

Functional Data Analysis (FDA) and Nonlinear Regression Models (NLR): an information quality perspective



March 22nd, 2022

Ron Kenett and Chris Gotwalt

Agenda

- A simple example – Ron
 - Intro to Functional Data Analysis (FDA)
 - Intro to Non-Linear Regression (NLR)
- An optimization example – Chris
 - Mixture experiments with profile responses
 - Designing tablets to match a reference profile

Dissolution
Curves of
12 tablets.
Test and
Reference

	Time	Label R	Data R	Label T	Data T
1	5	T1R	72.7	T1	46.6
2	5	T2R	78.8	T2	10.5
3	5	T3R	32.3	T3	10
4	5	T4R	38.8	T4	42.9
5	5	T5R	18.9	T5	61
6	5	T6R	52.1	T6	36.3
7	5	T7R	14.3	T7	6.4
8	5	T8R	67.8	T8	4.4
9	5	T9R	7.5	T9	5.4
10	5	T10R	8.5	T10	3.6
11	5	T11R	26.5	T11	6.4
12	5	T12R	10.2	T12	35
13	10	T1R	89.1	T1	74
14	10	T2R	94.4	T2	38.1
15	10	T3R	60.5	T3	30.9
16	10	T4R	63.7	T4	88.1
17	10	T5R	31.3	T5	84.3
18	10	T6R	79.6	T6	71.9
19	10	T7R	44.3	T7	39.4

Test

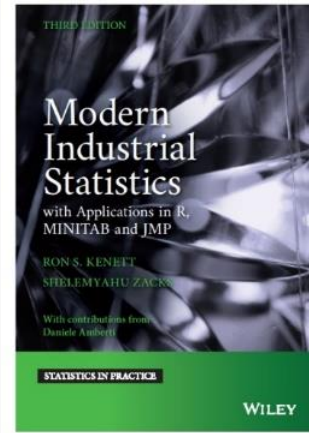
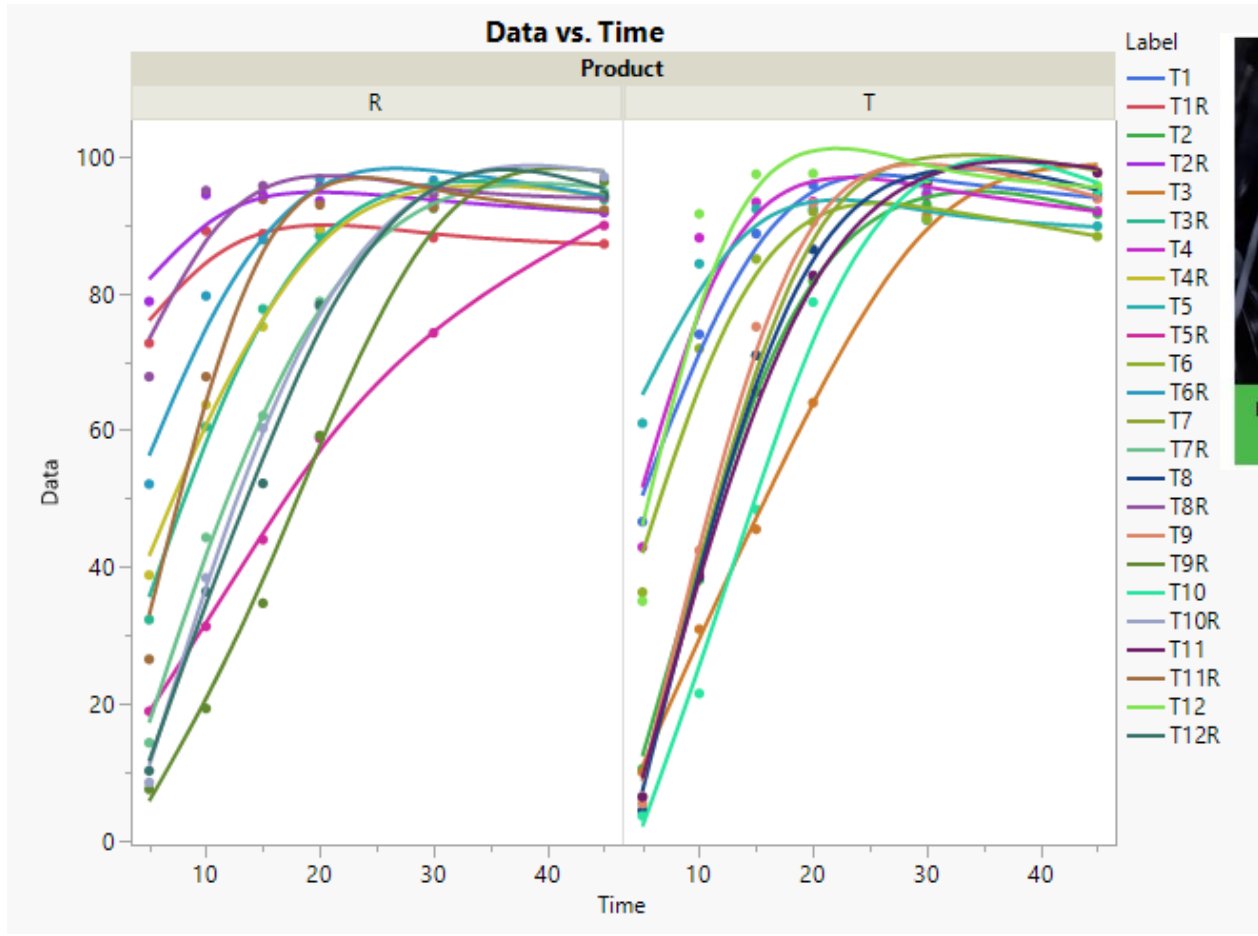
Level	Count
5	12
10	12
15	12
20	12
30	12
45	12
Total	72

Reference

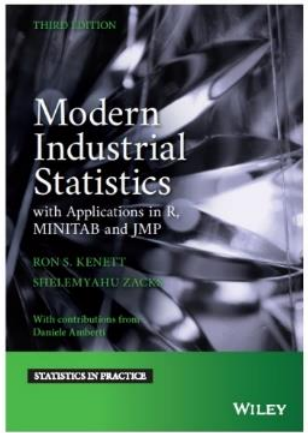
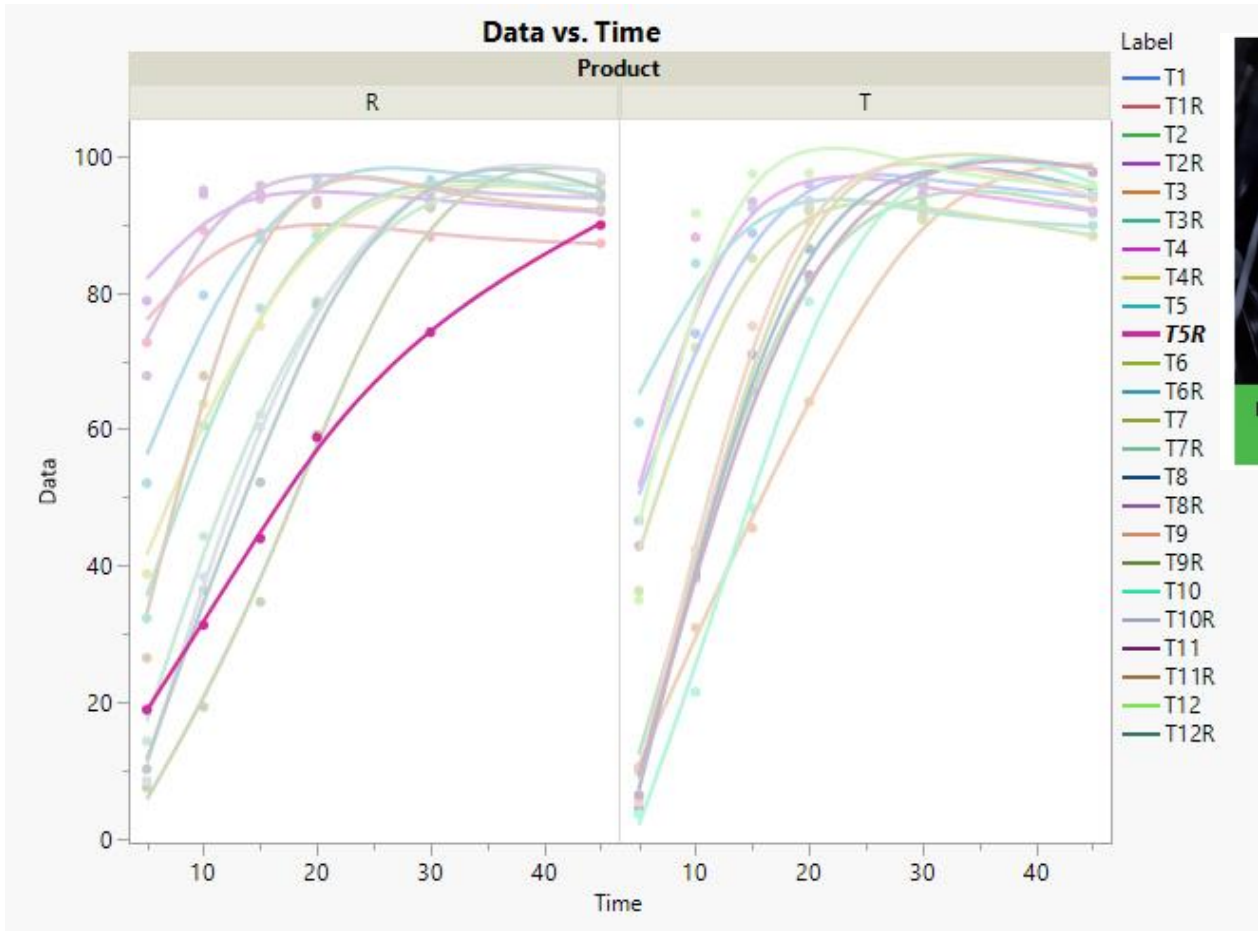
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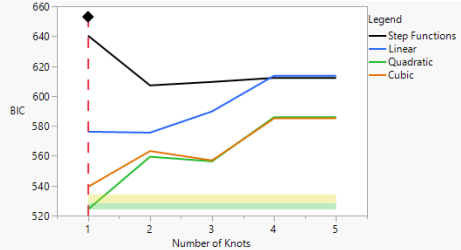
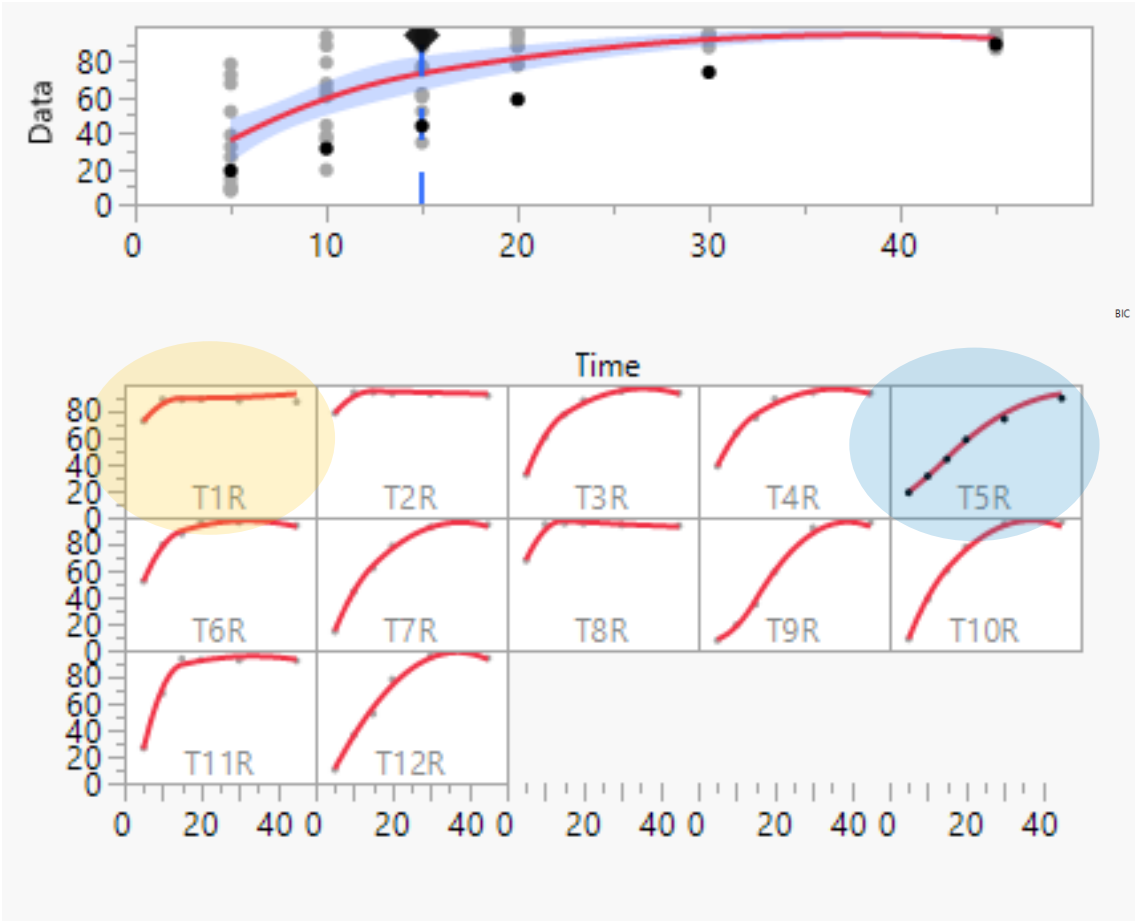
Dissolution
Curves of
12 tablets.
Test
T5R
Is different





Dissolution
Curves of
12 tablets.

Test T5R
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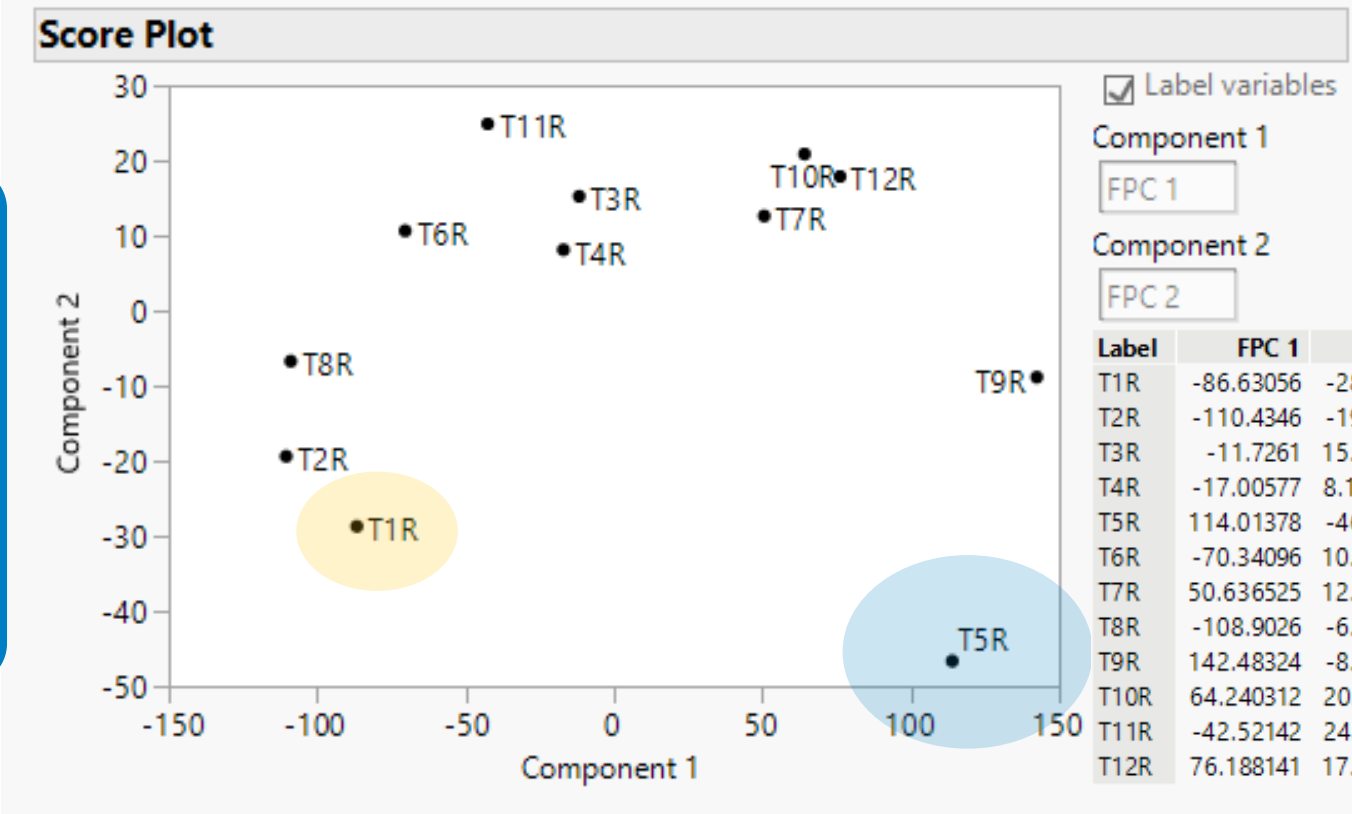


Quadratic B-spline
with 1 knot



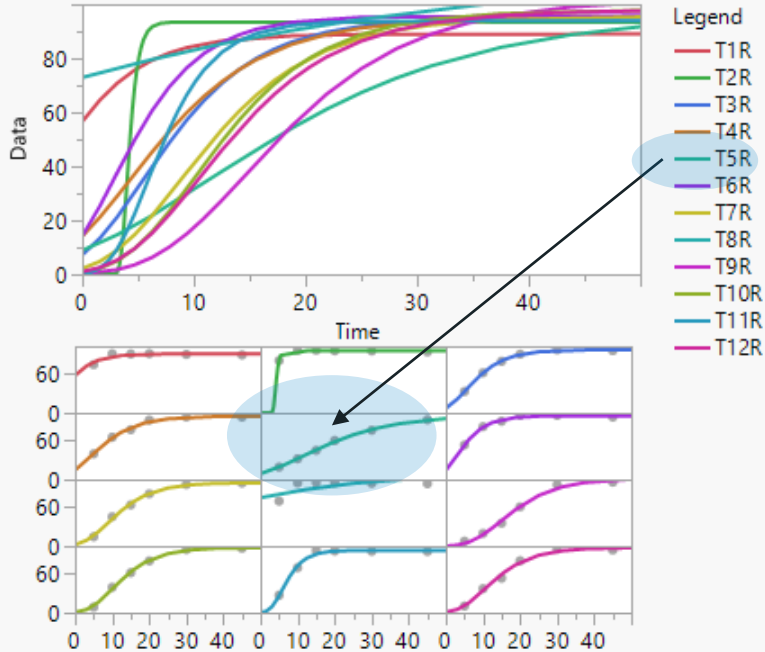
Dissolution
Curves of
12 tablets.

Test T5R
Is different



Gompertz 3P

Plot



Prediction Model

$$a \cdot \text{Exp} \left(- \text{Exp} \left(- b \cdot (\text{Time} - c) \right) \right)$$

a = Asymptote

b = Growth Rate

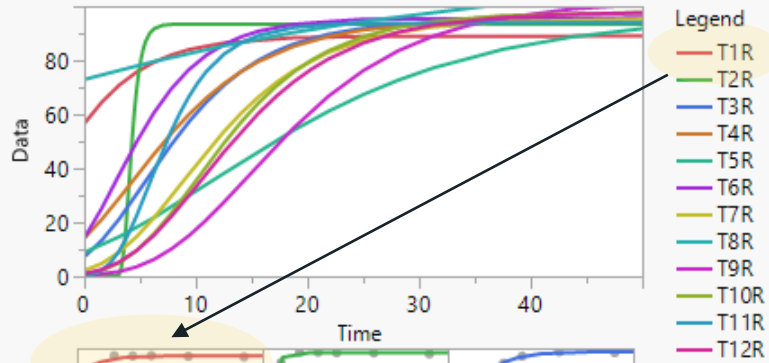
c = Inflection Point

NLR

Prediction Profiler

Gompertz 3P

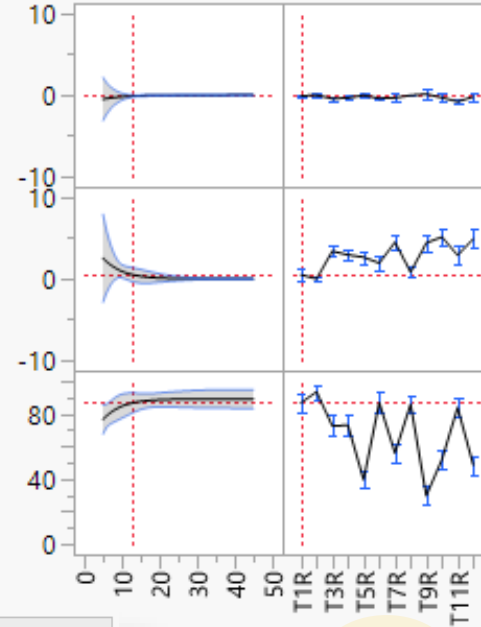
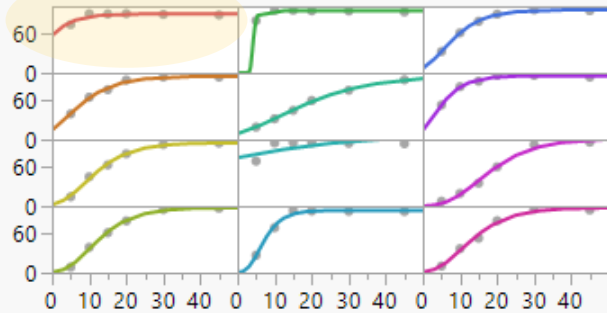
Plot



DERIVATIVE
 -0.10658
 [-0.21774,
 0.004582]

.50086
 -0.37387,
 .375584]

6.7501
 30.70902,
 2.79118]



Prediction Model

$$a \cdot \text{Exp} \left(- \text{Exp} \left(- b \cdot (\text{Time} - c) \right) \right)$$

a = Asymptote
 b = Growth Rate
 c = Inflection Point

13
 Time

T1R
 Label





		Label	Asymptote	Growth Rate	Inflection Point
T1R	1	T1R	89.072244404	0.2185624809	-3.625806907
	2	T2R	93.480399791	1.76758908	4.0002987548
	3	T3R	95.117117858	0.1732544061	5.4556204689
	4	T4R	95.393703545	0.1508168903	4.2794474042
T5R	5	T5R	97.047132531	0.0750862269	11.579937352
	6	T6R	95.886344295	0.2282099484	2.8239229453
	7	T7R	95.608682945	0.1500953986	8.8540204547
	8	T8R	113.26922091	0.0355126872	-23.11022674
	9	T9R	102.16502758	0.1201635618	14.766362121
	10	T10R	97.965019617	0.1562304451	10.087517474
	11	T11R	94.032980681	0.3037771891	5.8648755174
	12	T12R	97.966870258	0.1439240958	10.549169714

Prediction Model

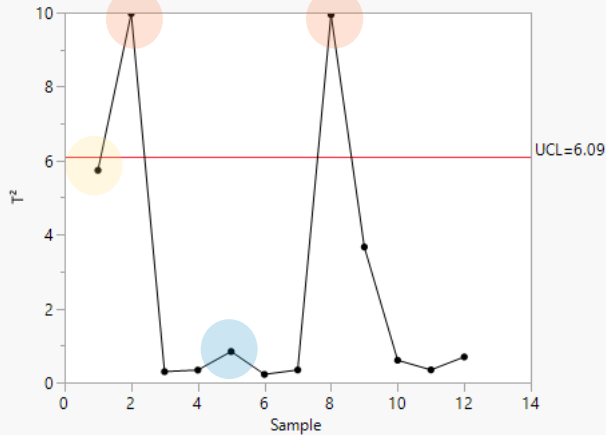
$$a \cdot \text{Exp} \left(- \text{Exp} \left(- b \cdot (\text{Time} - c) \right) \right)$$

- a = Asymptote
- b = Growth Rate
- c = Inflection Point

multivariate statistical distance (MSD)

Multivariate Control Chart

T Square with All Principal Components



Note: UCL is calculated based on Alpha=0.05

Principal Components: on Covariances

Eigenvalue	Percent	20	40	60	80	Cum Percent	ChiSquare	DF	Prob>ChiSq
109.6992	82.409					82.409	56.861	5.000	<.0001*
23.2208	17.444					99.853	37.506	2.000	<.0001*
0.1951	0.147					100.000	0.000	0.000	.

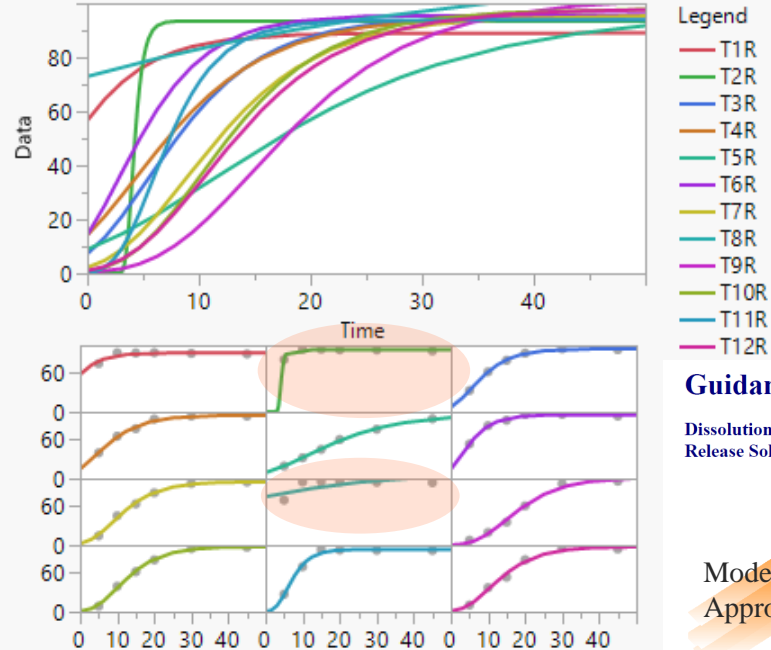
Eigenvectors

	Asymptote	Growth Rate	Inflection Point
	-0.03538	0.00038	0.08868
	0.19264	-0.00663	0.07689
	0.07053	2.26272	0.01853

Note: Eigenvectors were divided by square root of eigenvalues.

Gompertz 3P

Plot



NLR

Guidance for Industry

Dissolution Testing of Immediate Release Solid Oral Dosage Forms

Model Dependent Approaches

U.S. Department of Health and Human Services
Food and Drug Administration
Center for Drug Evaluation and Research (CDER)
August 1997

Information quality: what is the goal?

1. Data resolution
2. Data structure
3. Data integration
4. Temporal relevance
5. Chronology of data and goal
6. Generalizability
7. Operationalization
8. Communication

$$\text{InfoQ}(U, f, X, g) = U(f(X|g))$$

2021-EU-45MP-750

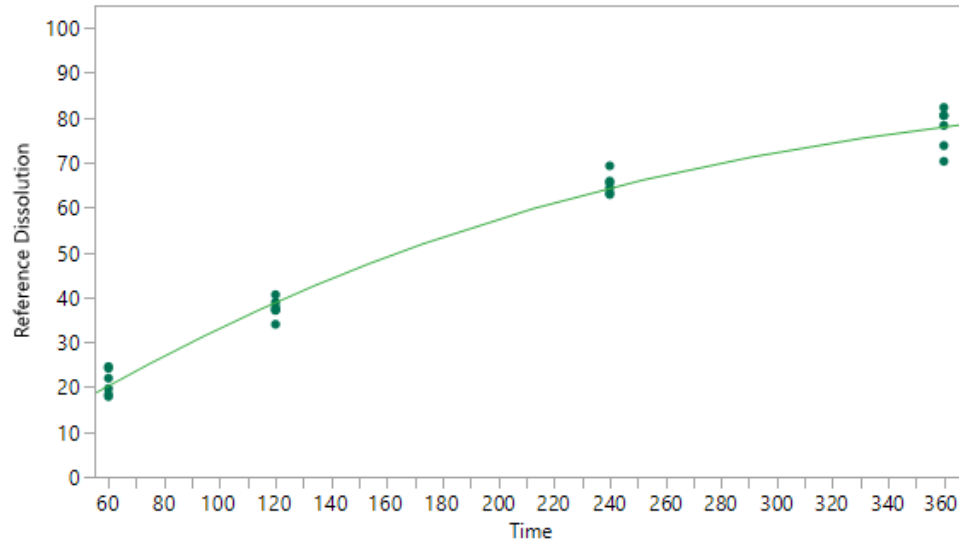
Maximizing Data Science Success with
Information Quality (InfoQ) and JMP®

<https://community.jmp.com/t5/Discovery-Summit-Europe-2021/Maximizing-Data-Science-Success-with-Information-Quality-InfoQ/ta-p/349217>

EUROPE 2021
DISCOVERY
SUMMIT
ONLINE

jmp

“After all, it is all about information quality.....”

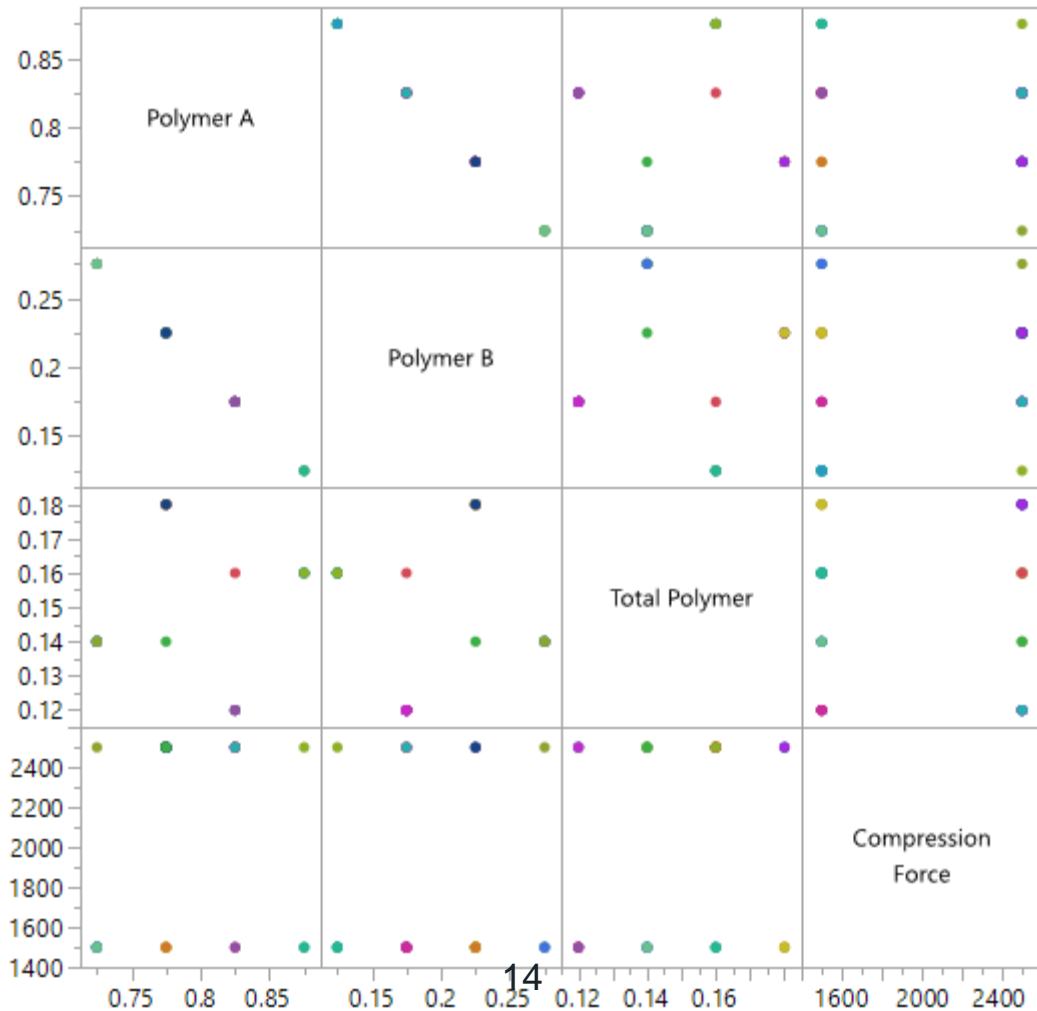


Goal:

Find Polymer & Compression Values leading to closest match to reference dissolution curve

Factors:

Polymer A (Mixture)
 Polymer B (Mixture)
 Total Polymer
 Compression Force



	Set	Batch	Rep	Polymer A	Polymer B	Total Polymer	Compression Force	Dissolution 60	Dissolution 120	Dissolution 240	Dissolution 360
1	R	R01	1	•	•	•	•	19.7	37.2	63.3	73.8
2	R	R01	2	•	•	•	•	24.2	34.0	64.4	70.3
3	R	R01	3	•	•	•	•	22.0	37.1	65.5	80.5
4	R	R01	4	•	•	•	•	18.4	40.6	62.9	78.3
5	R	R01	5	•	•	•	•	17.9	38.9	65.9	82.3
6	R	R01	6	•	•	•	•	24.6	37.8	69.3	80.5
7	A	A01	1	0.825	0.175	0.16	2500	17.0	26.7	39.6	54.6
8	A	A01	2	0.825	0.175	0.16	2500	22.3	25.9	44.8	57.5
9	A	A01	3	0.825	0.175	0.16	2500	12.7	28.5	45.1	52.9
10	A	A01	4	0.825	0.175	0.16	2500	18.7	28.0	43.9	52.5
11	A	A01	5	0.825	0.175	0.16	2500	19.0	25.8	44.0	54.3
12	A	A01	6	0.825	0.175	0.16	2500	16.1	28.8	44.1	58.0
13	A	A02	1	0.775	0.225	0.14	2500	19.1	36.5	59.9	73.5
14	A	A02	2	0.775	0.225	0.14	2500	18.4	36.1	58.9	75.0
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6 Tablets Per Formulation

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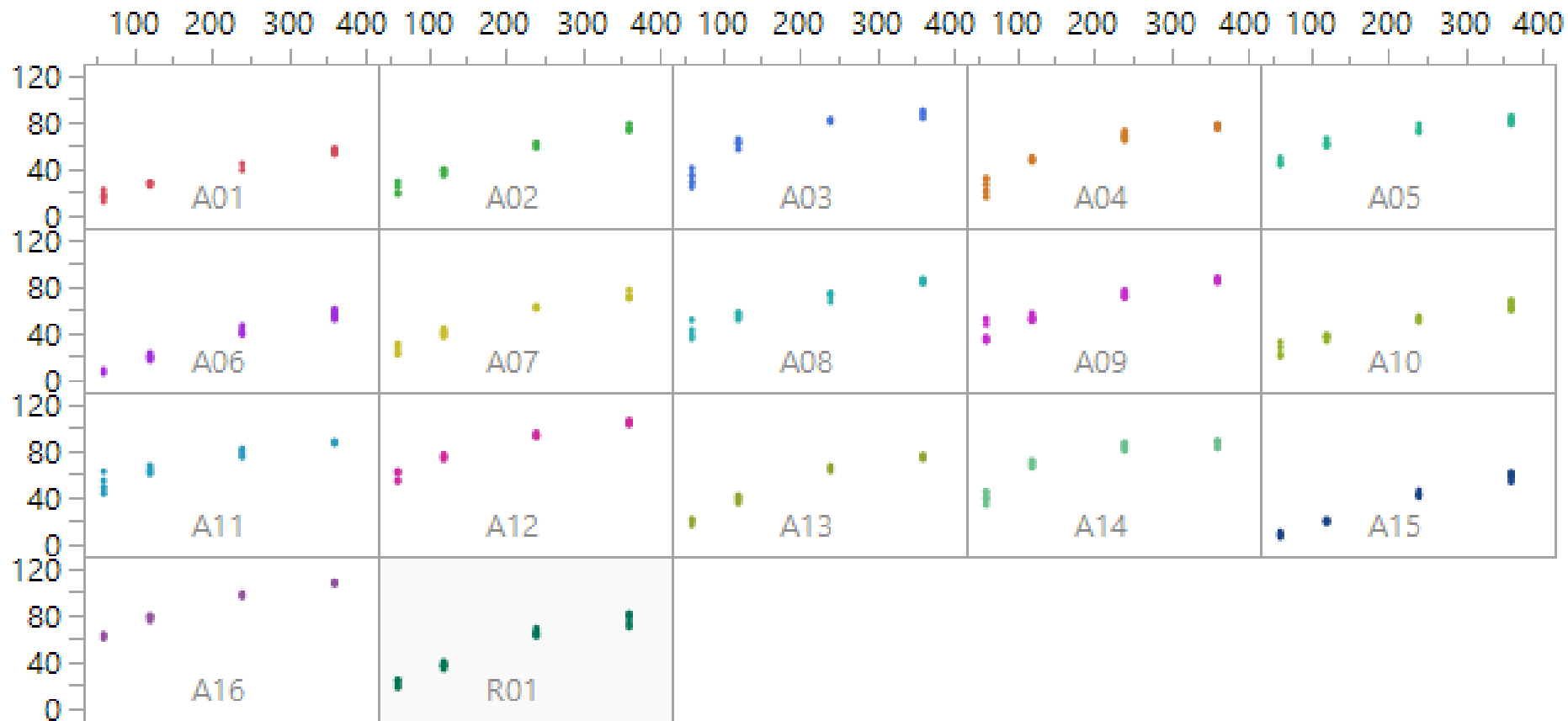
**4 Dissolution Measurements
Per Tablet**

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16 DoE Formulations

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← Reference we want to match



Data Resolution

- 1) Is the data scale used aligned with the stated goal? *Yes*
- 2) How reliable and precise are the measuring devices or data sources? *Yes*
- 3) Is the data analysis suitable for the data aggregation level? *yes, but...*

Data Structure

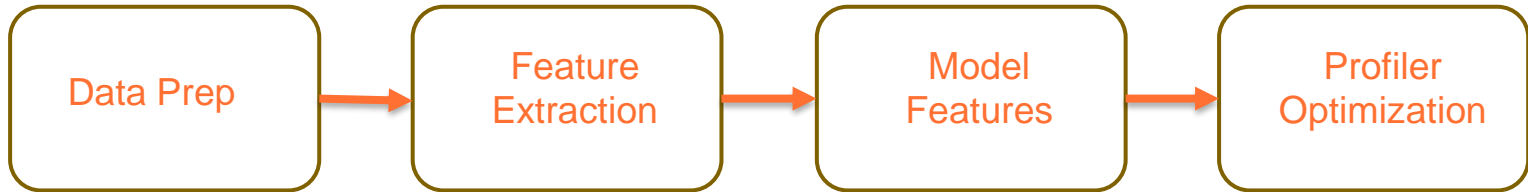
- 1) Is the type of the data used aligned with the stated goal? *Clearly yes*
- 2) Are data integrity details (corrupted/missing values) described and handled appropriately? *N/A (Yes)*
- 3) Are the analysis methods suitable for the data structure? *Yes, but...*

Data Integration

- 1) Are the data integrated from multiple sources? *Yes, mildly* -
If so, what is the credibility of each source? *N/A*
- 2) How is the integration done? *Feature extraction/Dimension reduction*
- 3) Are there linkage issues that lead to dropping crucial information? *TBD*
- 4) Does the data integration add value in terms of the stated goal? *TBD*
- 5) Does the data integration cause any privacy or confidentiality concerns? *No*

Three Analyses (f2, FDA, NLR)

$$\text{InfoQ}(U, f, X, g) = U(f(X/g))$$



Three Analyses (f2, FDA, NLR)

- 1) **f2** - Extract f2 scores and model them (GenReg)
- 2) **FDA** - Functional DoE: Extracted FPC scores (Functional Data Explorer, GenReg)
- 3) **NLR** - Curve DoE: Extract Weibull Growth parameters (Fit Curve, GenReg)

f2 DoE Analysis

Guidance for Industry

Dissolution Testing of Immediate
Release Solid Oral Dosage Forms

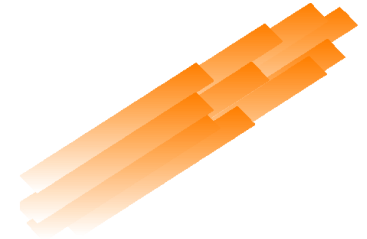
$$f2 = 50 \cdot \log \left(\frac{100}{\sqrt{1 + \frac{\sum(\bar{R}_t - T_t)^2}{n}}} \right)$$

R_t = Reference at time t

T_t = Test at time t

$$f2 \geq 50$$

Equivalence Region



U.S. Department of Health and Human Services
Food and Drug Administration
Center for Drug Evaluation and Research (CDER)
August 1997

f2 DoE Analysis

- 1) Calculate batch means of Dissolution
- 2) Create a formula column that calculates f2 relative to the reference batch
- 3) Model f2 using DoE factors as inputs
- 4) Profiler

f2 DoE Analysis

Dissolution DoE Split - JMP

File Edit **Tables** Rows Cols DOE Analyze Graph Tools Add-Ins View Window Help


Summary
Creates a new data table of summary statistics.

Subset
Sort
Stack
Split
Transpose
Join
Update
Concatenate
JMP Query Builder
Missing Data Pattern
Compare Data Tables
Anonymize

Set	Batch	Tablet	DoE Setting ID	Polymer A	Polymer B	Total Polymer	Compression Force
R	R01	1	•	•	•	•	•
R	R01	2	•	•	•	•	•
R	R01	3	•	•	•	•	•
R	R01	4	•	•	•	•	•
R	R01	5	•	•	•	•	•
R	R01	6	•	•	•	•	•
A	A01	1	1	0.825	0.175	0.16	2500
A	A01	2	1	0.825	0.175	0.16	2500
A	A01	3	1	0.825	0.175	0.16	2500
A	A01	4	1	0.825	0.175	0.16	2500
A	A01	5	1	0.825	0.175	0.16	2500

f2 DoE Analysis

Summary - JMP

 Creates a new data table of summary statistics.

Select Columns

12 Columns

- Set
- Batch
- Tablet
- DoE Setting ID
- Polymer A
- Polymer B
- Total Polymer
- Compression Force
- Dissolution 60
- Dissolution 120
- Dissolution 240
- Dissolution 360

Include marginal statistics

For quantile statistics, enter value (%)

statistics column name format

Output table name:

Link to original data table

Remove Excluded Groups

Prompt to save when closing summary tables

Keep dialog open

Save Script to Source Table

Statistics

- Mean(Dissolution 60)
- Mean(Dissolution 120)
- Mean(Dissolution 240)
- Mean(Dissolution 360)

Group

- Set
- Batch
- Tablet
- DoE Setting ID
- Polymer A
- Polymer B

Subgroup

Freq

Weight

Action

f2 DoE Analysis

Dissolution DoE Summarized - JMP

File Edit Tables Rows Cols DOE Analyze Graph Tools Add-Ins View Window Help

11/0 Cols

Design Custom Design

- Source
- Model
- Generalized Regression

Columns (12/0)

Polymer B *

Total Polymer *

Compression Force *

Dissolution 60 Mean

Dissolution 120 Mean

Dissolution 240 Mean

Dissolution 360 Mean

Rows

All rows 17

Selected 0

Excluded 1

Hidden 1

Labeled 0

	Set	Batch	DoE Setting ID	Polymer A	Polymer B	Total Polymer	Compression Force	Dissolution 60 Mean	Dissolution 120 Mean	Dissolution 240 Mean	Dissolution 360 Mean
1	R	R01	21.13	37.60	65.22	77.62
2	A	A01	1	0.825	0.175	0.16	2500	17.63	27.28	43.58	54.97
3	A	A02	2	0.775	0.225	0.14	2500	21.88	37.73	60.37	74.83
4	A	A03	3	0.725	0.275	0.14	1500	32.10	60.15	81.43	86.83
5	A	A04	4	0.775	0.225	0.18	1500	26.43	47.83	68.72	76.13
6	A	A05	5	0.875	0.125	0.16	1500	46.13	61.82	73.53	81.60
7	A	A06	6	0.775	0.225	0.18	2500	8.67	19.80	42.60	56.50
8	A	A07	7	0.775	0.225	0.18	1500	25.30	40.47	62.48	72.67
9	A	A08	8	0.825	0.175	0.12	2500	40.57	55.52	72.55	84.47
10	A	A09	9	0.825	0.175	0.12	2500	40.23	53.60	73.72	85.93
11	A	A10	10	0.875	0.125	0.16	2500	25.85	37.38	52.25	63.60
12	A	A11	11	0.875	0.125	0.16	1500	50.68	64.18	78.62	88.02
13	A	A12	12	0.825	0.175	0.12	1500	50.98	67.50	86.53	97.42
14	A	A13	13	0.725	0.275	0.14	2500	20.33	38.93	65.77	74.55
15	A	A14	14	0.725	0.275	0.14	1500	40.70	69.63	84.43	86.45
16	A	A15	15	0.775	0.225	0.18	2500	8.35	20.47	43.10	58.28
17	A	A16	16	0.825	0.175	0.12	1500	52.00	68.40	87.22	97.57

f2 DoE Analysis

$$50 \cdot \text{Log}_{10} \left(100 \cdot \left(1 + \frac{1}{4} \cdot \left(\begin{aligned} & \left(\text{Dissolution 60 Mean} - 21.13 \right)^2 \\ & + \left(\text{Dissolution 120 Mean} - 37.6 \right)^2 \\ & + \left(\text{Dissolution 240 Mean} - 65.22 \right)^2 \\ & + \left(\text{Dissolution 360 Mean} - 77.62 \right)^2 \end{aligned} \right) \right)^{-0.5}$$

f2 DoE Analysis

Dissolution DoE Summarized - JMP

File Edit Tables Rows Cols DOE Analyze Graph Tools Add-Ins View Window Help

Design Custom Design
 Source
 Model
 Generalized Regression

Columns (12/0)
 Polymer B *
 Total Polymer *
 Compression Force *
 Dissolution 60 Mean
 Dissolution 120 Mean
 Dissolution 240 Mean
 Dissolution 360 Mean

Rows
 All rows 17
 Selected 0
 Excluded 1
 Hidden 1
 Labeled 0

	Set	Batch	DoE Setting ID	Polymer A	Polymer B	Total Polymer	Compression Force	Dissolution 60 Mean	Dissolution 120 Mean	Dissolution 240 Mean	Dissolution 360 Mean	f2
1	R	R01						21.13	37.60	65.22	77.62	100
2	A	A01	1	0.825	0.175	0.16	2500	17.63	27.28	43.58	54.97	38.98
3	A	A02	2	0.775	0.225	0.14	2500	21.88	37.73	60.37	74.83	76.17
4	A	A03	3	0.725	0.275	0.14	1500	32.10	60.15	81.43	86.83	40.26
5	A	A04	4	0.775	0.225	0.18	1500	26.43	47.83	68.72	76.13	60.56
6	A	A05	5	0.875	0.125	0.16	1500	46.13	61.82	73.53	81.60	37.2
7	A	A06	6	0.775	0.225	0.18	2500	8.67	19.80	42.60	56.50	36.14
8	A	A07	7	0.775	0.225	0.18	1500	25.30	40.47	62.48	72.67	70.31
9	A	A08	8	0.825	0.175	0.12	2500	40.57	55.52	72.55	84.47	42.43
10	A	A09	9	0.825	0.175	0.12	2500	40.23	53.60	73.72	85.93	42.94
11	A	A10	10	0.875	0.125	0.16	2500	25.85	37.38	52.25	63.60	50.24
12	A	A11	11	0.875	0.125	0.16	1500	50.68	64.18	78.62	88.02	33.25
13	A	A12	12	0.825	0.175	0.12	1500	50.98	67.50	86.53	97.42	29.53
14	A	A13	13	0.725	0.275	0.14	2500	20.33	38.93	65.77	74.55	84.86
15	A	A14	14	0.725	0.275	0.14	1500	40.70	69.63	84.43	86.45	33.31
16	A	A15	15	0.775	0.225	0.18	2500	8.35	20.47	43.10	58.28	37
17	A	A16	16	0.825	0.175	0.12	1500	52.00	68.40	87.22	97.57	28.92

f2 DoE Analysis

The screenshot shows the 'Fit Model' dialog box in JMP, titled 'Fit Model - JMP'. The 'Model Specification' section is expanded, showing the following settings:

- Select Columns:** A list of 12 columns is shown, including 'Set', 'Batch', 'DoE Setting ID', 'Polymer A', 'Polymer B', 'Total Polymer', 'Compression Force', 'Dissolution 60 Mean', 'Dissolution 120 Mean', 'Dissolution 240 Mean', 'Dissolution 360 Mean', and 'f2'. The 'f2' column is selected.
- Pick Role Variables:** The response variable 'Y' is 'f2' (optional). The 'Freq' variable is 'optional numeric'. The 'Validation' variable is 'optional numeric'. The 'Censor' variable is 'optional'. The 'By' variable is 'optional'.
- Personality:** 'Generalized Regression'.
- Distribution:** 'Normal'.
- Censor Code:** An empty field with a dropdown arrow.
- Buttons:** 'Help', 'Run', 'Recall', and 'Remove'.
- Keep dialog open:** An unchecked checkbox.
- Construct Model Effects:** A list of effects is shown, including 'Polymer A & Mixture', 'Polymer B & Mixture', 'Polymer A*Total Polymer', 'Polymer A*Compression Force', 'Polymer B*Total Polymer', 'Polymer B*Compression Force', and 'Total Polymer*Compression Force'. The 'Degree' is set to 2. The 'Attributes' and 'Transform' checkboxes are unchecked. The 'No Intercept' checkbox is checked.

f2 DoE Analysis

Dissolution DoE Summarized - Generalized Regression - JMP

File Edit Tables Rows Cols DOE Analyze Graph Tools Add-Ins View Window Help

Generalized Regression for f2

Model Comparison

Show	Response Distribution	Estimation Method	Validation Method	Nonzero Parameters	AICc	BIC	Generalized RSquare
<input checked="" type="checkbox"/>	Normal	Standard Least Squares	None	8	155.59517	141.20445	0.6447116

Model Launch

Response Distribution: Normal

Estimation Method: Forward Selection

Advanced Controls

Validation Method: AICc

Early Stopping

Go

Standard Least Squares

Model Summary

Response	f2
Distribution	Normal
Estimation Method	Standard Least Squares
Validation Method	None
Mean Model Link	Identity
Scale Model Link	Identity

f2 DoE Analysis

Dissolution DoE Summarized - Generalized Regression - JMP

File Edit Tables Rows Cols DOE Analyze Graph Tools Add-Ins View Window Help

Generalized Regression for f2

Model Comparison

Show	Response Distribution	Estimation Method	Validation Method	Nonzero Parameters	AICc	BIC	Generalized RSquare
<input checked="" type="checkbox"/>	Normal	Standard Least Squares	None	8	155.59517	141.20445	0.6447116

Model Launch

Response Distribution
Normal

Estimation Method
Forward Selection
Standard Least Squares
Backward Elimination
Forward Selection
Pruned Forward Selection
Best Subset
Two Stage Forward Selection
SVEM-FS
Dantzig Selector
Lasso
Elastic Net
Ridge
Double Lasso
SVEM-Lasso

Mean Model Link Identity
Scale Model Link Identity

f2 DoE Analysis

Dissolution DoE Summarized - Generalized Regression - JMP

File Edit Tables Rows Cols DOE Analyze Graph Tools Add-Ins View Window Help

Generalized Regression for f2

Model Comparison

Show	Response Distribution	Estimation Method	Validation Method	Nonzero Parameters	AICc	BIC	Generalized RSquare
<input checked="" type="checkbox"/>	Normal	Standard Least Squares	None	8	155.59517	141.20445	0.6447116
<input checked="" type="checkbox"/>	Normal	Best Subset	AICc	5	136.86076	134.7237	0.6014858

Model Launch

Response Distribution
Normal

Estimation Method
Best Subset

Advanced Controls

Validation Method
AICc

Early Stopping

Go

f2 DoE Analysis

Dissolution DoE Summarized - Generalized Regression - JMP

File Edit Tables Rows Cols DOE Analyze Graph Tools Add-Ins View Window Help

Generalized Regression for f2

Model Comparison

Show	Response Distribution	Estimation Method	Validation Method	Nonzero Parameters	AICc	BIC	Generalized RSquare
<input checked="" type="checkbox"/>	Normal	Standard Least Squares	None	8	155.59517	141.20445	0.6447116
<input checked="" type="checkbox"/>	Normal	Best Subset	AICc	5	136.86076	134.7237	0.6014858

Model Launch

Response Distribution

- Normal
- Normal
- Cauchy
- t(5)
- Exponential
- Gamma
- Weibull
- LogNormal**
- Negative LogNormal
- Beta
- Quantile Regression
- Cox Proportional Hazards

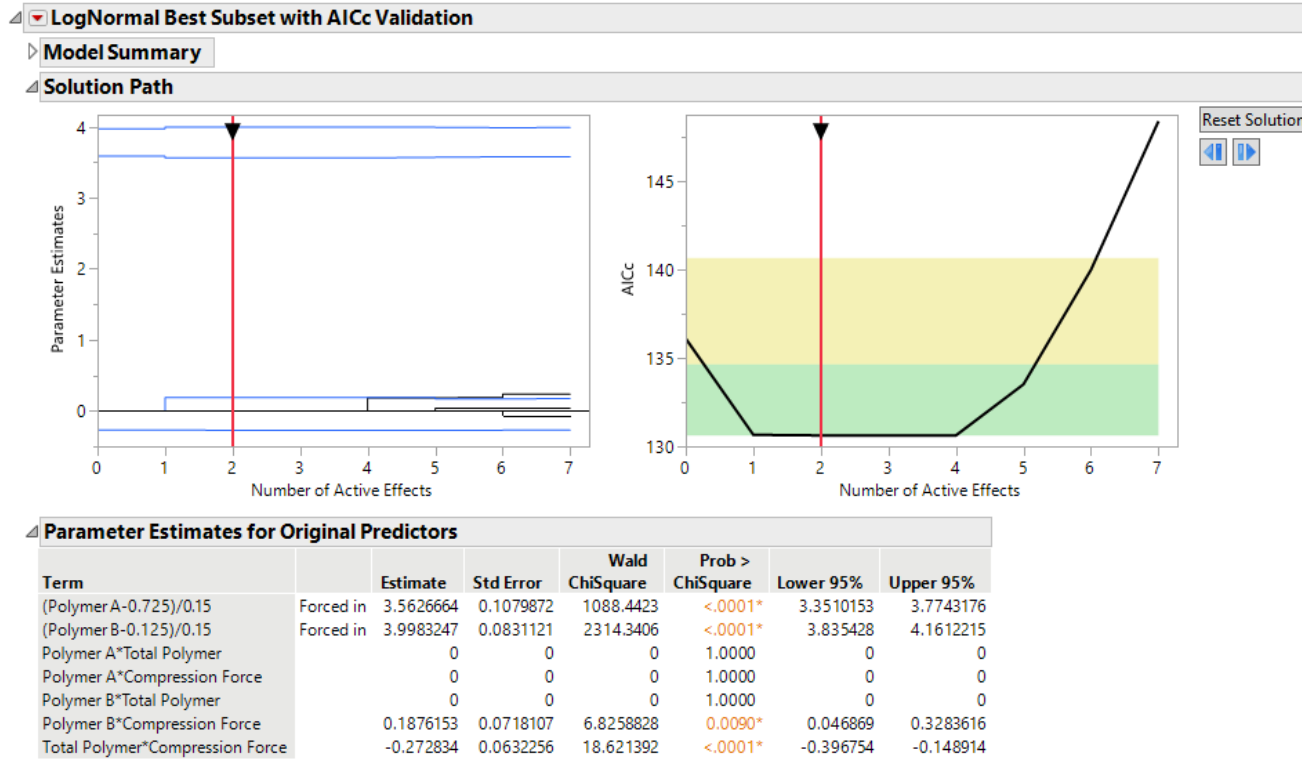
f2 DoE Analysis

Generalized Regression for f2

Model Comparison

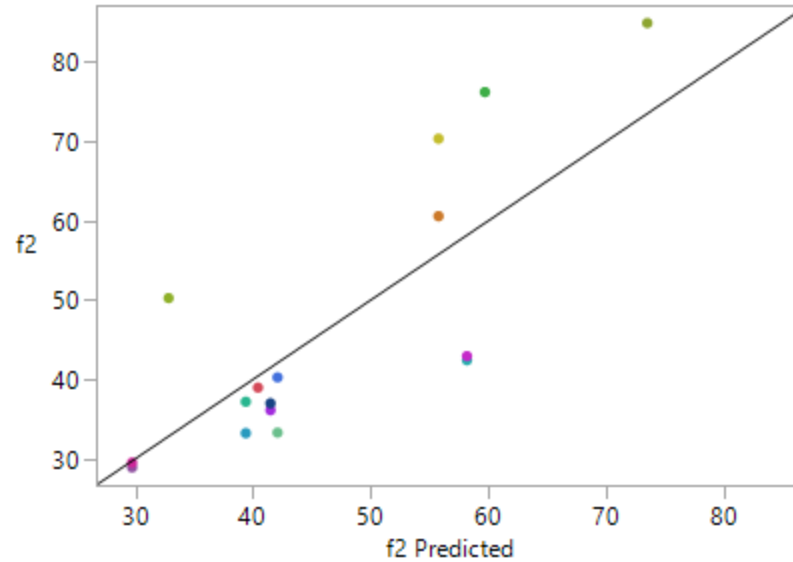
Show	Response Distribution	Estimation Method	Validation Method	Nonzero Parameters	AICc	BIC	Generalized RSquare
<input checked="" type="checkbox"/>	Normal	Standard Least Squares	None	8	155.59517	141.20445	0.6447116
<input checked="" type="checkbox"/>	Normal	Best Subset	AICc	5	136.86076	134.7237	0.6014858
<input checked="" type="checkbox"/>	LogNormal	Best Subset	AICc	5	130.6234	128.48635	0.9972659

f2 DoE Analysis

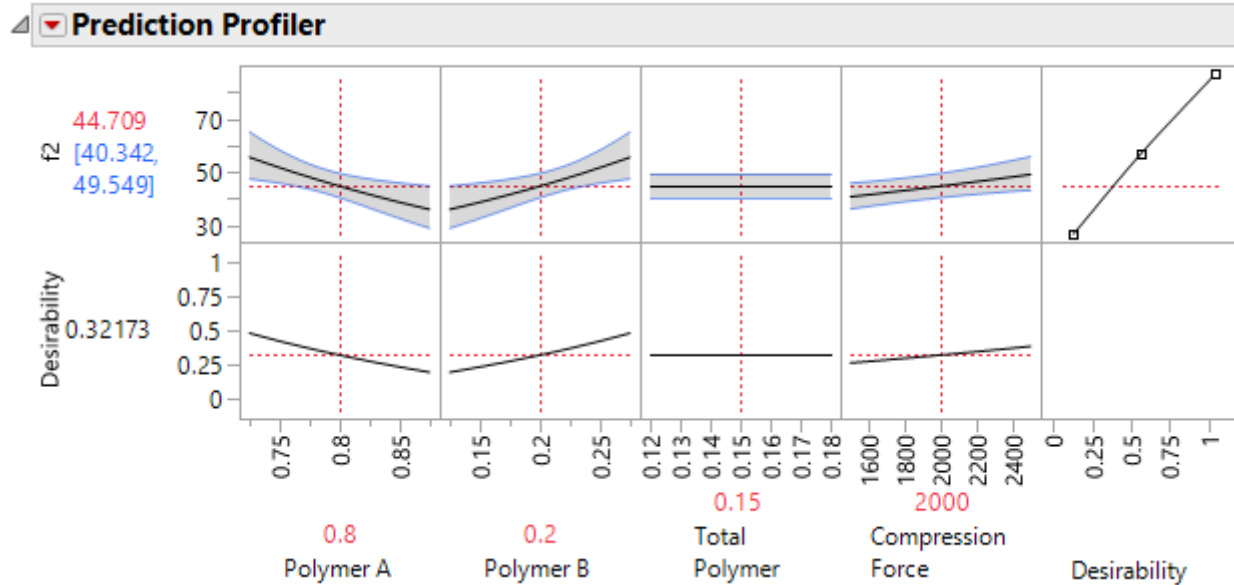


f2 DoE Analysis

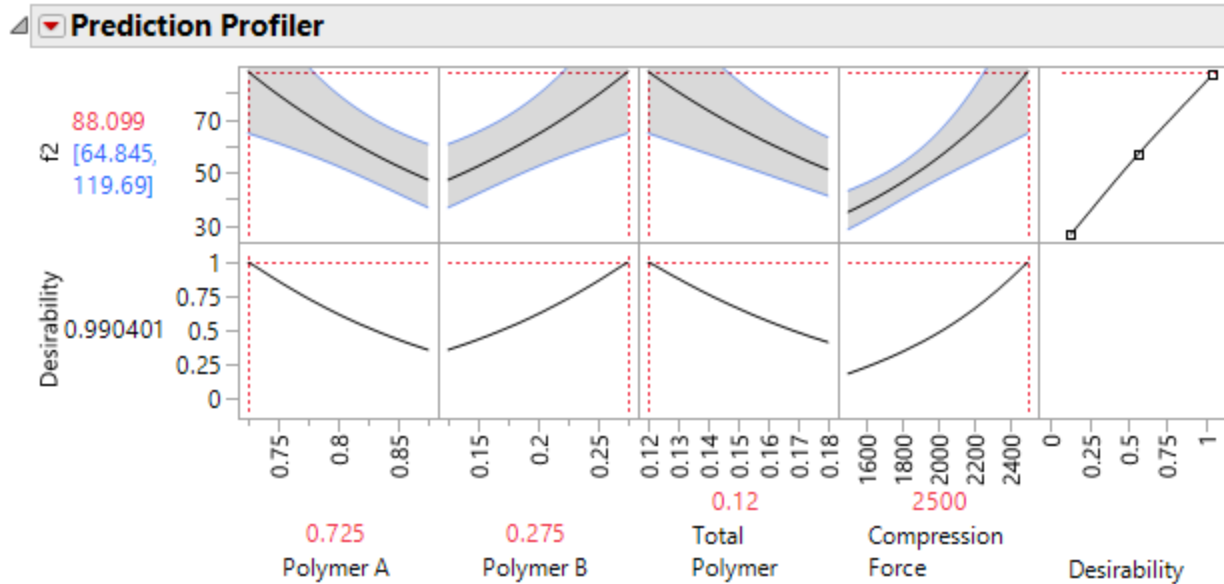
Actual by Predicted Plot



f2 DoE Analysis



f2 DoE Analysis



Functional DoE Analysis (FDA)

Dissolution DoE - JMP

File Edit Tables Rows Cols DOE Analyze Graph Tools Add-Ins View Window Help

Design Custom Design
Model
Generalized Regression

Columns (9/0)

- Set
- Batch
- Tablet
- Polymer A *
- Polymer B *
- Total Polymer *
- Compression Force *
- Time
- Dissolution

	Set	Batch	Tablet	Polymer A	Polymer B	Total Polymer	Compression Force	Time	Dissolution	
•	1	A	A01	1	0.825	0.175	0.16	2500	60	17.0
•	2	A	A01	1	0.825	0.175	0.16	2500	120	26.7
•	3	A	A01	1	0.825	0.175	0.16	2500	240	39.6
•	4	A	A01	1	0.825	0.175	0.16	2500	360	54.6
•	5	A	A01	2	0.825	0.175	0.16	2500	60	22.3
•	6	A	A01	2	0.825	0.175	0.16	2500	120	25.9
•	7	A	A01	2	0.825	0.175	0.16	2500	240	44.8
•	8	A	A01	2	0.825	0.175	0.16	2500	360	57.5
•	9	A	A01	3	0.825	0.175	0.16	2500	60	12.7
•	10	A	A01	3	0.825	0.175	0.16	2500	120	28.5
•	11	A	A01	3	0.825	0.175	0.16	2500	240	45.1
•	12	A	A01	3	0.825	0.175	0.16	2500	360	52.9

Functional DoE Analysis (FDA)

The screenshot shows the JMP software interface for a 'Dissolution DoE' project. The 'Analyze' menu is open, and 'Functional Data Explorer' is selected under the 'Specialized Modeling' submenu. A tooltip for 'Functional Data Explorer' is visible, stating: 'Explores and processes functional data, observed across a set of equally or unequally spaced points.'

The background data table is as follows:

Tablet	Polymer A	Polymer B	Total Polymer	Compression Force	Time	Dissolution
1	0.825	0.175	0.16	2500	60	17.0
				2500	120	26.7
				2500	240	39.6
				2500	360	54.6
				2500	360	57.5
				2500	60	12.7
				2500	120	28.5
				2500	240	45.1
				2500	360	52.9

Functional DoE Analysis (FDA)

Functional Data Explorer - JMP

Stacked Data Format Rows as Functions Columns as Functions

Stacked data format.

Select Columns

▼ 9 Columns

- Set
- Batch
- Tablet
- Polymer A
- Polymer B
- Total Polymer
- Compression Force
- Time
- Dissolution

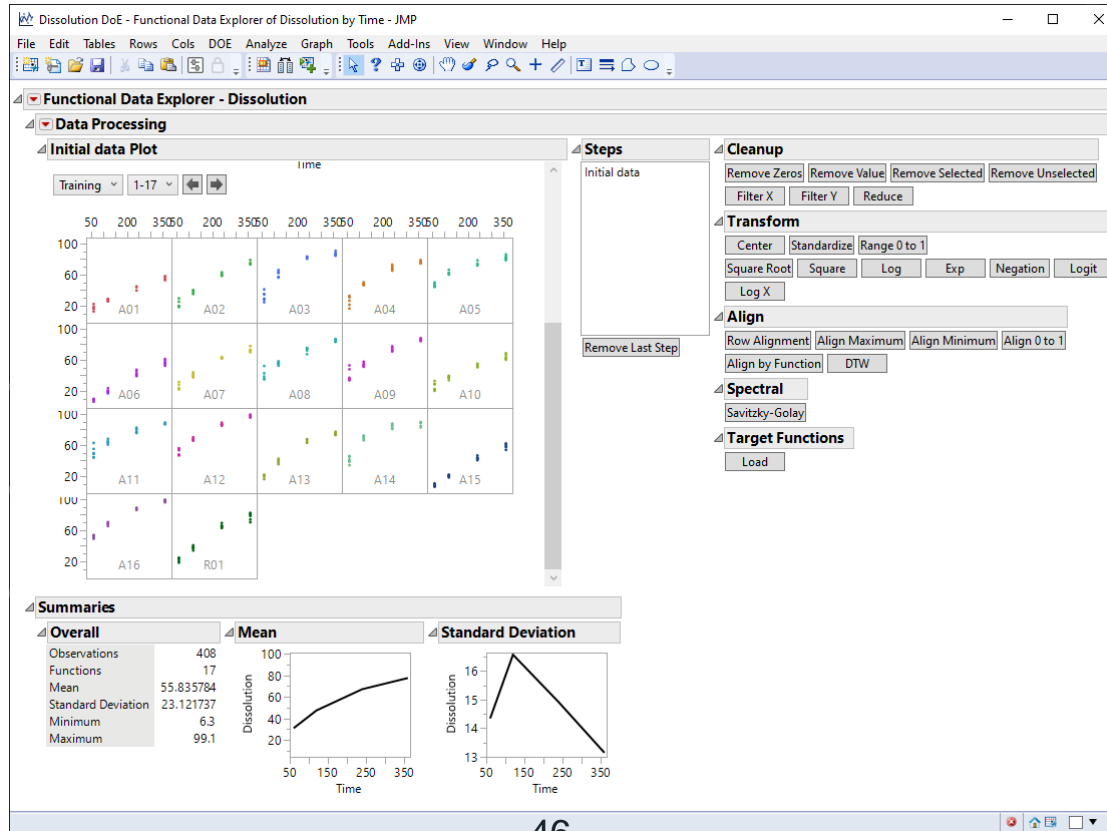
Cast Selected Columns into Roles

- Y, Output: Dissolution (optional numeric)
- X, Input: Time
- ID, Function: Batch
- Z, Supplementary: Polymer A, Polymer B, Total Polymer, Compression Force
- Freq: optional numeric
- Validation: optional numeric
- By: optional

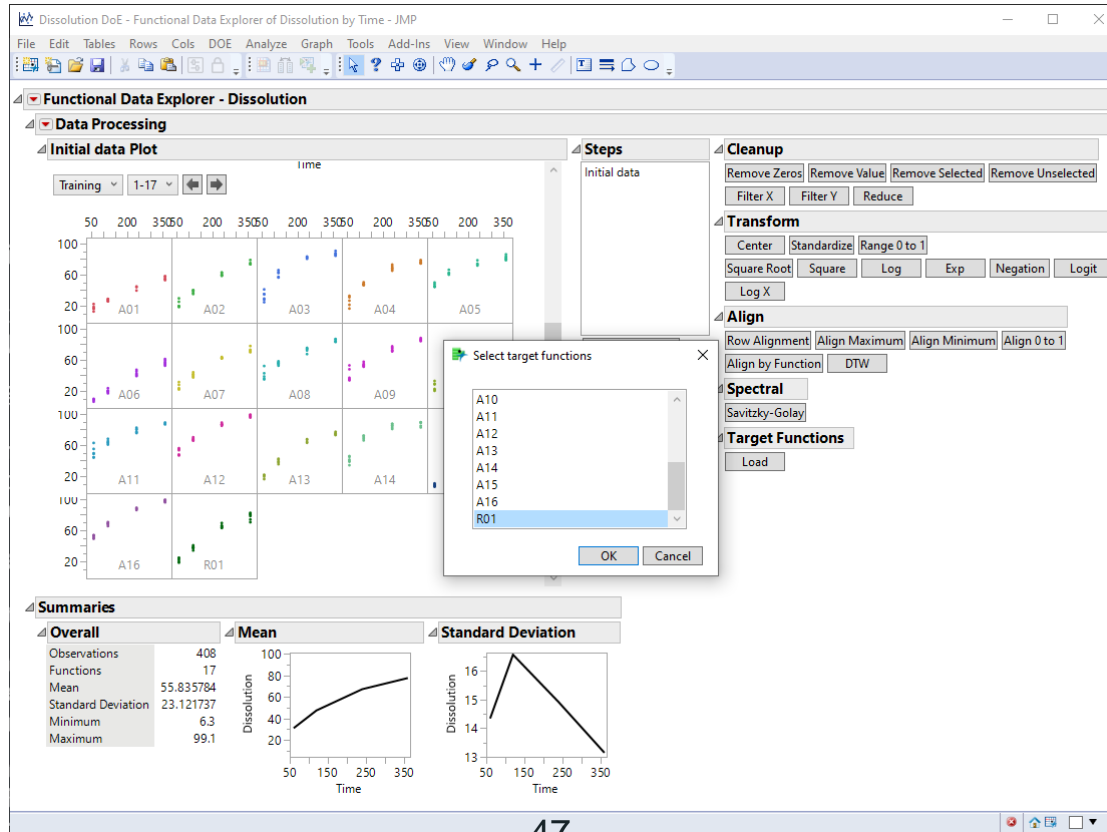
Action

- OK
- Cancel
- Remove
- Recall
- Help

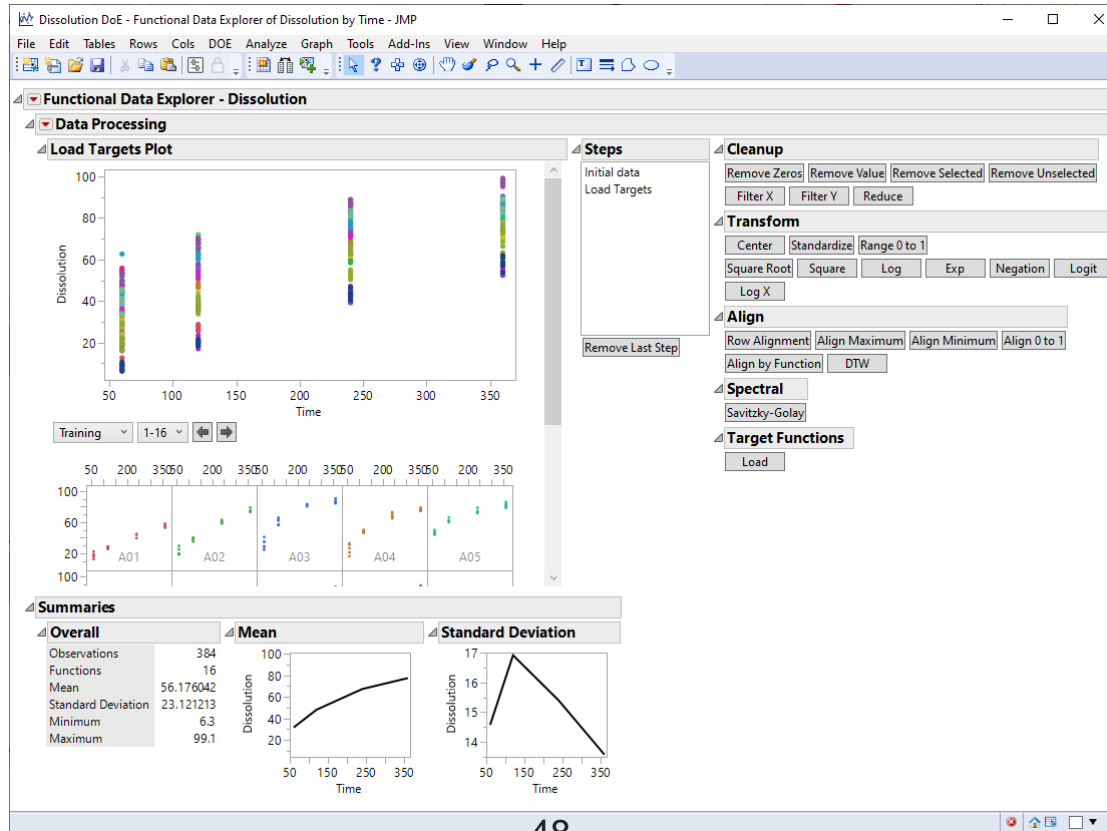
Functional DoE Analysis (FDA)



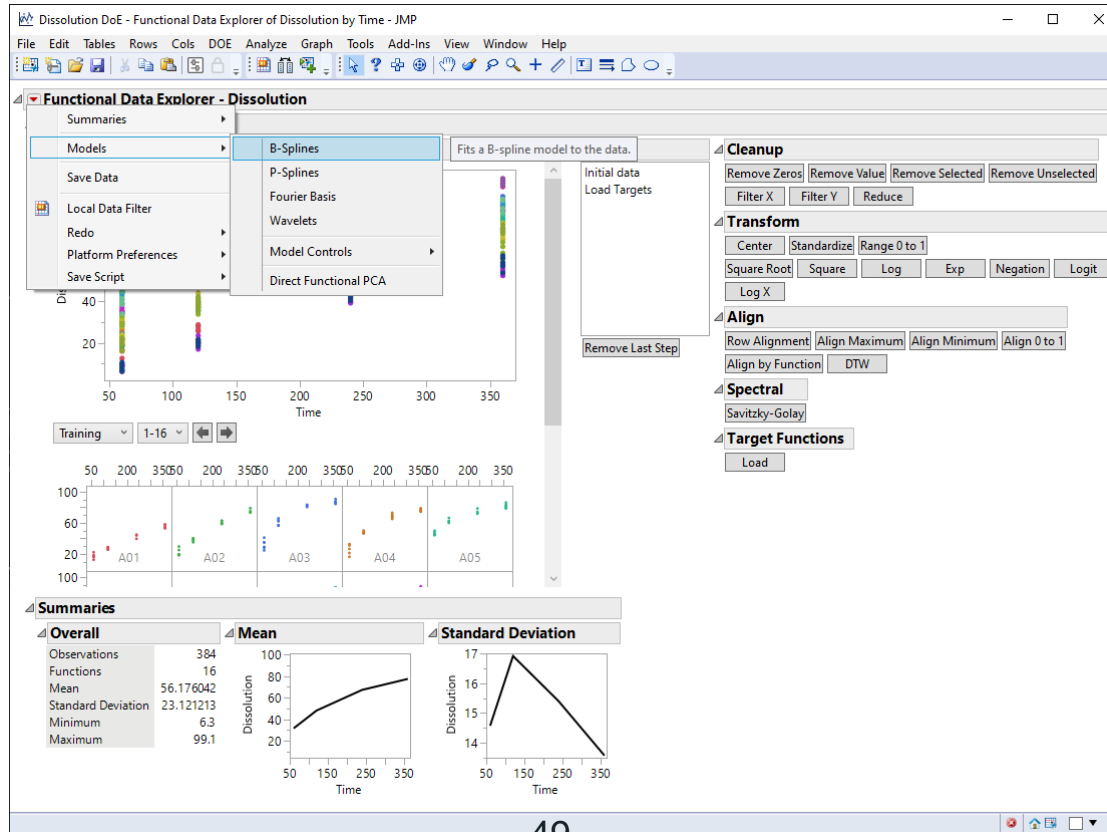
Functional DoE Analysis (FDA)



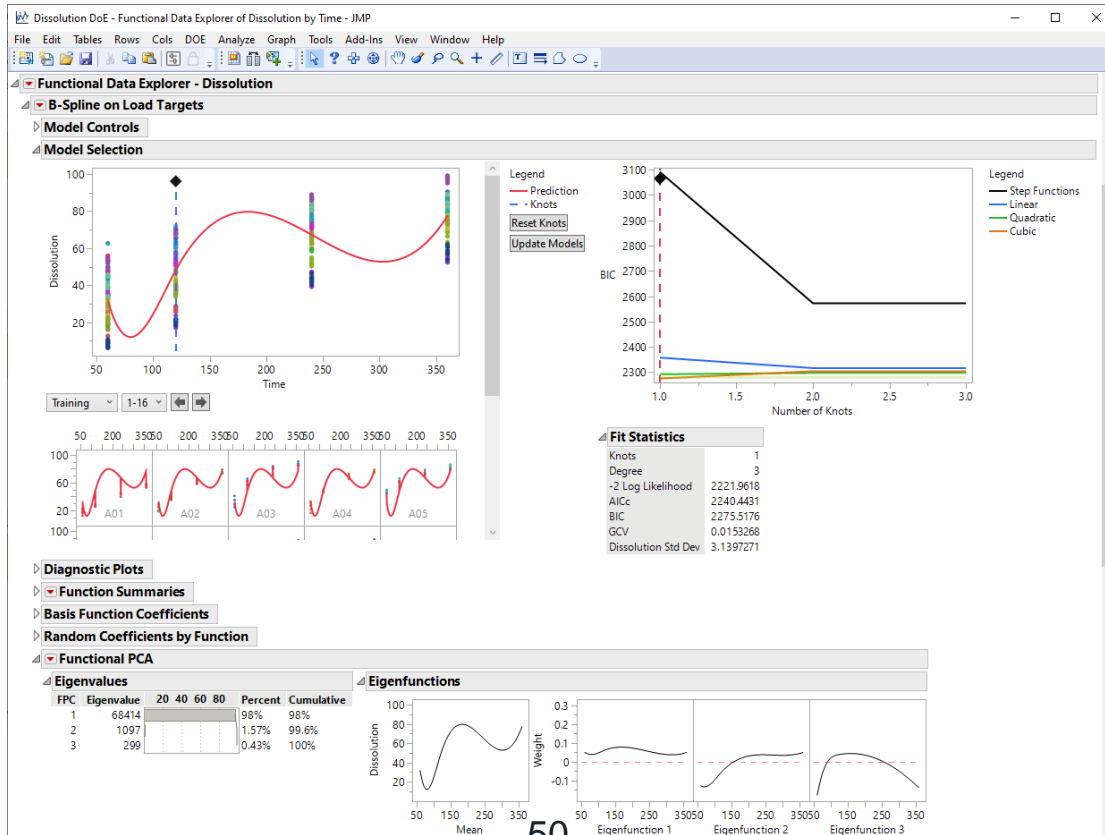
Functional DoE Analysis (FDA)



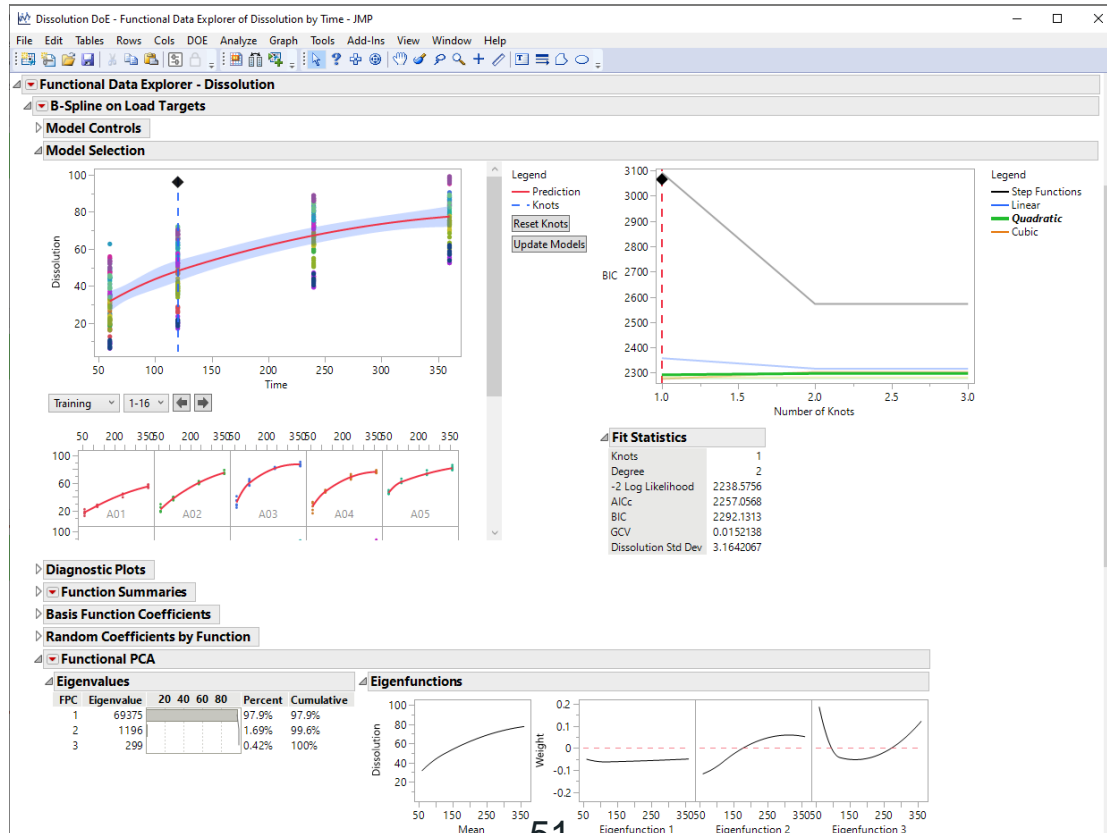
Functional DoE Analysis (FDA)



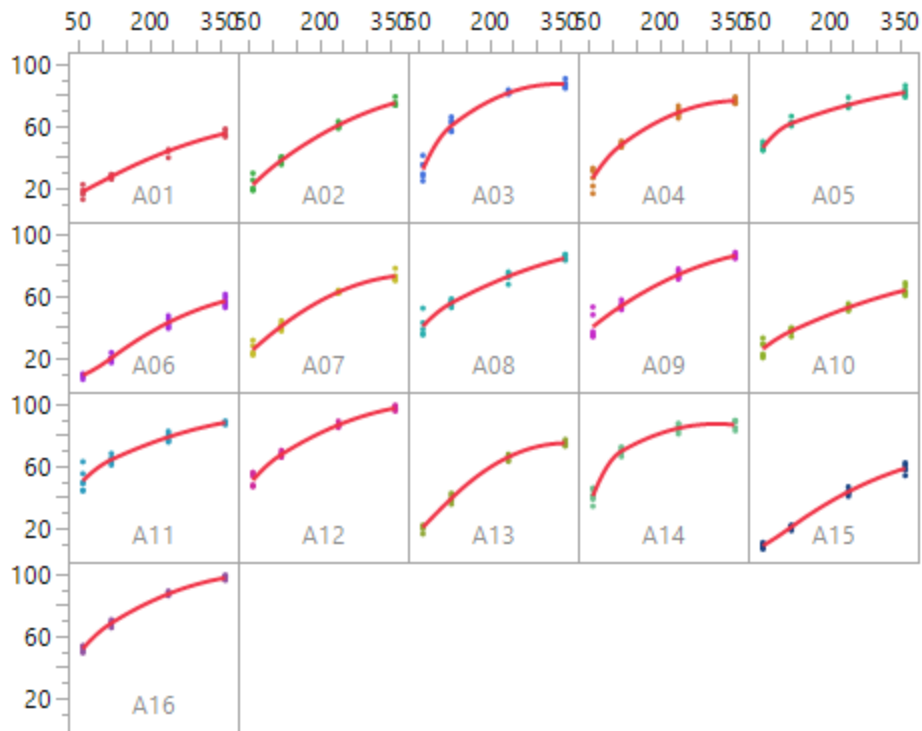
Functional DoE Analysis (FDA)



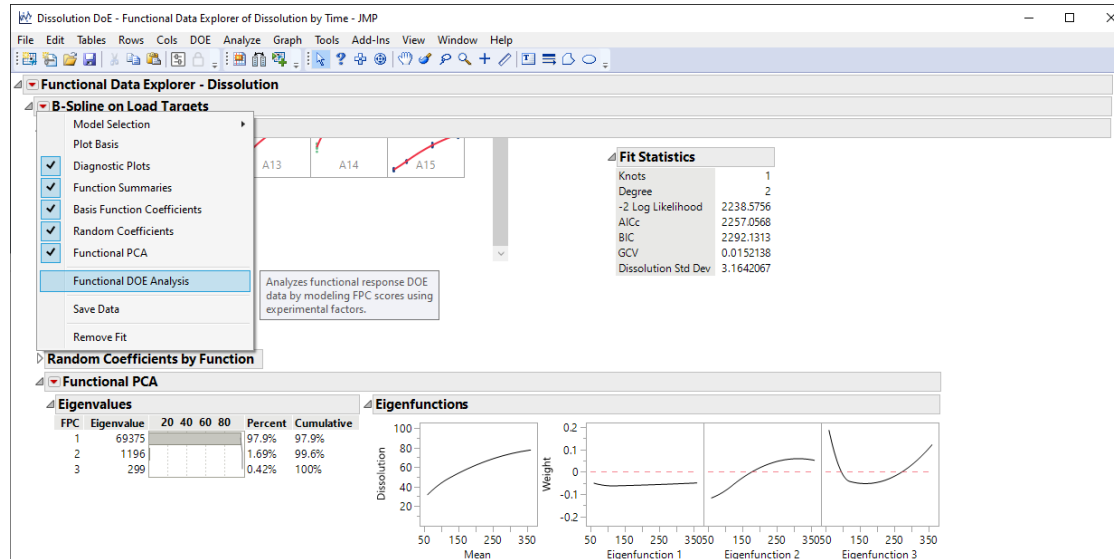
Functional DoE Analysis (FDA)



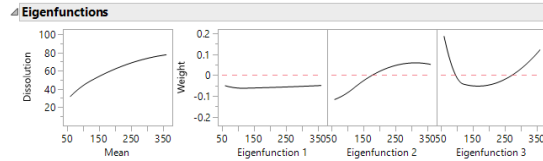
Functional DoE Analysis (FDA)



Functional DoE Analysis (FDA)



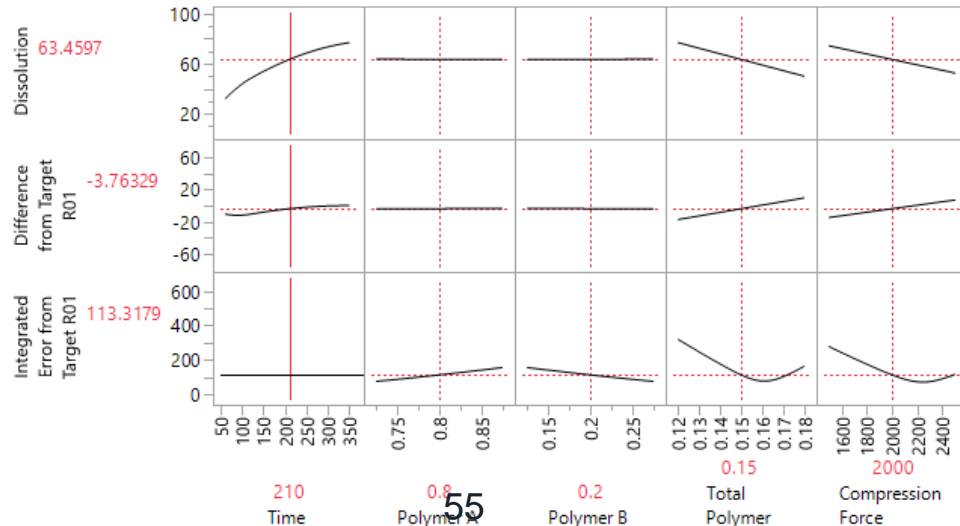
Functional DoE Analysis (FDA)



	Batch	Polymer A	Polymer B	Total Polymer	Compression Force	Dissolution FPC 1	Dissolution FPC 2	Dissolution FPC 3
1	A01	0.825	0.175	0.16	2500	377	-48.5	-5.36
2	A02	0.775	0.225	0.14	2500	131.6	32.75	11.98
3	A03	0.725	0.275	0.14	1500	-204	37.78	-26.7
4	A04	0.775	0.225	0.18	1500	-1.15	17.76	-18.2
5	A05	0.875	0.125	0.16	1500	-151	-61	-3.16
6	A06	0.775	0.225	0.18	2500	432.5	11.24	2.479
7	A07	0.775	0.225	0.18	1500	99.93	16.71	-1.11
8	A08	0.825	0.175	0.12	2500	-109	-11.6	13.62
9	A09	0.825	0.175	0.12	2500	-111	10.64	19.92
10	A10	0.875	0.125	0.16	2500	221.6	-50.2	-1.52
11	A11	0.875	0.125	0.16	1500	-226	-37.6	11.74
12	A12	0.825	0.175	0.12	1500	-331	13.58	20.37
13	A13	0.725	0.275	0.14	2500	82.16	59.97	-8.43
14	A14	0.725	0.275	0.14	1500	-290	-17.8	-40.6
15	A15	0.775	0.225	0.18	2500	421.2	15.66	5.832
16	A16	0.825	0.175	0.12	1500	-343	10.7	19.15

Functional DoE Analysis (FDA)

- Functional DOE Analysis
 - Generalized Regression for FPC Scores
 - Generalized Regression for Dissolution FPC 1
 - Generalized Regression for Dissolution FPC 2
 - Generalized Regression for Dissolution FPC 3
 - Diagnostic Plots
 - FDOE Profiler



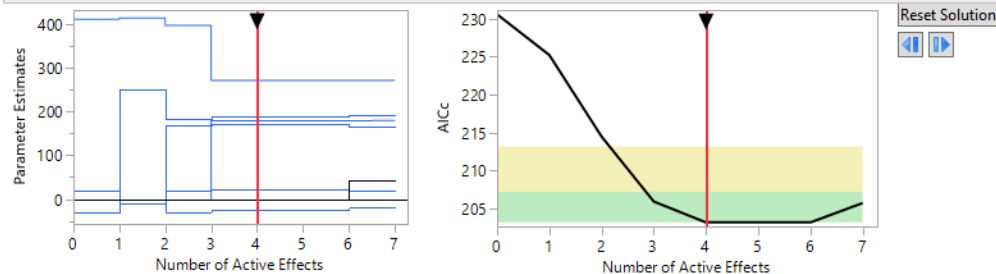
Functional DoE Analysis (FDA)

Generalized Regression for FPC Scores

Generalized Regression for Dissolution FPC 1

Normal Best Subset with AICc Validation

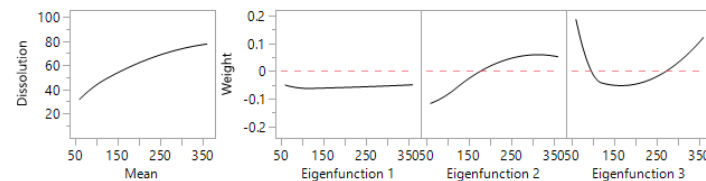
Solution Path



Parameter Estimates for Original Predictors

Term	Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%	
(Polymer A-0.725)/0.15	Forced in -23.91645	26.485753	0.8153964	0.3665	-75.82757	27.994671	
(Polymer B-0.125)/0.15	Forced in 21.35432	15.16401	1.9830943	0.1591	-8.366594	51.075233	
Polymer A*Total Polymer	179.73706	52.22562	11.844263	0.0006*	77.376723	282.09739	
Polymer A*Compression Force	188.51742	26.823659	49.393171	<.0001*	135.94401	241.09082	
Polymer B*Total Polymer	271.97377	36.417342	55.774737	<.0001*	200.59709	343.35044	
Polymer B*Compression Force	170.45066	15.599615	119.39045	<.0001*	139.87598	201.02535	
Total Polymer*Compression Force	0	0	0	1.0000	0	0	
Normal Distribution Parameters		Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%
Scale		73.066154	18.560994	15.496372	<.0001*	36.687275	109.44503

Eigenfunctions



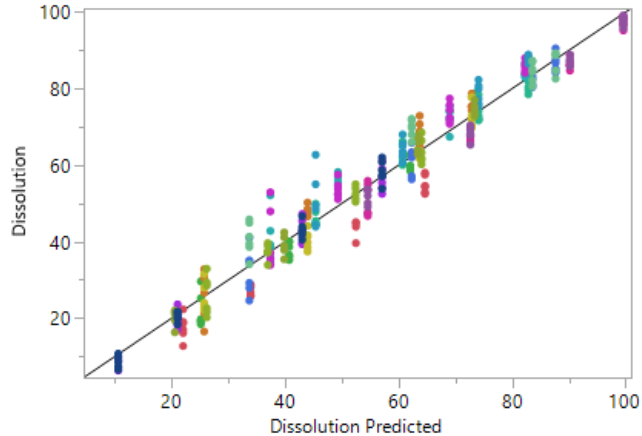
Generalized Regression for Dissolution FPC 2

Generalized Regression for Dissolution FPC 3

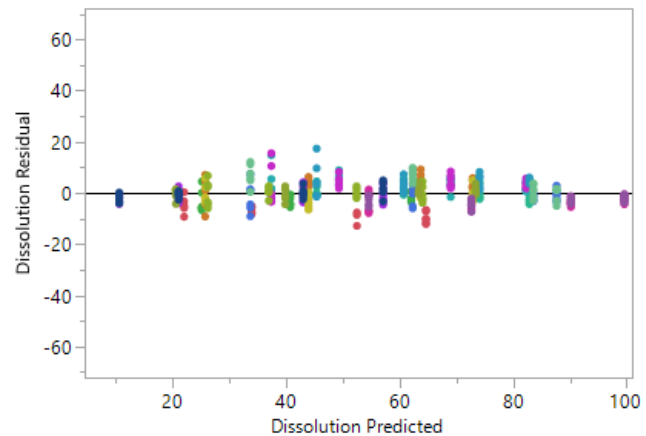
Functional DoE Analysis (FDA)

Diagnostic Plots

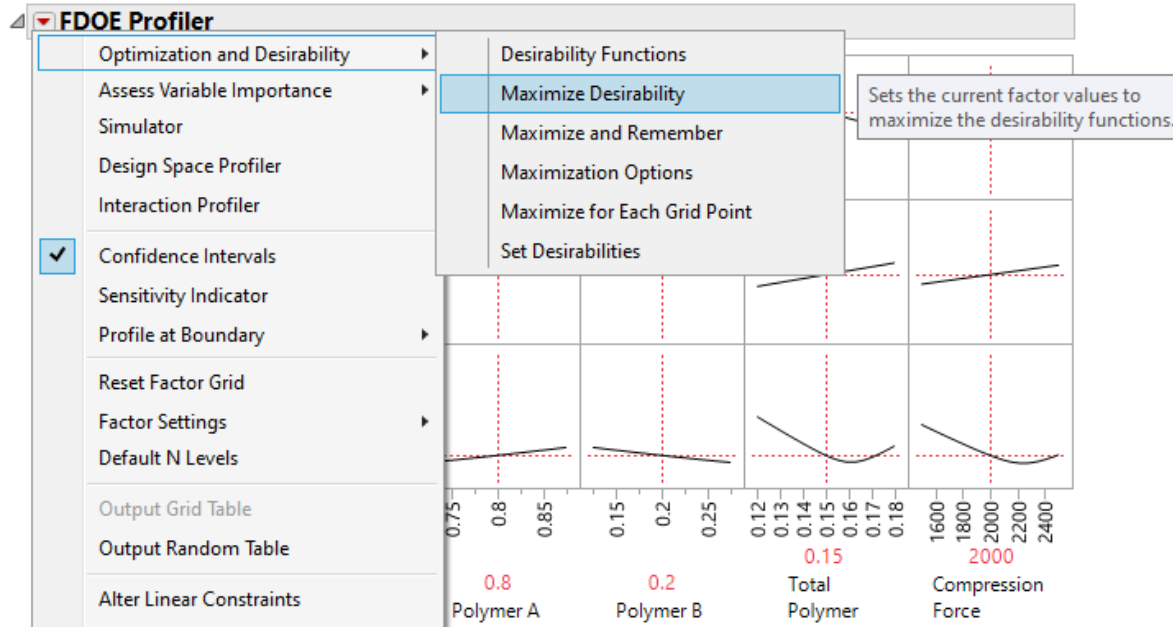
Actual by Predicted Plot



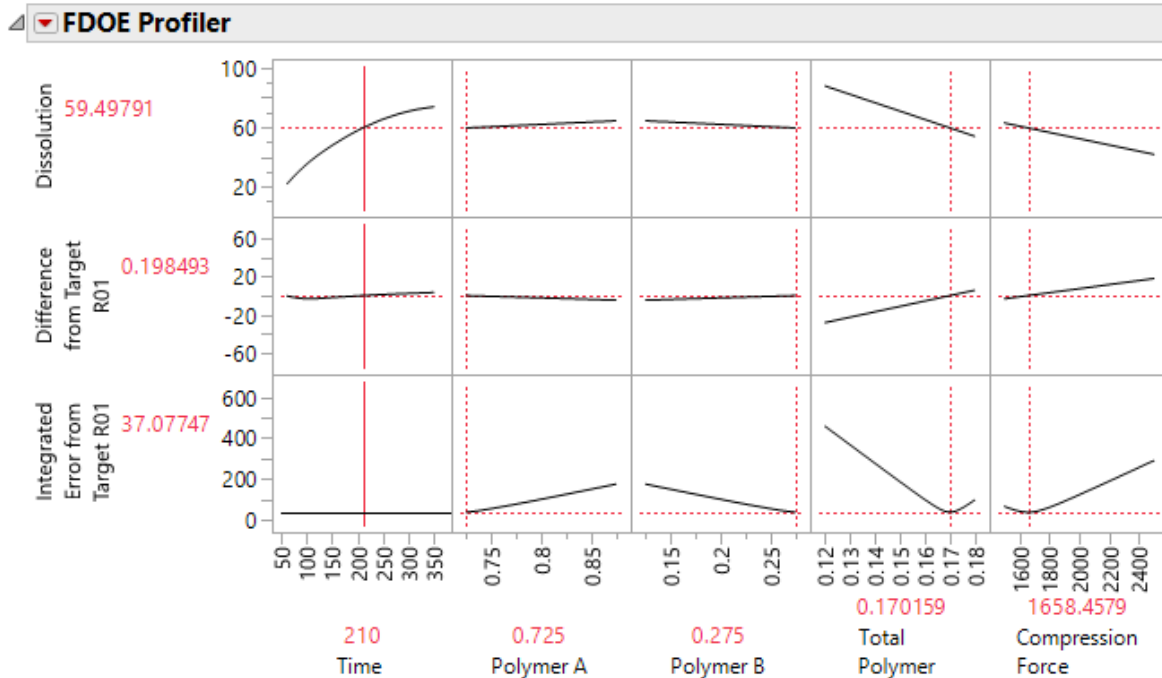
Residual by Predicted Plot



Functional DoE Analysis (FDA)



Functional DoE Analysis (FDA)



Functional DoE Analysis (FDA)

Formulation	Polymer A	Polymer B	Total Polymer	Compression Force
f2	0.725	0.275	0.12	2500
FDoE	0.725	0.275	0.17	1700

Curve DoE Analysis (NLR)

- 1) Fit the reference batch, save prediction formula
- 2) Curve DoE analysis of the design data, save prediction formula
- 3) Use Graph<<Profiler to find settings that best match the reference

Curve DoE Analysis (NLR)

▾ Weibull Growth

▾ Prediction Model

$$a \cdot \left(1 - \text{Exp} \left(- \left(\frac{\text{Time}}{b} \right)^c \right) \right)$$

a = Asymptote

b = Inflection Point

c = Growth Rate

Langenbucher, F. Letters to the Editor: Linearization of dissolution rate curves by the Weibull distribution. *J. Pharm. Pharmacol.* 1972, 24 (12), 979–981.

Curve DoE Analysis (NLR)

	Batch	Polymer A	Polymer B	Total Polymer	Compression Force	Asymptote	Inflection Point	Growth Rate
1	A01	0.825	0.175	0.16	2500	149.8	1043	0.733
2	A02	0.775	0.225	0.14	2500	104.7	282.5	0.938
3	A03	0.725	0.275	0.14	1500	87.08	107.5	1.311
4	A04	0.775	0.225	0.18	1500	78.78	128.1	1.17
5	A05	0.875	0.125	0.16	1500	91.69	104.5	0.622
6	A06	0.775	0.225	0.18	2500	68.95	248.1	1.454
7	A07	0.775	0.225	0.18	1500	87.61	193.8	0.938
8	A08	0.825	0.175	0.12	2500	150.7	521.5	0.534
9	A09	0.825	0.175	0.12	2500	257.6	2221	0.493
10	A10	0.875	0.125	0.16	2500	199.4	1963	0.565
11	A11	0.875	0.125	0.16	1500	139.6	365.3	0.44
12	A12	0.825	0.175	0.12	1500	135.8	235.2	0.553
13	A13	0.725	0.275	0.14	2500	79.21	158	1.296
14	A14	0.725	0.275	0.14	1500	86.17	83.28	1.356
15	A15	0.775	0.225	0.18	2500	73.12	260.2	1.438
16	A16	0.825	0.175	0.12	1500	131.6	207.9	0.555
17	R01	•	•	•	•	90.65	199.4	1.144

Curve DoE Analysis (NLR)

Dissolution DoE - JMP

File Edit Tables Rows Cols DOE Analyze Graph Tools Add-Ins View Window Help

Design Custom Design Model

Columns (9/0)

	Set	Batch	Tablet	Polymer A	Polymer B	Total Polymer	Compression Force	Time	Dissolution
376	A	A16	4	0.825	0.175	0.12	1500	360	95.8
377	A	A16	5	0.825	0.175	0.12	1500	60	53.5
378	A	A16	5	0.825	0.175	0.12	1500	120	69.2
379	A	A16	5	0.825	0.175	0.12	1500	240	87.8
380	A	A16	5	0.825	0.175	0.12	1500	360	98.0
381	A	A16	6	0.825	0.175	0.12	1500	60	53.7
382	A	A16	6	0.825	0.175	0.12	1500	120	69.6
383	A	A16	6	0.825	0.175	0.12	1500	240	88.9
384	A	A16	6	0.825	0.175	0.12	1500	360	99.1
385	R	R01	1	60	19.7
386	R	R01	1	120	37.2
387	R	R01	1	240	63.3
388	R	R01	1	360	73.8
389	R	R01	2	60	24.2
390	R	R01	2	120	34.0
391	R	R01	2	240	64.4
392	R	R01	2	360	70.3
393	R	R01	3	60	22.0
394	R	R01	3	120	37.1
395	R	R01	3	240	65.5
396	R	R01	3	360	80.5
397	R	R01	4	60	18.4

Rows: 408 (All rows), 0 (Selected), 0 (Excluded), 0 (Hidden), 0 (Labeled)

Curve DoE Analysis (NLR)

The screenshot displays the JMP software interface for a Dissolution DoE experiment. The main window shows a table with 11 columns: Set, Batch, Tablet, Polymer A, Polymer B, Total Polymer, Compression Force, Time, and Dissolution. A context menu is open over row 381, showing options like Fill, Color Cells, Select Matching Cells, Cut, Copy, Paste, Clear, and Edit. The left sidebar shows the design structure with factors like Set, Batch, Tablet, Polymer A, Polymer B, Total Polymer, Compression Force, Time, and Dissolution. The bottom status bar shows 408 total rows, with 1 selected, 0 excluded, 0 hidden, and 0 labeled.

	Set	Batch	Tablet	Polymer A	Polymer B	Total Polymer	Compression Force	Time	Dissolution
376	A	A16	4	0.825	0.175	0.12	1500	360	95.8
377	A	A16	5	0.825	0.175	0.12	1500	60	53.5
378	A	A16	5	0.825	0.175	0.12	1500	120	69.2
379	A	A16	5	0.825	0.175	0.12	1500	240	87.8
380	A	A16	5	0.825	0.175	0.12	1500	360	98.0
381	A	A16	6	0.825	0.175	0.12	1500	60	53.7
382	A				0.175	0.12	1500	120	69.6
383	A				0.175	0.12	1500	240	88.9
384	A				0.175	0.12	1500	360	99.1
385	R							60	19.7
386	R							120	37.2
387	R							240	63.3
388	R							360	73.8
389	R							60	24.2
390	R							120	34.0
391	R							240	64.4
392	R							360	70.3
393	R	R01	3					60	22.0
394	R	R01	3					120	37.1
395	R	R01	3					240	65.5
396	R	R01	3					360	80.5
397	R	R01	4					60	18.4

Curve DoE Analysis (NLR)

Dissolution DoE - JMP

File Edit Tables Rows Cols DOE Analyze Graph Tools Add-Ins View Window Help

Design Custom Design Model

Columns (9/1)

Set Batch Tablet Polymer A Polymer B Total Polymer Compression Force Time Dissolution

Rows: All rows 408, Selected 384, Excluded 0, Hidden 0, Labeled 0

	Set	Batch	Tablet	Polymer A	Polymer B	Total Polymer	Compression Force	Time	Dissolution	
•	376	A	A16	4	0.825	0.175	0.12	1500	360	95.8
•	377	A	A16	5	0.825	0.175	0.12	1500	60	53.5
•	378	A	A16	5	0.825	0.175	0.12	1500	120	69.2
•					0.825	0.175	0.12	1500	240	87.8
•					0.825	0.175	0.12	1500	360	98.0
•					0.825	0.175	0.12	1500	60	53.7
•					0.825	0.175	0.12	1500	120	69.6
•					0.825	0.175	0.12	1500	240	88.9
•					0.825	0.175	0.12	1500	360	99.1
•									60	19.7
•									120	37.2
•									240	63.3
•									360	73.8
•									60	24.2
•									120	34.0
•									240	64.4
•									360	70.3
•									60	22.0
•									120	37.1
•	395	R	R01	3					240	65.5
•	396	R	R01	3					360	80.5
•	397	R	R01	4					60	18.4

Curve DoE Analysis (NLR)

The screenshot displays the JMP software interface for a Dissolution DoE analysis. The 'Analyze' menu is open, and 'Fit Curve' is selected under 'Specialized Modeling'. A tooltip for 'Fit Curve' states: 'Fits a variety of built-in nonlinear models.' The data table in the background has the following structure:

	Polymer A	Polymer B	Total Polymer	Compression Force	Time	Dissolution
	0.825	0.175	0.12	1500	360	95.8
				1500	60	63.3
				1500	240	81.8
				1500	360	98.0
				1500	60	53.7
				1500	120	69.6
				1500	240	88.9
				1500	360	99.1
					60	19.7
					120	37.2
					240	63.3
					360	73.8
					60	24.2
					120	34.0
					240	64.4
					360	70.3
					60	22.0
					120	37.1
					240	65.5
					360	80.5
					60	18.4

Curve DoE Analysis (NLR)

Fit Curve - JMP

Fits a variety of built-in nonlinear models.

Select Columns

- 11 Columns
- Set
- Batch
- Tablet
- Polymer A
- Polymer B
- Total Polymer
- Compression Force
- Time
- Dissolution
- CDoE Dissolution Predictor
- Reference Predictor

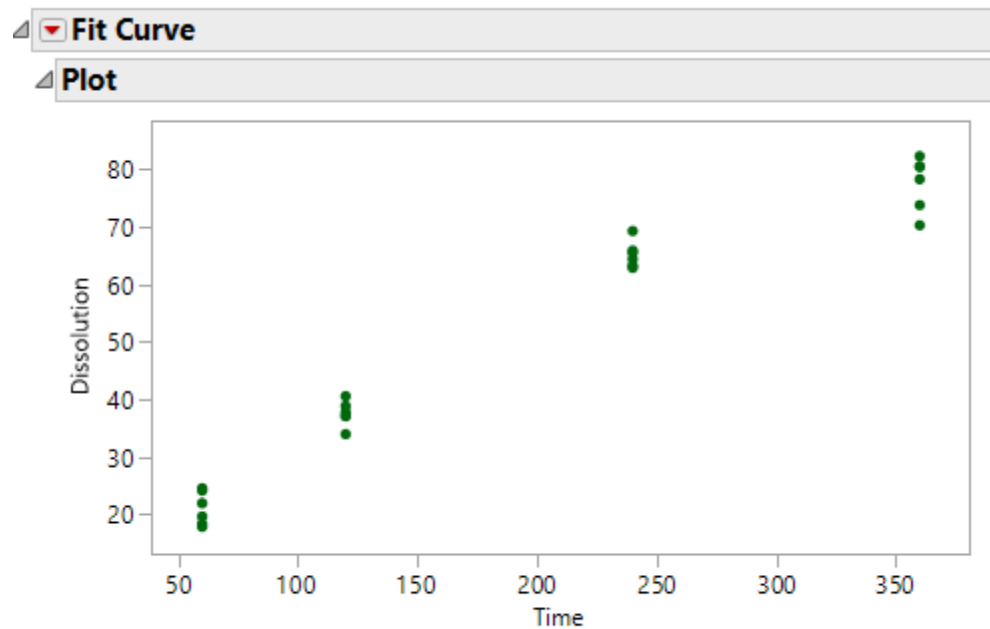
Cast Selected Columns into Roles

Role	Column
Y, Response	Dissolution
X, Regressor	Time
Group	Batch
Z, Supplementary	<i>optional</i>
Weight	<i>optional numeric</i>
Freq	<i>optional numeric</i>
By	<i>optional</i>

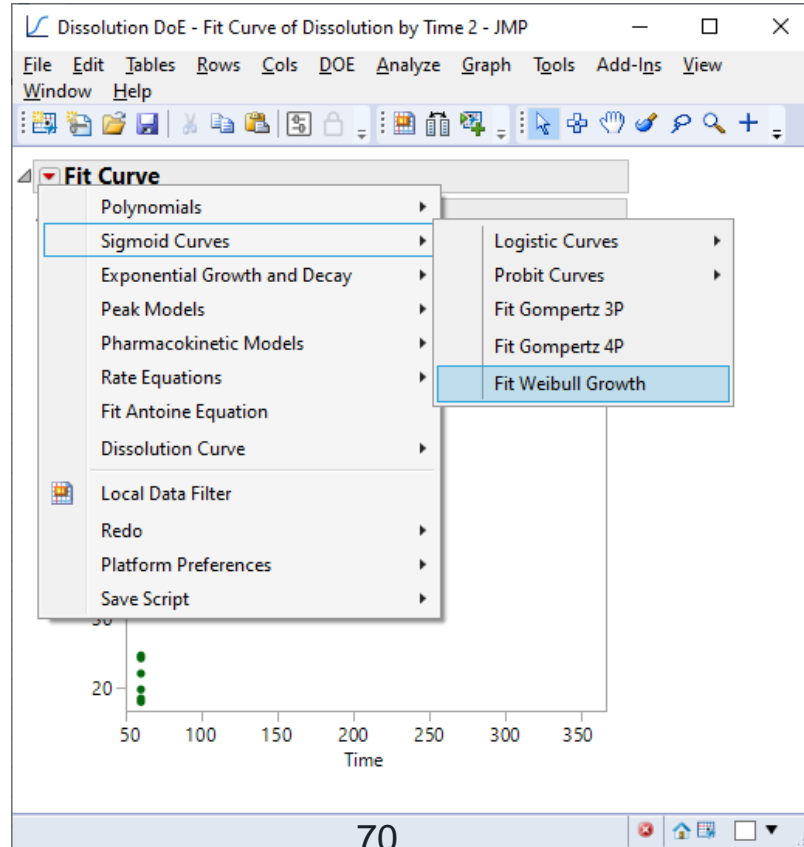
Action

- OK
- Cancel
- Remove
- Recall
- Help

Curve DoE Analysis (NLR)

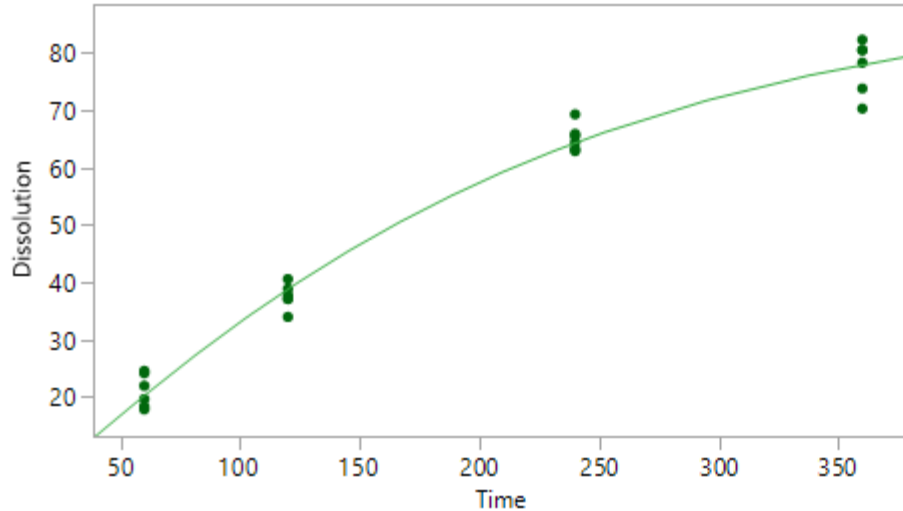


Curve DoE Analysis (NLR)



Curve DoE Analysis (NLR)

- Fit Curve
- Model Comparison
- Plot



Curve DoE Analysis (NLR)

Weibull Growth

- Plot Actual by Predicted
- Plot Residual by Predicted
- Profiler
- Save Formulas** ▶
 - Save Prediction Formula** (selected)
 - Save Std Error of Predicted
 - Save Parametric Prediction Formula
 - Save Residual Formula
 - Save Studentized Residual Formula
 - Save First Derivative
 - Save Std Error of First Derivative
 - Save Inverse Prediction Formula
- Custom Inverse Prediction
- Remove Fit













Growth Rate 1.144326 0.0998485

▶ **Correlation of Estimates**

▶ **Covariance of Estimates**

Create a new data column with current parameter estimates inserted into the prediction formula

Curve DoE Analysis (NLR)

	Set	Batch	Tablet	Polymer A	Polymer B	Total Polymer	Compression Force	Time	Dissolution	Reference Predictor	
	1	A	A01	1	0.825	0.175	0.16	2500	60	17.0	20.27
	2	A	A01	1	0.825	0.175	0.16	2500	120	26.7	38.84
	3	A	A01	1	0.825	0.175	0.16	2500	240	39.6	64.32
	4	A	A01	1	0.825	0.175	0.16	2500	360	54.6	77.96
	5	A	A01	2	0.825	0.175	0.16	2500	60	22.3	20.27
	6	A	A01	2	0.825	0.175	0.16	2500	120	25.9	38.84
	7	A	A01	2	0.825	0.175	0.16	2500	240	44.8	64.32
	8	A	A01	2	0.825	0.175	0.16	2500	360	57.5	77.96
	9	A	A01	3	0.825	0.175	0.16	2500	60	12.7	20.27
	10	A	A01	3	0.825	0.175	0.16	2500	120	28.5	38.84
	11	A	A01	3	0.825	0.175	0.16	2500	240	45.1	64.32
	12	A	A01	3	0.825	0.175	0.16	2500	360	52.9	77.96

Curve DoE Analysis (NLR)

	Set	Batch	Tablet	Polymer A	Polymer B	Total Polymer	Compression Force	Time	Dissolution	Reference Predictor
1	A	A01	1	0.825	0.175	0.16	2500	60	17.0	20.27
2	A	A01	1	0.825	0.175	0.16	2500	120	26.7	38.84
3	A	A01	1	0.825	0.175	0.16	2500	240	39.6	64.32
4	A	A01	1	0.825	0.175	0.16	2500	360	54.6	77.96
5	A	A01	2	0.825	0.175	0.16	2500	60	22.3	20.27
6	A	A01	2	0.825	0.175	0.16	2500	120	25.9	38.84
7	A	A01	2	0.825	0.175	0.16	2500	240	44.8	64.32
8	A	A01	2	0.825	0.175	0.16	2500	360	57.5	77.96
9	A	A01	3	0.825	0.175	0.16	2500	60	12.7	20.27
10	A	A01	3	0.825	0.175	0.16	2500	120	28.5	38.84
11	A	A01	3	0.825	0.175	0.16	2500	240	45.1	64.32
12	A	A01	3	0.825	0.175	0.16	2500	360	52.9	77.96

Curve DoE Analysis (NLR)

The screenshot shows the JMP software interface for a Dissolution DoE analysis. The 'Analyze' menu is open, and 'Fit Curve' is selected under 'Specialized Modeling'. A tooltip for 'Fit Curve' states: 'Fits a variety of built-in nonlinear models.' The data table below shows the experimental design and results.

				Polymer A	Polymer B	Total Polymer	Compression Force	Time	Dissolution	Reference Predictor
				0.825	0.175	0.16	2500	60	17.0	20.27
				0.825	0.175	0.16	2500	120	28.0	38.84
				0.825	0.175	0.16	2500	240	43.9	64.32
				0.825	0.175	0.16	2500	360	52.5	77.96
				0.825	0.175	0.16	2500	60	19.0	20.27

Curve DoE Analysis (NLR)

Fit Curve - JMP

Fits a variety of built-in nonlinear models.

Select Columns

10 Columns

- Set
- Batch
- Tablet
- Polymer A
- Polymer B
- Total Polymer
- Compression Force
- Time
- Dissolution
- Reference Predictor

Cast Selected Columns into Roles

Y, Response	Dissolution
X, Regressor	Time
Group	Batch
Z, Supplementary	Polymer A
	Polymer B
	Total Polymer
	Compression Force
Weight	<i>optional numeric</i>
Freq	<i>optional numeric</i>
By	<i>optional</i>

Action

OK

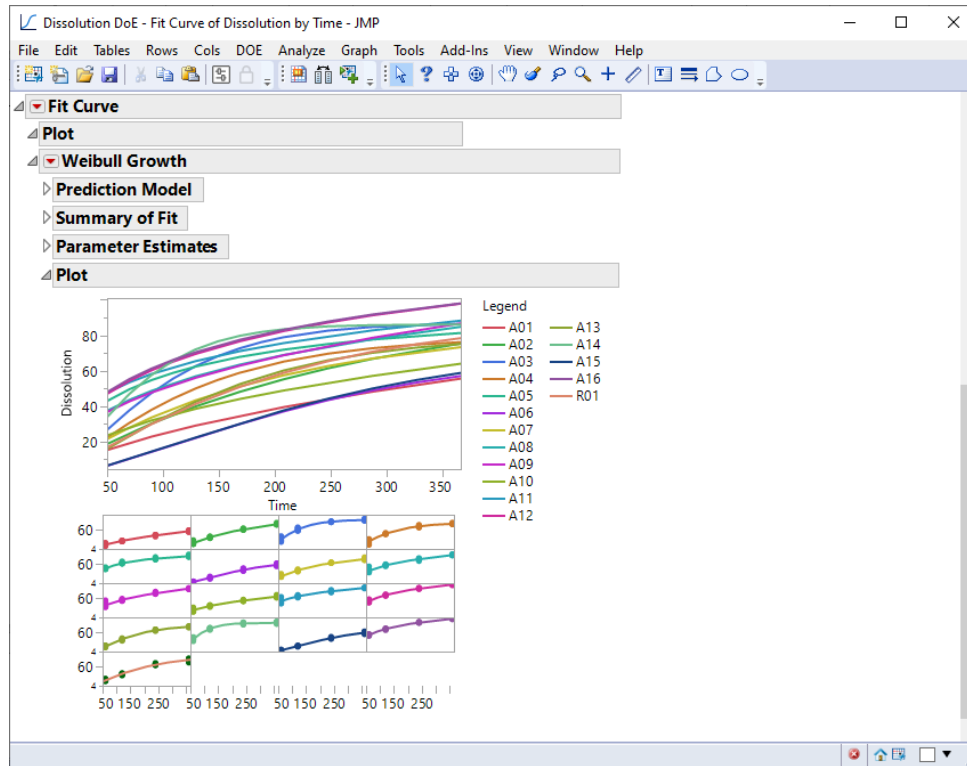
Cancel

Remove

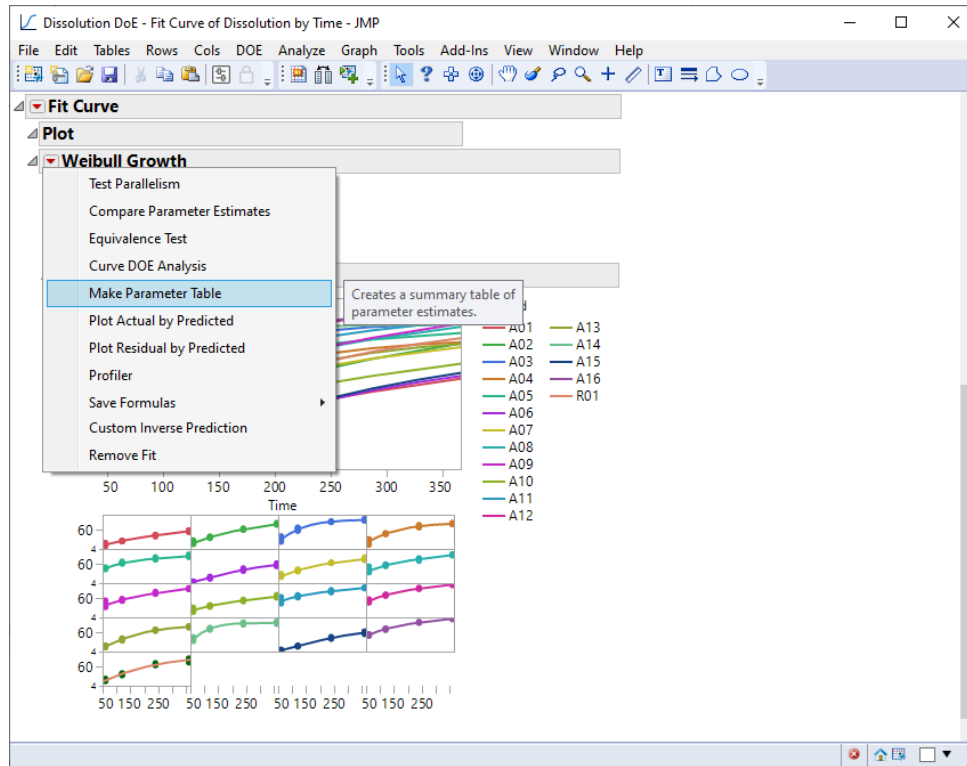
Recall

Help

Curve DoE Analysis (NLR)



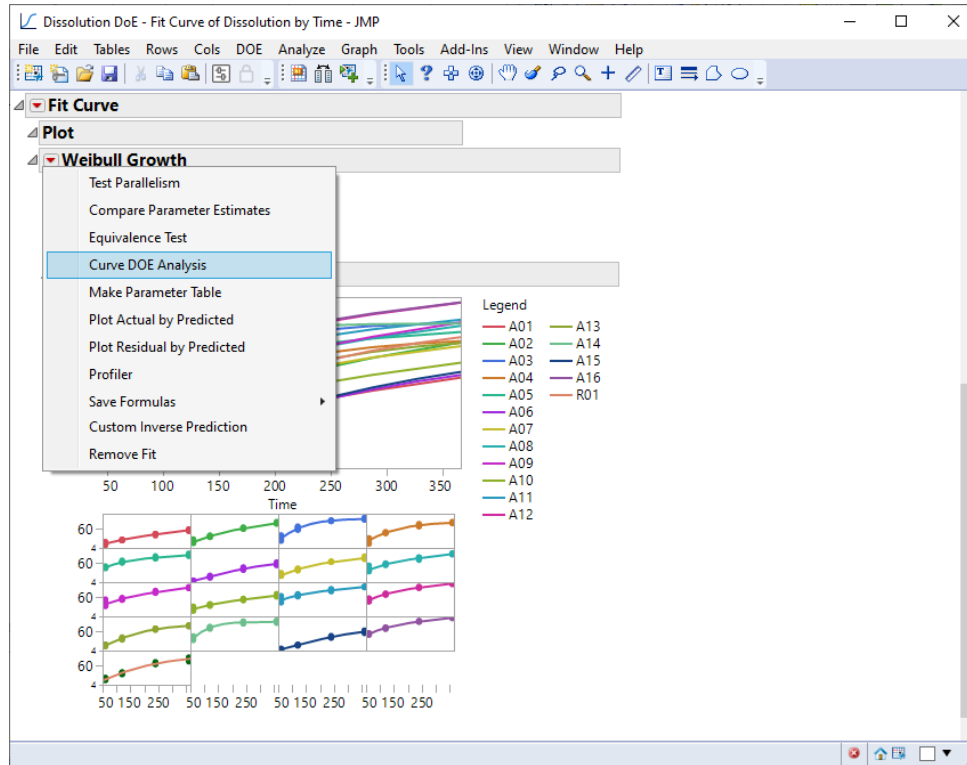
Curve DoE Analysis (NLR)



Curve DoE Analysis (NLR)

	Batch	Polymer A	Polymer B	Total Polymer	Compression Force	Asymptote	Inflection Point	Growth Rate
1	A01	0.825	0.175	0.16	2500	149.8	1043	0.733
2	A02	0.775	0.225	0.14	2500	104.7	282.5	0.938
3	A03	0.725	0.275	0.14	1500	87.08	107.5	1.311
4	A04	0.775	0.225	0.18	1500	78.78	128.1	1.17
5	A05	0.875	0.125	0.16	1500	91.69	104.5	0.622
6	A06	0.775	0.225	0.18	2500	68.95	248.1	1.454
7	A07	0.775	0.225	0.18	1500	87.61	193.8	0.938
8	A08	0.825	0.175	0.12	2500	150.7	521.5	0.534
9	A09	0.825	0.175	0.12	2500	257.6	2221	0.493
10	A10	0.875	0.125	0.16	2500	199.4	1963	0.565
11	A11	0.875	0.125	0.16	1500	139.6	365.3	0.44
12	A12	0.825	0.175	0.12	1500	135.8	235.2	0.553
13	A13	0.725	0.275	0.14	2500	79.21	158	1.296
14	A14	0.725	0.275	0.14	1500	86.17	83.28	1.356
15	A15	0.775	0.225	0.18	2500	73.12	260.2	1.438
16	A16	0.825	0.175	0.12	1500	131.6	207.9	0.555
17	R01	•	•	•	•	90.65	199.4	1.144

Curve DoE Analysis (NLR)



Curve DoE Analysis (NLR)

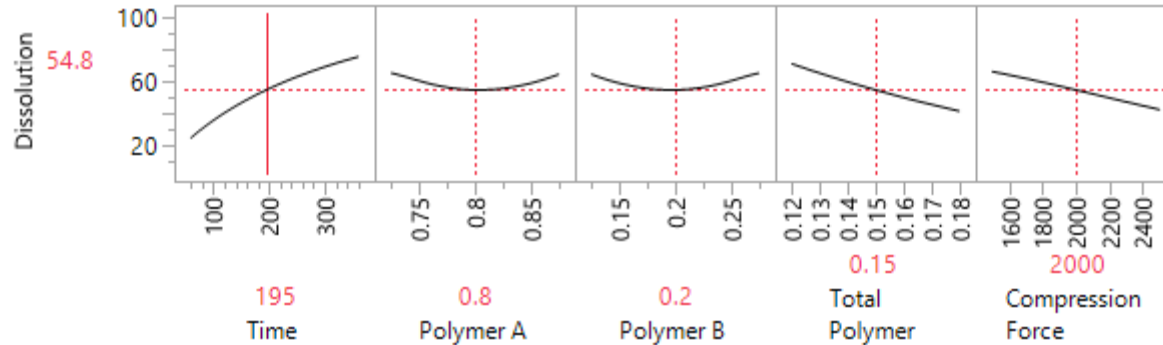
Curve DOE Analysis

Generalized Regression
for Model Parameters

Diagnostic Plots

CDOE Fit

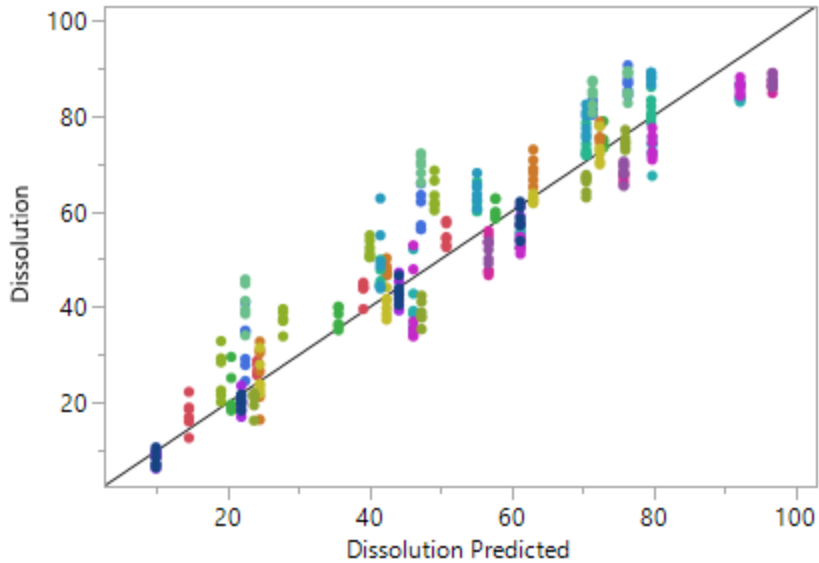
CDOE Profiler



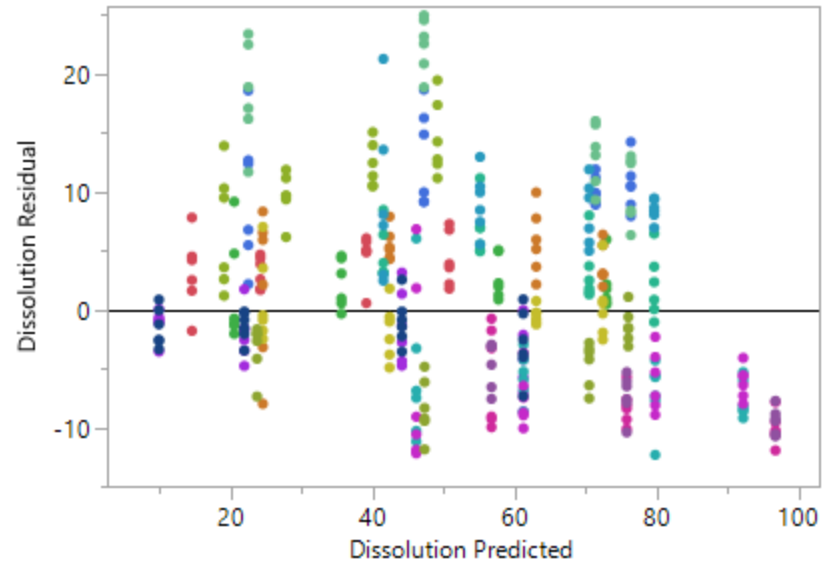
Curve DoE Analysis (NLR)

Diagnostic Plots

Actual by Predicted Plot



Residual by Predicted Plot



Curve DoE Analysis (NLR)

Generalized Regression for Asymptote

LogNormal Best Subset with AICc Validation

Solution Path

Parameter Estimates for Original Predictors

Term		Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%
(Polymer A-0.725)/0.15	Forced in	5.0876369	0.0793939	4106.3703	<.0001*	4.9320277	5.2432461
(Polymer B-0.125)/0.15	Forced in	4.3296224	0.0600676	5195.41	<.0001*	4.2118921	4.4473527
Polymer A*Total Polymer		-0.414667	0.1144104	13.136172	0.0003*	-0.638908	-0.190427
Polymer A*Compression Force		0.2397074	0.0718006	11.145676	0.0008*	0.0989808	0.3804341
Polymer B*Total Polymer		0	0	0	1.0000		
Polymer B*Compression Force		0	0	0	1.0000		
Total Polymer*Compression Force		0	0	0	1.0000		
LogNormal Distribution Parameters		Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%
Scale		0.1681744	0.0210398	63.890567	<.0001*	0.1269372	0.2094117

$$a \cdot \left(1 - \text{Exp} \left(- \left(\frac{\text{Time}}{b} \right)^c \right) \right)$$

a = Asymptote
 b = Inflection Point
 c = Growth Rate

Generalized Regression for Inflection Point

Generalized Regression for Growth Rate

Curve DoE Analysis (NLR)

Generalized Regression for Inflection Point

LogNormal Best Subset with AICc Validation

Solution Path

Parameter Estimates for Original Predictors

Term		Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%
(Polymer A-0.725)/0.15	Forced in	6.6114613	0.2254624	859.89753	<.0001*	6.1695632	7.0533595
(Polymer B-0.125)/0.15	Forced in	4.7439783	0.1219589	1513.0678	<.0001*	4.5049432	4.9830133
Polymer A*Total Polymer		0	0	0	1.0000	0	0
Polymer A*Compression Force		1.1778766	0.2041102	33.30198	<.0001*	0.7778279	1.5779254
Polymer B*Total Polymer		0	0	0	1.0000		
Polymer B*Compression Force		0	0	0	1.0000		
Total Polymer*Compression Force		0	0	0	1.0000		

LogNormal Distribution Parameters	Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%
Scale	0.3991865	0.0737269	29.315666	<.0001*	0.2546845	0.543688

$$a \cdot \left(1 - \text{Exp} \left(- \left(\frac{\text{Time}}{b} \right)^c \right) \right)$$

a = Asymptote
 b = Inflection Point
 c = Growth Rate

Curve DoE Analysis (NLR)

Generalized Regression for Growth Rate							
LogNormal Best Subset with AICc Validation							
Solution Path							
Parameter Estimates for Original Predictors							
Term		Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%
(Polymer A-0.725)/0.15	Forced in	-0.716675	0.0561331	163.0071	<.0001*	-0.826694	-0.606656
(Polymer B-0.125)/0.15	Forced in	0.3420244	0.0434337	62.009753	<.0001*	0.2568958	0.4271529
Polymer A*Total Polymer		0.4241638	0.0594451	50.913822	<.0001*	0.3076536	0.5406739
Polymer A*Compression Force		0	0	0	1.0000	0	0
Polymer B*Total Polymer		0	0	0	1.0000		
Polymer B*Compression Force		0	0	0	1.0000		
Total Polymer*Compression Force		0.0928903	0.0337311	7.5836617	0.0059*		
LogNormal Distribution Parameters		Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%
Scale		0.1035127	0.0140294	54.439018	<.0001*	0.0760156	0.1310098

$$a \cdot \left(1 - \exp \left(- \left(\frac{\text{Time}}{b} \right)^c \right) \right)$$

a = Asymptote
 b = Inflection Point
 c = Growth Rate

Curve DoE Analysis (NLR)

```
Exp(
  5.08763690244406 * ((:Polymer A - 0.725) / 0.15) + 4.32962237609893 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
  :Total Polymer - 0.15) / 0.03) * -0.414667337719225) + ((:Polymer A - 0.725) / 0.15) * (((:Compression Force - 2000) / 500) * 0.239707444419611)
  + 0.168174449903471 ^ 2 / 2
) * (1 - Exp(
  -(:Time / Exp(
    6.61146132683894 * ((:Polymer A - 0.725) / 0.15) + 4.74397829394421 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
    :Compression Force - 2000) / 500) * 1.17787664936899) + 0.399186546036449 ^ 2 / 2
  )) ^ Exp(
    -0.716674955680227 * ((:Polymer A - 0.725) / 0.15) + 0.342024361999155 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
    :Total Polymer - 0.15) / 0.03) * 0.424163753840414) + ((:Total Polymer - 0.15) / 0.03) * (((:Compression Force - 2000) / 500) *
    0.0928902831533859) + 0.103512708322975 ^ 2 / 2
  ))
))
))
```

$$a \cdot \left(1 - \exp \left(- \left(\frac{\text{Time}}{b} \right)^c \right) \right)$$

a = Asymptote

b = Inflection Point

c = Growth Rate

Curve DoE Analysis (NLR)

```

Exp(
  5.08763690244406 * ((:Polymer A - 0.725) / 0.15) + 4.32962237609893 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
  :Total Polymer - 0.15) / 0.03) * -0.414667337719225) + ((:Polymer A - 0.725) / 0.15) * (((:Compression Force - 2000) / 500) * 0.239707444419611)
  + 0.168174449903471 ^ 2 / 2
) * (1 - Exp(
  -(:Time / Exp(
    6.61146132683894 * ((:Polymer A - 0.725) / 0.15) + 4.74397829394421 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
    :Compression Force - 2000) / 500) * 1.17787664936899) + 0.399186546036449 ^ 2 / 2
  ))) * Exp(
  -0.716674955680227 * ((:Polymer A - 0.725) / 0.15) + 0.342024361999155 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
  :Total Polymer - 0.15) / 0.03) * 0.424163753840414) + ((:Total Polymer - 0.15) / 0.03) * (((:Compression Force - 2000) / 500) *
  0.0928902831533859) + 0.103512708322975 ^ 2 / 2
)
)
)
)

```

$$a \cdot \left(1 - \exp \left(- \left(\frac{\text{Time}}{b} \right)^c \right) \right)$$

a = Asymptote

b = Inflection Point

c = Growth Rate

Curve DoE Analysis (NLR)

```
Exp(
  5.08763690244406 * ((:Polymer A - 0.725) / 0.15) + 4.32962237609893 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
  :Total Polymer - 0.15) / 0.03) * -0.414667337719225) + ((:Polymer A - 0.725) / 0.15) * (((:Compression Force - 2000) / 500) * 0.239707444419611)
  + 0.168174449903471 ^ 2 / 2
) * (1 - Exp(
  -(:Time / Exp(
    6.61146132683894 * ((:Polymer A - 0.725) / 0.15) + 4.74397829394421 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
    :Compression Force - 2000) / 500) * 1.17787664936899) + 0.399186546036449 ^ 2 / 2
  )) ^ Exp(
    -0.716674955680227 * ((:Polymer A - 0.725) / 0.15) + 0.342024361999155 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
    :Total Polymer - 0.15) / 0.03) * 0.424163753840414) + ((:Total Polymer - 0.15) / 0.03) * (((:Compression Force - 2000) / 500) *
    0.0928902831533859) + 0.103512708322975 ^ 2 / 2
  ))
))
```

$$a \cdot \left(1 - \exp \left(- \left(\frac{\text{Time} + c}{b} \right) \right) \right)$$

a = Asymptote
 b = Inflection Point
 c = Growth Rate

Curve DoE Analysis (NLR)

$$100 \cdot \left(\frac{\left| \text{CDoE Dissolution Predictor} - \text{Reference Predictor} \right|}{\text{Reference Predictor}} \right)$$

Curve DoE Analysis (NLR)

Profiler - JMP

Explores how the factors affect the response formulas.

Select Columns

12 Columns

- Set
- Batch
- Tablet
- Polymer A
- Polymer B
- Total Polymer
- Compression Force
- Time
- Dissolution
- CDoE Dissolution Predictor
- Reference Predictor
- Percent Difference**

Expand Intermediate Formulas

Cast Selected Columns into Roles

Y, Prediction Formula **Percent Difference**
optional numeric

Noise Factors *optional numeric*

All Y Columns must have formulas. Specify Noise Factors only if you want to study robustness (flatness) with respect to transmitted variation from these factors.

Action

OK

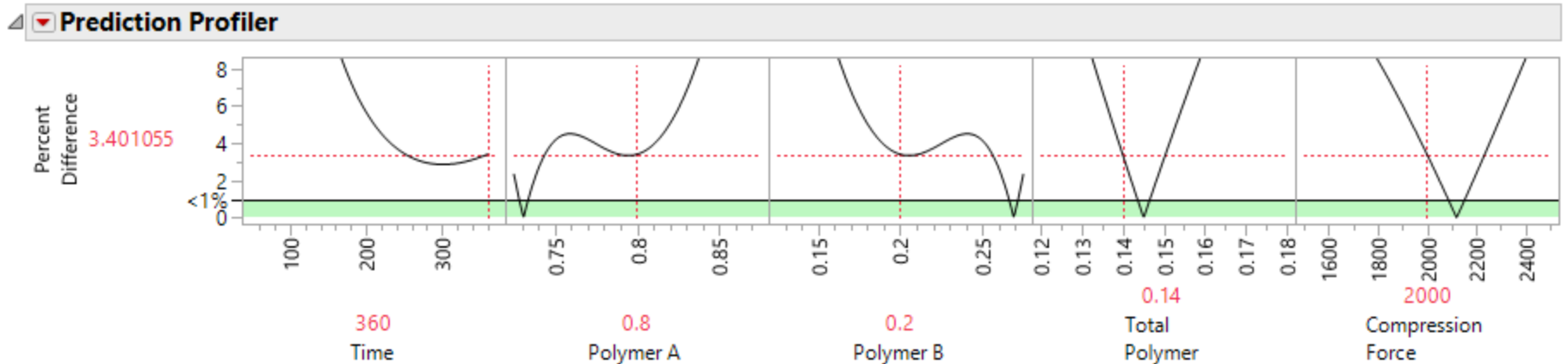
Cancel

Remove

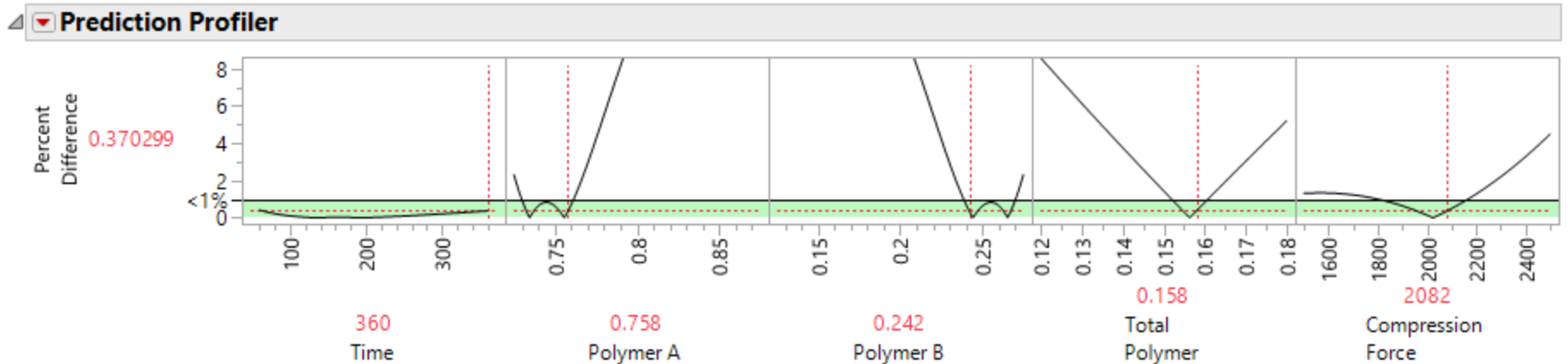
Recall

Help

Curve DoE Analysis (NLR)



Curve DoE Analysis (NLR)



Verification Results

	Formulation	Polymer A	Polymer B	Total Polymer	Compression Force
1	Ref	•	•	•	•
2	f2	0.725	0.275	0.12	2500
3	FDoE	0.725	0.275	0.17	1700
4	CDoE	0.758	0.242	0.16	2100

f2

FDA

NLR

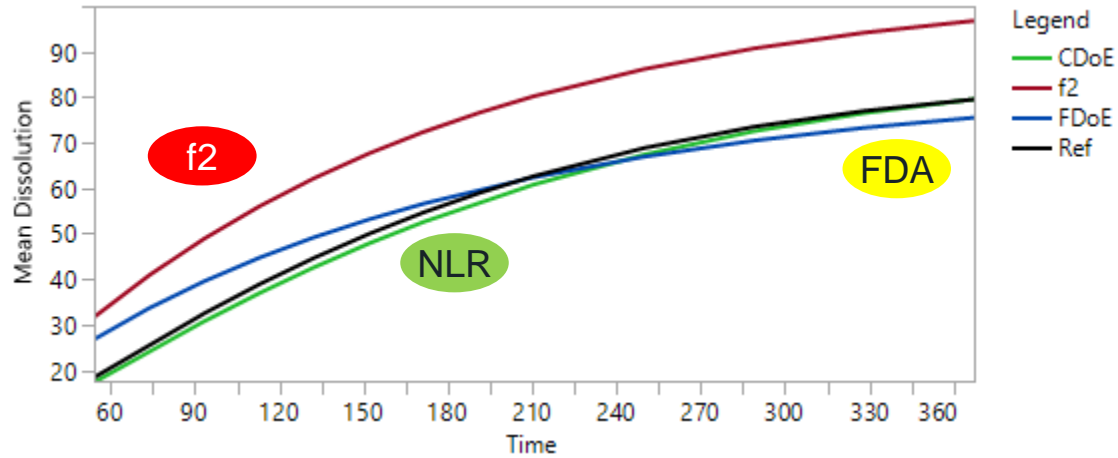
Verification Results

	Formulation	Rep	Polymer A	Polymer B	Total Polymer	Compression Force	Dissolution 60	Dissolution 120	Dissolution 240	Dissolution 360
1	Ref	1	•	•	•	•	22.9	41.1	71.9	82.1
2	Ref	2	•	•	•	•	17.7	40.7	66.8	77
3	Ref	3	•	•	•	•	22.7	42.9	68.7	79.1
4	Ref	4	•	•	•	•	21.8	39.8	68.5	79.6
5	Ref	5	•	•	•	•	19.3	39.7	65.8	79.2
6	Ref	6	•	•	•	•	20.9	40.1	64.7	77.1
7	CDoE	1	0.758	0.242	0.16	2100	17.8	43	67.2	80.2
8	CDoE	2	0.758	0.242	0.16	2100	23.4	38.8	66.7	78.3
9	CDoE	3	0.758	0.242	0.16	2100	20.3	36.3	63.1	77.3
10	CDoE	4	0.758	0.242	0.16	2100	18.9	42.2	66.6	79
11	CDoE	5	0.758	0.242	0.16	2100	18.9	39.3	67	81.1
12	CDoE	6	0.758	0.242	0.16	2100	15.6	37.2	63.1	79.2
13	FDoE	1	0.725	0.275	0.17	1700	31.6	52.1	62.8	75.5
14	FDoE	2	0.725	0.275	0.17	1700	28.8	49.2	60.5	76
15	FDoE	3	0.725	0.275	0.17	1700	23.3	48.4	64.3	75.7
16	FDoE	4	0.725	0.275	0.17	1700	29.2	50.3	64.4	76.8
17	FDoE	5	0.725	0.275	0.17	1700	24.9	46.7	61.7	74.1
18	FDoE	6	0.725	0.275	0.17	1700	24.9	52.3	63.3	80.8
19	f2	1	0.725	0.275	0.12	2500	31.3	57.8	86.4	96
20	f2	2	0.725	0.275	0.12	2500	25.6	54.2	79.7	94.7
21	f2	3	0.725	0.275	0.12	2500	36.1	57.6	83.6	95.7
22	f2	4	0.725	0.275	0.12	2500	38.3	59.4	84.5	96.8
23	f2	5	0.725	0.275	0.12	2500	32.2	61.9	91.8	98.2
24	f2	6	0.725	0.275	0.12	2500	45.3	57.3	85.1	96.1
25	BCV	1	0.725	0.275	0.17	1750	17	46.9	69.1	84.1
26	BCV	2	0.725	0.275	0.17	1750	23.6	45.6	72.7	88.9
27	BCV	3	0.725	0.275	0.17	1750	20.4	41.8	75.5	87.5
28	BCV	4	0.725	0.275	0.17	1750	16.9	47.6	72.9	82.9
29	BCV	5	0.725	0.275	0.17	1750	25.4	46	65.2	83.9
30	BCV	6	0.725	0.275	0.17	1750	21	47	67.8	77.5

Verification Results

	Formulation	Polymer A	Polymer B	Total Polymer	Compression Force	Dissolution 60 Mean	Dissolution 120 Mean	Dissolution 240 Mean	Dissolution 360 Mean	f2
1	Ref	•	•	•	•	20.88	40.72	67.73	79.02	100
f2	2 f2	0.725	0.275	0.12	2500	34.80	58.03	85.18	96.25	39.03
FDA	3 FDoE	0.725	0.275	0.17	1700	27.12	49.83	62.83	76.48	60.2
NLR	4 CDoE	0.758	0.242	0.16	2100	19.15	39.47	65.62	79.18	87.16

Verification Results



InfoQ Assessment of Results

	f2	FDoE	CDoE
Generalizability	Insufficient	Good	Best
Operationalization	Good/Easy	Good/Easy	Good/Harder
Communication	Good	Good	Best

f2 FDA NLR



Calculate 'InfoQ' score with JMP

Created: JAN 24, 2017 09:26 AM | Last Modified: JAN 24, 2017 12:15 PM

InfoQ.jmpaddin

InfoQ - JMP Pro

Help

This is a rating-based approach to quantifying InfoQ that scores each of the eight dimensions. This coarse grained approach rates each dimension on a 5 point scale, with 5 indicating "Very High" achievement in that dimension.

The ratings are then normalized into a desirability function for each dimension, which are then combined to produce an overall InfoQ score using the geometric mean of the individual desirabilities.

By dragging the slider handles, each dimension can be assigned a plausible range of ratings, or a specific rating.

InfoQ

Lower Bound: Undefined
Upper Bound: Undefined

Data Resolution

Very Low Very High

Data Structure

Very Low Very High

Data Integration

Very Low Very High

Temporal Relevance

Very Low Very High

Chronology of Data and Goal

Very Low Very High

Generalizability

Very Low Very High

Operationalization

Very Low Very High

Communication

Very Low Very High

Information Quality Dimension	Questions	JMP Features
1. Data Resolution	1.1 to the data scale used aligned with the stated goal?	Analyzer<<Distribution Format
	1.2 How reliable and precise are the measuring devices or data sources?	Analyzer<<Measurement Systems Analysis
	1.3 to the data analysis suitable for the data aggregation level?	Analyzer<<Control Chart Builder: IHR Chart, Xbar&R Chart Variable Clustering Analyzer<<Principal Components
2. Data Structure	2.1 to the type of the data used aligned with the stated goal?	Set up variable types and Format Analyzer<<Explore Patterns Analyzer<<Explore Outliers
	2.2 Are data integrity details (corrected/misring values) described and handled appropriately?	Tables<<Missing Data Patterns Analyzer<<Explore Missing Values
	2.3 Are the analysis methods suitable for the data structures?	Check the data type Analyzer<<Distribution<<Quantiles
3. Data Integration	3.1Are the data integrated from multiple sources? If so, what is the credibility of each source?	Analyzer<<Distribution Analyzer<<Explore Patterns Tables<<Join
	3.2 How is the integration done? Are there linkage issues that lead to dropping crucial information?	Latest variable methods: SEM, Factor Analysis
	3.3 Does the data integration add value in terms of the stated goal?	Analyzer<<Model Comparison (JMP Pro) Modeling: It is possible to predict the sensitive information using the associated information. Remove features that predict sensitive information. You want models that are unproductive of the sensitive information.
4. Temporal Relevance	4.1 Considering the data collection, data analysis and deployment stages, is any of them time-cositive?	Analyzer<<Model Comparison (JMP Pro)
	4.2 Does the time gap between data collection and analysis cause any concern?	Data should be standardized Analyzer<<Structural Equations Model (JMP Pro) Logit (Column Formula)
	4.3 Is the time gap between the data collection and analysis and the intended use of the model (e.g., in terms of policy recommendations) of any concern?	
5. Chronology of Data & Goal	5.1 If the stated goal is predictive, are all the predictor variables expected to be available at the time of 5.2	
	5.2 If the stated goal is causal, do the causal variables precede the effects?	
	5.3 In a causal study, are there issues of endogeneity (reverse-causation)?	
6. Generalizability	6.1 In the stated goal statistical or scientific generalizability?	validation column using selected rows as training set, the rest as validation set (JMP Pro) Analyzer<<Measurement Systems Analysis Analyzer<<Fit Model<<EMM
	6.2 For statistical generalizability in the case of inference, does the paper answer the question "What population does the sample represent?"	
	6.3 For generalizability in the case of a stated predictive goal (predicting the values of new observations; forecasting future values), are the results generalizable to the to-be-predicted data?	
7. Operationalization	6.4 Does the paper provide sufficient detail for the type of needed reproducibility and/or repeatability, and/or replicability?	
	7.1 Are the measured variables themselves of interest to the study goal, or is their underlying construct?	If the underlying construct is of interest then use Analyzer<<Structural Equations Model (JMP Pro) Analyzer<<Fit Model<<Generalized Regression (JMP Pro) Analyzer<<Bootstrap Forest (JMP Pro) Graphs<<Profiler
	7.2 What are the justifications for the choice of variables?	
	7.3 What action items can be derived from the findings?	
	7.4 Who can be affected (positively or negatively) by the findings?	
	7.5 What can the affected parties do about it?	
7.6 How would you know if you achieved your post study objectives?	Analyzer<<Model Comparison Graphs<<Profiler Graphs<<Graph Builder Analyzer<<Model Comparison	
8. Communication	8.1 to the exposition of the goal, data and analysis clear?	
	8.2 Is the exposition level appropriate for the readership?	
	8.3 Are there any confusing details or statements that might lead to confusion or misunderstanding?	

<https://community.jmp.com/t5/Discovery-Summit-Europe-2021/Maximizing-Data-Science-Success-with-Information-Quality-InfoQ/ta-p/349217?attachment-id=12709>

Thank you for your attention