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Software Documentation For TRU Certification Program

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Abstract:
The document provides validation information for software used to support TRU operational activities. Calculations were performed using a spreadsheet application.

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Software Documentation for TRU Certification Program

Software Documentation: MICROSOFT ®EXCEL
Version 97 SR-1, Copyright © 1985 - 1997

1.0 INTRODUCTION

This document provides information about the usage of the software application, Microsoft ® Excel. Microsoft ® Excel spreadsheets were used to perform specific calculations to determine the amount of containers to visually examine and to perform analyses on container head-gas data. Contained in this document are definitions of formulas and variables with relation to the Excel codes used. Also, a demonstration is provided using predetermined values to obtain predetermined results.

2.0 DESCRIPTION OF FORMULAS

This section provides a description of the formulas used to obtain the values for visual examination and head-gas data analyses.

2.1 Determination of Visual Exam Drum Amount Using Hypergeometric Distribution

<u>Hypergeometric Equations:</u>
(Note: The variables, a through f, were not originally used in the Excel spreadsheet. Since it is difficult to illustrate the performance of the calculation, these variables help make the calculations easier to track. See Attachment 1 for formulas and hand calculations and Excel results using dummy data.)

Microsoft Excel Filename: Hypergeo

$$\sum_{k=0}^{x} (M_{est} .. k)(N-M_{est} .. n_I - k)/(N .. n_I)$$

where:

$A = M_{est} .. k$
$B = N-M_{est} .. n_I - k$
$C = N .. n_I$

$$a_I = \sum_{k=0}^{x} (M_{UCL} .. k)(N-M_{UCL} .. n_I - k)/(N .. n_I)$$

where:

$D = M_{UCL} .. k$
$E = N-M_{UCL} .. n_I - k$
$F = N .. n_I$

Formula Variable	Variable Description	Microsoft Excel Equivalent
N	Population of containers	Cell E6
M	Miscertified containers	Assumed to be 2%.
P_{ucl90}	The true proportion of miscertified containers in the population.	14%; a given value as per CAO-94-1010
M_{ucl90}	$N \times P_{ucl90}$	Cell G6 = E6 x 0.14
M_{est}	N x 0.02	Cell C5 = E6 x 0.02
A	M_{est}.. k	Cell C10 = COMBIN(C6, A10) and Cell C11 = COMBIN(C6, A11)
B	N-M_{est} .. $n_I - k$	Cell D10 = COMBIN(G5, E5 – A10) and Cell D11 = COMBIN(C6, E5 – A11)
C	N .. n_I	Cell E10 = COMBIN(E6, E5) and Cell E11 = COMBIN(E6, E5)
D	M_{UCL}.. k	Cell C15 = COMBIN(G6, A15) and Cell C16 = COMBIN(G6, A16)
E	N-M_{UCL} .. $n_I - k$	Cell D15 = COMBIN(G7, E5 – A15) and Cell D16 = COMBIN(G7, E5 – A16)
F	N .. n_I	Cell E15 = COMBIN(E6, E5) and Cell E16 = COMBIN(E6, E5)

2.2 Head-gas Analyses to Determine Shapiro-Wilk Tests and UCL_{90}

Shapiro-Wilk Normality Test Equations:
(Note: See Attachment 2 for formulas and hand calculations and Excel results using dummy data)

Microsoft Excel Filename: HeadAnalRMA and HeadAnalRMC

Reference: Shapiro, S.S. and Wilk, M.B. (1965). "An Analysis of Variance Test for Normality (Complete Samples)." Biometrika, No. 52, pp. 591-611

Constants:

Equations:

$$b = \Sigma a_{n-i+1}(y_{n-i+1} - yi)$$

$$S^2 = \Sigma (y_i)^2 - 1/n(\Sigma y_i)^2$$

$$W = b^2/S^2$$

Where:

a_n = some constant dependent upon the number of samples
y_n = the constituent concentration
n = the number of observations
i = iteration

Shapiro-Wilk W-Test Formulas	**Microsoft Excel Equivalent**
$(y_{n-I+1} - yi)$	Cell B6 = B3 – B2
$a_{n-i+1}(y_{n-i+1} - yi)$	Cell A6 = PRODUCT(B6, 0.7071)
$b = \Sigma\, a_{n-i+1}(y_{n-i+1} - yi)$	Cell B9 = SUM(A6:A6)
$\Sigma\,(y_I)^2$	Cell B10 = SUM(C2:C3)
$\Sigma\, y_I$	Cell B11 = SUM(B2:B3)
$(\Sigma\, y_I)^2$	Cell B12 = POWER(B11,2)
$1/n(\Sigma\, y_i)^2$	Cell B13 = B12/n (n = sample number)
$S^2 = \Sigma\,(y_i)^2 - 1/n(\Sigma\, y_i)^2$	Cell B14 = B10 – B13
b^2	Cell B15 = POWER(B9,2)
W	Cell B16 = B15/B14

UCL_{90} Test:
(Note: See Attachment 3 for formulas and hand calculations and Excel results using dummy data)

Equations:

Mean X = $(\Sigma\, x_i)/n$

StDev = $(\sqrt{1/n-1})\,(\sqrt{\Sigma(x_i - \text{Mean X})^2}$

$T_{90,n-1}$ = a value from Student T Distribution from Newnan, D.G., Engineering –In-Training License Review, 14th edition, 1997, pp. 5-21.

UCL_{90} = Mean X + $(T_{90,n-1})$(StDev)/ $\sqrt{n}$

Where:

Mean X = the sum of all constituent values divided by the total sample population.

UCL_{90} Formulas	**Microsoft Excel Equivalent**
Mean X	Cell B7 = SUM(B3:B4)
Standard Deviation	Cell B8 = STDEV(B3:B4)
$T_{90,n-1}$	Dependent on number of samples
$(T_{90,n-1})$(StDev)	Cell B10 = PRODUCT(B8:B9)
$\sqrt{n}$	Cell B11 = SQRT(n)
$(T_{90,n-1})$(StDev)/ $\sqrt{n}$	Cell B12 = B10/B11
UCL_{90} = Mean X + $(T_{90,n-1})$(StDev)/ $\sqrt{n}$	Cell B13 = SUM(B12:B7)

ATTACHMENT 1

Hypergeometric Distribution Using Pre-Selected Data

**Consisting of 6 pages,
Including the coversheet**

Hypergeometric Distribution Test Formulas							
	Miscert=	0.02	n1=	26	N - Mest=	=E6-C6	
	Mest=	=PRODUCT(C5, E6)	N=	844	Mucl=	=PRODUCT(E6,0.14)	Pucl90 = .14; 14%
					N - Mucl=	=E6 - G6	
0		=COMBIN(C6,A10)	=COMBIN(G5,E5-A10)	=COMBIN(E6,E5)	=C10*D10/E10		
1		=COMBIN(C6,A11)	=COMBIN(G5,E5-A11)	=COMBIN(E6,E5)	=C11*D11/E11	=SUM(F10:F11)	
				Sum of x=	=SUM(F10:F11)		
0		=COMBIN(G6,A15)	=COMBIN(G7,E5-A15)	=COMBIN(E6,E5)	=C15*D15/E15		
1		=COMBIN(G6,A16)	=COMBIN(G7,E5-A16)	=COMBIN(E6,E5)	=C16*D16/E16		
				alpha=	=SUM(F15:F16)		GOOD
	Miscert=	0.02	n1=	25	N - Mest=	=E22-C22	
	Mest=	=PRODUCT(C21, E22)	N=	844	Mucl=	=PRODUCT(E22, 0.14)	Pucl90 = .14; 14%
					N - Mucl=	=E22 - G22	
0		=COMBIN(C22,A26)	=COMBIN(G21,E21 -A26)	=COMBIN(E22,E21)	=C26*D26/E26		
1		=COMBIN(C22,A27)	=COMBIN(G21,E21 -A27)	=COMBIN(E22,E21)	=C27*D27/E27	=SUM(F26:F27)	

Hypergeometric Distribution Test Formulas

				Sum of x=	=SUM(F26:F27)		
0		=COMBIN(G22,A31)	=COMBIN(G23,E21-A31)	=COMBIN(E22,E21)	=C31*D31/E31		
1		=COMBIN(G22,A32)	=COMBIN(G23,E21-A32)	=COMBIN(E22,E21)	=C32*D32/E32		
				alpha=	=SUM(F31:F32)		
	Miscert=	0.02	n1=	27	N - Mest=	=E37-C37	
	Mest=	=PRODUCT(C36,E37)	N=	844	Mucl=	=PRODUCT(E37,0.14)	Pucl90 = .14; 14%
					N - Mucl=	=E37 - G37	
0		=COMBIN(C37,A41)	=COMBIN(G36,E36 -A41)	=COMBIN(E37,E36)	=C41*D41/E41		
1		=COMBIN(C37,A42)	=COMBIN(G36,E36 –A42)	=COMBIN(E37,E36)	=C42*D42/E42	=SUM(F41:F42)	
				Sum of x=	=SUM(F41:F42)		
0		=COMBIN(G37,A46)	=COMBIN(G38,E36-A46)	=COMBIN(E37,E36)	=C46*D46/E46		
1		=COMBIN(G37,A47)	=COMBIN(G38,E36-A47)	=COMBIN(E37,E36)	=C47*D47/E47		
				alpha=	=SUM(F46:F47)		

Hypergeometric Distribution Using Pre-Selected Data								
	Miscert=	2%	n1=	30	N - Mest=	49		
	Mest=	1	N=	50	Mucl=	7	**Pucl90 = .14; 14%**	
					N - Mucl=	43		
0		1	1.89E+13	4.71E+13	0.4			
1		1.00	2.83E+13	4.71E+13	0.6	1		
				Sum of x=	1			
0		1	3.66E+10	4.71E+13	0.000776			
1		7	7.84E+10	4.71E+13	0.011641			
				Alpha=	0.012418			

Validation Equation for HyperGeo Spreadsheet

$$\binom{N}{X} = \frac{N!}{(N-X)X!} \qquad \frac{\sum_{K=0}^{X}\binom{M_{est}}{K}\binom{N-M_{est}}{n_i-K}}{\binom{N}{n_i}}$$

$$M_{est}(N)\left(\frac{M}{N}\right) = (50)(0.02)$$

$$M_{est} = 1$$

$K = 0$

$$\binom{M_{est}}{K} = \binom{1}{0} = \frac{1!}{(1-0)0!} = \frac{1}{(1)(1)} = 1$$

$$\binom{N-M_{est}}{n_i-K} = \binom{50-1}{30-0} = \binom{49}{30} = 1.885168e13$$ using nCr (Texas Instruments, TI60)

$$\binom{N}{n_i} = \binom{50}{30} = 4.712921e13$$

$$\sum_{K=0}^{X}\frac{(1)(1.885168e13)}{4.712921e13} = 0.399$$ or ≈0.4

K=1

$$\binom{M_{est}}{K} = \binom{1}{1} = \frac{1!}{(1-1)1!} = 1$$

$$\binom{N-M_{est}}{n_i-K} = \binom{50-1}{30-1} = \binom{49}{29} = 2.827753e13$$

$$\binom{N}{n_i} = \binom{50}{30} = 4.712921e13$$

$$\sum_{K=1}^{X}\frac{(1)(2.827753e13)}{4.712921e13} = 0.6$$

- Sum of both iterations = 0.4 + 0.6 = 1
- Sum is greater 80% (α=0.80), so X_{max} = 1

Validation Equation for HyperGeo Spreadsheet

$$a = \frac{\sum_{K=0}^{X_{max}} \binom{M_{ucl}}{K}\binom{N - M_{ucl}}{n_i - K}}{\binom{N}{n_i}}$$

$M_{ucl} = (50)(0.14) = 7$

$P_{ucl} = 0.14$; given 14% miscertification

K=0

$$\binom{m_{ucl}}{K} = \binom{7}{0} = 1$$

$$\binom{N - M_{ucl}}{n_i - K} = \binom{50-7}{30-0} = \binom{43}{30} = 3.657685e10$$

$$\binom{N}{n_i} = 4.712921e13$$

$$a_0 = \frac{(1)(3.657685e10)}{4.712921e13} = 0.000776$$

K=1

$$\binom{M_{ucl}}{K} = \binom{7}{1} = 7$$

$$\binom{N - M_{ucl}}{n_i - K} = \binom{50-7}{30-1} = \binom{43}{29} = 7.837896e10$$

$$a_1 = \frac{(7)(7.837896e10)}{4.712921e13} = 0.011641$$

$$\binom{N}{n_i} = 4.712921e13$$

$a = a_0 + a_1 \Rightarrow 0.000776 + 0.011641 = 0.012417$

Value is approximately the same as the value calculated in the MS Excel spreadsheet, HyperGeo.

ATTACHMENT 2

Shapiro-Wilk Test Using Pre-Selected Data

Consisting of 4 pages,
Including the coversheet

Shapiro-Wilk Formulas			
PIN	BENZENE	y sq	y cu.
9601092	0.18	=POWER(B2,2)	=POWER(B2,3)
9601950	1.1	=POWER(B3,2)	=POWER(B3,3)
An(Yn-Yi)	Yn - Yi	An(Yn-Yi)	Yn - Yi
=PRODUCT(B6,0.7071)	=B3 - B2	=PRODUCT(D6,0.70 71)	=D3 - D2
b =	=SUM(A6:A6)	b =	=SUM(C6:C6)
SumYsq	=SUM(C2:C3)	SumYsq	=SUM(E2:E3)
Sum Y	=SUM(B2:B3)	Sum Y	=SUM(D2:D3)
Yi sq	=POWER(B11,2)	Yi sq	=POWER(D11,2)
Yi sq/2	=B12/2	Yi sq/2	=D12/2
S sq =	=B10 - B13	S sq =	=D10 - D13
b sq	=POWER(B9,2)	b sq	=POWER(D9,2)
W =	=B15/B14	W =	=D15/D14

Shapiro-Wilk Test Using Pre-Selected Data		
PIN	BENZENE	y sq
9601092	0.35	0.1225
9601950	0.85	0.7225
An(Yn-Yi)	Yn - Yi	
0.35355	0.5	
b =	0.35355	
SumYsq	0.845	
Sum Y	1.2	
Yi sq	1.44	
Yi sq/2	0.720	
S sq =	0.125	
b sq	0.124998	
W =	1.000	

Validation Equation for Shapiro-Wilk Spreadsheet

$y_1 = 0.35$ $a_2 = 0.7071$

$y_2 = 0.85$ $n = 2$

$$b = \sum a_{2-1+1}(y_{2-1+1} - y_1) = a_2(y_2 - y_1) \Rightarrow (0.7071)(0.85 - 0.35) = 0.35355$$

$$s^2 = \sum (y_1)^2 - \frac{1}{n}\left(\sum y_1\right)^2$$

$$y_1 = 0.35; y_1^2 = (0.35)^2 = .1225$$
$$y_2 = 0.85; y_2^2 = (0.85)^2 = 0.7225$$

$$\sum yi^2 = y_1^2 + y_2^2 \Rightarrow 0.1225 + 0.7225 = 0.845$$

$$\sum y_i = y_1 + y_2 \Rightarrow 0.35 + 0.85 = 1.2$$
$$\left(\sum y_i\right)^2 = (1.2)^2 = 1.44$$
$$\frac{\left(\sum y_i\right)^2}{n} = \frac{1.44}{2} = 0.72$$

$$s^2 = 0.845 - 0.72 = 0.125$$
$$b^2 = (0.35355)^2 = 0.12499$$

$$W = \frac{b^2}{s^2} = \frac{0.12499}{0.125} = 0.999 \approx 1$$

Value is approximately the same as the value from the MS Excel spreadsheet, Shapiro-Wilk.

ATTACHMENT 3

UCL90 Test Using Pre-Selected Data

Consisting of 4 pages,
Including the coversheet

UCL90 Test Formulas	
	Benzene
	0.18
	1.1
Mean X=	=SUM(B3:B4)/2
StDev=	=STDEV(B3:B4)
t90n-1=	3.078
t90n-1 x StD	=PRODUCT(B8:B9)
sqrt n	=SQRT(2)
t90StD/sqrt n	=B10/B11
UCL90	=SUM(B12,B7)
PQRL(ppmv)	10
Transfomed	N/A

UCL90 Test Using Pre-Selected Data	
	Benzene
	0.35
	0.85
Mean X=	0.6
StDev=	0.353553
t90n-1=	3.078
t90n-1 x StD	1.088237
sqrt n	1.414214
t90StD/sqrt n	0.7695
UCL90	1.3695
PQRL(ppmv)	10
Transformed	N/A

Validation Equation for UCL90 Spreadsheet

$$UCL_{90} = MeanX + \frac{(T_{90,\,n-1})(StDev)}{\sqrt{n}}$$

$$MeanX = \frac{(0.35 + 0.85)}{2} = 0.6$$

$T_{90,\,n-1} = 3.078$ at $\propto = 90$ n=2

$$\text{Standard Deviation} = \sqrt{\frac{\sum\left(X_1 - \bar{X}\right)^2}{n-1}} = \sqrt{\frac{\sum X_1^2 - \frac{\left(\sum X_i\right)^2}{n}}{n-1}}$$

$$\sum X_i = 0.35 + 0.85 = 1.2$$

$$\sum X_i^2 = (0.35)^2 + (0.85)^2 = 0.1225 + 0.7725 = 0.845$$

$$S = \sqrt{\frac{0.845 - \frac{(1.2)^2}{n}}{n-1}} = \sqrt{\frac{0.845 - 0.72}{2-1}} = 0.35355$$

$$\sqrt{n} = \sqrt{2} = 1.4142$$

$$UCL_{90} = 0.6 + \frac{(3.078)(0.35355)}{1.4142} = 1.36949$$