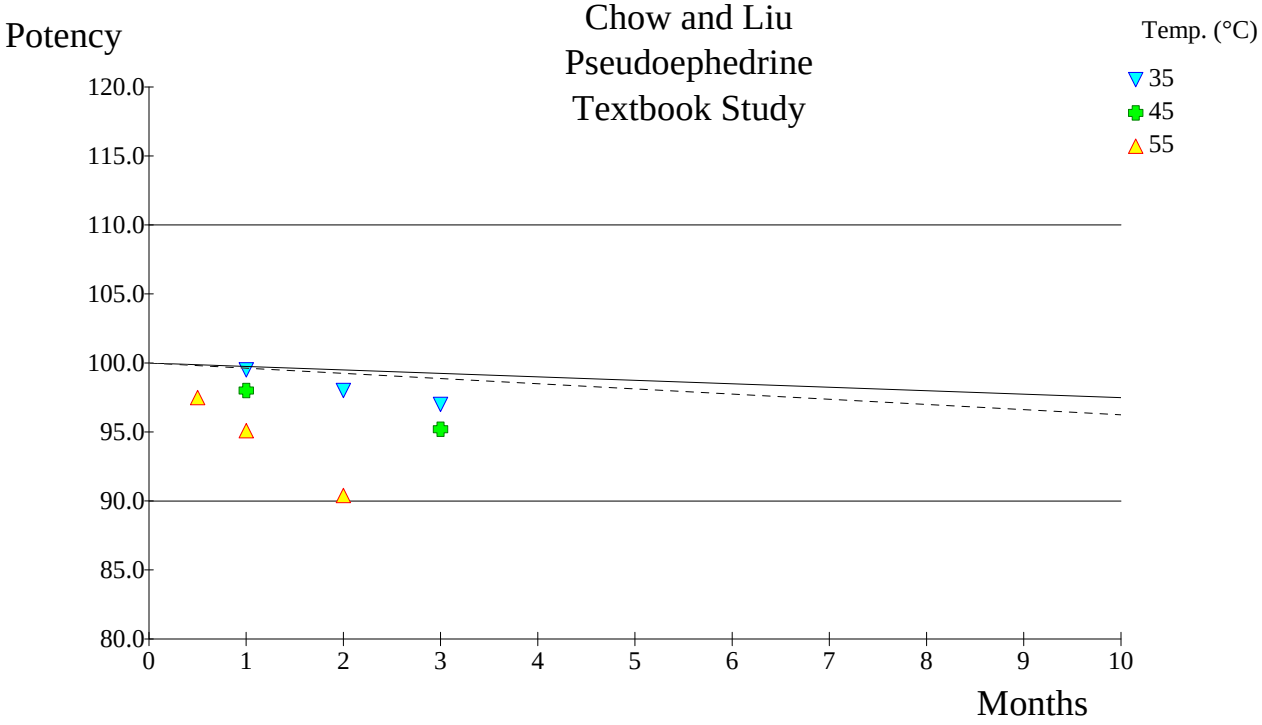
Shelf Life Projection

Chow and Liu
Pseudoephedrine
Textbook Study



Arrhenius Projection (Zero-Order) at 25.0 °C = 40 Months. Shelf life = 26 Months. (95.0% CI)
Test Category: Assay High Spec: 110.0 Low Spec: 90.0
Test Data
File: C:\Program Files (x86)\SLIM\Demo\Accelerated Conditions.SST User: Craig Hamilton

Zero-Order fit substituted into the Arrhenius equation.

Initial Purity = 100.0 Potency.

Original Raw Data (Time in units of Months):

Temp. (1) 35 °C			
Time :	1.0	2.0	3.0
Results:	99.50	98.00	97.00
Temp. (2) 45 °C			
Time :	1.0	3.0	
Results:	98.00	95.20	
Temp. (3) 55 °C			
Time :	0.5	1.0	2.0
Results:	97.50	95.10	90.40

Original Raw Data Treatment:
a. Less than (<) results are ignored.
b. Greater than (>) results are ignored.
c. Values that are not between 0.0 and 100.0 are ignored.

Data Points used in Calculations:

Temp. (1) 35 °C			
Time :	1.0	2.0	3.0
Results:	99.50	98.00	97.00
Temp. (2) 45 °C			
Time :	1.0	3.0	
Results:	98.00	95.20	
Temp. (3) 55 °C			
Time :	0.5	1.0	2.0
Results:	97.50	95.10	90.40

STATISTICAL ANALYSIS

LOWER ONE-TAILED CONFIDENCE INTERVAL
PROBABILITY LEVEL = 95.0% (equivalent to two-tail 90.0% probability)

ANOVA Table Under Model $D(h) = \sum_{i=1}^{I} \beta(h)X(h) + e_{ij}$

Order of reaction	Source of variation	df	Sum of squares	Mean squares	F value	p-value	R^2
0	Regression	3	162.31814	54.10605	690.37975	0.00000	99.75917
	Residual	5	0.39186	0.07837			
	Total	8	162.71000				
1	Regression	3	0.01750	0.00583	778.29613	0.00000	99.78631
	Residual	5	0.00004	0.00001			
	Total	8	0.01754				

Zero Order : Product degrades at a constant rate which is independent of concentration.

The Arrhenius equation is K = A * exp(-E/RT), where:
K : Rate Constant E : Activation Energy
A : Frequency Factor R : Gas Constant (8.31441 J/(K mol))
T : Absolute Temperature

Initial estimates using Simple Linear Regression:
A = 7.01506E+012 E = 76479.088
Refined estimates using Taylor series expansion:
A = 3.20451E+013 E = 80545.898

Using the refined estimates, let alpha = ln(A), beta = -E/R, and X = 1/T. The Arrhenius equation can be rewritten as K = exp(alpha + beta*X), where
alpha = 31.098167 and beta = -9687.506180.

Summary of Residuals for Lack of Fit for the Arrhenius Equation

Source of variation	df	Sum of squares	Mean squares	F value	p-value
Residual from Arrhenius	6	2.09523			
Residual from Model	5	0.39186	0.07837		
Lack of Fit	1	1.70337		21.73461	0.00552

Additional Statistics...
Sum of Squares of the Error = 0.341060
Variance of A = 4.583206
Variance of b = 489670.277601
Variance in K = 0.042960

Zero Order Results:
(By convention, projections are rounded and expiration dates are truncated.)
Arrhenius Projection at 25.0 °C = 40 Months.
Expiration Date (95.0% CI) at 25.0 °C = 26 Months.

First Order: Product degrades at a constant rate that is proportional to the log of the concentration.

The Arrhenius equation is K = A * exp(-E/RT), where:
K : Rate Constant E : Activation Energy
A : Frequency Factor R : Gas Constant (8.31441 J/(K mol))
T : Absolute Temperature

Initial estimates using Simple Linear Regression:
A = 9.81508E+010 E = 77317.544
Refined estimates using Taylor series expansion:
A = 4.76832E+011 E = 81551.079

Using the refined estimates, let alpha = ln(A), beta = -E/R, and X = 1/T. The Arrhenius equation can be rewritten as ln(K) = alpha + beta*X, where
alpha = 26.890430 and beta = -9808.402460.

Summary of Residuals for Lack of Fit for the Arrhenius Equation

Source of variation	df	Sum of squares	Mean squares	F value	p-value
Residual from Arrhenius	6	0.00021			
Residual from Model	5	0.00004	0.00001		
Lack of Fit	1	0.00017		23.11188	0.00485

Additional Statistics...
Sum of Squares of the Error = 0.000033
Variance of A = 4.291514
Variance of b = 458610.844716
Variance in K = 0.040308

First Order Results:
(By convention, projections are rounded and expiration dates are truncated.)
Arrhenius Projection at 25.0 °C = 42 Months.
Expiration Date (95.0% CI) at 25.0 °C = 28 Months.

Analysis Complete.

HISTORY INFORMATION
File Version: 1
File Status : ACTIVE
File Name : C:\Program Files (x86)\SLIM\Demo\Accelerated Conditions.SST
Created : 02 December 2010 at 17:51:28 by Administrator (User ID = 1)
Last Saved : 26 February 2011 at 23:06:13 by Administrator (User ID = 1)