K
      X = ABS(A(K))
      DO 4 J=KP,L
          IF(ABS(A(J)).LE.X) GO TO 4
          I = J
          X = ABS(A(J))
      4 CONTINUE
      INT(K) = I
      IF(I.EQ.K) GO TO 6
C  ** INTERCHANGE ROWS OF ** IF NECESSARY
      IJ = I
      KJ = K
      DO 5 J=1,LL
          X = A(KJ)
          A(KJ) = A(IJ)
          A(IJ) = X
          IJ = IJ + MA
          KJ = KJ + MA
      5 DET = -DET
C  ** BEGIN THE EXCHANGE STEP LOOP
      6 X = A(K)
      IF(X.EQ.0.) GO TO 11
      X = -1./X
      IK = K + MA
      KJ = K + IL
      DO 7 I=KP,L
          KJ = KJ + MA
          XX = A(I)*X
          A(KJ) = XX
          CALL ADDVEC(KK,XX,A(IK),MA,A(I+MA),MA,A(I),MA)
      7 A(I+IL) = 0.
      8 CONTINUE
C  ** END GAUSS ELIMINATION LOOP
      IF(A(N).EQ.0.) GO TO 11
      INT(N) = 0
      RETURN
C  ** IN THIS CASE ** IS UPPER TRIANGULAR
      9 DO,10 K=1,N
          IF(A(K).EQ.0.) GO TO 11
      10 INT(K) = K
      DET = 1.
      INT(N) = 0
      RETURN
C  ** MATRIX ** MAY BE SINGULAR
      11 DET = 0.
      INT(N) = K
      RETURN
C  ** ERROR IN THE SYSTEM PARAMETERS **,*ML*,*MU*
      12 DET = XND
      RETURN
END

```

1. THE BOARD OF DIRECTORS OF THE COMPANY HAS APPROVED THE
 DIVIDEND PAYMENT OF \$0.10 PER SHARE FOR THE QUARTER ENDED
 MARCH 31, 1964. THE DIVIDEND IS BEING PAID TO THE SHAREHOLDERS
 OF RECORD AS OF MARCH 15, 1964. THE CHECKS WILL BE MAILED
 TO YOU BY FIRST CLASS MAIL ON MARCH 20, 1964. IF YOU
 HAVE ANY QUESTIONS CONCERNING YOUR DIVIDEND CHECK, PLEASE
 CONTACT THE INVESTOR SERVICES DEPARTMENT AT (212) 850-0100.
 2. THE BOARD OF DIRECTORS HAS ALSO APPROVED THE
 PURCHASE OF AN ADDITIONAL \$1,000,000 OF COMMON STOCK
 UNDER THE AUTHORITY GRANTED BY THE SHAREHOLDERS AT THE
 ANNUAL MEETING HELD ON DECEMBER 15, 1963. THE PURCHASE
 WILL BE MADE FROM TIME TO TIME IN SUCH MANNER AS THE BOARD
 DEEMES APPROPRIATE. THE PURCHASES WILL BE MADE AT THE
 MARKET PRICE OR AT SUCH OTHER PRICE AS THE BOARD MAY
 DETERMINE. THE PURCHASES WILL BE MADE IN SUCH MANNER AS
 TO AVOID THE NEED FOR SECURITIES REGISTRATION UNDER THE
 SECURITIES ACT OF 1933 AND THE SECURITIES ACT OF 1934.
 3. THE BOARD OF DIRECTORS HAS ALSO APPROVED THE
 AMENDMENT TO THE CHARTER OF THE COMPANY TO BE EFFECTIVE
 AS OF MARCH 15, 1964. THE AMENDMENT IS BEING FILED
 WITH THE SECRETARY OF STATE OF THE STATE OF NEW YORK
 ON MARCH 15, 1964. A COPY OF THE AMENDMENT IS BEING
 FURNISHED TO YOU BY FIRST CLASS MAIL ON MARCH 15, 1964.
 IF YOU HAVE ANY QUESTIONS CONCERNING THE AMENDMENT,
 PLEASE CONTACT THE INVESTOR SERVICES DEPARTMENT AT
 (212) 850-0100.

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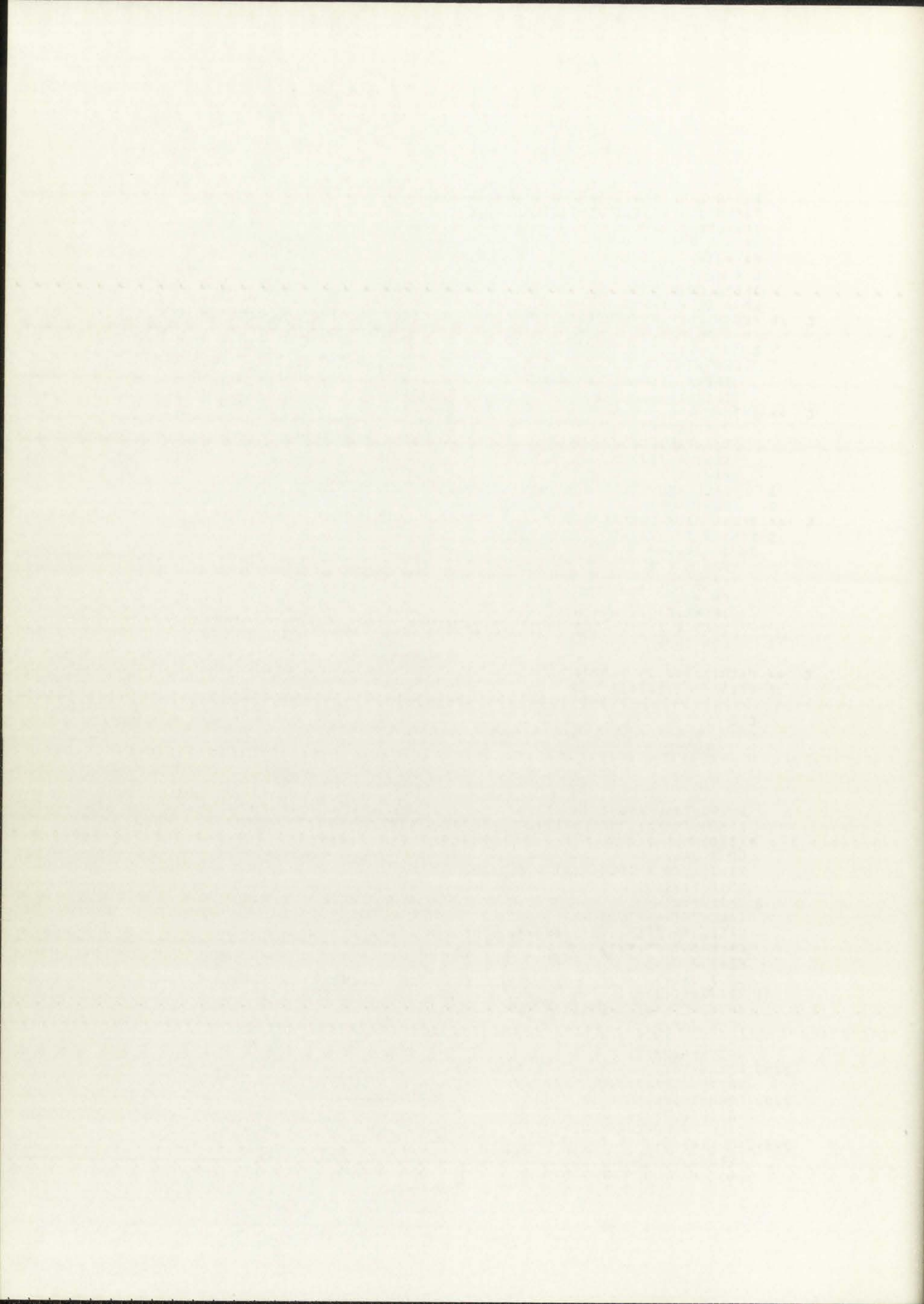
SUBROUTINE BANS1(N,ML,MU,A,IA,INT,Y)
DIMENSION A(IA,1),INT(1),Y(1)
IF(N.EQ.1) GO TO 5
NM = N - 1
MA = IA
L = ML + MU
IF(ML.EQ.0) GO TO 3
LP = (L + 1)*MA
C ** BEGIN FORWARD SUBSTITUTION LOOP FOR COMPUTING THE SOLUTION **
KK = ML
DO 2 K=1,NM
  KP = K + 1
  IF(KK.GT.N-K) KK = N - K
  IF(INT(K).EQ.K) GO TO 1
C ** INTERCHANGE ROWS OF ** JUST AS WITH **
  J = INT(K)
  X = Y(K)
  Y(K) = Y(J)
  Y(J) = X
  1 CALL ADDVEC(KK,Y(K),A(K+LP),MA,Y(KP),1,Y(KP),1)
  2 CONTINUE
C ** BEGIN BACK SUBSTITUTION
  3 Y(N) = Y(N)/A(N)
  DO 4 I=1,NM
    K = N - I
    KP = K + 1
    KK = L
    IF(KK.GT.I) KK = I
    Y(K) = (Y(K) - DOTPRO(KK,A(K+MA),MA,Y(KP),1))/A(K)
  4 CONTINUE
  RETURN
C ** MATRIX ** IS 1 BY 1
  5 Y(1) = Y(1)/A(1)
  RETURN
END

```

```

SUBROUTINE PROG2 (B,N)
DIMENSION XI(100),DXI(100),A(100),B(100),X(100),TEMP(500),WW(100),
*XSI(100)
DO 3 J=1,N
  XI(J)=.05 + (FLOAT(J) - 1.)/10.
  XSI(J)=XI(J)
  3 DXI(J)=.1
  CALL FCT(A,XI,DXI,N)
  CALL UNSLIT(N,1,A,N,B,N,X,N,TEMP,DET,IEX,L)
  CALL OUTP(N,X,1)
  F3=1.0/B(4)
  DO 1 J=1,N
  1 XI(J)=XI(J)**3
  WW(1)=F3*XI(1)*DXI(1)*X(1)
  DO 2 J=2,N
  2 WW(J)=WW(J-1)+F3*XI(J)*DXI(J)*X(J)
  WRITE(6,2005)
2005 FORMAT(5X,19HWEIGHT DISTRIBUTION)
  WRITE(6,2002)(WW(J),J=1,N)
2002 FORMAT(10X,5E14.7)
  WRITE(6,2001)
  CALL PRNPLT(XSI,WW,1.,.01,1.2,.025,0,0,N)
2001 FORMAT(1H1)
  RETURN
END

```



```

SUBROUTINE FCT(A,XI,DXI,N)
DIMENSION A(N,1),XI(N),DXI(N)
DO 10 J=1,N
T=XI(J)
A(1,J)=DXI(J)
DO 10 I=2,N
10 A(I,J)=A(I-1,J)*T
RETURN
END

```

```

SUBROUTINE OUTP(N,X,IX)
DIMENSION X(1)
NX=(N-1)*IX+1
WRITE(6,3000)(X(J),J=1,NX,IX)
3000 FORMAT(10X,5E14.7)
RETURN
END

```

```

SUBROUTINE UNSLIT(N,M,A,IA,B,IB,X,IX,SCR,DET,IEX,L)
C GIVES CORRECTLY ROUNDED SOLUTIONS OF  $A \cdot X = B$ , WHERE A IS
C UNSYMMETRIC AND H IS N BY M, PROVIDED A IS NOT TOO
C ILL-CONDITIONED. USES PROCEDURES UNSDET, UNSACC, UNSSOL,
C INRPRO. COMPUTES THE DETERMINANT OF A IN THE FORM
C  $DET * 2^{**IEX}$ . L IS THE NUMBER OF REFINEMENT STEPS.
C SCR IS WORKING STORAGE OF LENGTH AT LEAST  $N*(IA + 1) + M*IB$ .
C THE PROCEDURE FAILS, AND PRINTS ERROR MESSAGES, IF THE LU
C FACTORIZATION OF A OR THE ITERATIVE REFINEMENT OF X FAILS.
10 FORMAT(1H0,37HMATRIX HAS ZERO ROW IN UNSDET AT STEP,I4/)
11 FORMAT(1H0,43HMATRIX IS NEARLY SINGULAR IN UNSDET AT STEP,I4/)
12 FORMAT(1H0,32HNO CONVERGENCE IN UNSACC AT STEP,I4/)
DIMENSION A(IA,1),B(IB,1),X(IX,1),SCR(1)
C AA STARTS IN SCR(LA), BB IN SCR(LB), INT IN SCR(LI)
DO 1 J=1,N
K = (J - 1)*IA
DO 1 I=1,N
L = K + I
1 SCR(L) = A(I,J)
LA = 1
LB = LA + IA*N
LI = LB + IB*M
C FORM LU FACTORS
CALL UNSDET(N,SCR(LA),IA,DET,IEX,SCR(LI),SCR(LI),ILL)
IF(ILL.NE.0) GO TO 2
C ITERATIVE REFINEMENT
CALL UNSACC(N,M,A,SCR(LA),IA,B,SCR(LB),IB,X,IX,SCR(LI),L,ILL)
IF(ILL.EQ.0) RETURN
C ITERATIVE REFINEMENT FAILED
PRINT 12,ILL
RETURN
C LU FACTORIZATION FAILED
2 IF(ILL.GT.0) PRINT 11,ILL
ILL = -ILL
IF(ILL.GT.0) PRINT 10,ILL
RETURN
END

```

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SUBROUTINE INRPRO(L,C1,C2,X,IX,Y,IY,D1,D2)
C ACCUMULATES THE SUM OF PRODUCTS X(K)*Y(K) AND ADDS IT
C TO THE INITIAL VALUE C1 + C2 IN DOUBLE PRECISION.
C D1 IS THE SINGLE PRECISION VALUE OF THE DOUBLE PRECISION
C SUM D. D2 IS THE SINGLE PRECISION DIFFERENCE D - D1.
C IF THE VECTOR LENGTH L IS NOT POSITIVE, THEN D = C1 + C2,
C SPEED OF EXECUTION OF THIS ROUTINE CAN BE GREATLY INCREASED
C BY HAND CODING. WHAT IS REQUIRED IS THAT THE SUMS AND
C MULTIPLICATIONS BE PERFORMED IN DOUBLE PRECISION.
  DIMENSION X(1),Y(1)
  DOUBLE PRECISION D,DX,DY
  DX = C1
  DY = C2
  D = DX + DY
  IF (L.LE.0) GO TO 2
  I = 1
  J = 1
  DO 1 K=1,L
    DX = X(I)
    DY = Y(J)
    D = D + DX*DY
    I = I + IX
  1 J = J + IY
  2 D1 = D
  D2 = D - D1
  RETURN
END

```

```

SUBROUTINE UNSDET(N,A,IA,DET,IEX,INT,SCA,ILL)
C FORMS LU FACTORS OF A BY CROUT METHOD WITH ROW EQUILIBRATION
C AND PARTIAL PIVOTING. OVERWRITES L AND U ON A, OMITTING
C UNIT DIAGONAL OF U, AND RECORDS ROW INTERCHANGES IN INT.
C COMPUTES THE DETERMINANT OF A IN THE FORM DET * 2**IEX.
C THE PROCEDURE FAILS IF A, AS MODIFIED BY ROUNDING ERRORS, IS
C SINGULAR OR NEARLY SINGULAR. USES PROCEDURE INRPRO. EPS IS
C THE (MACHINE-DEPENDENT) LEAST NUMBER X SO THAT 1. + X .GT. 1.
  DIMENSION A(IA,1),INT(1),SCA(1)
  DATA EPS /2.0**(-47)/
  COMMON/FPSILON/EPS,EPS2
  ILL = 0
  C SCALE SO THAT SCA(I)*(A(I,)) HAS UNIT SUP NORM LENGTH
  DO 2 I=1,N
    X = 0.
    DO 1 J=1,N
  1 IF(ABS(A(I,J)).GT.X) X = ABS(A(I,J))
    IF(X) 2,11,2
  2 SCA(I) = 1./X
  DET = 1.
  IEX = 0
  DO 10 K=1,N
  C COMPUTE ENTRIES OF L IN COLUMN K
  L = K
  X = 0.
  DO 3 I=K,N
    CALL INRPRO(K-1,-A(I,K),0.,A(I,1),IA,A(1,K),1,Y,YY)
    A(I,K) = -Y
    Y = ABS(Y*SCA(I))
    IF(Y.LE.X) GO TO 3
    X = Y
    L = I
  3 CONTINUE
  IF(L.EQ.K) GO TO 5
  C INTERCHANGE ROWS IF NECESSARY, SAVING INTERCHANGE INFORMATION
  DET = -DET

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      DO 4 J=1,N
        Y = A(K,J)
        A(K,J) = A(L,J)
4      A(L,J) = Y
      SCA(L) = SCA(K)
5      INT(K) = L
C      UPDATE DETERMINANT AND CHECK FOR NEARLY SINGULAR A
      DET = DET*A(K,K)
      IF(X.LT.8.0*EPS) GO TO 12
C      A IS OK THROUGH ROW K
C      SCALE DETERMINANT TO AVOID OVERFLOW
6      IF(ABS(DET).LT.1.) GO TO 7
      DET = DET*0.0625
      IEX = IEX + 4
      GO TO 6
7      IF(ABS(DET).GE.0.0625) GO TO 8
      DET = DET*16.0
      IEX = IEX - 4
      GO TO 7
C      COMPUTE ENTRIES OF U IN ROW K
8      IF(K.EQ.N) GO TO 10
      X = -1./A(K,K)
      KP = K + 1
      DO 9 J=KP,N
        CALL INRPRO(K-1,-A(K,J),0.,A(K,1),IA,A(1,J),1,Y,YY)
9      A(K,J) = X*Y
10     CONTINUE
      RETURN
C      A IS SINGULAR
11     ILL = -I
      RETURN
C      A IS NEARLY SINGULAR
12     ILL = K
      RETURN
      END

      SUBROUTINE UNSSOL(N,M,A,IA,B,IB,INT)
C      SOLVES A*X = B WHERE A IS UNSYMMETRIC AND B IS N BY M.
C      MUST BE PRECEDED BY PROCEDURE UNSDET TO PRODUCE LU FACTORS
C      IN A WITH RECORD OF ROW INTERCHANGES IN INT. OVERWRITES
C      X ON B. USES PROCEDURE INRPRO,
      DIMENSION A(IA,1),B(IB,1),INT(1)
C      INTERCHANGE ROWS OF B
      DO 2 I=1,N
        IF(INT(I).EQ.1) GO TO 2
        J = INT(I)
        DO 1 K=1,M
          X = B(I,K)
          B(I,K) = B(J,K)
1         B(J,K) = X
2        CONTINUE
      DO 5 K=1,M
C      SOLVE L*Y = B
      DO 3 I=1,N
        CALL INRPRO(I-1,B(I,K),0.,A(I,1),IA,B(1,K),1,X,XX)
3        B(I,K) = -X/A(I,I)
C      SOLVE U*X = Y
      B(N,K) = -B(N,K)
      DO 4 II=2,N
        I = N + 1 - II
        CALL INRPRO(II-1,B(I,K),0.,A(I,I+1),IA,B(I+1,K),1,X,XX)
4        B(I,K) = -X
5      CONTINUE
      RETURN
      END

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SUBROUTINE UNSACC(N,M,A,AA,IA,B,BB,IB,X,IX,INT,L,ILL)
C SOLVES A*X = B WHERE A IS UNSYMMETRIC AND B IS N BY M,
C USING PROCEDURE UNSSOL, MUST BE PRECEDED BY PROCEDURE UNSDET
C TO PRODUCE LU FACTORS OF A IN AA WITH RECORD OF ROW
C INTERCHANGES IN INT. COMPUTES RESIDUALS BB = B - A*X USING
C PROCEDURE INRPRO, AND SOLVES A*D = BB, OVERWRITING D ON BB,
C THEN OVERWRITES THE REFINEMENT X + D ON X. REPEATS THE
C REFINEMENT SO LONG AS THE MAX CORRECTION AT ANY STEP IS LESS THAN
C HALF THAT AT THE PREVIOUS STEP, UNTIL THE MAX CORRECTION IS LESS
C THAN 2*EPS*(SUP NORM OF X). EXITS WITH ILL .NE. 0 IF THE
C SOLUTION FAILS TO IMPROVE. L IS THE NUMBER OF ITERATIONS.
C EPS IS THE (MACHINE-DEPENDENT) LEAST NUMBER T SUCH THAT
C 1. + T .GT. 1., AND EPS2 IS THE (MACHINE-DEPENDENT) GREATEST
C NUMBER T SUCH THAT 1. + T .EQ. 1.
C DIMENSION A(IA,1),AA(IA,1),B(IB,1),BB(IB,1),X(IX,1),INT(1)
C DATA EPS /2.0**(-47)/ , EPS2 /((2.0**(-48))*(1.0 + 2.0**(-48)))/
COMMON/EPSILON/EPS,EPS2
ILL = 0
C SET UP FOR FIRST APPROXIMATE SOLUTION
DO 1 J=1,M
DO 1 I=1,N
X(I,J) = 0.
1 BB(I,J) = B(I,J)
L = 0
D0 = 0.0

C COMPUTE AND ADD THE CORRECTION
2 CALL UNSSOL(N,M,AA,IA,BB,IB,INT)
L = L + 1
ID = 0
D1 = 0.0
DO 3 J=1,M
DO 3 I=1,N
3 X(I,J) = X(I,J) + BB(I,J)
C COMPUTE NEW RESIDUALS
DO 5 J=1,M
XMAX = 0.0
BBMAX = 0.0
DO 4 I=1,N
IF(ABS(X(I,J)).GT.XMAX) XMAX = ABS(X(I,J))
IF(ABS(BB(I,J)).GT.BBMAX) BBMAX = ABS(BB(I,J))
CALL INRPRO(N,-B(I,J),0.,A(I,1),IA,X(I,J),1,C,CC)
4 BB(I,J) = -C
IF(BBMAX.GT.D1*XMAX) D1 = BBMAX/XMAX
5 IF(BBMAX.GT.2.0*EPS*XMAX) ID = 1
IF(2.0*D1.GT.D0 .AND. L.NE.1) ILL = L
D0 = D1
IF(ID.EQ.1) GO TO 2
RETURN
END

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SUBROUTINE PRNPLT(X,Y,XMAX,XINCR,YMAX,YINCR,ISX,ISY,NPTS)
C PRINTER PLOT ROUTINE M.S.ITZKOWITZ MAY,1967
C
C PLOTS THE 'NPTS' POINTS GIVEN BY 'X(I),Y(I)' ON A 51 X 101 GRID
C USING A TOTAL OF 56 LINES ON THE PRINTER
C IF 'ISX' OR 'ISY' ARE NON-ZERO, THE CORRESPONDING MAXIMUM AND

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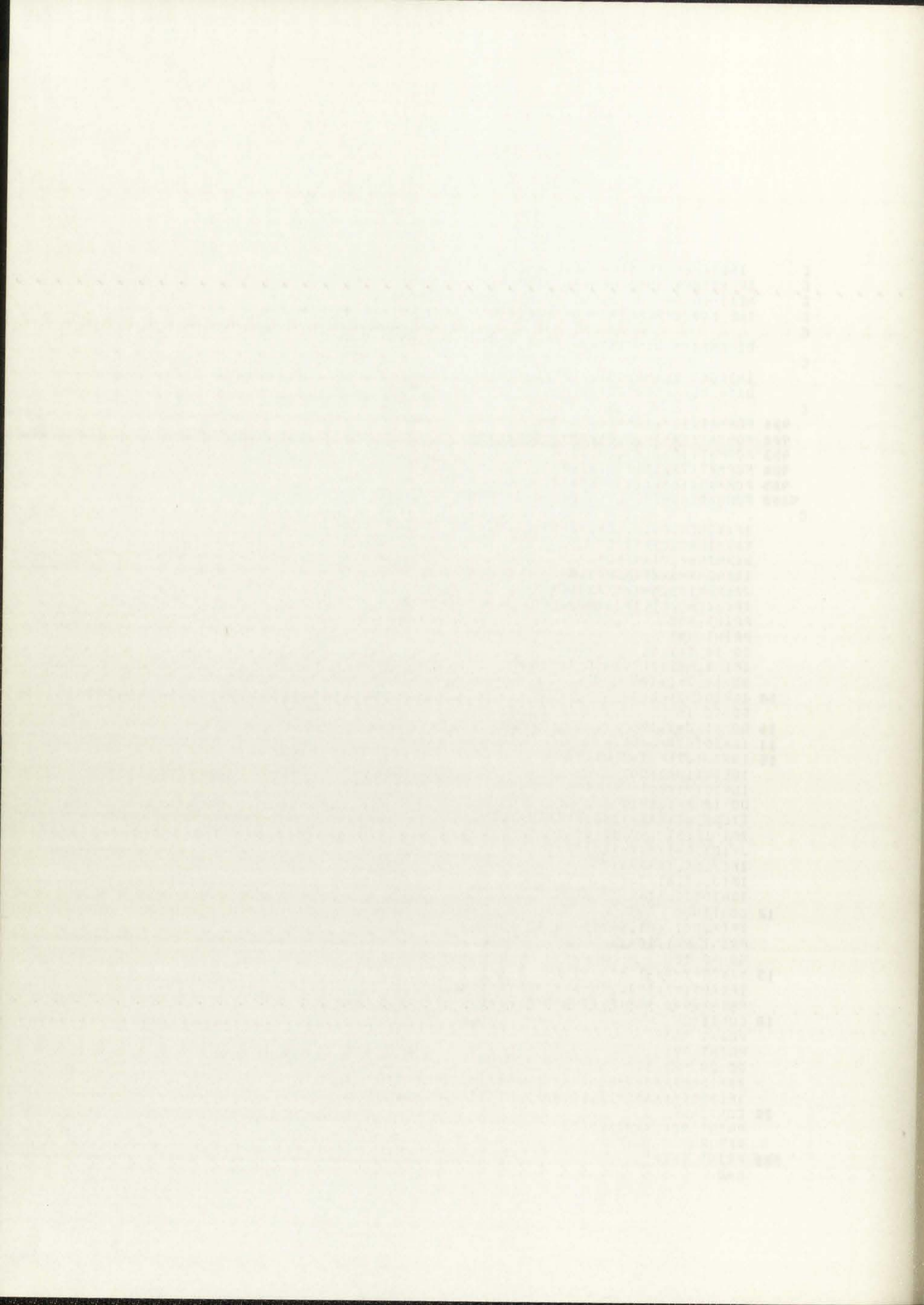
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C      INCREMENTAL STEP SIZE ARE COMPUTED
C      IF EITHER INCREMENTAL STEP SIZE IS ZERO, THE PROGRAM EXITS
C      NEITHER OF THE INPUT ARRAYS ARE DESTROYED, IF SCALING IS DONE
C      THE CORRESPONDING NEW VALUES OF MAXIMUM AND STEP SIZE ARE RETURNED
C
C      DIMENSION X(NPTS),Y(NPTS),IGRID(105),XAXIS(11)
C
C      INTEGER BLANK,DOT,STAR,IGRID,PLUS
C      DATA BLANK,DOT,STAR,PLUS / 1H ,1H,,1H*,1H+ /
C
901  FORMAT(14X,105A1)
902  FORMAT(1XE10.3,2X,1H+,105A1,1H+)
903  FORMAT(15X,103(1H,))
904  FORMAT(7X,11(F10.2),2H (,14,5H PTS) )
905  FORMAT(16X,11(1H+,9X))
9800 FORMAT(46H1SCALING ERROR IN PRNPLT, EXECUTION TERMINATED )
C
      IF(XINCR.EQ.0..OR.YINCR.EQ.0.) GO TO 800
      YAXMIN=0.01*YINCR
      XAXMIN=0.01*XINCR
      IZERO=YMAX/YINCR+1.5
      JZERO=103.5-XMAX/XINCR
      IF(JZERO.GT.103.OR.JZERO.LT.4) JZERO=2
      PRINT 905
      PRINT 903
      DO 10 I=1,51
      IF( I.NE.IZERO) GO TO 16
      DO 14 J=1,105
14  IGRID(J)=PLUS
      GO TO 15
16  DO 11 J=1,105
11  IGRID(J)=BLANK
15  IGRID(JZERO)=PLUS
      IGRID(104)=DOT
      IGRID(2)=DOT
      DO 12 K=1,NPTS
      ITEST =(YMAX-Y(K))/YINCR+1.5
      IF( ITEST .NE.I) GO TO 12
      J=103.5-(XMAX-X(K))/XINCR
      IF(J.GT.103)J=105
      IF(J.LT.3) J=1
      IGRID(J)=STAR
12  CONTINUE
      IF(MOD(I,10).EQ.1) GO TO 13
      PRINT 901,IGRID
      GO TO 10
13  YAXIS=YMAX-(I-1)*YINCR
      IF(ABS(YAXIS).LT.YAXMIN) YAXIS=0.
      PRINT 902,YAXIS,(IGRID(J),J=1,105)
10  CONTINUE
      PRINT 903
      PRINT 905
      DO 20 M=1,11
      XAXIS(M)=XMAX-XINCR*(FLOAT(11-M))*10.0
      IF(ABS(XAXIS(M)).LT.XAXMIN)XAXIS(M)=0.
20  CONTINUE
      PRINT 904,XAXIS,NPTS
      RETURN
800  PRINT 9800
      END

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Subsequent to the above, the following is a list of the items...

Location: [illegible] (see page 11 for details) - these are in the...

These items are listed below:

1. [illegible]

2. [illegible]

3. [illegible]

4. [illegible]

5. [illegible]

6. [illegible]

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23. [illegible]

24. [illegible]

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30. [illegible]

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CURRICULUM VITAE

Thomas Rivera was born on December 16, 1940 in Santa Fe, New Mexico. He graduated from St. Michaels High School in 1958 and received his B.S. in Chemistry from the College of Santa Fe in 1962. From 1962 to 1966 he was employed as an analytical chemist by The Dow Chemical Company, Rocky Flats Division, Golden, Colorado during which time he attended the University of Colorado as a part-time graduate student. He attended the New Mexico Highlands University, Las Vegas, New Mexico from 1966 to 1967 as a graduate student and also served as a Teaching Assistant in the Department of Chemistry. In 1971 he received his M.S. in Chemistry from the University of New Mexico in Albuquerque. During the time he was a graduate student at the University of New Mexico, he served as a graduate assistant for four years, and held a NASA Traineeship for one year and a University Fellowship for one year. In the summers of 1968, 1969, and 1971 he was a Summer Research Assistant at the Los Alamos Scientific Laboratory (LASL), Los Alamos, New Mexico. At the present time, he is a process engineer for the Materials Engineering Section, Group WX-3 at LASL where he began employment in August 1973. He is the author of the LASL report, LA-5313, entitled "Study to Determine the Phase Diagram of the BDNPA/F System."

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Thomas Brown was born on December 16, 1940 in Santa Fe, New Mexico. He graduated from St. Michael's High School in 1958 and transferred to the University of Colorado at Boulder in 1959. From 1958 to 1960 he was employed as an analytical chemist by the Dow Chemical Company, Rocky State District, Golden, Colorado. During which time he attended the University of Colorado as a part-time graduate student. He attended the New Mexico Institute of Mining and Technology, Las Vegas, New Mexico from 1960 to 1961 as a graduate student and also served as a Teaching Assistant in the Department of Chemistry. In 1961 he received the M.S. in Chemistry from the University of New Mexico in Albuquerque. During the time he was a graduate student at the University of New Mexico, he served as a graduate assistant for four years, and held a NASA Fellowship for one year and a University Fellowship for one year. In the summer of 1962, 1963, and 1964 he was a Summer Research Assistant at the Los Alamos Scientific Laboratory (LASL), Los Alamos, New Mexico. At the present time, he is a process engineer for the Materials Engineering Section, Group W-5 at LASL where he began employment in August 1973. He is the author of the LASL report LA-3333, "Study to Determine the Feasibility of the BENTON System".

