RECORDS ADMINISTRATION
R0061034

DP-MS-87-148

STATISTICAL ESTIMATION OF PROCESS HOLDUP

by

S. P. Harris

E. I. du Pont de Nemours and Company
Savannah River Laboratory
Aiken, SC 29808

SRL
RECORD COPY

A paper proposed for presentation at the
INMM Workshop on Process Holdup
Rockville, MD
March 2-4, 1988

This paper was prepared in connection with work done under Contract No. DE-AC09-76SR00001 with the U.S. Department of Energy. By acceptance of this paper, the publisher and/or recipient acknowledges the U.S. Government's right to retain a nonexclusive, royalty-free license in and to any copyright covering this paper, along with the right to reproduce and to authorize others to reproduce all or part of the copyrighted paper.

DP-MS-87-148

STATISTICAL ESTIMATION of PROCESS HOLDUP

S.P. Harris, Jr.

Savannah River Laboratory

Aiken, S.C.

SUMMARY

Estimates of potential process holdup and their random and systematic error variances are derived to improve the inventory difference(ID) estimate and its associated measure of uncertainty for a new process at the Savannah River Plant.

Since the process is in a start-up phase, data have not yet accumulated for statistical modelling. Therefore, early on, we were faced with an interesting problem: to develop statistical holdup models with no data available from the process.

The material produced in the facility will be a very pure, highly enriched 235U with very small isotopic variability. Therefore, data published in LANL's unclassified report on Estimation Methods for Process Holdup of Special Nuclear Materials(NUREG/CR - 3678) was used as a starting point for the modelling process.

LANL's data were gathered through a series of designed measurements of special nuclear material(SNM) holdup at two

of their materials - processing facilities. Also, they had taken steps to improve the quality of data through controlled, larger scale, experiments outside of LANL at highly enriched uranium processing facilities. The data they have accumulated are on an equipment component basis. For example, holdup estimates for different levels of throughput are available for air filters, dissolvers, pumps, pipes, elbows, etc.

Our modelling has been restricted to the wet chemistry area. We have developed predictive models for each of our process components based on the LANL data. These models are typically non-linear functions of throughput(e.g., negative exponential growth curves). The SAS - PROC NLIN software was used to fit the models to the data using non-linear least squares. Additionally, an asymptotic variance-covariance matrix for the parameters results which is used for estimating predictive accuracy through propagation of error methods.

In many cases, the LANL components were not of the same dimensions as in our facility. Therefore, a constant multiplicative factor, based on engineering diagrams, is used to correct for equivalent surface area.

The models are currently fully developed on a unit process area(UPA) basis, at least as far as possible without our own process specific data. To start, we have counted the total

number of components, lengths of pipe, etc., and determined recirculation factors for SNM initially input into the UPA. For each component - recirculation factor model, projections are generated and summed to estimate total UPA holdup. To calculate the variance, all like components are first summed. Independence is assumed between the different components. However, different recirculation factors for the same component type yield correlated estimates. The variance for these components is estimated by error propagation.

Conceptually, a facility estimate of holdup is not much more difficult to obtain. However, estimating the facility holdup variance poses a much more difficult problem. This arises because of a cascade effect of holdup among the UPAs. Specifically, the SNM hold-up in a UPA is not passed to the next UPA in a continuous production process.

Work is continuing to assess ways of determining model adequacy and total facility holdup error propagation.

The information contained in this article was developed during the course of work under Contract No. DE-AC09-76SR00001 with the U.S. Department of Energy.

Statistical Estimation of Process Holdup

S. P. Harris
Savannah River Laboratory
Aiken, S. C.

M802117

Summary

1. Overview

2. Caveats

3. LANL Data
   a. Aquacol
   b. Horizontal Duct
      Predictive Equation
      Random and Systematic Variance

4. Exponential Growth Curves (EGC)

5. Nonlinear Least Squares

M802118

Summary (Contd)

6. Propagation of Errors for EGC

7. LANL Data
   a. Aquacol
   b. Pump
   c. Tees & Unions

8. Adjustments to Models

9. UPA Example
   a. Aquacol Total Holdup
   b. Aquacol Error Variances
   c. Total UPA Estimates

1. Overview

a. Develop holdup models for each process component based on LANL data.

b. Adjust the models to correspond with SRP components.

c. Determine UPA makeup of components.

d. Use holdup models for forecasts as a function of throughput.

e. Propagate the errors for each UPA for sigma limits.

M802120

2. Caveats

a. Systematic errors are present in the LANL data due to the same NDA devices and calibration curves.

b. Be aware of LANL's throughput range when forecasting.

c. Our example is based on part of a liquid system.

d. Throughput assumed to be known.

e. Recirculation factors assumed to be constant.

2. Caveats (Contd)

f. Multiplicative factors were used to adjust for equivalent surface areas.

g. No process data are yet available for model validation.

h. Data for updating the models are not likely to be developed for some time.

i. A cascade effect among UPA's presents a problem for calculating MBA estimates.

j. The MBA estimates as a function of throughput seem intractable. However, steady state estimates are easily obtained.

NUREG/CR-3678

Estimation Methods for Process Holdup of Special Nuclear Materials

K. K. S. Pillay
R. R. Picard
R. S. Marshall

Los Alamos

Los Alamos National Laboratory
Los Alamos, New Mexico 87547

M802123

3.a.

Table C-XXII. Holdup of Uranium in the Dissolver Vessel

Throughput (kg of U)	Holdup (g of U)	Error (g of U)[a]	Throughput (kg of U)	Holdup (g of U)	Error (g of U)[a]
1	0.31	0.01	27	0.71	0.01
2	0.66	0.01	28	0.80	0.01
3	1.32	0.01	29	0.96	0.01
4	0.92	0.01	30	0.58	0.01
5	0.81	0.01	31	1.13	0.02
6	0.84	0.01	32	0.80	0.01
7	1.62	0.01	33	0.77	0.02
8	0.88	0.01	34	0.80	0.02
9	0.92	0.01	35	0.65	0.02
10	0.73	0.01	36	0.62	0.02

3.b. Horizontal Duct

$$Y = (A + B F) X + \varepsilon$$

where Y = Holdup (mg/cm^2)

F = Air Flow Rate

X = Throughput (KG)

ε = Random error

M802125

3.c. Least Squares Results

$a = 0.003286$

$b = 0.006184 / 10^2$

$\text{std err}(a) = \sigma(a) = 0.047414 / 10^2$

$\text{std err}(b) = \sigma(b) = 0.0008075 / 10^2$

$\text{Corr}(a,b) = -0.7656$

$\text{Var_rnd} = 0.023744 / 10^2$

M802126

Predictive Model

$$y = (a + b\,F)\,x$$

$$\text{Var_sys} = x^2 \{ \text{Var}(a) + F^2\,\text{Var}(b) + 2F\,\text{Cov}(a,b) \}$$

where $\text{Var}(a) = [\,\sigma(a)\,]^2$

$\text{Var}(b) = [\,\sigma(b)\,]^2$

$\text{Cov}(a,b) = \sigma(a)\;\sigma(b)\;\text{Corr}(a,b)$

M802127

Define: Ratio = (Var_sys) / (Var_rnd)

<u>For F = 45</u>

$$\text{Var_sys} = 0.0930387\ x^2\ /\ 1000^2$$

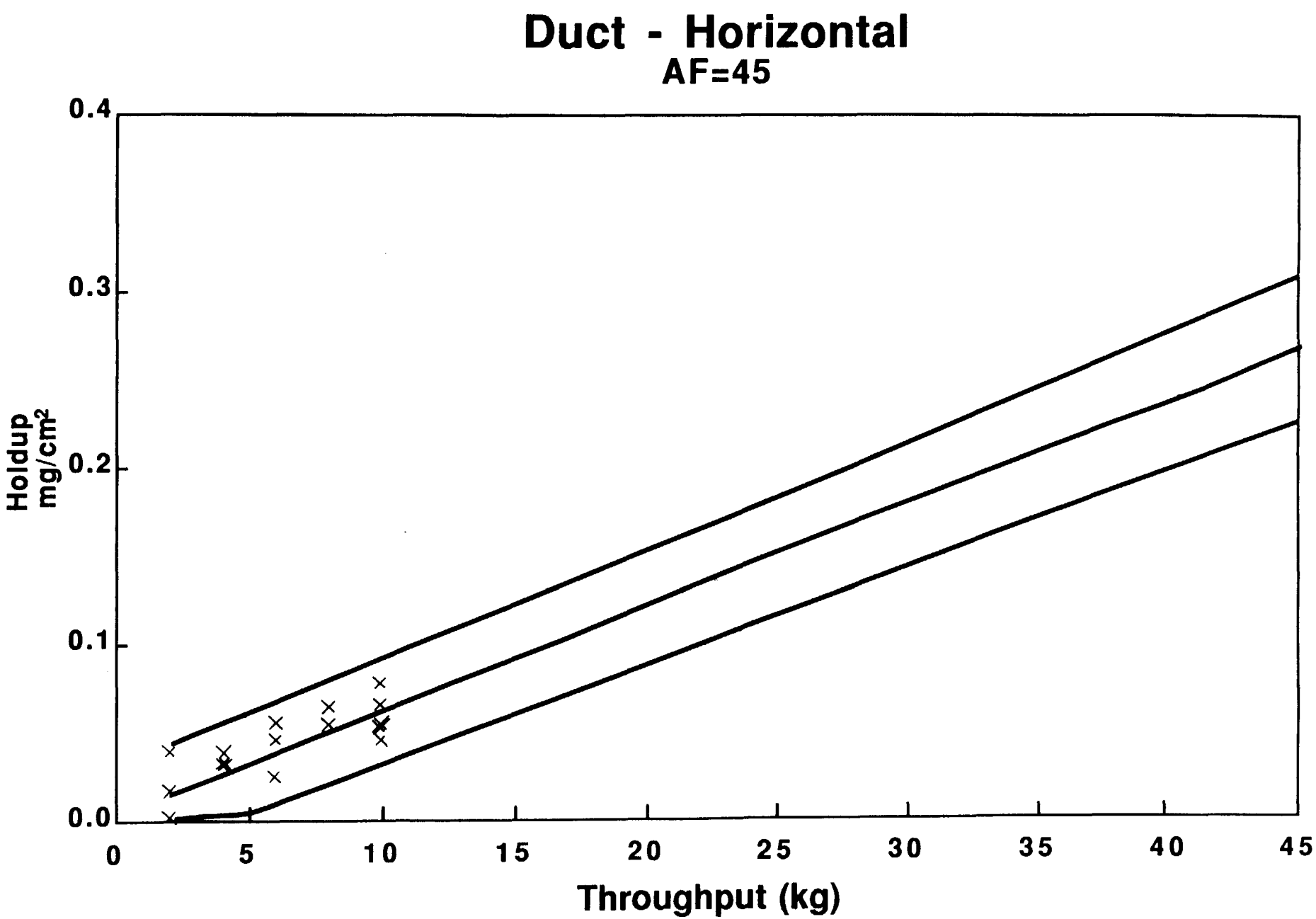
$$\text{Ratio} = 0.0391841\ x^2\ /\ 10^2$$

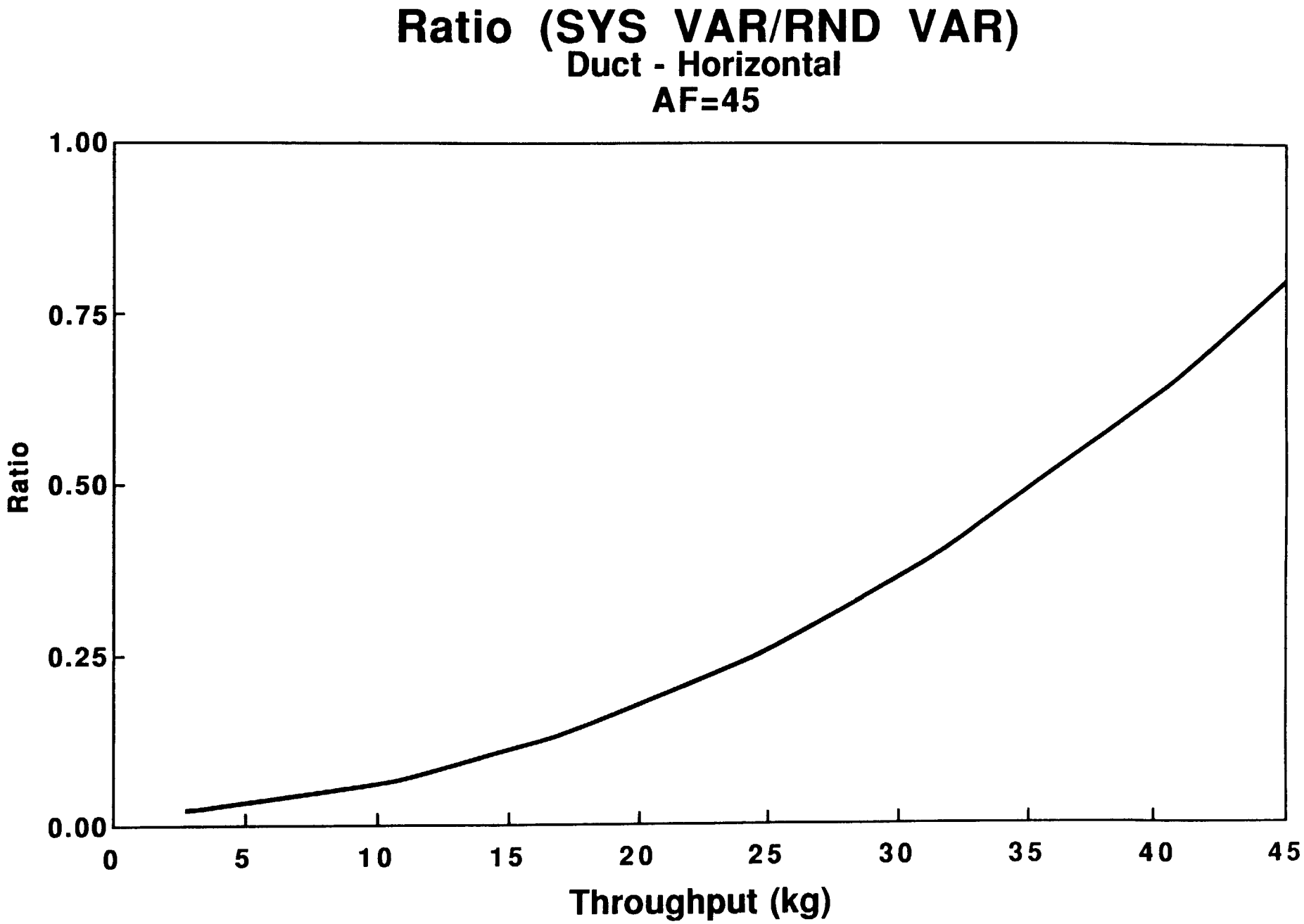
<u>For F = 100</u>

$$\text{Var_sys} = 0.2906170\ x^2\ /\ 1000^2$$

$$\text{Ratio} = 0.1223960\ x^2\ /\ 10^2$$

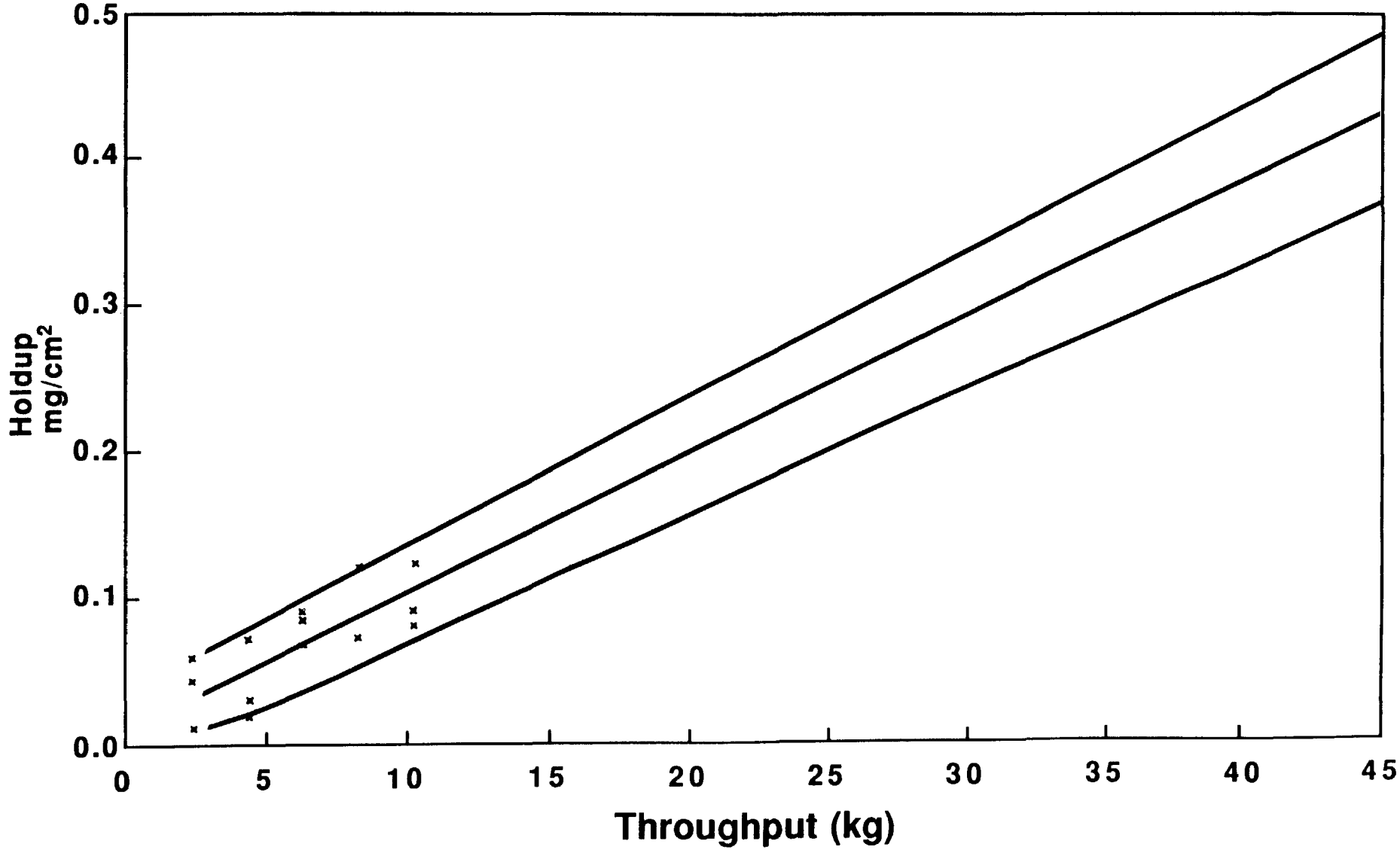
M802128

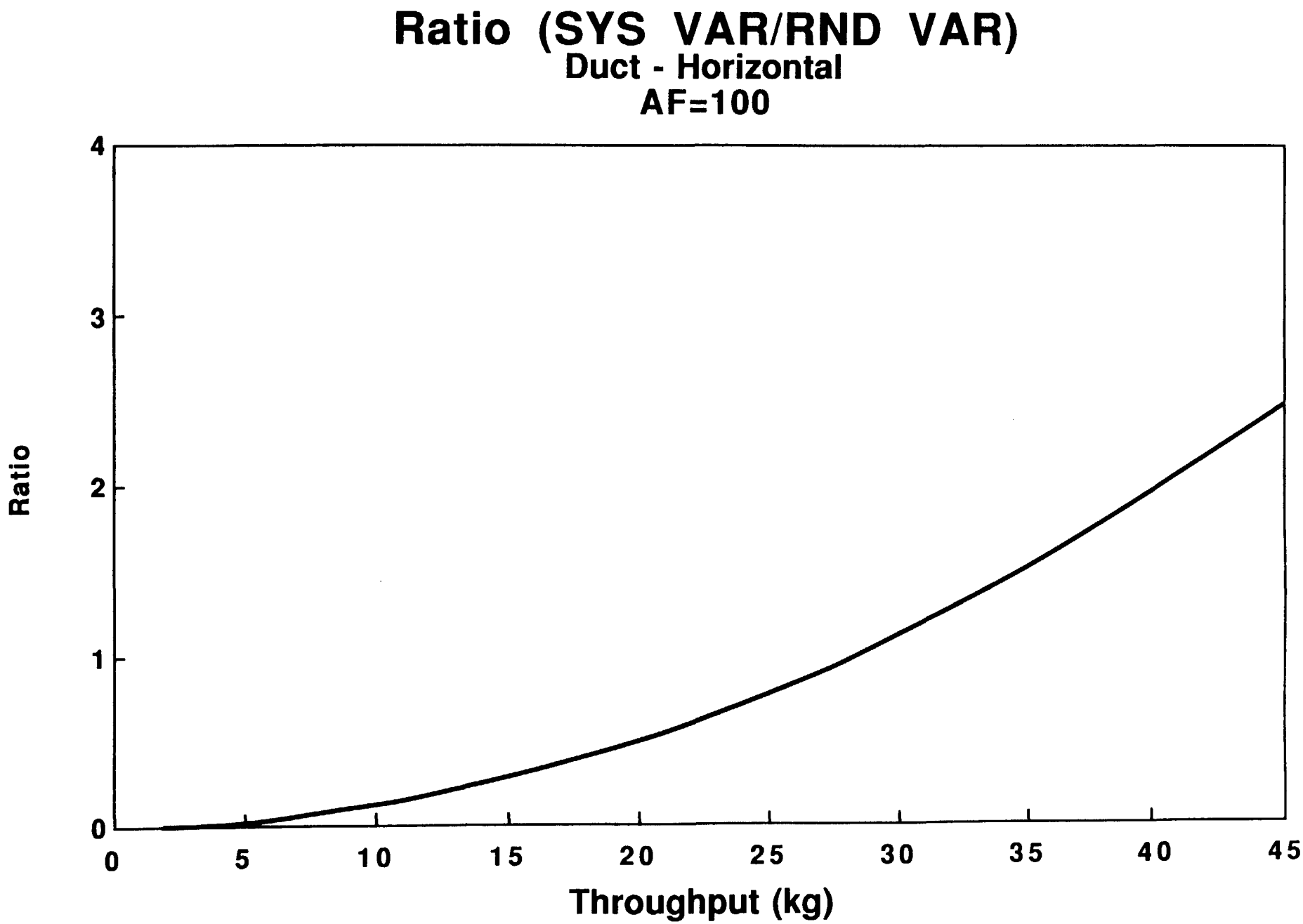

Duct - Horizontal
AF=45
Holdup
mg/cm²
0.4
0.3
0.2
0.1
0.0
0
5
10
15
20
25
30
35
40
45
Throughput (kg)


Ratio (SYS VAR/RND VAR)
Duct - Horizontal
AF=45
1.00
0.75
0.50
0.25
0.00
Ratio
0
5
10
15
20
25
30
35
40
45
Throughput (kg)

Duct - Horizontal

AF=100




Ratio (SYS VAR/RND VAR)
Duct - Horizontal
AF=100
Ratio
0
1
2
3
4
0
5
10
15
20
25
30
35
40
45
Throughput (kg)

4. Exponential Growth Curves

(EGC)

$$Y = A\ (1 - e^{-BX}) + \varepsilon$$

where A & B are constants and

$A > 0,\ B > 0$

Y = Holdup

X = Throughput

ε = Random error

M802129

EGC Component Models:

$$Y = A\,(1 - e^{-BX}) + \varepsilon$$

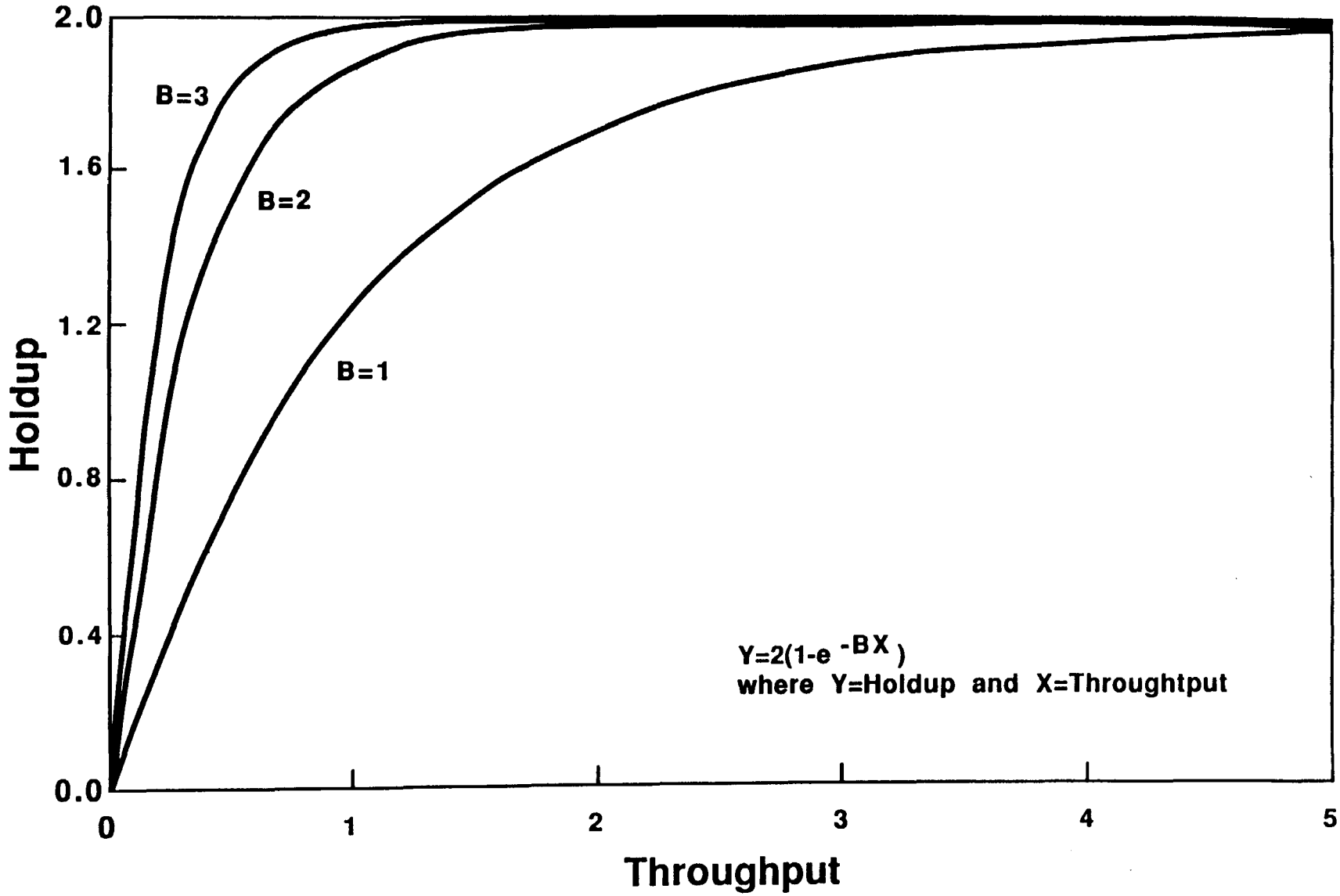
- Aquacol
- Orgacol
- Furnace
- Filters
- Pump
- Pipe, Tees and Unions, Elbows, Valves:

$$A = (C_1 D + C_2 D^2)$$

where C_1 and C_2 are constants and D is pipe diameter.

M802130

EG Curves


2.0
1.6
1.2
0.8
0.4
0.0
Holdup
B=3
B=2
B=1
Y=2(1-e -BX)
where Y=Holdup and X=Throughtput
0
1
2
3
4
5
Throughput

5. Nonlinear Least Squares:

Sum of Squares

$$SS(A,B) = \sum_{i=1}^{N} [\, Y_i - A\,(1 - \exp(-BX_i))\,]^2$$

Estimates of

- A & B
- Var (a) & Var (b)
- Cov (a,b)
- Random Variance

SAS PROC NLIN

Marquardt's Method

(SIAM 1963)

M802131

Aquacol

Nonlinear Least Squares Summary Statistics — Dependent Variable Y

Source	DF	Sum of Squares	Mean Square
Regression	2	26.009213898	13.004606949
Residual	44	0.632086102	0.014365593
Uncorrected Total	46	26.641300000	
(Corrected Total)	45	0.811280435	

M802132A

Aquacol (Contd)

Parameter	Estimate	Asymptotic Std. Error	Asymptotic 95% Confidence Interval Lower	Upper
A	0.7614362	0.01828530	0.72458472	0.7982877
B	834.0999957	268.51745785	292.94050366	1375.2594877

M802132B

Asymptotic Correlation Matrix of the Parameters

CORR	A	B
A	1.0000	-0.2055
B	-0.2055	1.0000

M802124

6. Propagation of Errors

$$x = \phi(x_1, x_2, \ldots, x_n)$$

$$\mu_x \approx \phi(\mu_1, \ldots, \mu_n)$$

$$\sigma_x^2 \approx \left(\frac{\partial \phi}{\partial x_1}\right)^2 \sigma_1^2 + \left(\frac{\partial \phi}{\partial x_2}\right)^2 \sigma_2^2 + \ldots + \left(\frac{\partial \phi}{\partial x_n}\right)^2 \sigma_n^2$$

$$+ 2\left(\frac{\partial \phi}{\partial x_1}\right)\left(\frac{\partial \phi}{\partial x_2}\right)\sigma_{12} + \ldots + 2\left(\frac{\partial \phi}{\partial x_1}\right)\left(\frac{\partial \phi}{\partial x_n}\right)\sigma_{1n}$$

$$+ \ldots +$$

$$\vdots$$

$$2\left(\frac{\partial \phi}{\partial x_{n-1}}\right)\left(\frac{\partial \phi}{\partial x_n}\right)\sigma_{n-1,n}$$

EGC Variance Estimates

Random Variance

$$Var_rnd = SS(a,b) / (N-2)$$

Systematic Variance

"Propagation of errors"

$$Var_sys = Var(y) \text{ where}$$

$y = a(1 - e^{-bx})$ and a and b are random

M802133

$$DER_a = (1 - e^{-bx})$$

$$DER_b = a \times e^{-bx}$$

$$Var(y) \approx (1 - e^{-bx})^2 \; Var(a)$$

$$+ (a \times e^{-bx})^2 \; Var(b)$$

$$+ 2 \, (1 - e^{-bx}) \; a \times e^{-bx} \; Cov(a,b)$$

At equilibrium: $y \approx a$

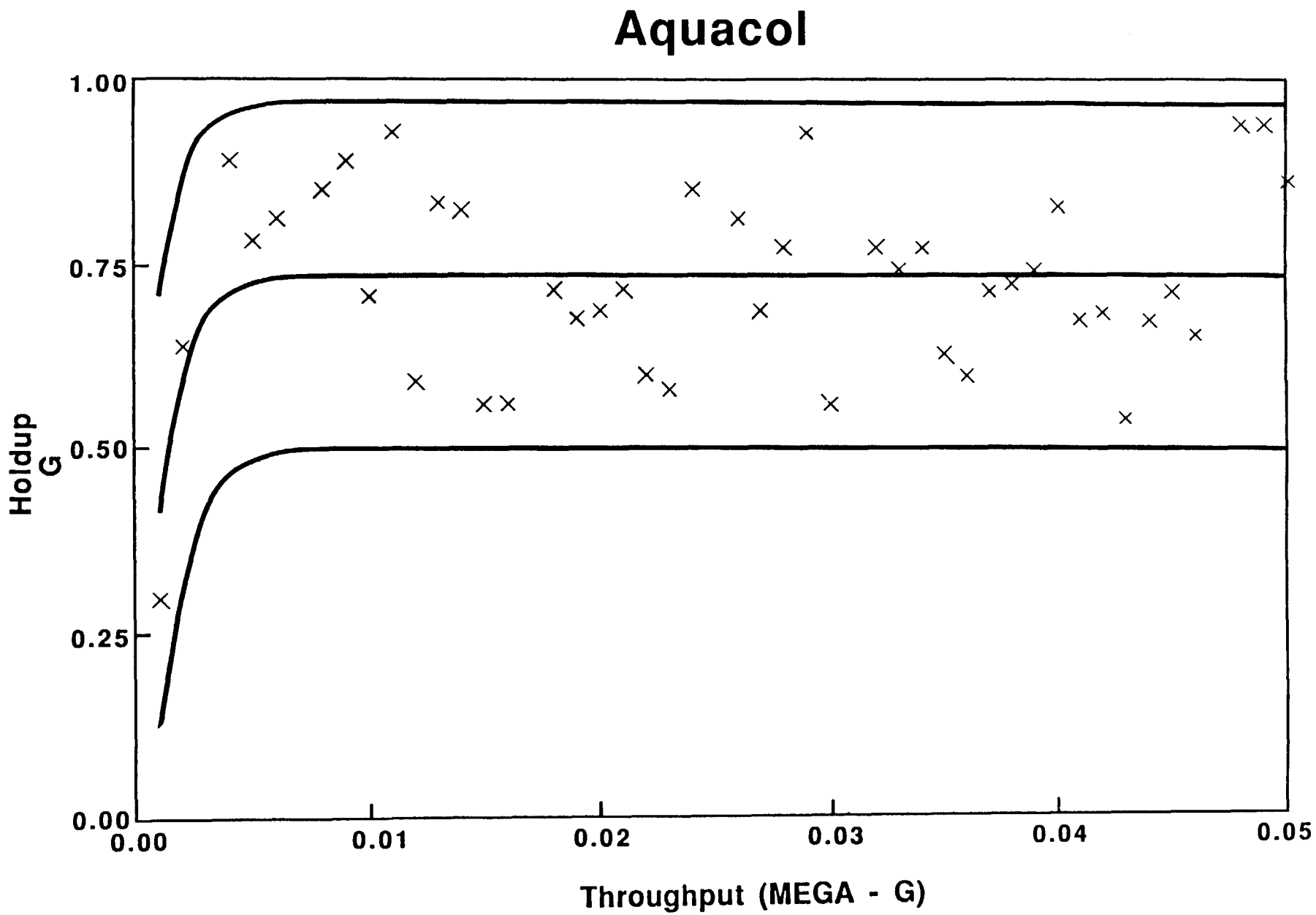
$$Var_sys \approx Var(a)$$

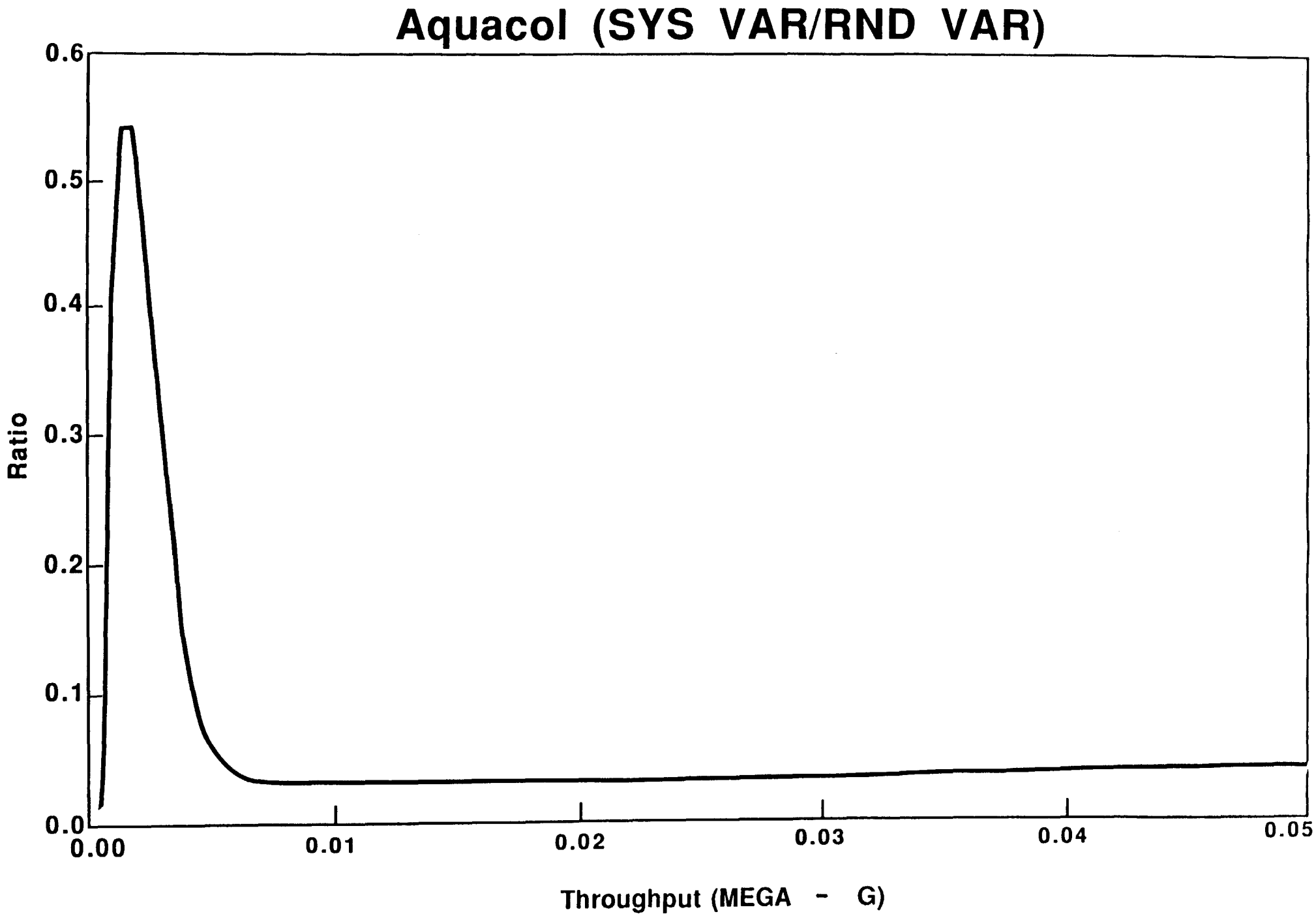
Prediction Variance

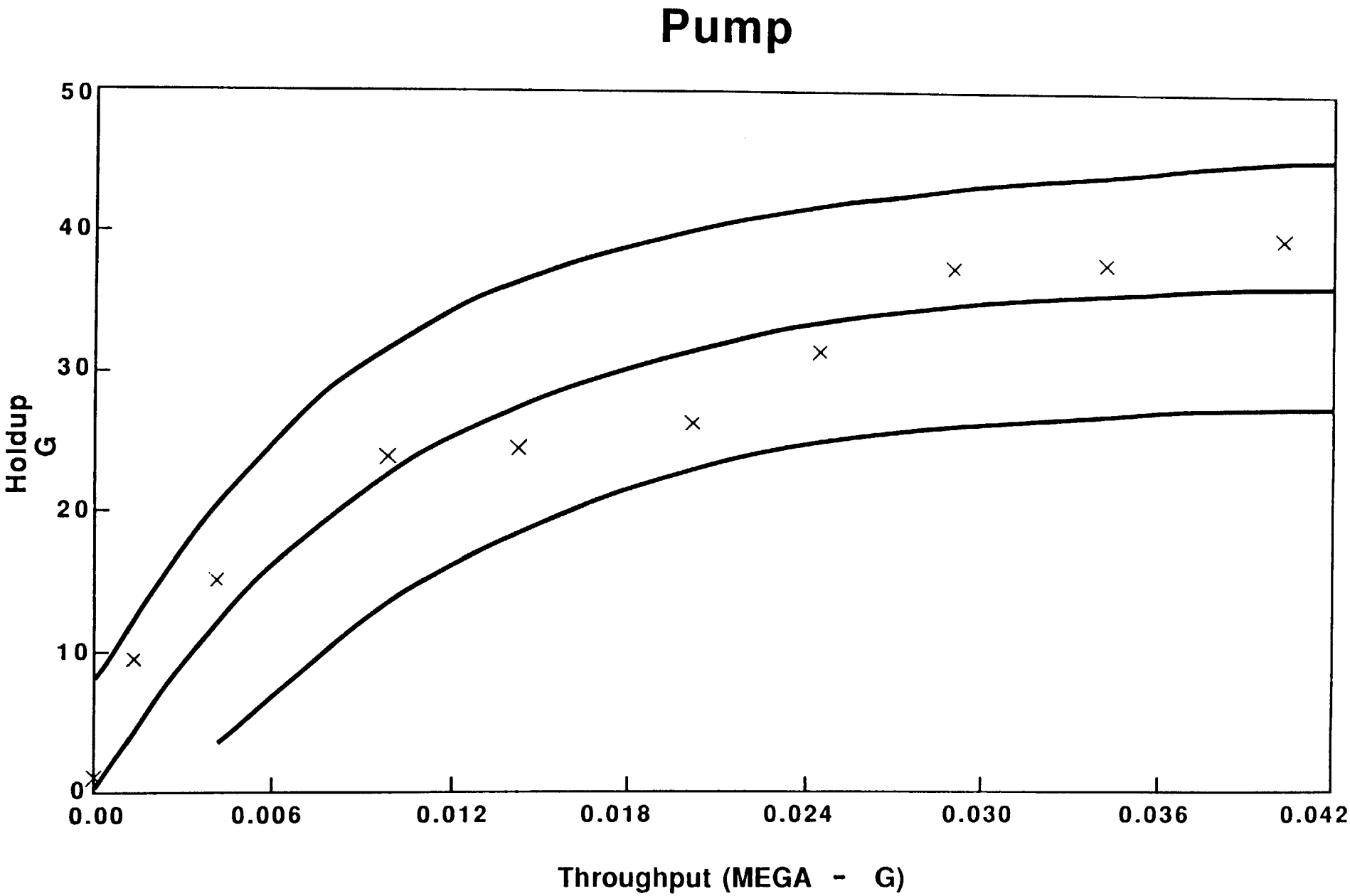
$$Var_prd = Var_sys + Var_rnd$$

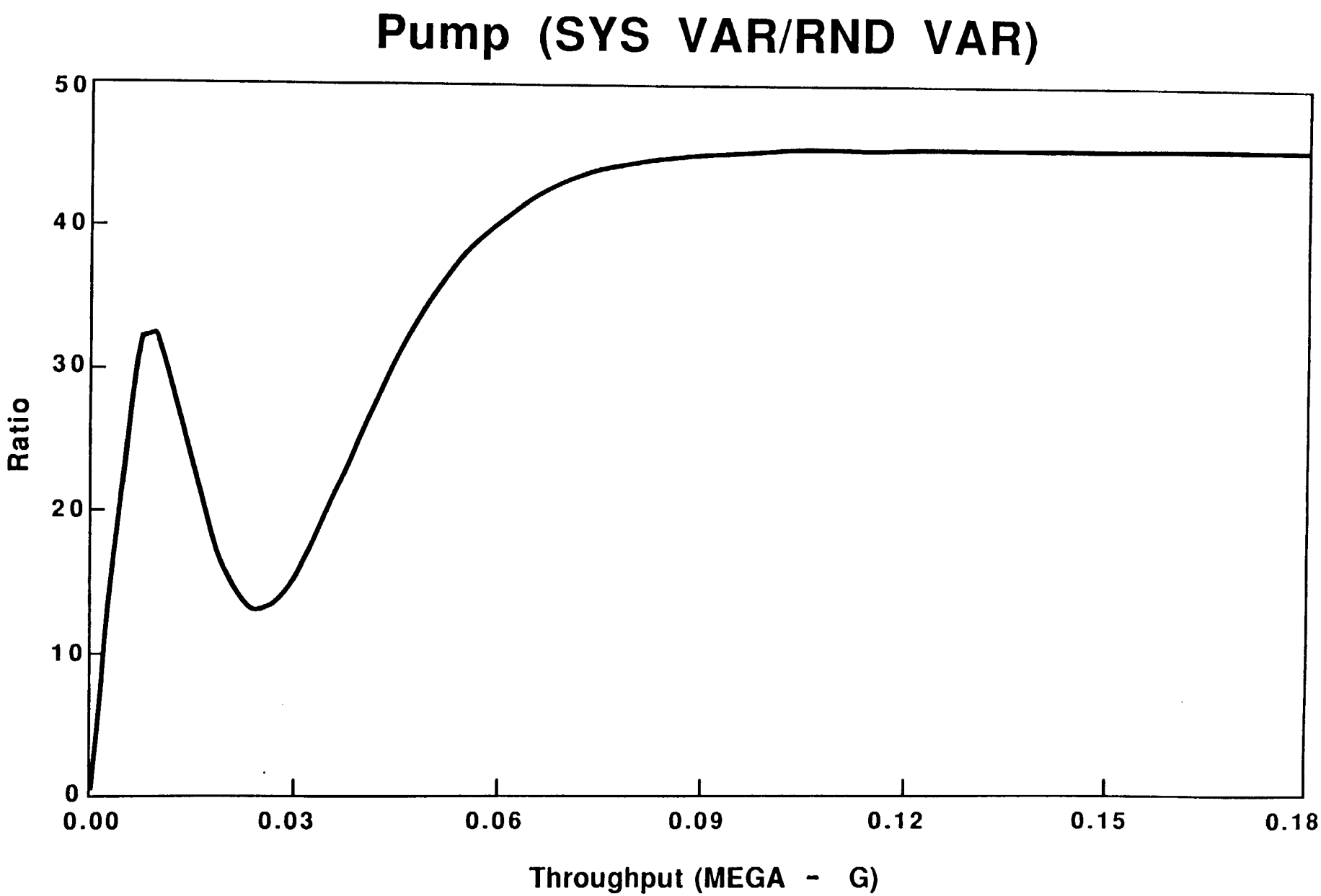
M802134

7.


Aquacol
1.00
0.75
0.50
0.25
0.00
Holdup
G
0.00
0.01
0.02
0.03
0.04
0.05
Throughput (MEGA - G)

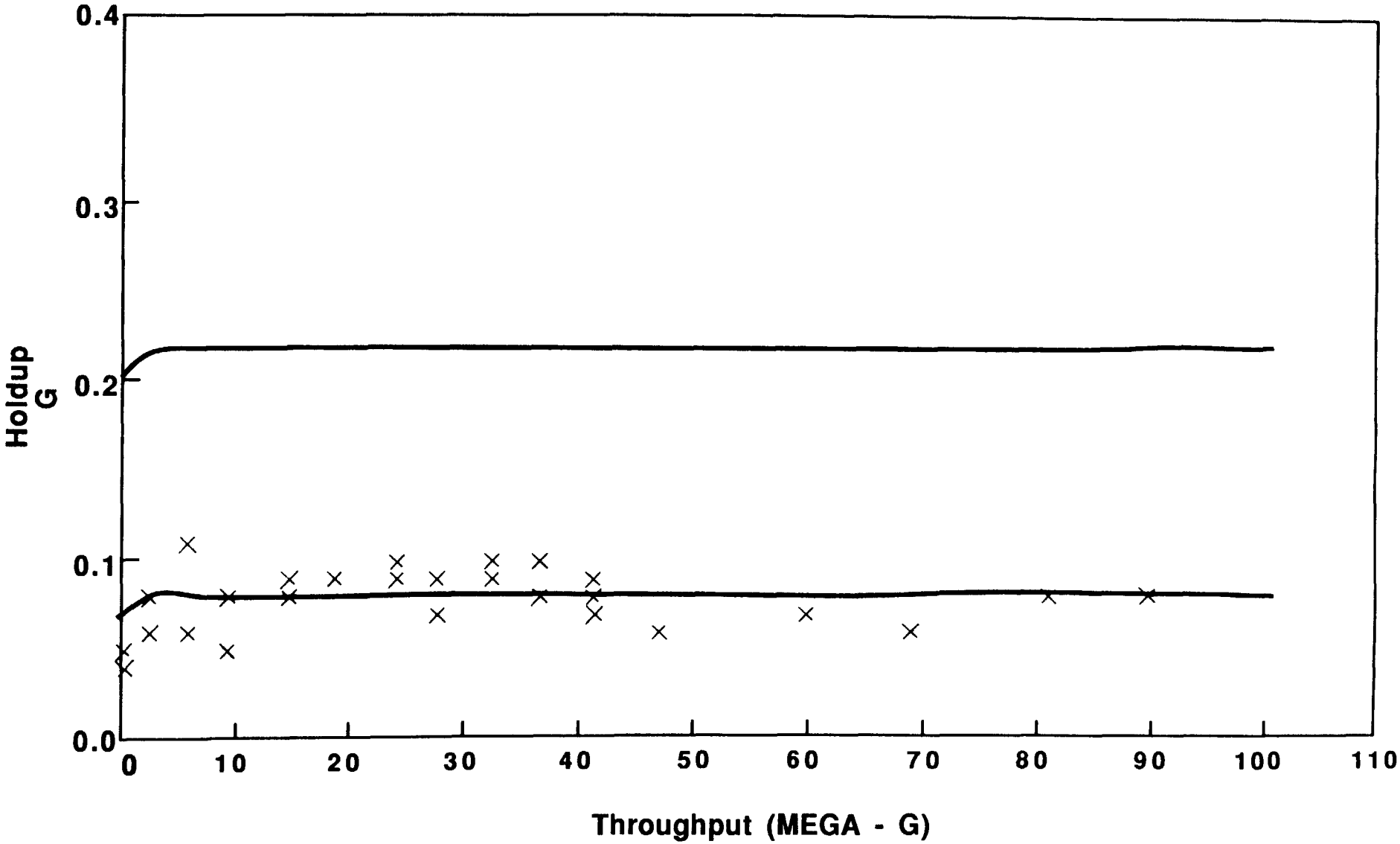

Aquacol (SYS VAR/RND VAR)
Ratio
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.00
0.01
0.02
0.03
0.04
0.05
Throughput (MEGA - G)


Pump
Holdup
G
50
40
30
20
10
0
0.00
0.006
0.012
0.018
0.024
0.030
0.036
0.042
Throughput (MEGA - G)


Pump (SYS VAR/RND VAR)
Ratio
50
40
30
20
10
0
0.00
0.03
0.06
0.09
0.12
0.15
0.18
Throughput (MEGA - G)

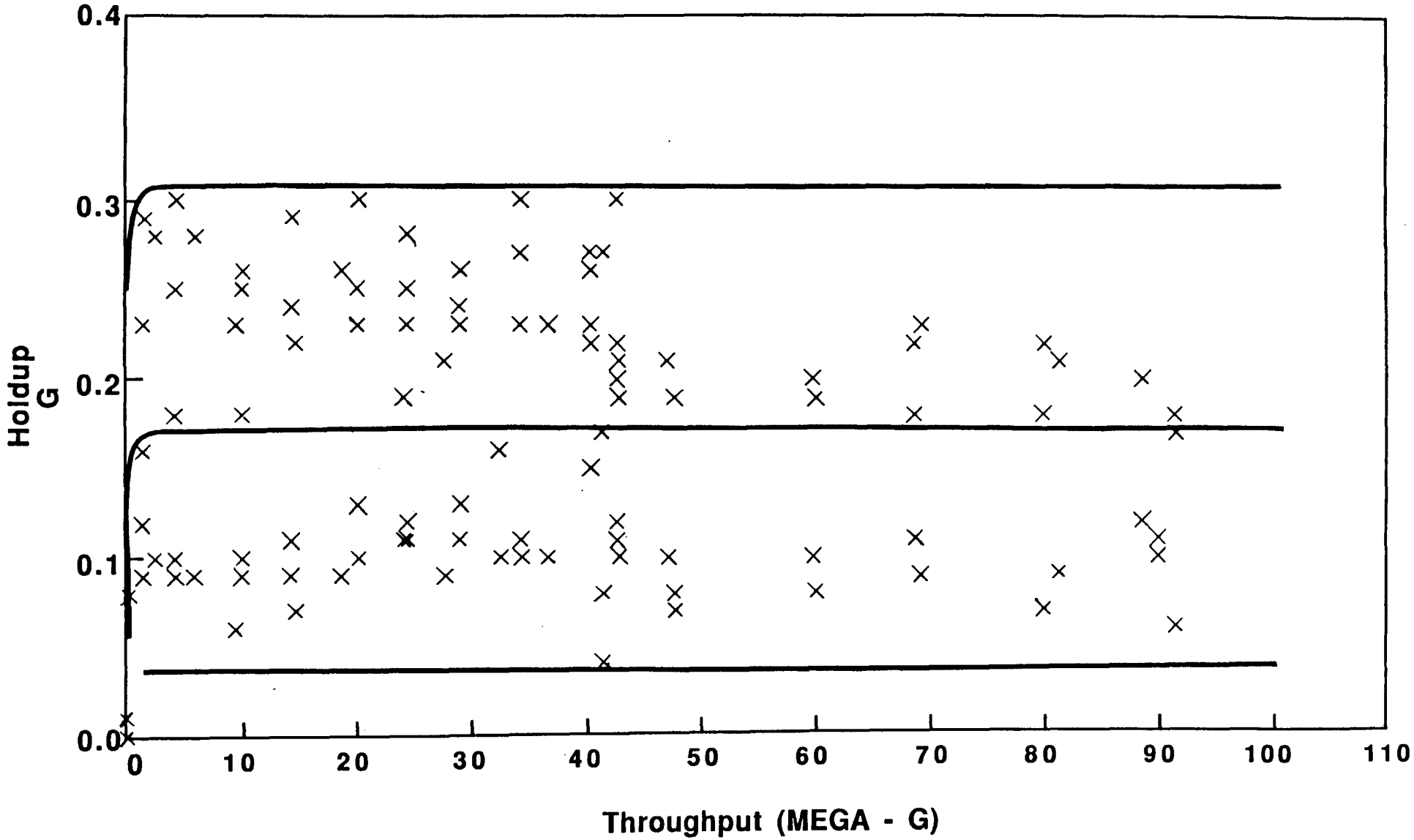
Line - Tee Union

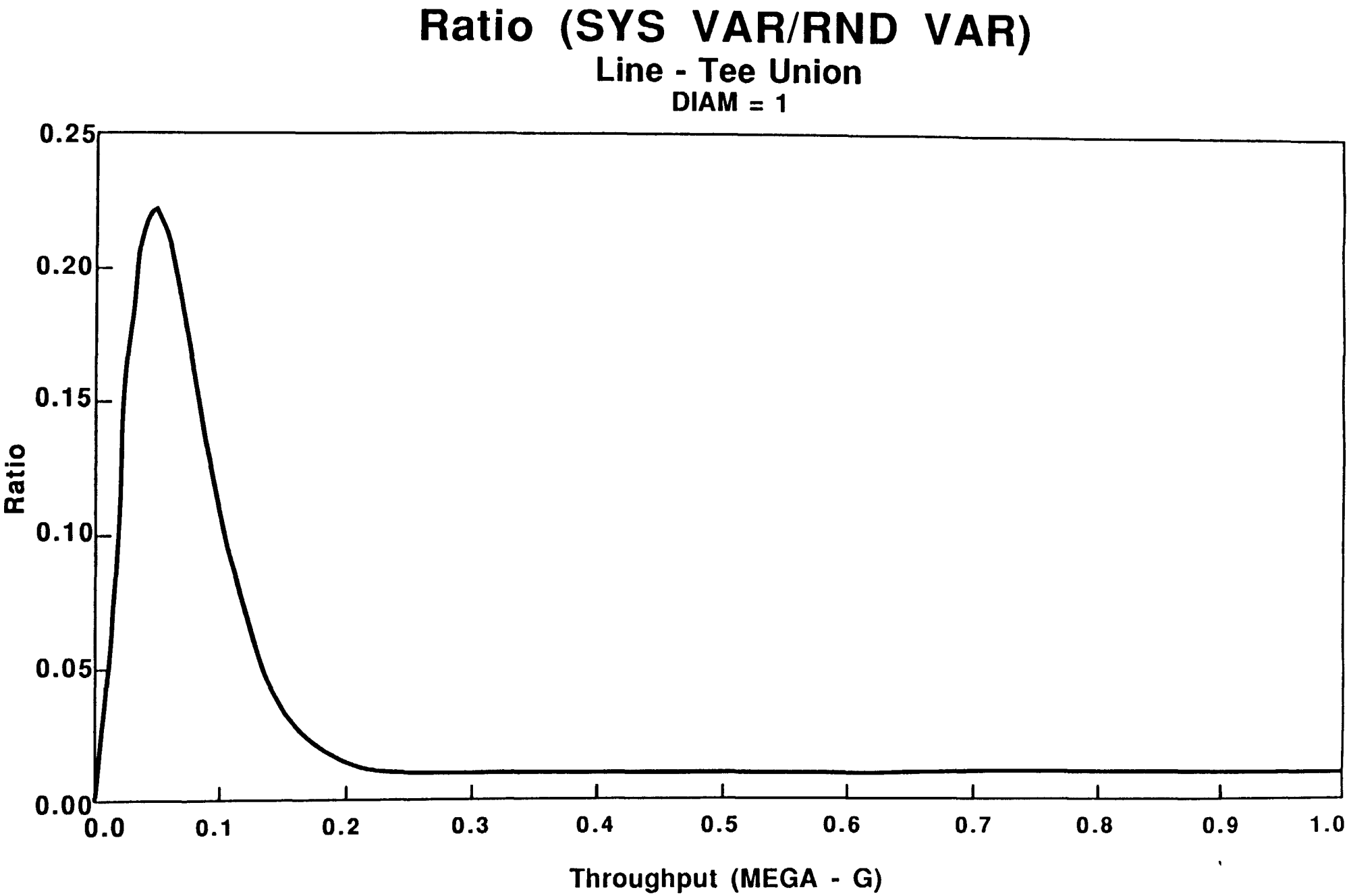
DIAM = 0.75



Line - Tee Union

DIAM = 1




Ratio (SYS VAR/RND VAR)
Line - Tee Union
DIAM = 1
Ratio
0.25
0.20
0.15
0.10
0.05
0.00
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Throughput (MEGA - G)

8. Adjustments to LANL Models

Usually $Y_{SRP} = k\ Y_{LANL}$

where k is a constant correction factor for surface area

$$Var\ (Y_{SRP}) = k^2\ Var\ (Y_{LANL})$$

Eg. Aquacol:

$$k = D\,L / 310$$

M802135

Aquacol

LANL

Diameter $D = 20 \text{ cm} = 7.874 \text{ in.}$

Length $L = 100 \text{ cm} = 39.370 \text{ in.}$

Surface Area

$$\text{Area} = \pi D L$$

$$= 3.1416 (7.874) (39.370)$$

$$= 973.9 \text{ in}^2$$

M802136

Aquacol (Contd)

SRP:

$$k = \pi D L / 973.9 = D L / 310$$

$$y = k a (1 - e^{-bx})$$

where $a = 0.7614$

$b = 834.1$

x = throughput in mega-grams

M802137

---- 9. ---------- UPA ----------

OBS	ID	TP_MULT	DIAM	NUMBER	CONC
1	AQUACOL	0.0001	6.0	96.000	.
2	AQUACOL	0.0313	6.0	132.000	.
3	AQUACOL	1.0000	6.0	560.000	.
4	ELBOW	0.0001	1.0	11.000	.
5	ELBOW	0.0002	1.0	11.000	.
6	ELBOW	0.0004	1.0	5.000	.
7	ELBOW	0.0273	1.0	6.000	.
8	ELBOW	0.0313	1.0	25.000	.
9	ELBOW	0.0400	1.0	4.000	
10	ELBOW	1.0000	1.0	[illegible]	
11	ELBOW	3.1250	1.0		
12	ELBOW	10.0000	1[illegible]		.
13	ELBOW	0.0004		[illegible]	.
14	ELBOW	0.5000		25.355	.
15	ELBOW	1.00[illegible]	[illegible]	0.991	.
16	ELBOW	10.[illegible]	1.5	7.074	.
17	ELBOW	[illegible]	1.5	0.610	.
18	ELBOW	[illegible]	1.5	16.408	.
19	ELBOW	[illegible]13	2.0	2.940	.
20	ELBOW	[illegible].0000	2.0	3.111	.
21	ELBOW	0.0001	3.0	4.572	.
22	ORGACO[illegible]	0.0313	3.0	1.448	.
23	ORGA[illegible]	1.0000	3.0	1.956	.
24	OR[illegible]	3.1250	.	1.000	130
25	[illegible]	10.0000	.	1.000	135
[illegible]	[illegible]	10.0000	.	1.000	50
[illegible]	[illegible]UNION	0.0001	1.0	5.000	.
[illegible]	[illegible]E_UNION	0.0002	1.0	1.000	.
[illegible]	TEE_UNION	0.0004	1.0	3.000	.
49	TEE_UNION	0.0273	1.0	1.000	.
50	TEE_UNION	0.0313	1.0	3.000	.
51	TEE_UNION	0.0400	1.0	1.000	.
52	TEE_UNION	3.1250	1.0	8.000	.
53	TEE_UNION	10.0000	1.0	9.000	.
54	TEE_UNION	0.0004	1.5	2.000	.

9.a. Aquacol Example

(UPA)

$$H = \{ 96\ (6)\ a\ (1 - e^{-.0001bx}) +$$
$$132\ (6)\ a\ (1 - e^{-.0313bx}) +$$
$$560\ (6)\ a\ (1 - e^{-bx})\ \} / 310 =$$

$$1.8581\ a\ (1 - e^{-.0001bx}) +$$
$$2.5548\ a\ (1 - e^{-.0313bx}) +$$
$$10.8387\ a\ (1 - e^{-1.0\ bx})$$

M802138

9.b. Estimation of Error Variances

$$\begin{aligned} DER_a = {} & 1.8581\ (1 - e^{-.0001bx}) + \\ & 2.5548\ (1 - e^{-.0313bx}) + \\ & 10.8387\ (1 - e^{-bx}) \end{aligned}$$

$$\begin{aligned} DER_b = {} & a\ \{ 1.8581\ (.0001x\, e^{-.0001bx}) \\ & + 2.5548\ (.0313x\ e^{-.0313bx}) \\ & + 10.8387\ (x\ e^{-bx})\ \} = \end{aligned}$$

$$\begin{aligned} & a\ \{ .00018581\ x\ e^{-.0001bx} + \\ & .07996524\ x\ e^{-.0313bx} + \\ & 10.8387\ x\ e^{-bx}\ \} \end{aligned}$$

M802139

Example

Let x = 0.002 mega-grams (2 KG)

H = 6.796 g

DER_a = 8.9250

DER_b = 0.0032287

$$\text{Var_sys} \approx (8.9250)^2 \ \text{Var}(a) + (0.0032287)^2 \ \text{Var}(b) + 2\,(8.925)\,(0.00323)\ \text{Cov}(a,b)$$

M802140

Example (Contd)

where $\mathrm{Var}(a) = (0.0183)^2$,

$\mathrm{Var}(b) = (268.518)^2$,

$\mathrm{Cov}(a,b) = -0.2055\ (0.0183)\ (268.518)$.

$\mathrm{Var_sys} \approx 0.7201$

$\mathrm{Var_rnd} = \{1.858 + 2.555 + 10.839\}^2\ \mathrm{MSE}$

where $\mathrm{MSE} = 0.01437$.

$\mathrm{Var_rnd} = 3.3416$

M802141

9.c. Total UPA Estimates

(Fixed Throughput)

$$\text{HOLDUP} = \sum_{\text{all } j} (\text{component holdup})_j$$

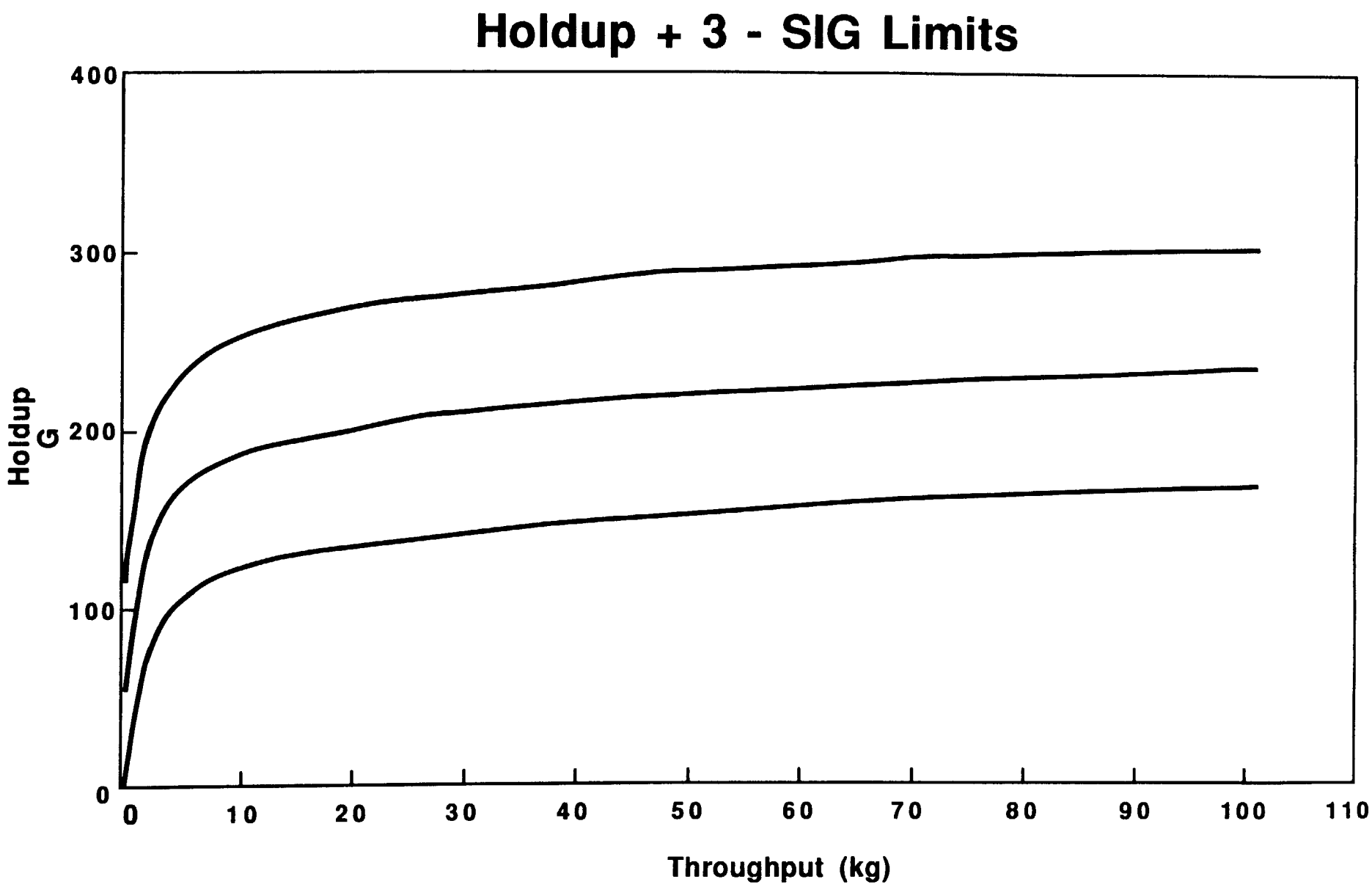
$$\text{VAR_SYS} = \sum_{\text{all } j} (\text{component Var_sys})_j$$

$$\text{VAR_RND} = \sum_{\text{all } j} (\text{component Var_rnd})_j$$

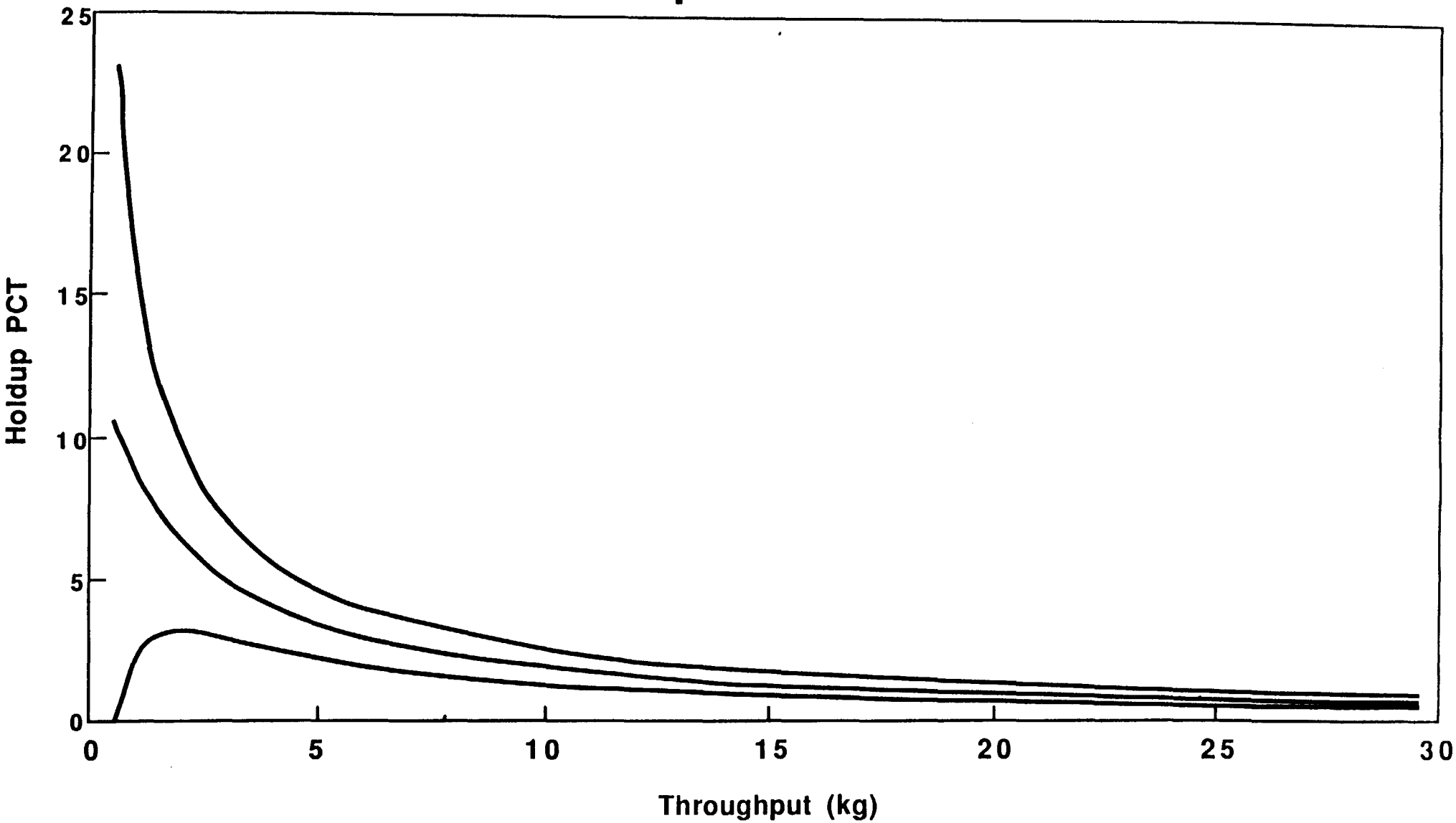
<u>Assumptions</u>

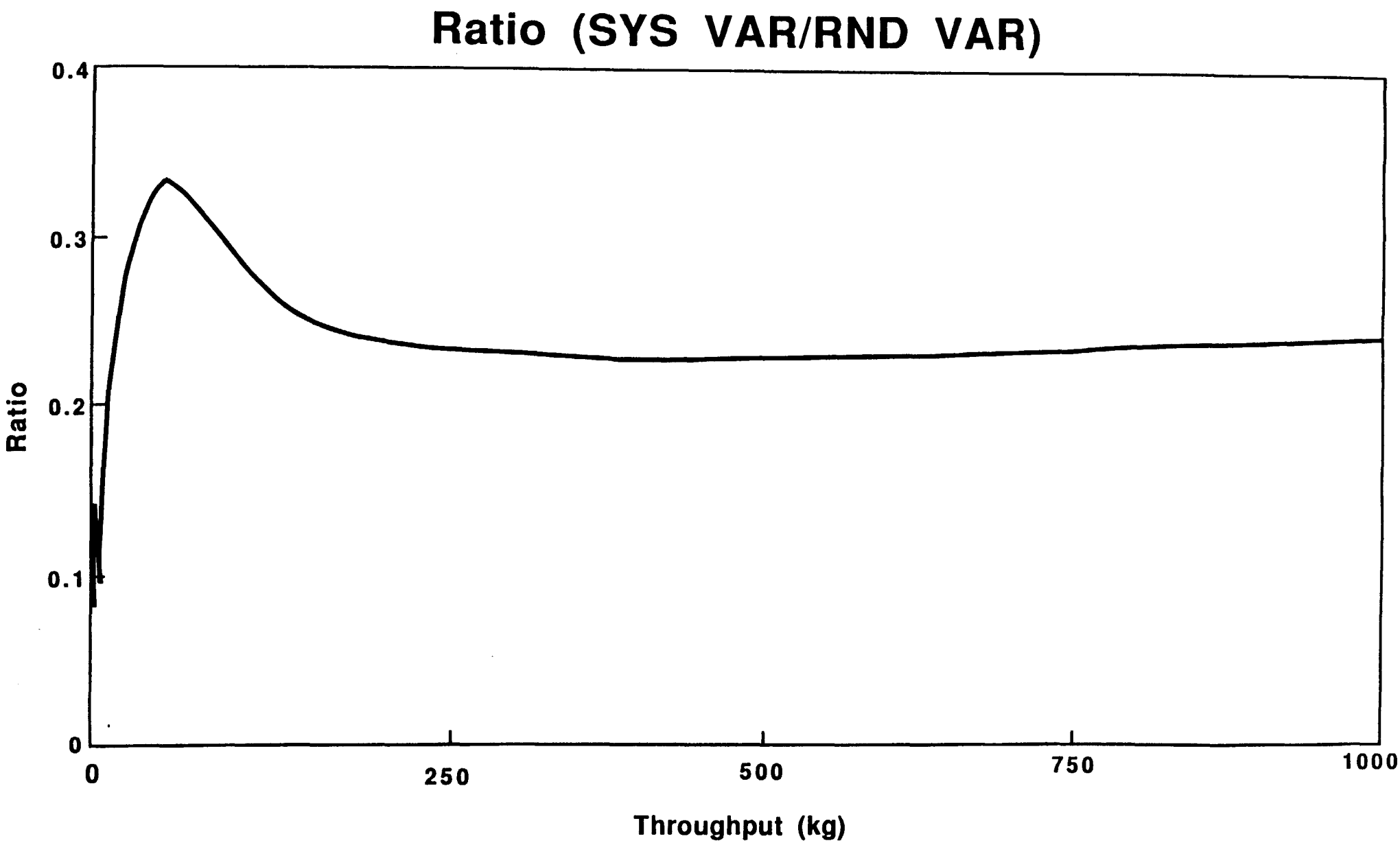
Data from different components are uncorrelated

M802142


Holdup + 3 - SIG Limits
400
300
200
100
0
Holdup
G
0
10
20
30
40
50
60
70
80
90
100
110
Throughput (kg)

PCT Holdup + 3 SIG Limits




Ratio (SYS VAR/RND VAR)
0.4
0.3
0.2
0.1
0
Ratio
0
250
500
750
1000
Throughput (kg)