LUBRICANT RESEARCH USING JMP NON-LINEAR REGRESSION

Discovery Summit Americas 2020
13 – 15 October 2020

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2020-US-45MP-580

Performance you can rely on.

Infineum

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AGENDA

INTRODUCTIONS

BACKGROUND OF LUBRICANT RESEARCH

TYPES OF QUESTIONS WE WANT TO ANSWER

NON-LINEAR MODEL EXAMPLES

NON-LINEAR ANALYSIS EXAMPLES

CONCLUSIONS AND FUTURE

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Introductions

Introduction: Who am I?

- Fred W. Girshick
- Researcher for a specialty chemical company
  - Manufacturer of chemical additives for lubricants and fuels
  - Have a global Statistics Group, for help with more complicated situations
- Experience with various forms of (reciprocating internal combustion) engine oils
  - Passenger Car, On- and off-highway trucks, railroad, aviation, stationary engines
- My specialty – for the past 19 years – is Large Engines
  - I'll show you what they are later
- Previous user of SAS and currently JMP
- Not a sophisticated user
  - Tend to do the same type of analyses over and over
  - Still learning
- Better at Microsoft Excel than JMP
  - Use Excel to prepare dataset for import into JMP
  - Often export results to Excel for graphing and export to PowerPoint or Word
- No real-time "live action" demonstrations today
  - Screen shots and pointing

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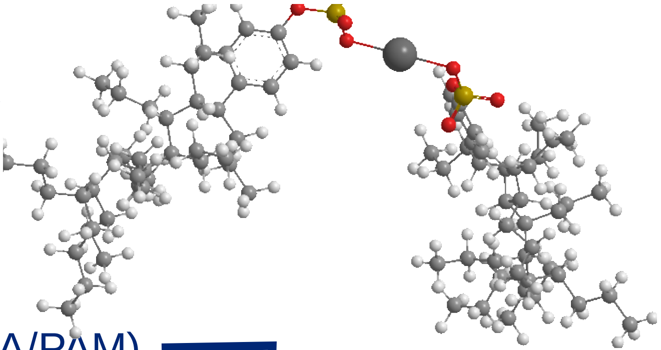
Introduction: Lubricants

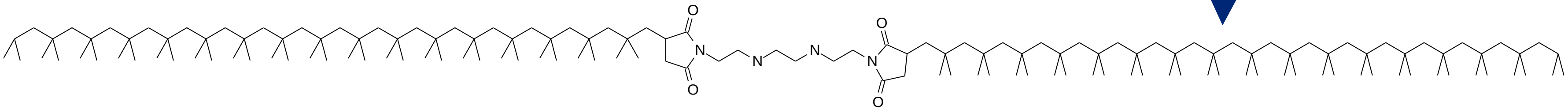
- Lubricants are needed any time or place there are moving parts
  - Engines
  - Transmissions
  - Gears
  - Pumps
  - Motors
  - *etc*.
- Lubricants can be solid, liquid, or gas
- Engine oils contain:
  - Base stock: the “oil” stream refined from crude oil
  - Additives: detergent, dispersant, anti-oxidant, anti-wear, friction modifier, anti-foam, corrosion inhibitor, viscosity modifier, *etc*.
  - Each additive type has many different chemical options
  - Not all engine oils contain all additive types: only what’s needed
- Today’s talk addresses:
  - Liquid lubricants (engine oils)
  - For Reciprocating Internal Combustion Engines (RICE)

Introduction: Components (examples)

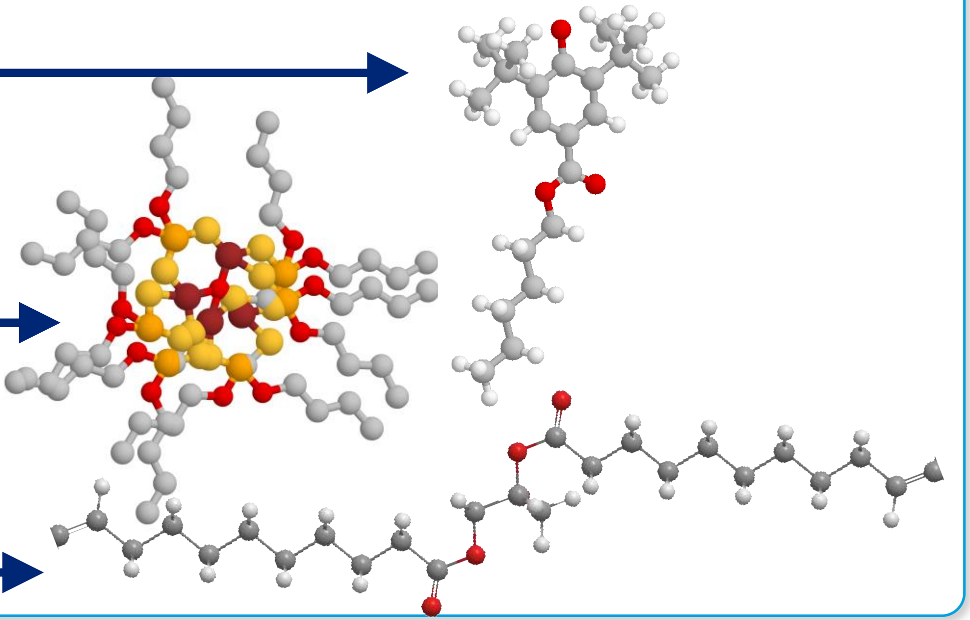
- Detergent
  - Calcium sulphonate



- Dispersant
  - Polyisobutylene Succinic Anhydride PolyAmine (PIBSA/PAM)



- Anti-oxidant
  - Hindered phenol
- Anti-wear
  - Zinc dialkyl dithio phosphate (ZDDP)
- Friction modifier
  - Glycerol dioleate



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Large Engines

Large engines

- Not large engines:

200 Hp

500 Hp

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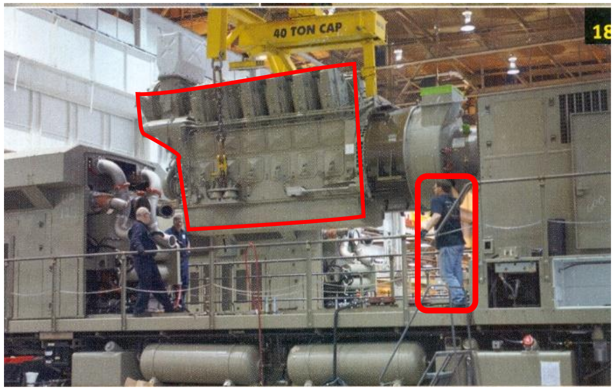
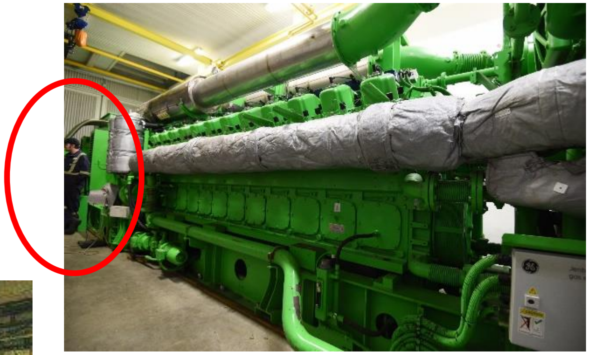
Large engines

- Railroad
  - Locomotives



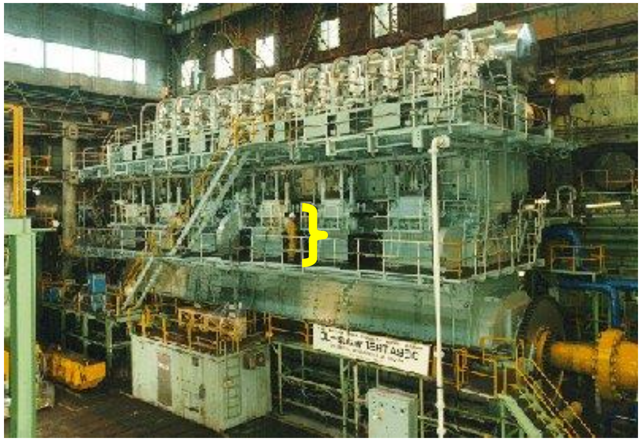
4400 Hp

- Stationary natural gas engines
  - Compressing natural gas in pipelines
    - To get it from where it exists to your house
  - Recycling household garbage (landfill)
  - Recycling farm waste (biogas)



5900 Hp

- Marine
  - Ships at sea



98,000 Hp

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Types of Questions We Want to Answer

Types of questions

- How well does this bench test predict real-world performance?
- How does performance depend on concentration of this additive?
- How does the structure of this additive affect performance?
  - *e.g.*, If I make the chain longer or more branched?
  - *e.g.*, If I change the ratio of polar and non-polar parts?
- Can I predict performance from composition?
- How long will this product last before it needs to be changed?
  - *e.g.*, passenger cars are either 3000 miles; 5000 miles; 7500 miles; 10,000 miles (depending who you ask)
- How much better is my premium product than my “mainline” product?
- How does my product compare to my competitor’s product?

Non-Linear

Linear or Non-Linear

- “Non-linear” means non-linear in the **parameters**, not the **variables**

Linear or **Non-linear**

$$y = m * x + b$$

$$y = a * x^2 + b * x + c$$

$$y = a * x^3 + b * x^2 + c * x + d$$

$$y = a * e^{b*x}$$

$$Ln(y) = Ln(a) + b * x$$

$$y = \frac{a}{(x+b)}$$

$$\frac{1}{y} = \frac{(x+b)}{(a)} = \frac{x}{a} + c$$

$$y = a + b * x^c$$

$$y = \frac{(a * x)}{(b + x)}$$ Michaelis-Menten

$$y = a + b * \left[1 + \ e^{\left(\frac{-x}{c}\right)}\right]$$ This paper

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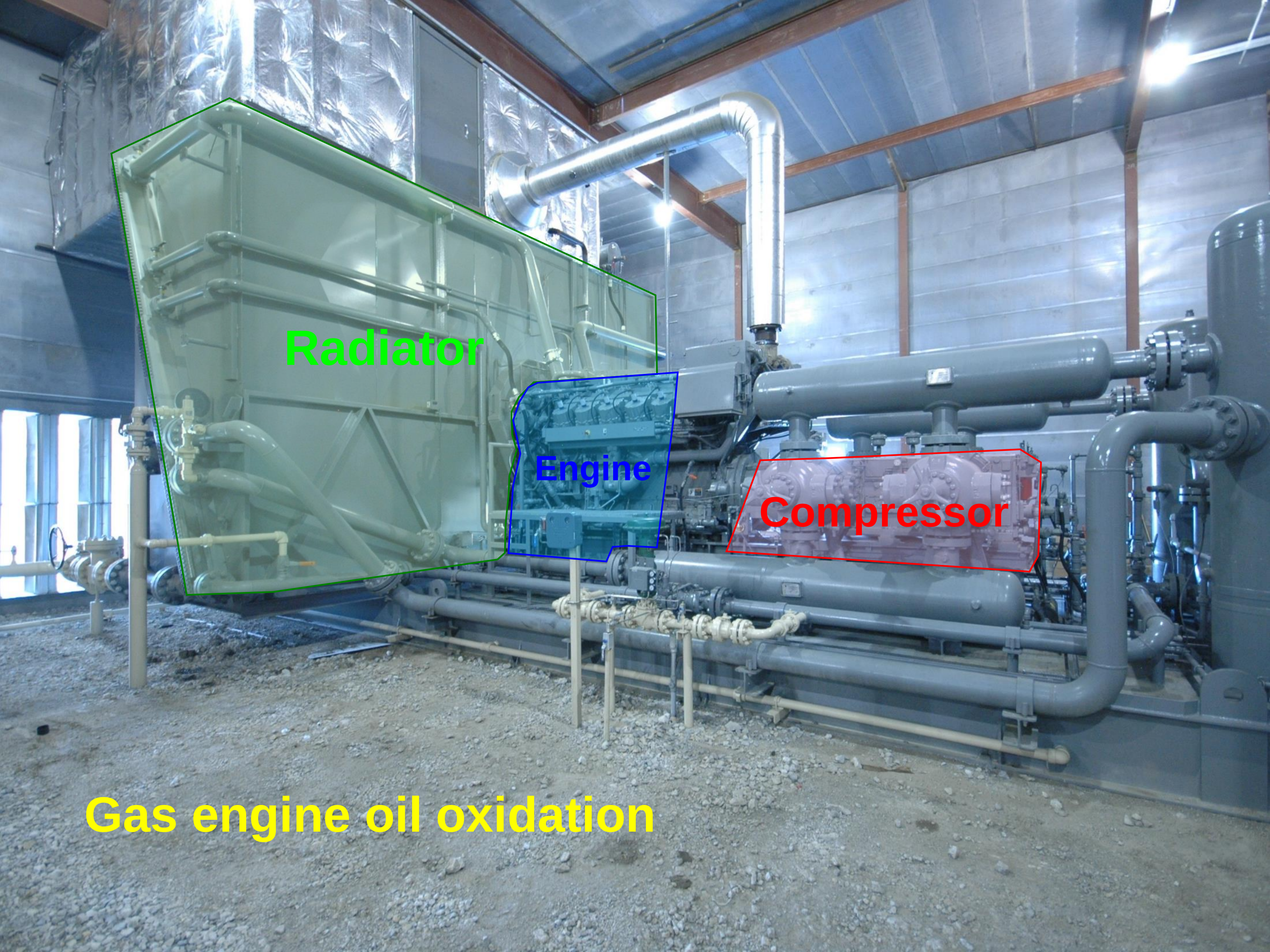

Gas engine oil oxidation

Engine oil oxidation

- For our purposes, oxidation is degradation caused by reaction with oxygen
  - Strictly speaking, chemical oxidation can occur without oxygen
- Common examples are when apple slices turn brown or old milk goes sour
- Engine oils are mostly hydrocarbon molecules
  - They are exposed to high temperatures during engine operation
  - Fuel combustion generates free radicals, which promote oxidation
    - Free radicals are molecular fragments with unpaired electrons
    - Unstable and reactive, they “attack” other molecules to pair their electrons
- Oxidation of engine oil leads to undesirable consequences:

– Oil thickening	higher viscosity than engine design needs & lower fuel economy
– Acid formation	acid corrodes metal parts
– Deposit formation	deposits can block oil passages and impede moving parts

- Oxidation is often measured by Infrared (IR)
  - Units: Absorbance *per* centimeter (A/cm)
  - Engine manufacturers publish limits at which oil must be changed

Engine oil oxidation – test design

- Two natural gas engine manufacturers
  - Called XXX and YYY for the example
- Three oils
  - Called **BLUE**, **RED**, and **GREEN** for the example
- 2 x 3 design
  - Each oil in each engine design
- Run for about 14 months
  - 10,000 operating hours
  - At ≥95% of maximum load
- Oil samples taken every week to 10 days
  - Total 600 samples
- Many parameters measured
  - About 20 oil properties
  - Physical measurements of wear
  - Physical measurements of deposits
- Concentrate on oxidation for this example

Today, only analyzing one engine model in detail

If you drove near maximum engine output, and averaged 70 mph, that would be 700,000 miles

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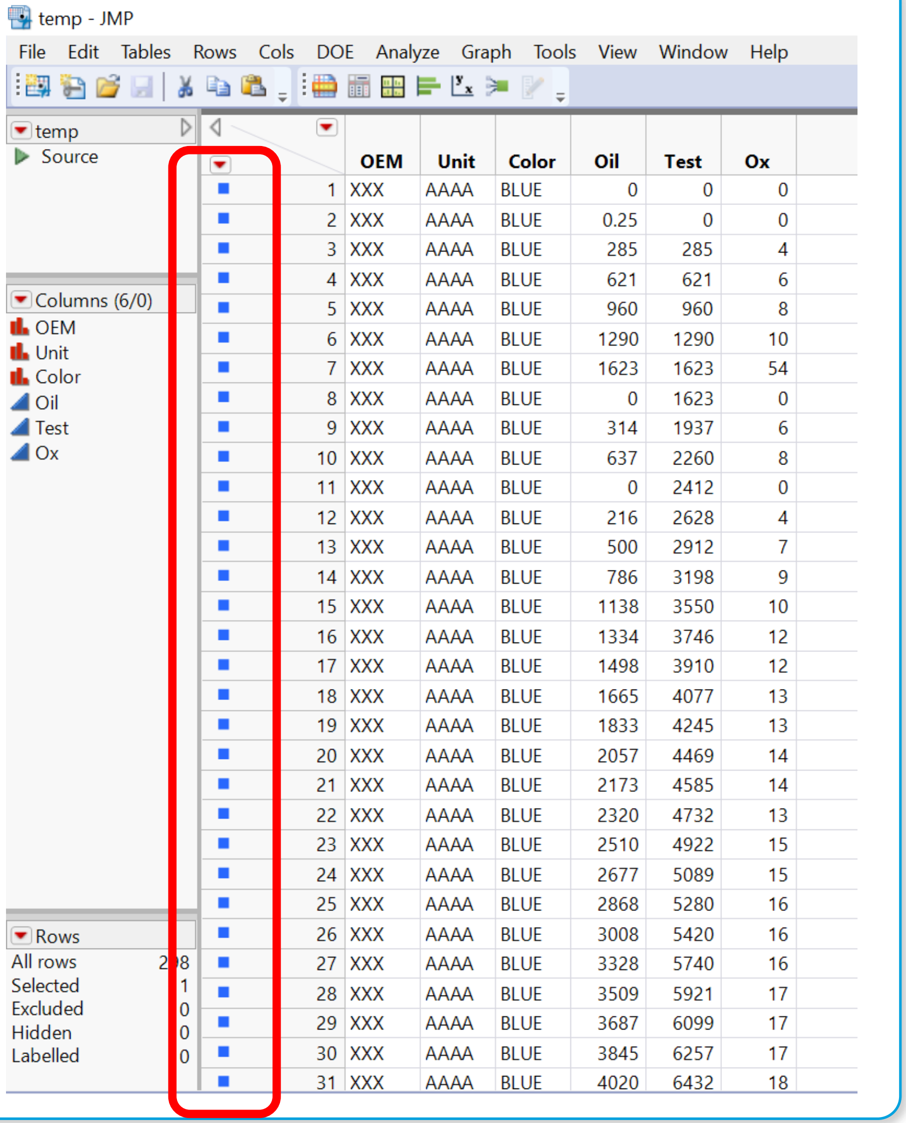
Engine oil oxidation – dataset

- Showing simplified JMP dataset
  - Color = oil formulation
  - Oil = age of oil since last change, hours
  - Test = duration of test, hours
  - Ox = oxidation in A/cm
- Rows are color-coded *per* Color variable
- Rows are assigned markers:
  - Square for XXX
  - Circle for YYY
- Full dataset contains many more measurements of oil properties
  - And parameters of oil composition
  - And physical engine measurements



Rows

All rows 2[illegible]8
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Excluded 0
Hidden 0
Labelled 0

		OEM	Unit	Color	Oil	Test	Ox
■	1	XXX	AAAA	BLUE	0	0	0
■	2	XXX	AAAA	BLUE	0.25	0	0
■	3	XXX	AAAA	BLUE	285	285	4
■	4	XXX	AAAA	BLUE	621	621	6
■	5	XXX	AAAA	BLUE	960	960	8
■	6	XXX	AAAA	BLUE	1290	1290	10
■	7	XXX	AAAA	BLUE	1623	1623	54
■	8	XXX	AAAA	BLUE	0	1623	0
■	9	XXX	AAAA	BLUE	314	1937	6
■	10	XXX	AAAA	BLUE	637	2260	8
■	11	XXX	AAAA	BLUE	0	2412	0
■	12	XXX	AAAA	BLUE	216	2628	4
■	13	XXX	AAAA	BLUE	500	2912	7
■	14	XXX	AAAA	BLUE	786	3198	9
■	15	XXX	AAAA	BLUE	1138	3550	10
■	16	XXX	AAAA	BLUE	1334	3746	12
■	17	XXX	AAAA	BLUE	1498	3910	12
■	18	XXX	AAAA	BLUE	1665	4077	13
■	19	XXX	AAAA	BLUE	1833	4245	13
■	20	XXX	AAAA	BLUE	2057	4469	14
■	21	XXX	AAAA	BLUE	2173	4585	14
■	22	XXX	AAAA	BLUE	2320	4732	13
■	23	XXX	AAAA	BLUE	2510	4922	15
■	24	XXX	AAAA	BLUE	2677	5089	15
■	25	XXX	AAAA	BLUE	2868	5280	16
■	26	XXX	AAAA	BLUE	3008	5420	16
■	27	XXX	AAAA	BLUE	3328	5740	16
■	28	XXX	AAAA	BLUE	3509	5921	17
■	29	XXX	AAAA	BLUE	3687	6099	17
■	30	XXX	AAAA	BLUE	3845	6257	17
■	31	XXX	AAAA	BLUE	4020	6432	18

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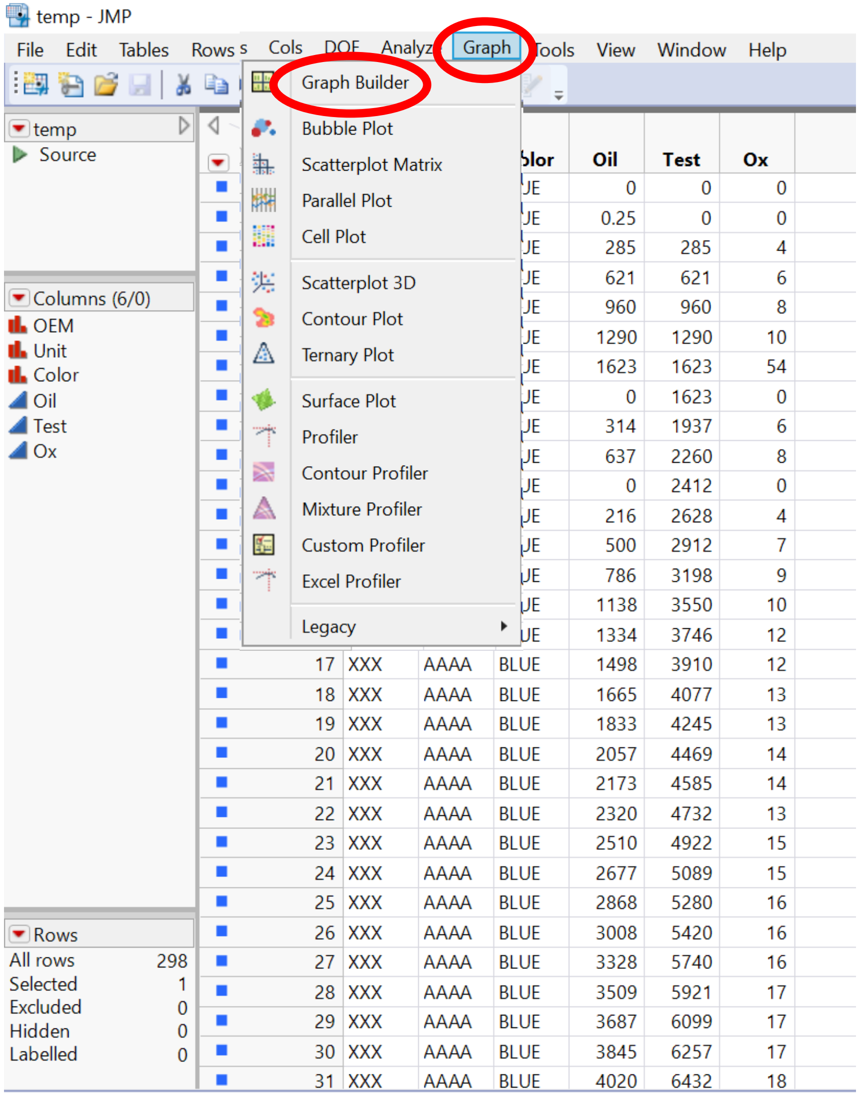
Engine oil oxidation – analysis

- What to do first?
  - (A trick question)
- **Plot The Data!**

- Graph ➔
- Graph Builder ➔



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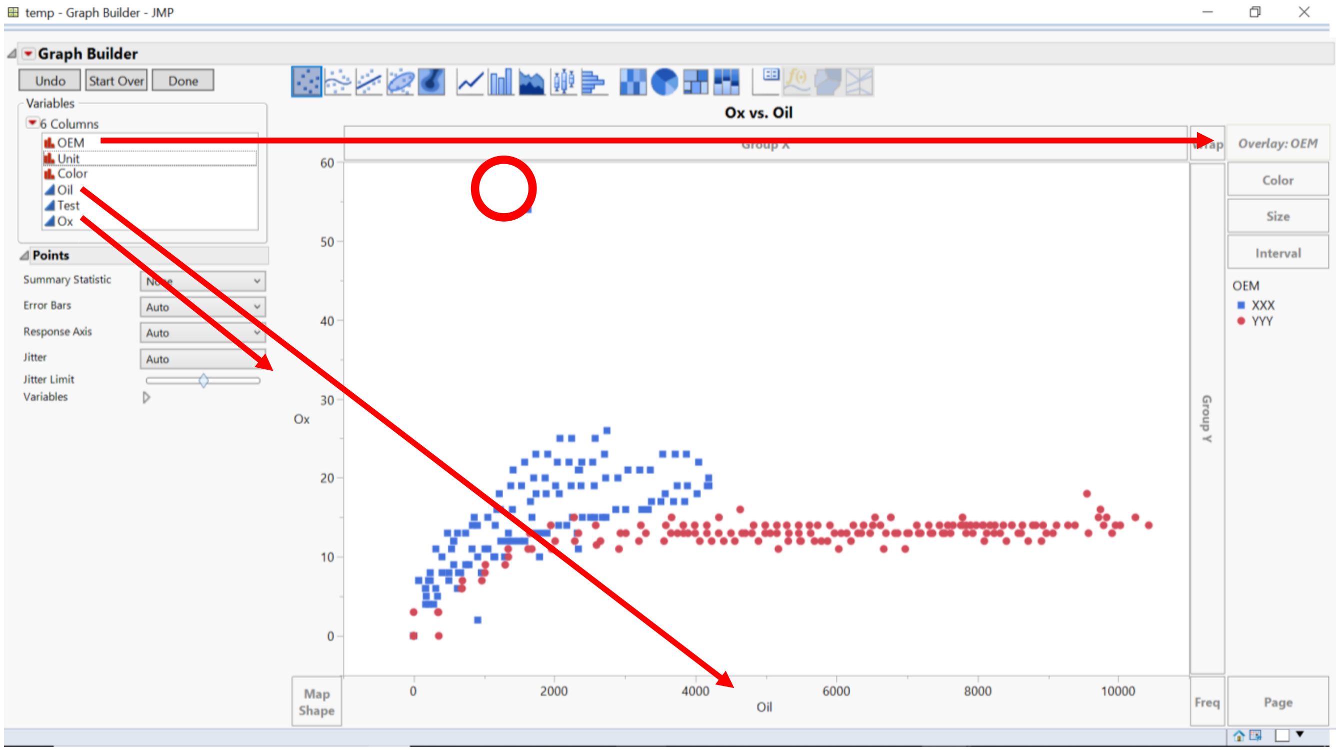
Labelled	0

			lor	Oil	Test	Ox
			JE	0	0	0
			JE	0.25	0	0
			JE	285	285	4
			JE	621	621	6
			JE	960	960	8
			JE	1290	1290	10
			JE	1623	1623	54
			JE	0	1623	0
			JE	314	1937	6
			JE	637	2260	8
			JE	0	2412	0
			JE	216	2628	4
			JE	500	2912	7
			JE	786	3198	9
			JE	1138	3550	10
			JE	1334	3746	12
17	XXX	AAAA	BLUE	1498	3910	12
18	XXX	AAAA	BLUE	1665	4077	13
19	XXX	AAAA	BLUE	1833	4245	13
20	XXX	AAAA	BLUE	2057	4469	14
21	XXX	AAAA	BLUE	2173	4585	14
22	XXX	AAAA	BLUE	2320	4732	13
23	XXX	AAAA	BLUE	2510	4922	15
24	XXX	AAAA	BLUE	2677	5089	15
25	XXX	AAAA	BLUE	2868	5280	16
26	XXX	AAAA	BLUE	3008	5420	16
27	XXX	AAAA	BLUE	3328	5740	16
28	XXX	AAAA	BLUE	3509	5921	17
29	XXX	AAAA	BLUE	3687	6099	17
30	XXX	AAAA	BLUE	3845	6257	17
31	XXX	AAAA	BLUE	4020	6432	18

Engine oil oxidation – graphing

- Oil → X
- Ox → Y
- Obvious outlier
  - Deal with it for later
- Looks messy
- OEM → Overlay

- For illustration, let’s pick AAAA (Blue) in XXX for further examination



temp - Graph Builder - JMP

Graph Builder

Variables

6 Columns: OEM, Unit, Color, Oil, Test, Ox

Points

Summary Statistic: None

Error Bars: Auto

Response Axis: Auto

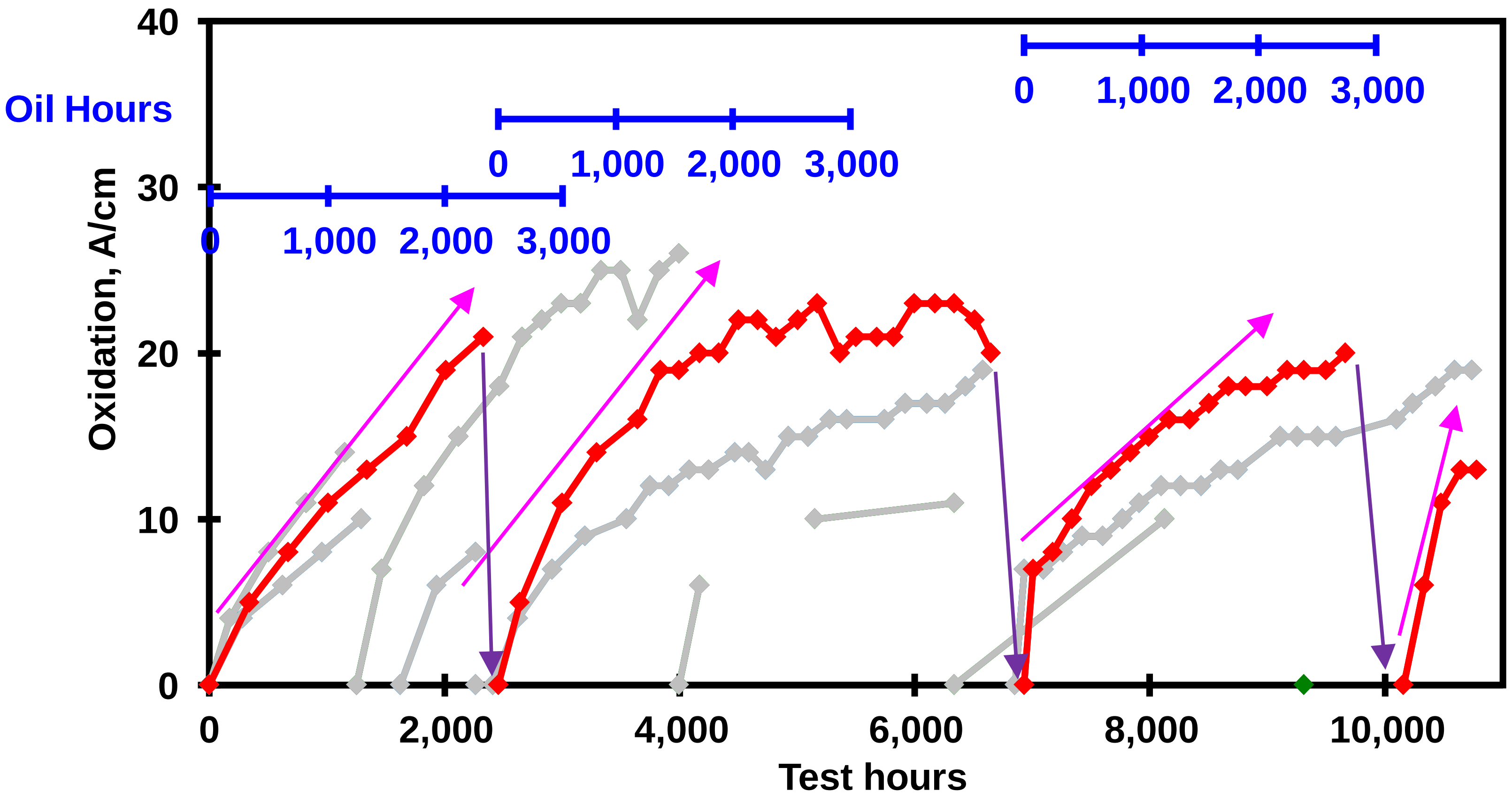
Jitter: Auto

Jitter Limit

Variables

Engine oil oxidation – “Oil hours” *vs*. “Test hours”

- Oxidation vs. Test hours reveals oil changes
  - – In “Oil Hours” space, each oil change can be considered a replicate



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Engine oil oxidation – AAAA (Blue) in XXX only

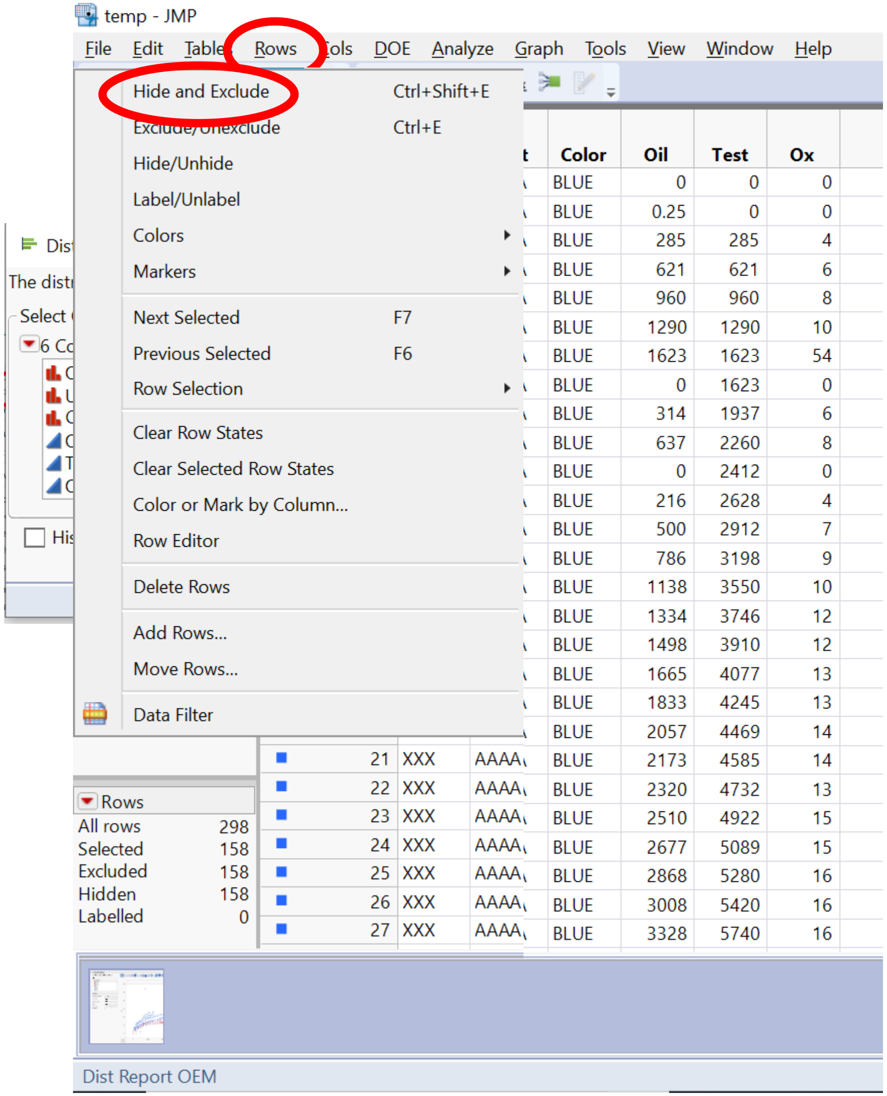
- Back to the dataset
- Analyze ➔
- Distribution ➔

- OEM → Y, Columns
- OK

- Click on YYY

- Back to dataset
- Rows ➔
- Hide and Exclude ➔

- Go to Graph Builder

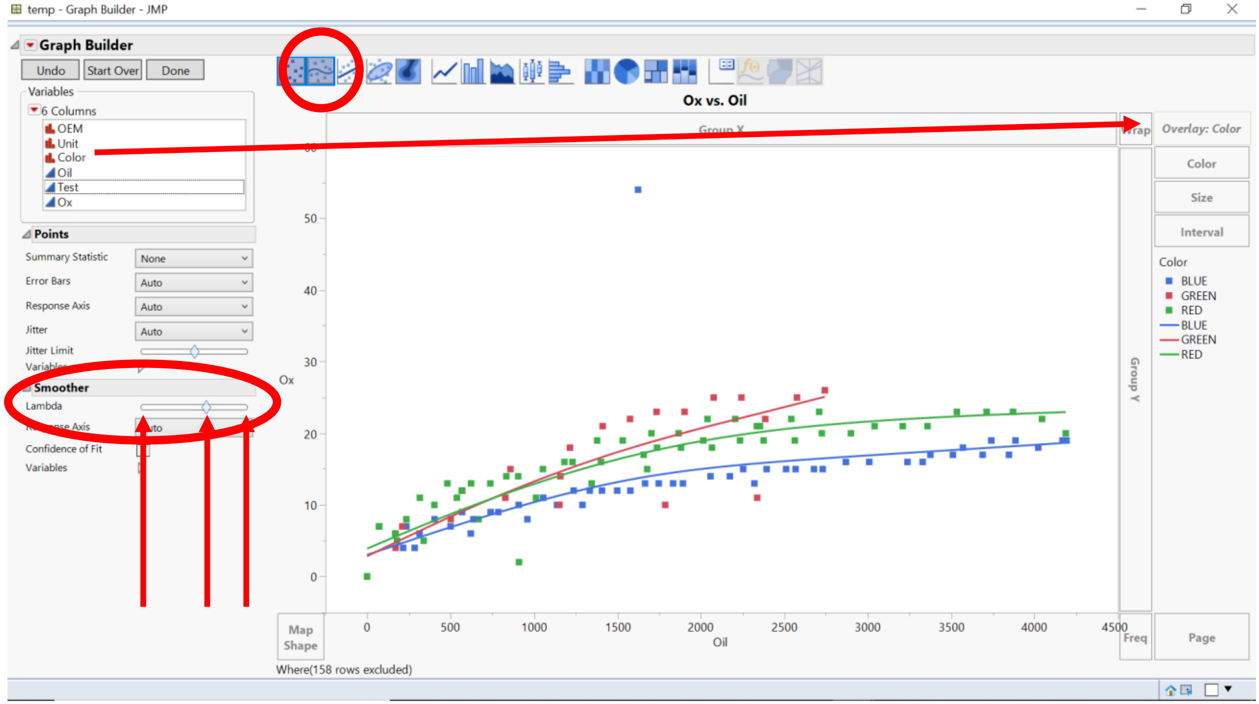


			Color	Oil	Test	Ox
			BLUE	0	0	0
			BLUE	0.25	0	0
			BLUE	285	285	4
			BLUE	621	621	6
			BLUE	960	960	8
			BLUE	1290	1290	10
			BLUE	1623	1623	54
			BLUE	0	1623	0
			BLUE	314	1937	6
			BLUE	637	2260	8
			BLUE	0	2412	0
			BLUE	216	2628	4
			BLUE	500	2912	7
			BLUE	786	3198	9
			BLUE	1138	3550	10
			BLUE	1334	3746	12
			BLUE	1498	3910	12
			BLUE	1665	4077	13
			BLUE	1833	4245	13
			BLUE	2057	4469	14
21	XXX	AAAA	BLUE	2173	4585	14
22	XXX	AAAA	BLUE	2320	4732	13
23	XXX	AAAA	BLUE	2510	4922	15
24	XXX	AAAA	BLUE	2677	5089	15
25	XXX	AAAA	BLUE	2868	5280	16
26	XXX	AAAA	BLUE	3008	5420	16
27	XXX	AAAA	BLUE	3328	5740	16

Rows	
All rows	298
Selected	158
Excluded	158
Hidden	158
Labelled	0

Engine oil oxidation – exploring shape

- Because the rows are color-coded with the “Color” variable, it looks like there are three separate responses
- But JMP doesn’t know that yet
- Color → Overlay
- Smoother ➔
- Lambda ➔
  - Slide until you like the look of the curves
  - Left tries to fit more closely
  - Right is smoother
  - Find the one you like
  - This is one way to decide what shape curve to fit



temp - Graph Builder - JMP

Graph Builder

Variables

6 Columns: OEM, Unit, Color, Oil, Test, Ox

Points

Summary Statistic: None

Error Bars: Auto

Response Axis: Auto

Jitter: Auto

Jitter Limit

Variables

Smoother

Lambda

Response Axis: Auto

Confidence of Fit: □

Variables

Where(158 rows excluded)

Quirk: JMP assigns
Blue (points) is Blue (oil)
Red (points) is Green (oil)
Green (points) is Red (oil)
Can be fixed, but it doesn’t bother me

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Engine oil oxidation – choosing a model

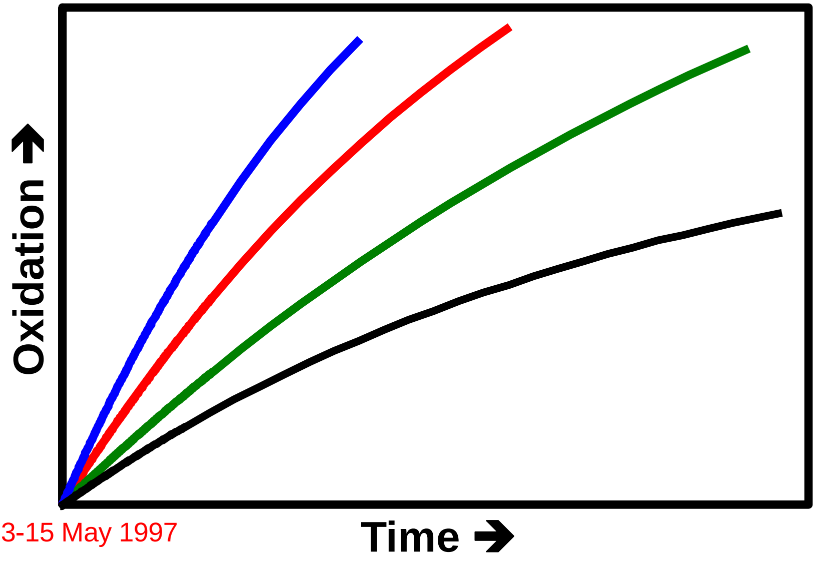
- Graphical analysis can inform the appropriate curve shape
  - Or, from fundamental physical principles
- Engine oil oxidation, under these conditions, generally follows*:

$$Oxidation = A + B\left[1 - e^{(-t/C)}\right]$$

- JMP has a built-in library of non-linear functions, including "Mechanistic Growth Model (3P)"

$$Oxidation = theta1 * [1 - theta2 * \mathrm{Exp}(-theta3 * t)]$$

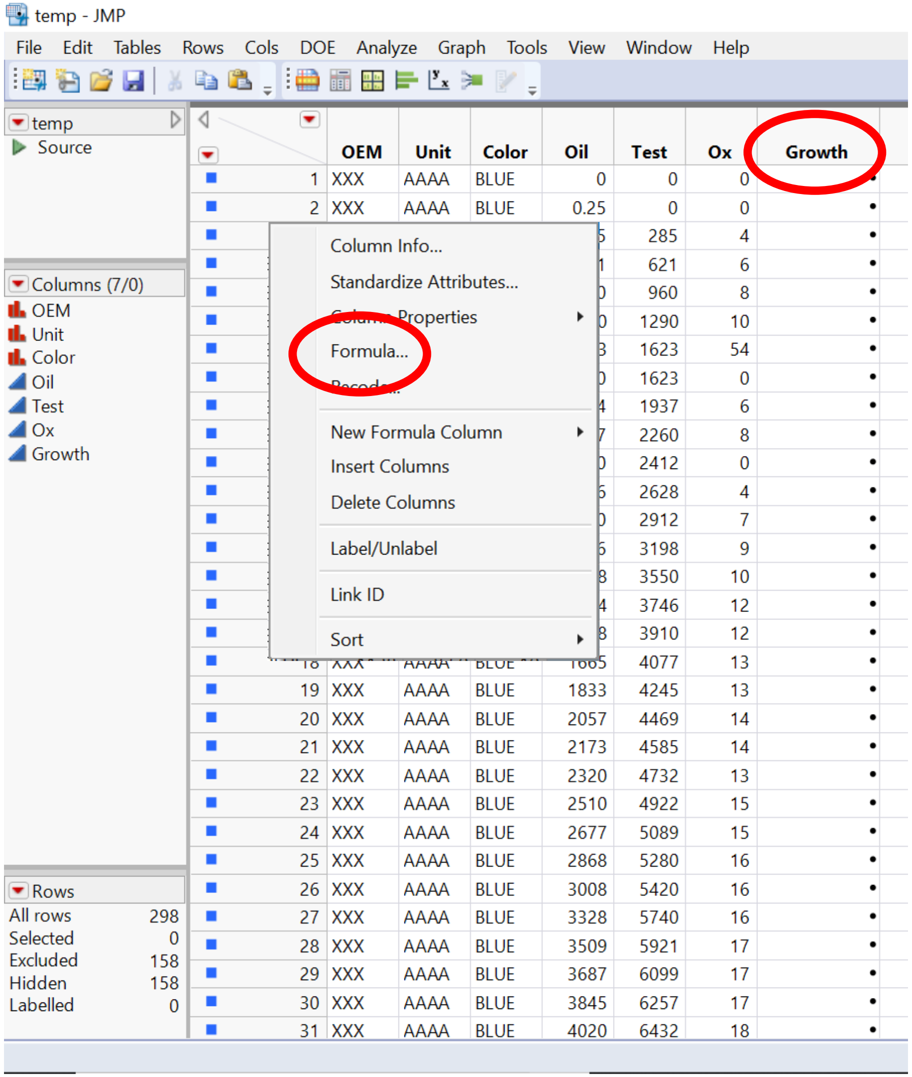
- Equivalent, with
  - A = theta1 – theta1 * theta2
  - B = theta1 * theta2
  - C = 1/theta3
- But, I prefer my parameterization
  - A,B,C have physical meanings



*M. J. Cannon, *et. al.*, CEC97-EL09, Fifth CEC Symposium, Göteborg, Sweden, 13-15 May 1997

Engine oil oxidation – fitting a model

- Simple first
  - One engine-oil at a time
- Create a new column ➔
  - I always call it “Growth”
- Right click on column name ➔
- Formula ➔



Rows	
All rows	298
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Labelled	0

	OEM	Unit	Color	Oil	Test	Ox	Growth
1	XXX	AAAA	BLUE	0	0	0	•
2	XXX	AAAA	BLUE	0.25	0	0	•
				5	285	4	•
				1	621	6	•
				0	960	8	•
				0	1290	10	•
				3	1623	54	•
				0	1623	0	•
				4	1937	6	•
				7	2260	8	•
				0	2412	0	•
				6	2628	4	•
				0	2912	7	•
				6	3198	9	•
				8	3550	10	•
				4	3746	12	•
				8	3910	12	•
18	XXX	AAAA	BLUE	1665	4077	13	•
19	XXX	AAAA	BLUE	1833	4245	13	•
20	XXX	AAAA	BLUE	2057	4469	14	•
21	XXX	AAAA	BLUE	2173	4585	14	•
22	XXX	AAAA	BLUE	2320	4732	13	•
23	XXX	AAAA	BLUE	2510	4922	15	•
24	XXX	AAAA	BLUE	2677	5089	15	•
25	XXX	AAAA	BLUE	2868	5280	16	•
26	XXX	AAAA	BLUE	3008	5420	16	•
27	XXX	AAAA	BLUE	3328	5740	16	•
28	XXX	AAAA	BLUE	3509	5921	17	•
29	XXX	AAAA	BLUE	3687	6099	17	•
30	XXX	AAAA	BLUE	3845	6257	17	•
31	XXX	AAAA	BLUE	4020	6432	18	•

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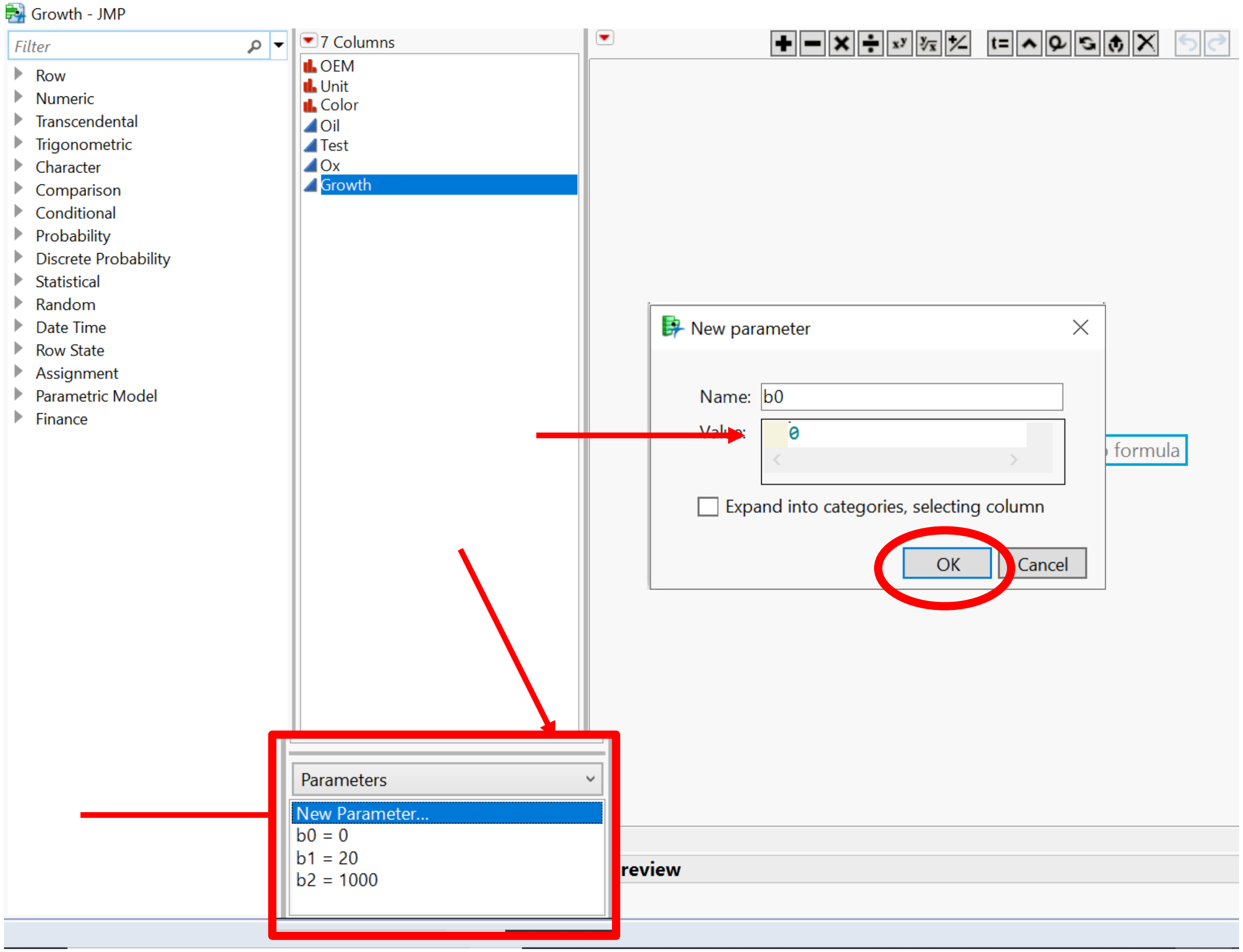
Engine oil oxidation – creating parameters

- Define parameters
  - Constants ➔
  - Parameters ➔
- New parameter ➔
- Value ➔
- OK ➔
- Repeat for other parameters
- A, B, C = b0, b1, b2
  - Use values suggested from the graphs
  - Makes it easier later
- b0 = 0
- b1 = 20
- b2 = 1000



Growth - JMP

New parameter

Name: b0

Value: 0

□ Expand into categories, selecting column

Parameters

New Parameter...

b0 = 0

b1 = 20

b2 = 1000

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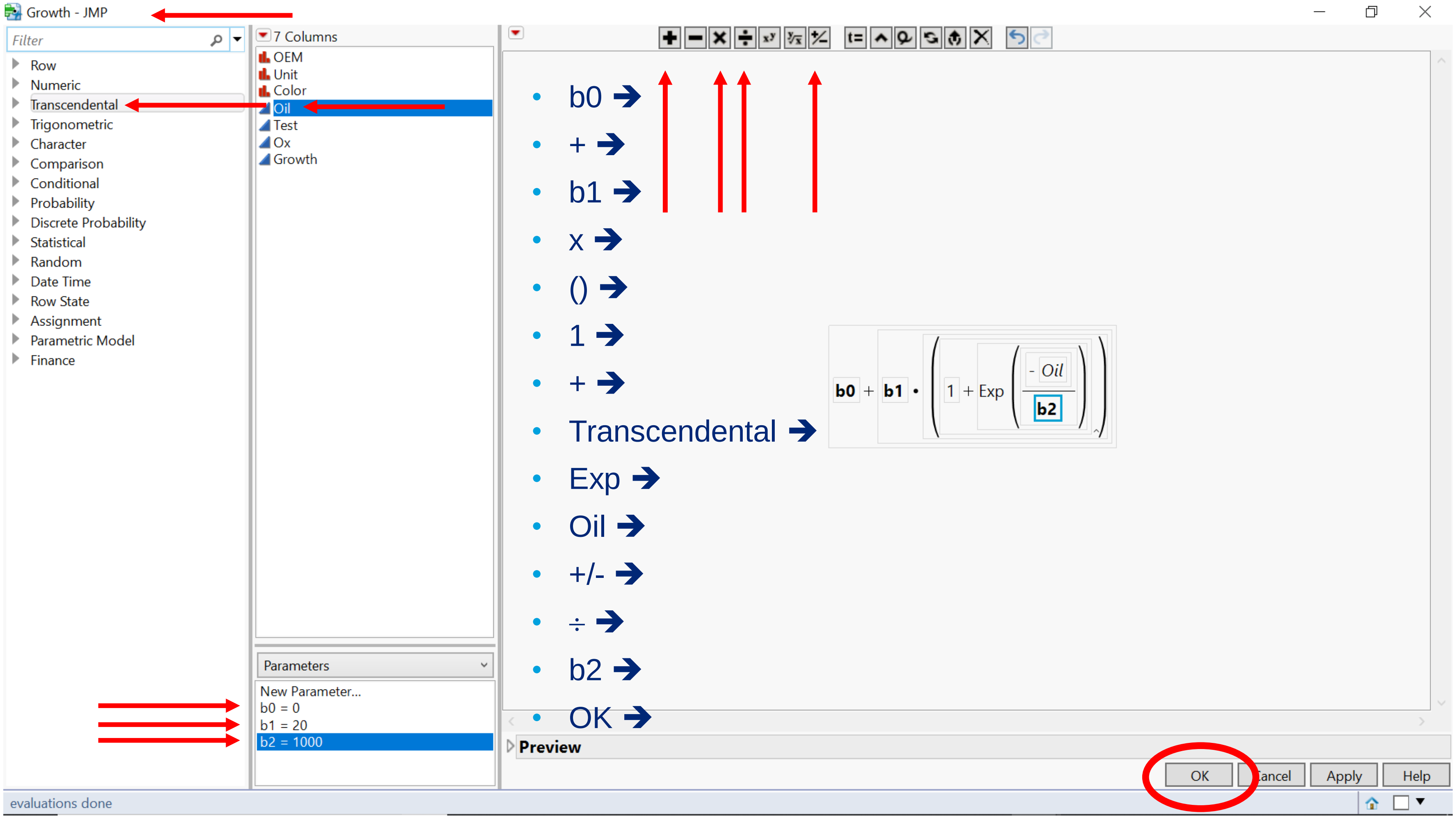
Engine oil oxidation – creating a formula



b0 = 0
b1 = 20
b2 = 1000

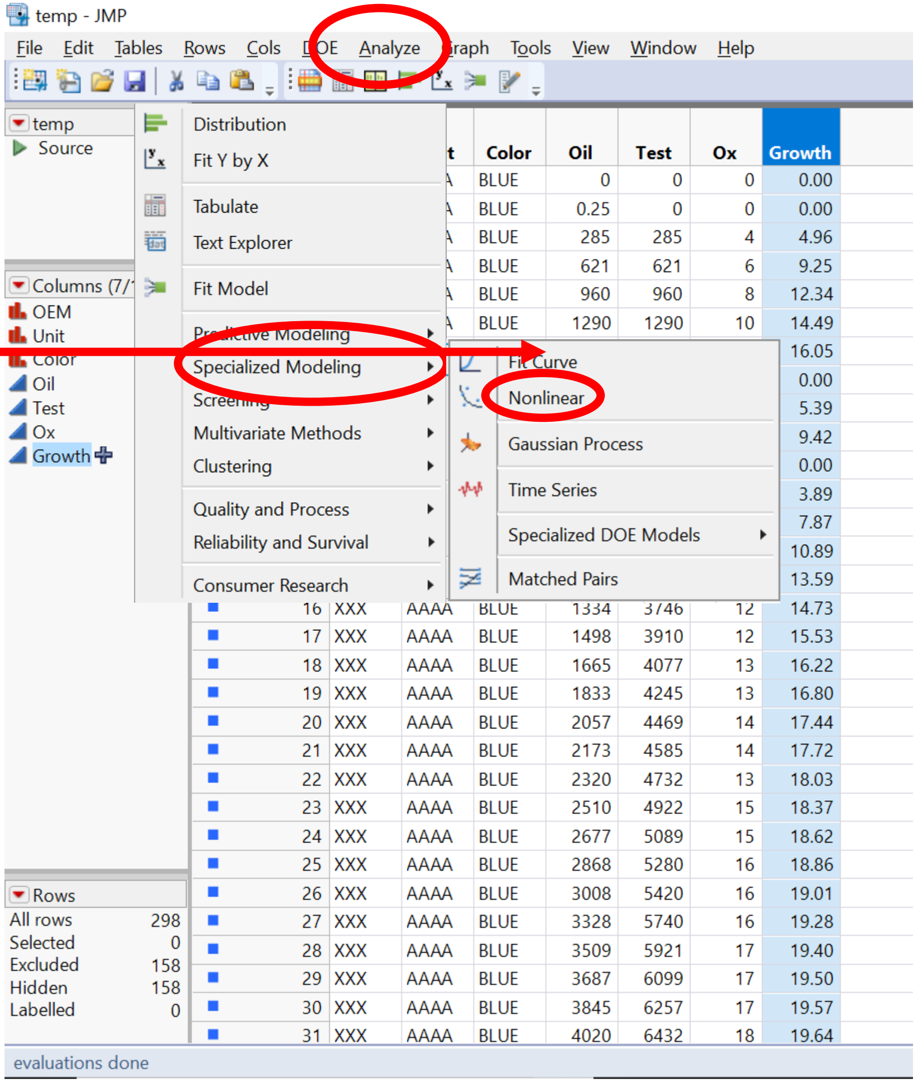
$$b0 + b1 \cdot \left(\left(1 + \mathrm{Exp}\left(\frac{-\,Oil}{b2} \right) \right) \right)$$

- b0 →
- + →
- b1 →
- x →
- () →
- 1 →
- + →
- Transcendental →
- Exp →
- Oil →
- +/- →
- ÷ →
- b2 →
- OK →

Engine oil oxidation – entering nonlinear platform

- “Growth” function is populated
- Analyze ➔
- Specialized Modeling ➔
- Nonlinear ➔

$$Growth = 0 + 20 * \left[1 + e^{\left(\frac{-1623}{1000}\right)}\right] = 16.05$$

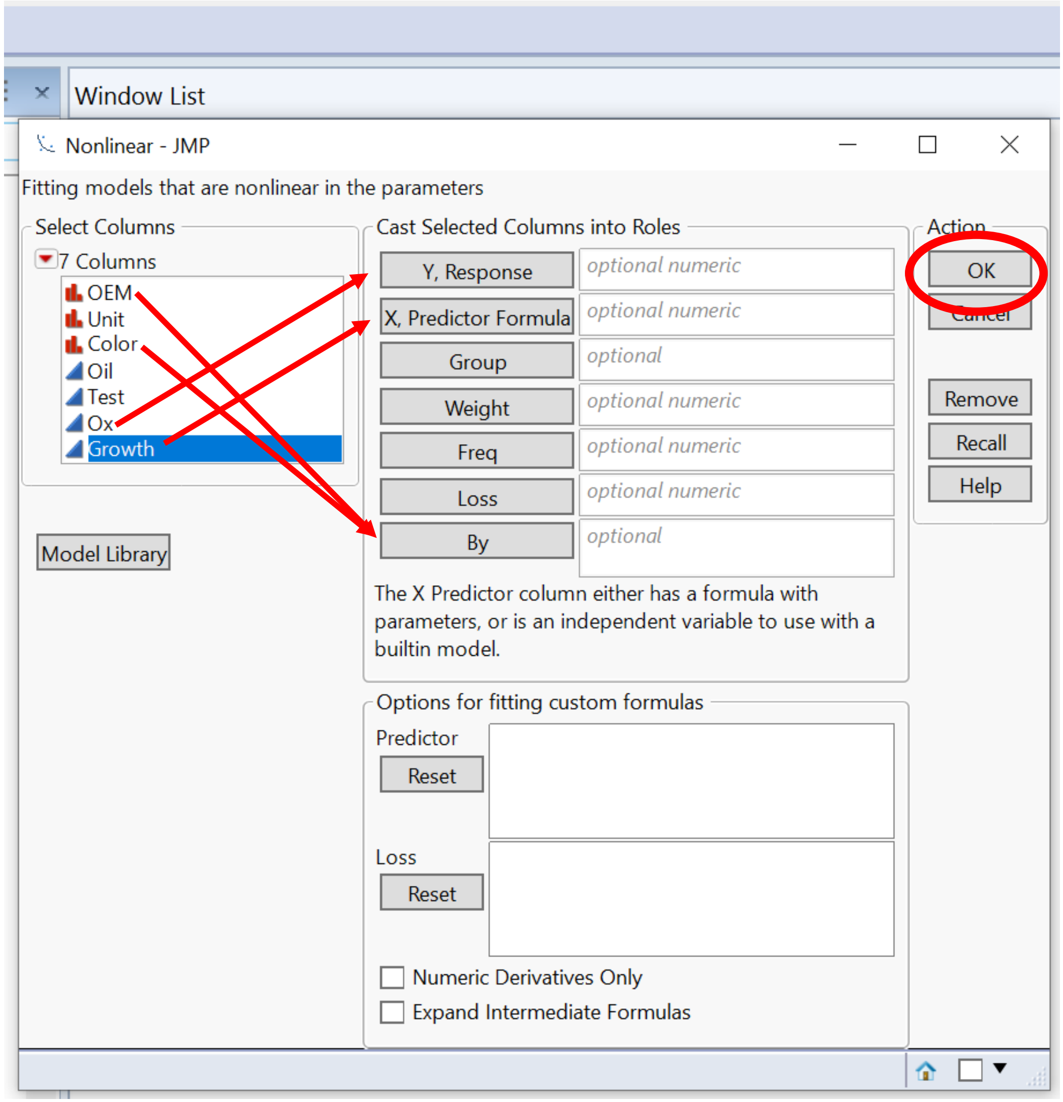


Rows	
All rows	298
Selected	0
Excluded	158
Hidden	158
Labelled	0

		t	Color	Oil	Test	Ox	Growth
		A	BLUE	0	0	0	0.00
		A	BLUE	0.25	0	0	0.00
		A	BLUE	285	285	4	4.96
		A	BLUE	621	621	6	9.25
		A	BLUE	960	960	8	12.34
		A	BLUE	1290	1290	10	14.49
							16.05
							0.00
							5.39
							9.42
							0.00
							3.89
							7.87
							10.89
							13.59
16	XXX	AAAA	BLUE	1334	3746	12	14.73
17	XXX	AAAA	BLUE	1498	3910	12	15.53
18	XXX	AAAA	BLUE	1665	4077	13	16.22
19	XXX	AAAA	BLUE	1833	4245	13	16.80
20	XXX	AAAA	BLUE	2057	4469	14	17.44
21	XXX	AAAA	BLUE	2173	4585	14	17.72
22	XXX	AAAA	BLUE	2320	4732	13	18.03
23	XXX	AAAA	BLUE	2510	4922	15	18.37
24	XXX	AAAA	BLUE	2677	5089	15	18.62
25	XXX	AAAA	BLUE	2868	5280	16	18.86
26	XXX	AAAA	BLUE	3008	5420	16	19.01
27	XXX	AAAA	BLUE	3328	5740	16	19.28
28	XXX	AAAA	BLUE	3509	5921	17	19.40
29	XXX	AAAA	BLUE	3687	6099	17	19.50
30	XXX	AAAA	BLUE	3845	6257	17	19.57
31	XXX	AAAA	BLUE	4020	6432	18	19.64

Engine oil oxidation – nonlinear analysis

- Ox → Y, response
- Growth → X, Predictor Formula
- OEM → By
- Color → By
- OK ➔



The X Predictor column either has a formula with parameters, or is an independent variable to use with a builtin model.

□ Numeric Derivatives Only

□ Expand Intermediate Formulas

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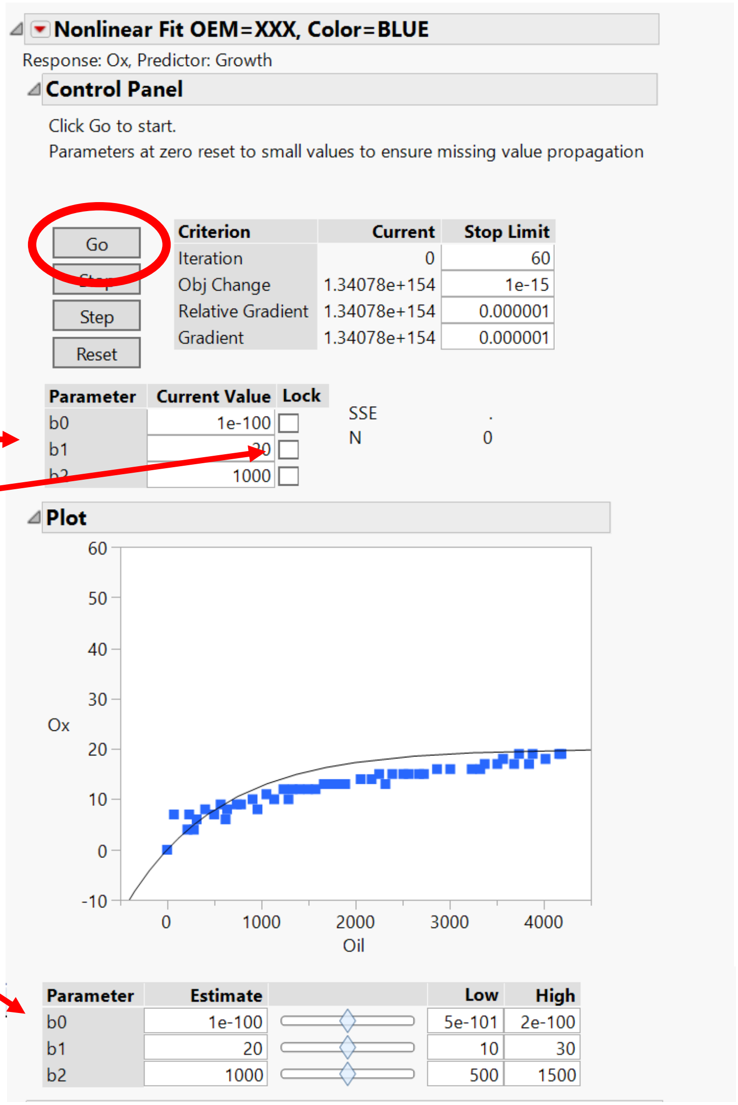
Engine oil oxidation – initial view

- For OEM = XXX, Color = Blue
- Shows data points
- Shows “Growth” function using initial parameter estimates
  - Can manually adjust parameters for a “See What Happens” exploration
  - Digitally
  - Sliders
- Can enter fixed parameter(s), not to be fitted
  - For example, if there is a physical reason curve should start at zero
- Go ➔



Response: Ox, Predictor: Growth

Click Go to start.

Parameters at zero reset to small values to ensure missing value propagation

Criterion	Current	Stop Limit
Iteration	0	60
Obj Change	1.34078e+154	1e-15
Relative Gradient	1.34078e+154	0.000001
Gradient	1.34078e+154	0.000001

Parameter	Current Value	Lock
b0	1e-100	□
b1	20	□
b2	1000	□

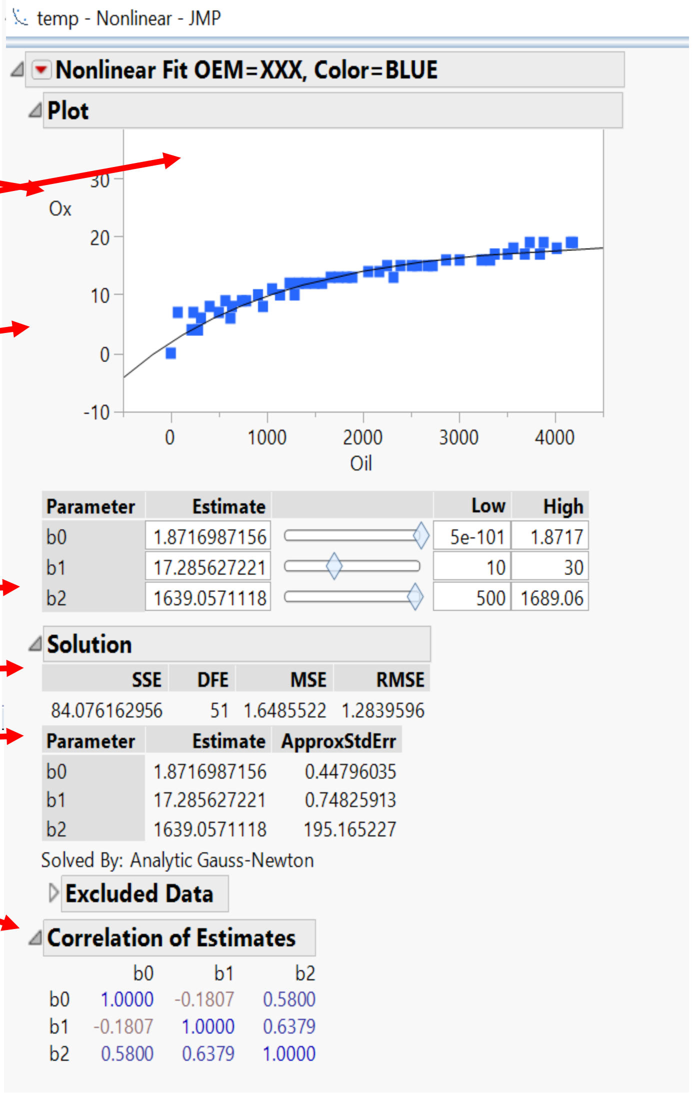
SSE .

N 0

Parameter	Estimate		Low	High
b0	1e-100		5e-101	2e-100
b1	20		10	30
b2	1000		500	1500

Engine oil oxidation – results

- Expand each section
- Converged in Gradient
  - The fit was successful
  - If not, there are things to do
- Various diagnostics
  - How long it took to fit, *etc*.
- Parameter fits
  - You can change them and run again
  - Example later
- Plot showing fitted line
- Goodness-of-fit statistics
- Parameters with errors
- Correlation of parameter estimates



Parameter	Estimate	Low	High
b0	1.8716987156	5e-101	1.8717
b1	17.285627221	10	30
b2	1639.0571118	500	1689.06

Solution

SSE	DFE	MSE	RMSE
84.076162956	51	1.6485522	1.2839596

Parameter	Estimate	ApproxStdErr
b0	1.8716987156	0.44796035
b1	17.285627221	0.74825913
b2	1639.0571118	195.165227

Solved By: Analytic Gauss-Newton

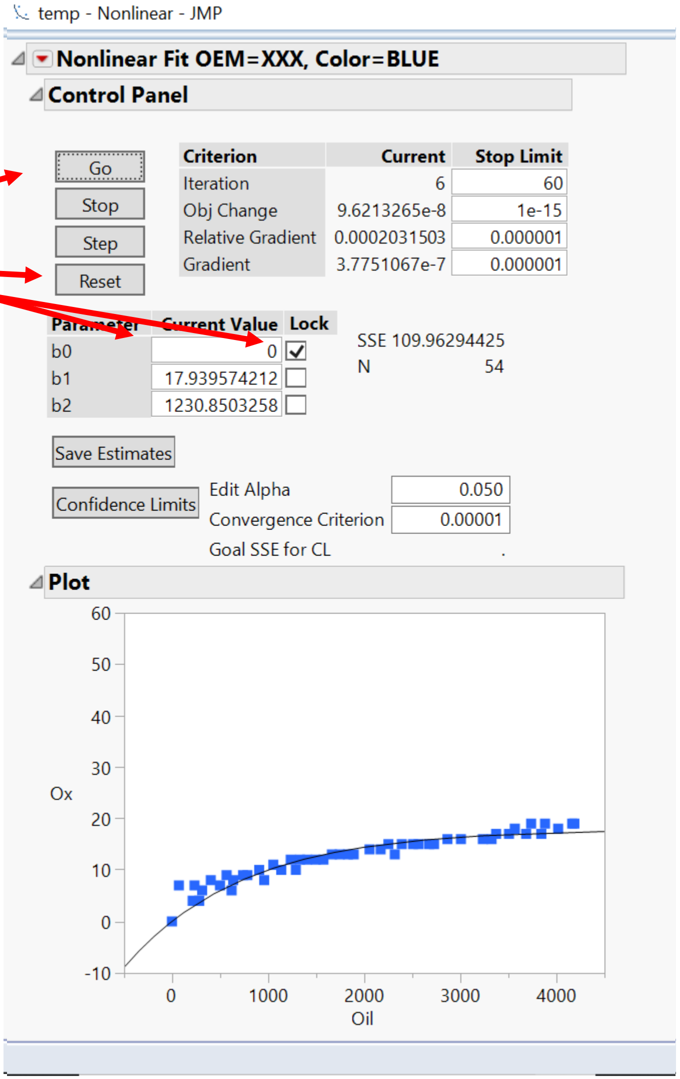
Excluded Data

Correlation of Estimates

	b0	b1	b2
b0	1.0000	-0.1807	0.5800
b1	-0.1807	1.0000	0.6379
b2	0.5800	0.6379	1.0000

Engine oil oxidation – change a parameter

- Change and fix parameter
- b0 = 0 ➔
  - Belief: fresh oil has no oxidation, by definition
- Check ➔
- Reset ➔
  - Fitting diagnostics change
  - Plot changes
- Go ➔
  - Diagnostics change
  - Plot changes
  - Summary statistics change



temp - Nonlinear - JMP

Nonlinear Fit OEM=XXX, Color=BLUE

Control Panel

Go

Stop

Step

Reset

Criterion	Current	Stop Limit
Iteration	6	60
Obj Change	9.6213265e-8	1e-15
Relative Gradient	0.0002031503	0.000001
Gradient	3.7751067e-7	0.000001

Parameter	Current Value	Lock
b0	0	☑
b1	17.939574212	□
b2	1230.8503258	□

SSE 109.96294425
N 54

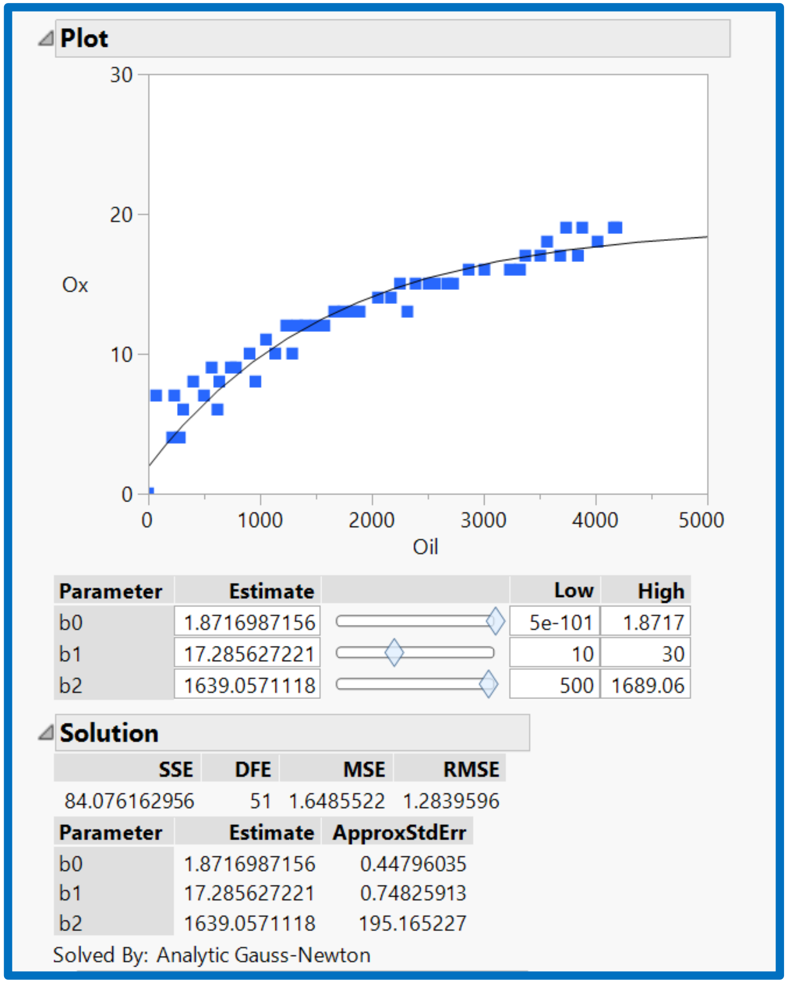
Save Estimates

Confidence Limits

Edit Alpha 0.050
Convergence Criterion 0.00001
Goal SSE for CL .

Plot

Engine oil oxidation – compare fits



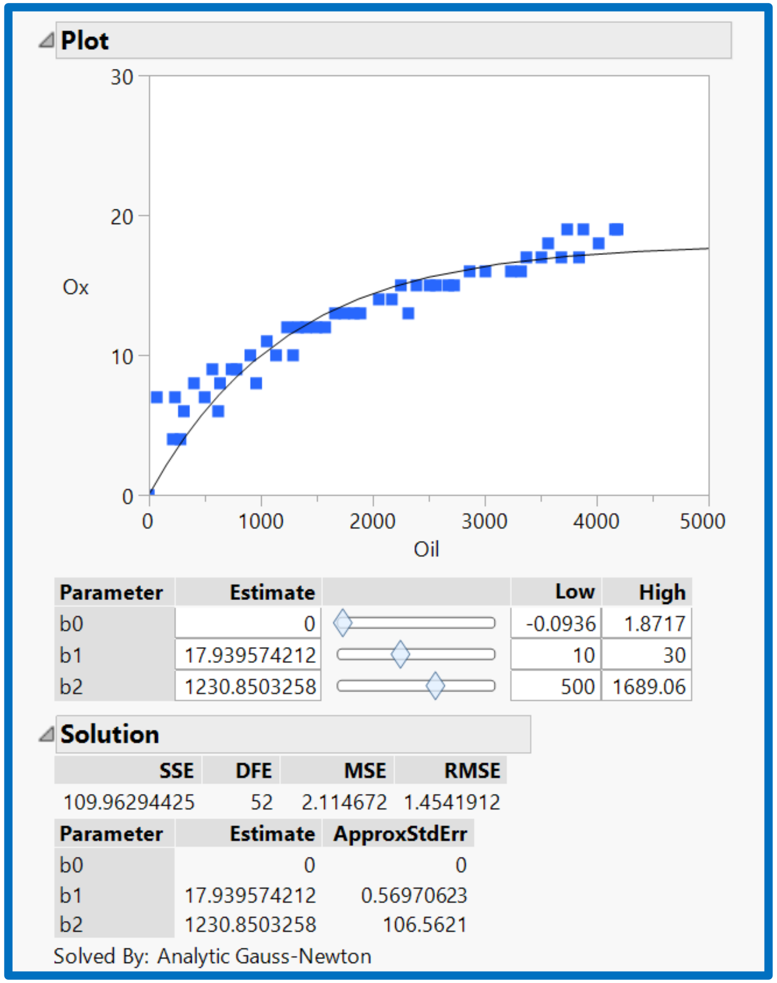
Parameter	Estimate		Low	High
b0	1.8716987156		5e-101	1.8717
b1	17.285627221		10	30
b2	1639.0571118		500	1689.06

Solution

SSE	DFE	MSE	RMSE
84.076162956	51	1.6485522	1.2839596

Parameter	Estimate	ApproxStdErr
b0	1.8716987156	0.44796035
b1	17.285627221	0.74825913
b2	1639.0571118	195.165227

Solved By: Analytic Gauss-Newton



Parameter	Estimate		Low	High
b0	0		-0.0936	1.8717
b1	17.939574212		10	30
b2	1230.8503258		500	1689.06

Solution

SSE	DFE	MSE	RMSE
109.96294425	52	2.114672	1.4541912

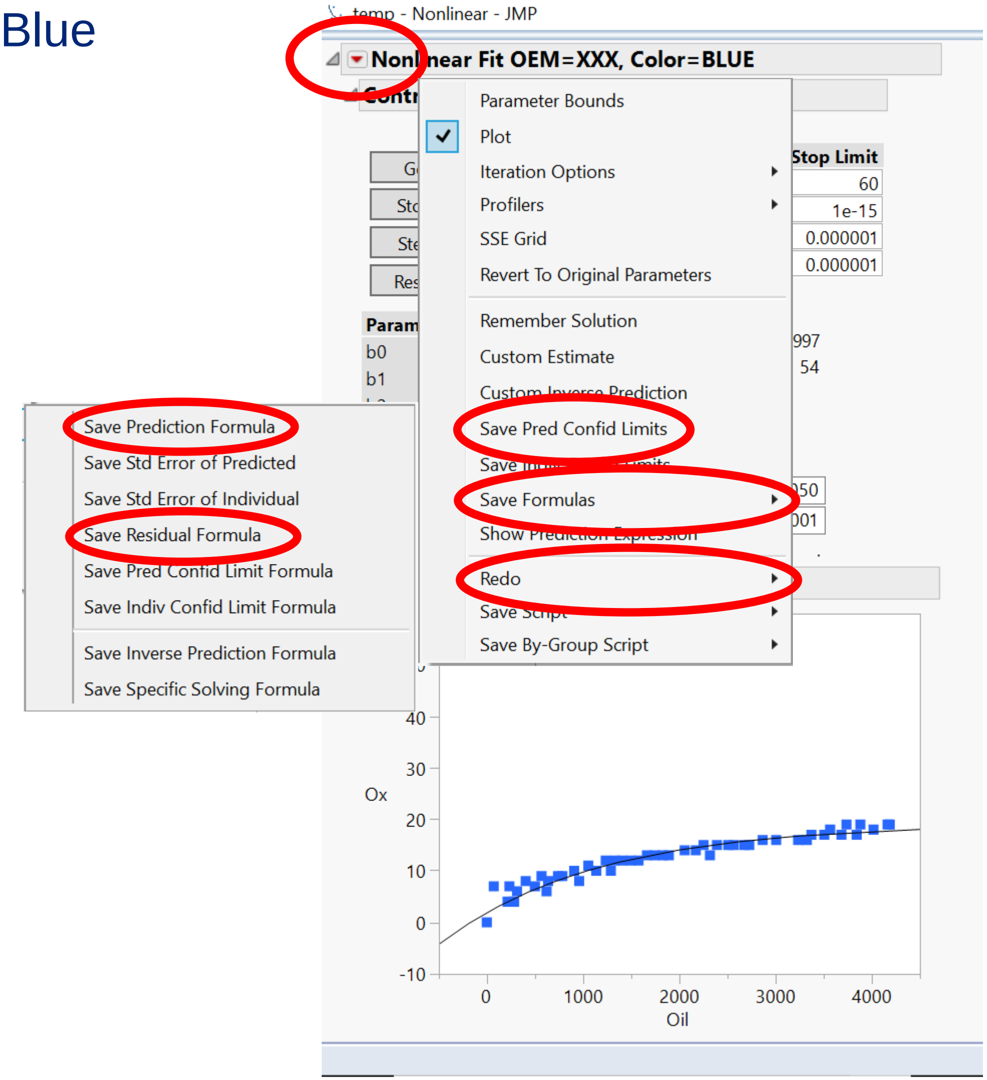
Parameter	Estimate	ApproxStdErr
b0	0	0
b1	17.939574212	0.56970623
b2	1230.8503258	106.5621

Solved By: Analytic Gauss-Newton

Engine oil oxidation – diagnostics

- ▼Nonlinear Fit OEM=XXX, Color=Blue

- Selected options I find useful
  - Save Confid Limits
    - xx% confidence intervals
    - Mean values
    - Individual values
  - Save Formulas
    - Save Residual Formula
    - Save Prediction Formula
  - Redo
    - Redo the same analysis
    - *e.g.*, After deleting outliers
    - Saves entering model over again
    - Example later

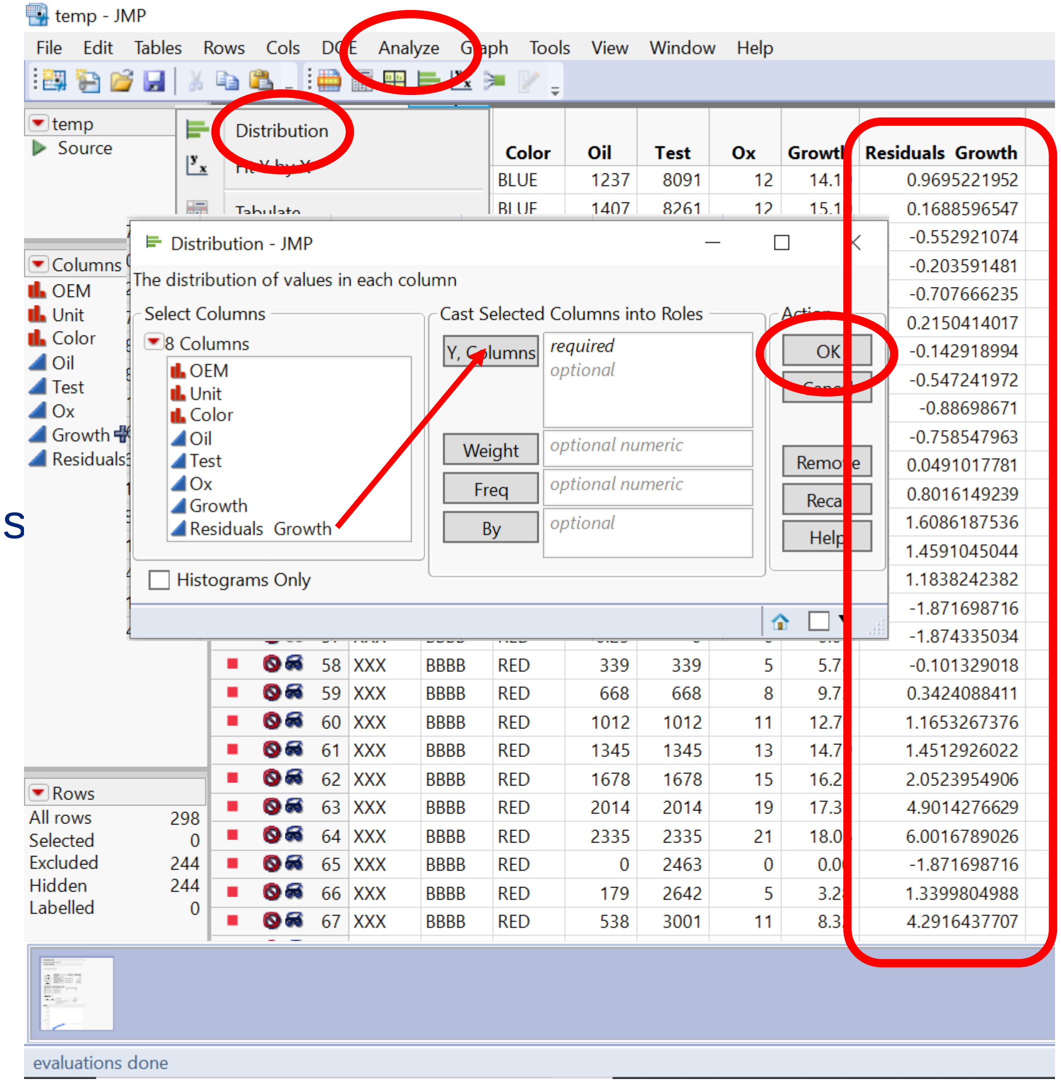


Engine oil oxidation – residuals

- ▼Nonlinear Fit
- Save Formulas
- Save Residual Formula
  - New column appears

- Analyze ➔
- Distribution ➔
- Residuals Growth → Y, Columns
- Go ➔

- Similar process to save predicted values



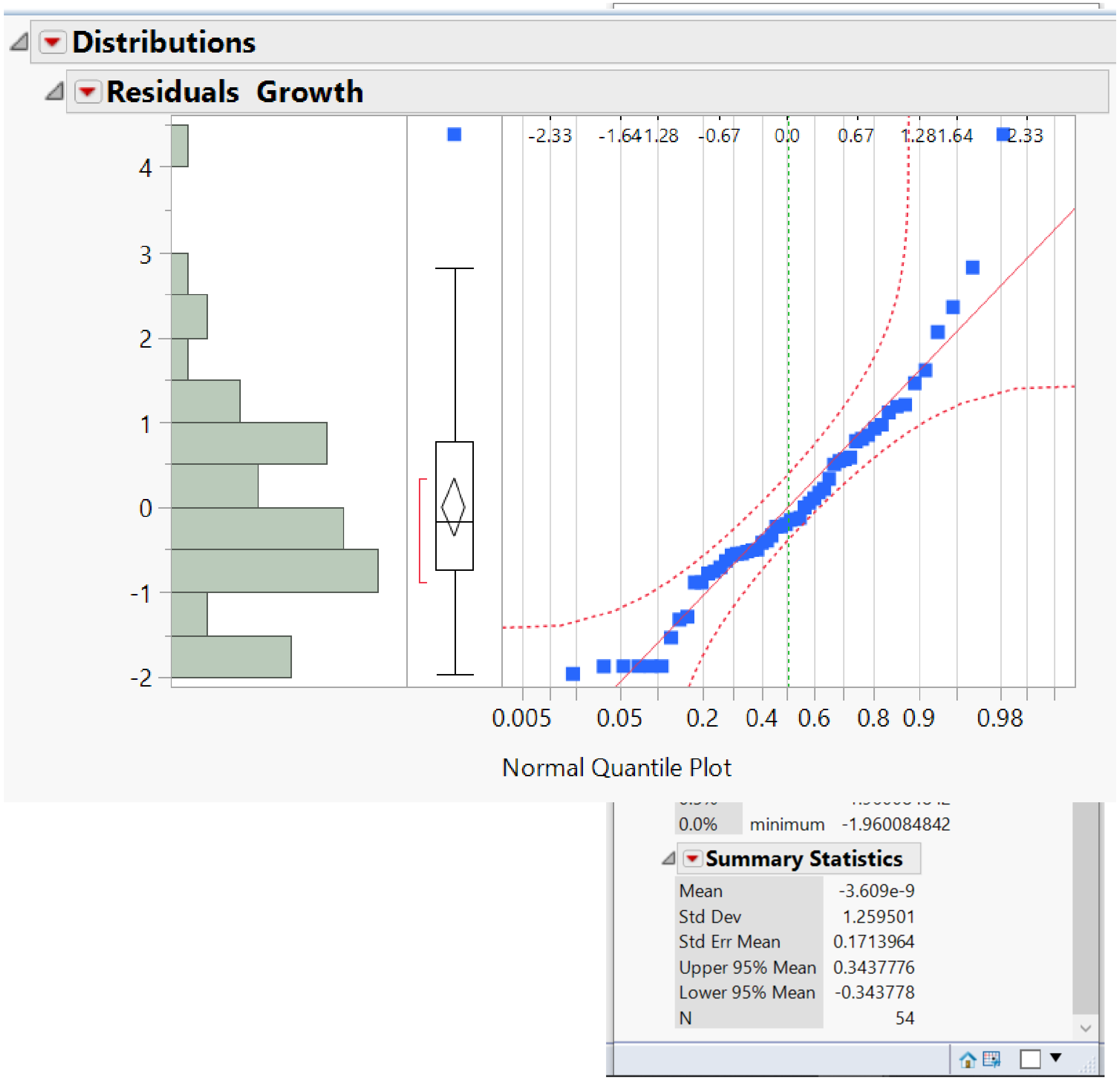
Rows	
All rows	298
Selected	0
Excluded	244
Hidden	244
Labelled	0

			Color	Oil	Test	Ox	Growth	Residuals Growth
			BLUE	1237	8091	12	14.1	0.9695221952
			BLUE	1407	8261	12	15.1	0.1688596547
								-0.552921074
								-0.203591481
								-0.707666235
								0.2150414017
								-0.142918994
								-0.547241972
								-0.88698671
								-0.758547963
								0.0491017781
								0.8016149239
								1.6086187536
								1.4591045044
								1.1838242382
								-1.871698716
								-1.874335034
58	XXX	BBBB	RED	339	339	5	5.7	-0.101329018
59	XXX	BBBB	RED	668	668	8	9.7	0.3424088411
60	XXX	BBBB	RED	1012	1012	11	12.7	1.1653267376
61	XXX	BBBB	RED	1345	1345	13	14.7	1.4512926022
62	XXX	BBBB	RED	1678	1678	15	16.2	2.0523954906
63	XXX	BBBB	RED	2014	2014	19	17.3	4.9014276629
64	XXX	BBBB	RED	2335	2335	21	18.0	6.0016789026
65	XXX	BBBB	RED	0	2463	0	0.0	-1.871698716
66	XXX	BBBB	RED	179	2642	5	3.2	1.3399804988
67	XXX	BBBB	RED	538	3001	11	8.3	4.2916437707

Engine oil oxidation – residual inspection

- Residuals distribution
- Histogram
  - Doesn’t look Normal
  - Don’t expect it to
- Various quantiles
- Summary statistics

- ▼Residuals Growth ➔
- Normal Quantile Plot ➔
  - Looks OK to me



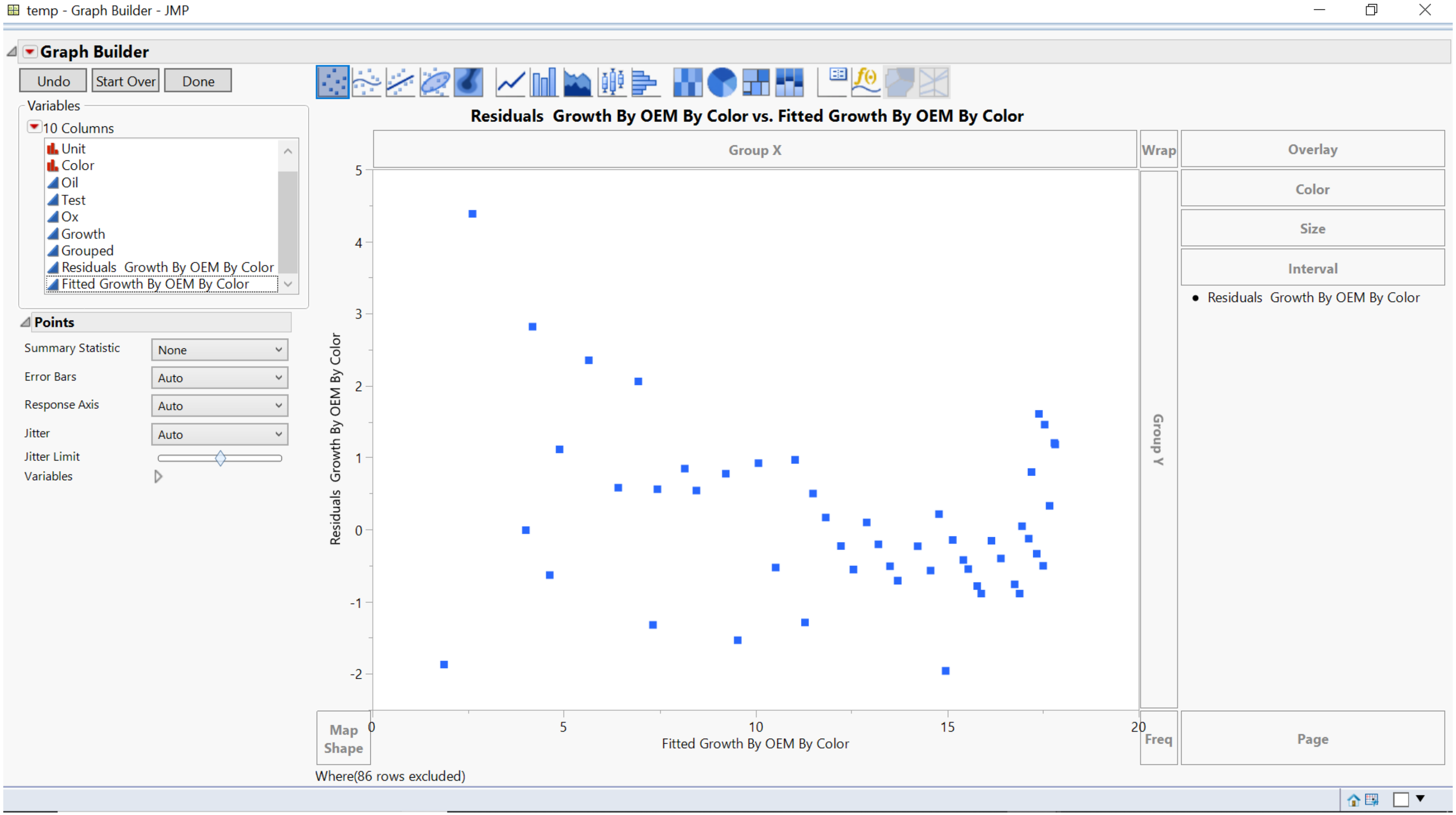
0.0%	minimum	-1.960084842

Summary Statistics

Mean	-3.609e-9
Std Dev	1.259501
Std Err Mean	0.1713964
Upper 95% Mean	0.3437776
Lower 95% Mean	-0.343778
N	54

Engine oil oxidation – residual inspection

- Residuals vs. Predicted: usually more unclear than linear analysis
  - Normal quantile plot probably more useful



temp - Graph Builder - JMP

Graph Builder

Variables

10 Columns

- Unit
- Color
- Oil
- Test
- Ox
- Growth
- Grouped
- Residuals Growth By OEM By Color
- Fitted Growth By OEM By Color

Points

Summary Statistic	None
Error Bars	Auto
Response Axis	Auto
Jitter	Auto
Jitter Limit	
Variables	

Residuals Growth By OEM By Color vs. Fitted Growth By OEM By Color

Where(86 rows excluded)

Undo
Start Over
Done
Group X
Wrap
Overlay
Color
Size
Interval
● Residuals Growth By OEM By Color
Group Y
Residuals Growth By OEM By Color
5
4
3
2
1
0
-1
-2
0
5
10
15
20
Fitted Growth By OEM By Color
Map Shape
Freq
Page

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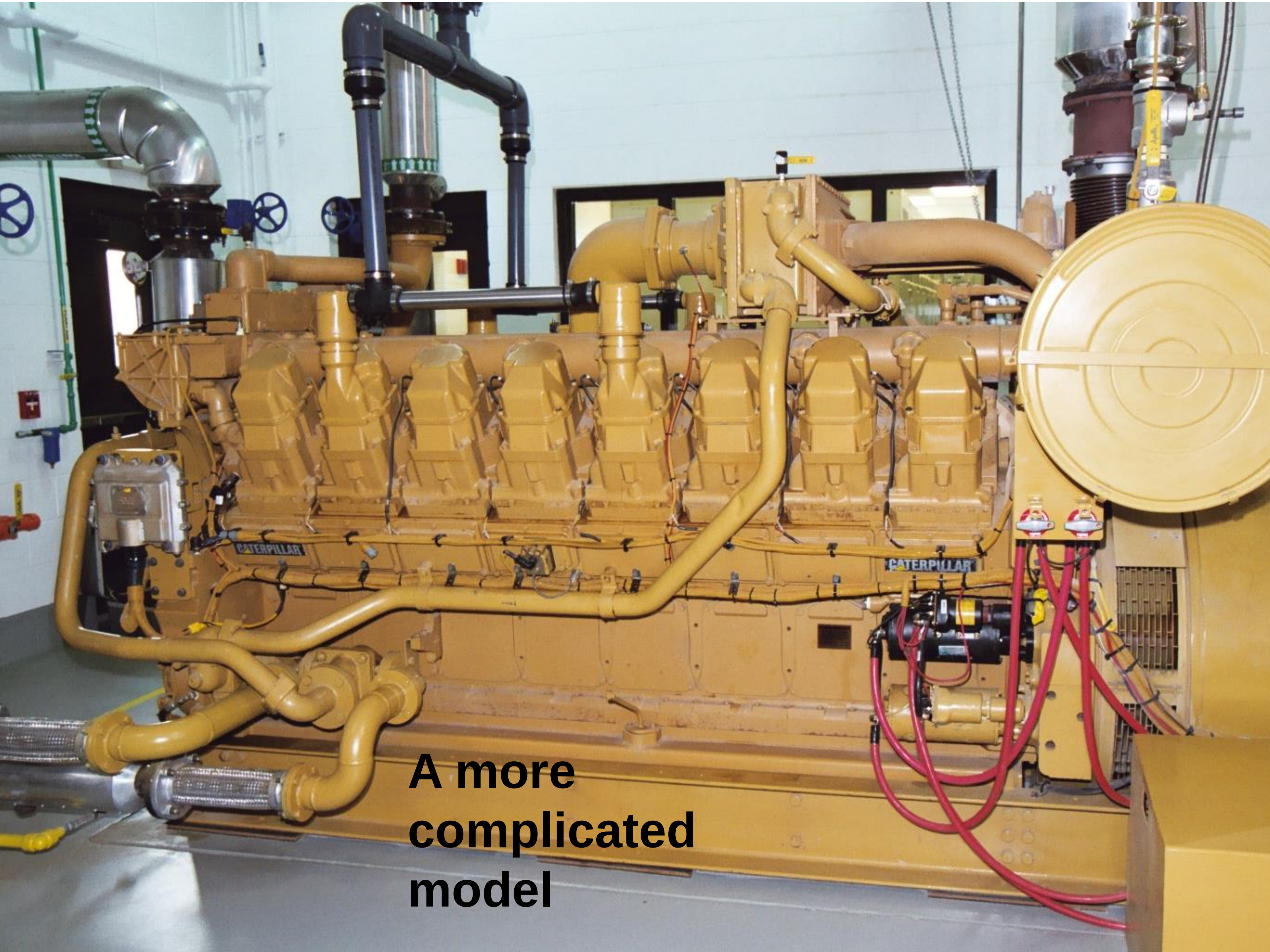

A more complicated model

A more complicated model

- Non-linear regression
  - One case at a time

$$Y = A + B * \left[1 - e^{\left(\frac{-t}{C}\right)}\right]$$

- Non-linear ANOVA
  - Multiple simultaneous comparisons

$$Y_i = A_i + B_i * \left[1 - e^{\left(\frac{-t}{C_i}\right)}\right]$$

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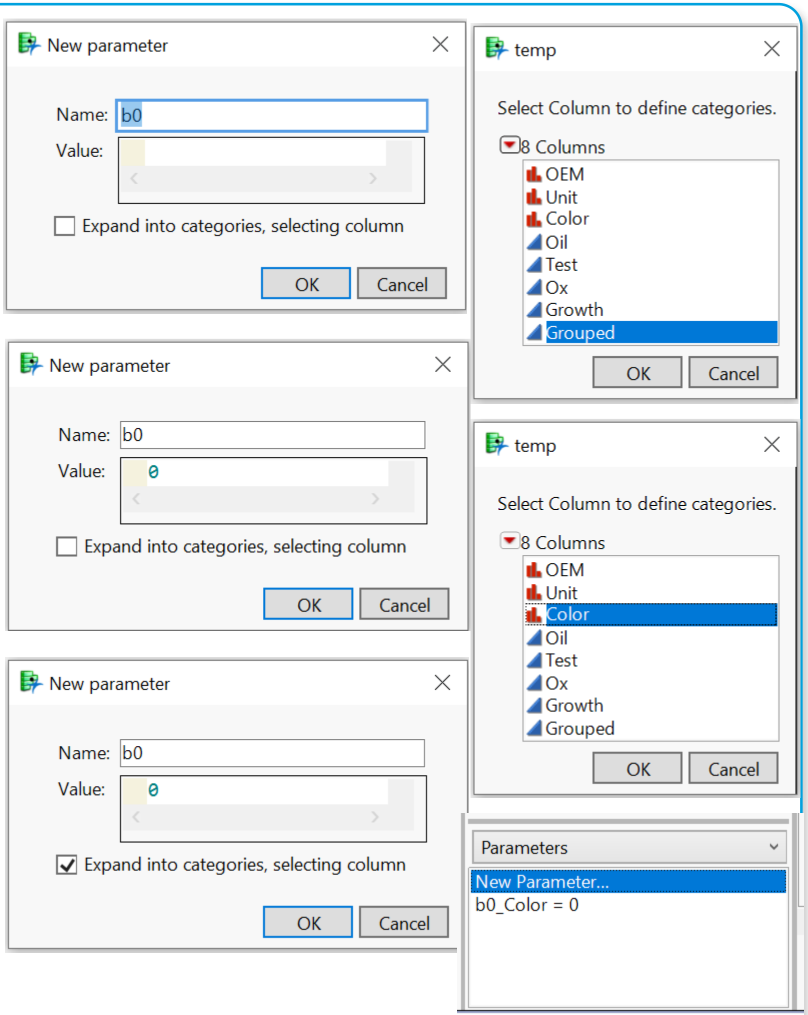
Engine oil oxidation – simultaneous fitting

- Fit all three “Colors” at once
  - Easier to make comparisons
- Create new column
  - I called it “Grouped”
  - Define a Formula
- Define Parameters ➔
  - b0 = 0 ➔
- Expand into categories, selecting column ➔
- OK ➔
- Want to select “Color” as category
- Color ➔
- OK ➔
- Do the same for the other parameters
- Define the equation, as before ➔



New parameter

Name: b0

Value:

☐ Expand into categories, selecting column

New parameter

Name: b0

Value: 0

☐ Expand into categories, selecting column

New parameter

Name: b0

Value: 0

☑ Expand into categories, selecting column

temp

Select Column to define categories.

8 Columns: OEM, Unit, Color, Oil, Test, Ox, Growth, Grouped (selected: Grouped)

temp

Select Column to define categories.

8 Columns: OEM, Unit, Color, Oil, Test, Ox, Growth, Grouped (selected: Color)

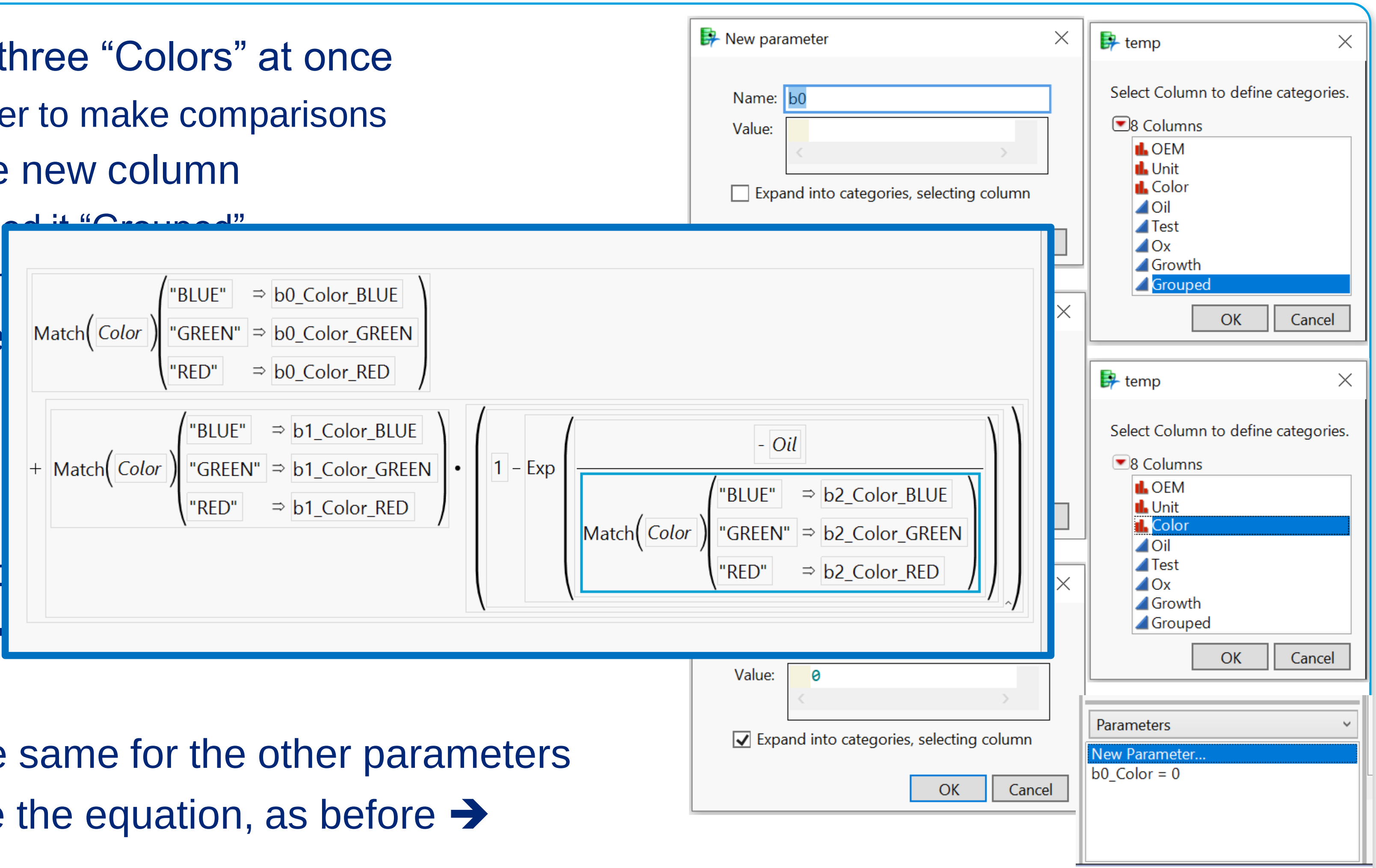
Parameters

New Parameter...

b0_Color = 0

Engine oil oxidation – simultaneous fitting

- Fit all three “Colors” at once
  - Easier to make comparisons
- Create new column
  - I called it “Grouped”
  - Defi
- Define
  - b0 =
- Expan
- OK ➔
- Want t
- Color
- OK ➔
- Do the same for the other parameters
- Define the equation, as before ➔



New parameter

Name: b0

Value:

□ Expand into categories, selecting column

temp

Select Column to define categories.

8 Columns: OEM, Unit, Color, Oil, Test, Ox, Growth, Grouped (selected)

OK Cancel

temp

Select Column to define categories.

8 Columns: OEM, Unit, Color (selected), Oil, Test, Ox, Growth, Grouped

OK Cancel

Value: 0

☑ Expand into categories, selecting column

OK Cancel

Parameters

New Parameter...

b0_Color = 0

$$\mathrm{Match}(Color)\begin{pmatrix}\text{"BLUE"} \Rightarrow \text{b0\_Color\_BLUE}\\ \text{"GREEN"} \Rightarrow \text{b0\_Color\_GREEN}\\ \text{"RED"} \Rightarrow \text{b0\_Color\_RED}\end{pmatrix} + \mathrm{Match}(Color)\begin{pmatrix}\text{"BLUE"} \Rightarrow \text{b1\_Color\_BLUE}\\ \text{"GREEN"} \Rightarrow \text{b1\_Color\_GREEN}\\ \text{"RED"} \Rightarrow \text{b1\_Color\_RED}\end{pmatrix} \bullet \left(1 - \mathrm{Exp}\left(\frac{-\,Oil}{\mathrm{Match}(Color)\begin{pmatrix}\text{"BLUE"} \Rightarrow \text{b2\_Color\_BLUE}\\ \text{"GREEN"} \Rightarrow \text{b2\_Color\_GREEN}\\ \text{"RED"} \Rightarrow \text{b2\_Color\_RED}\end{pmatrix}}\right)\right)$$

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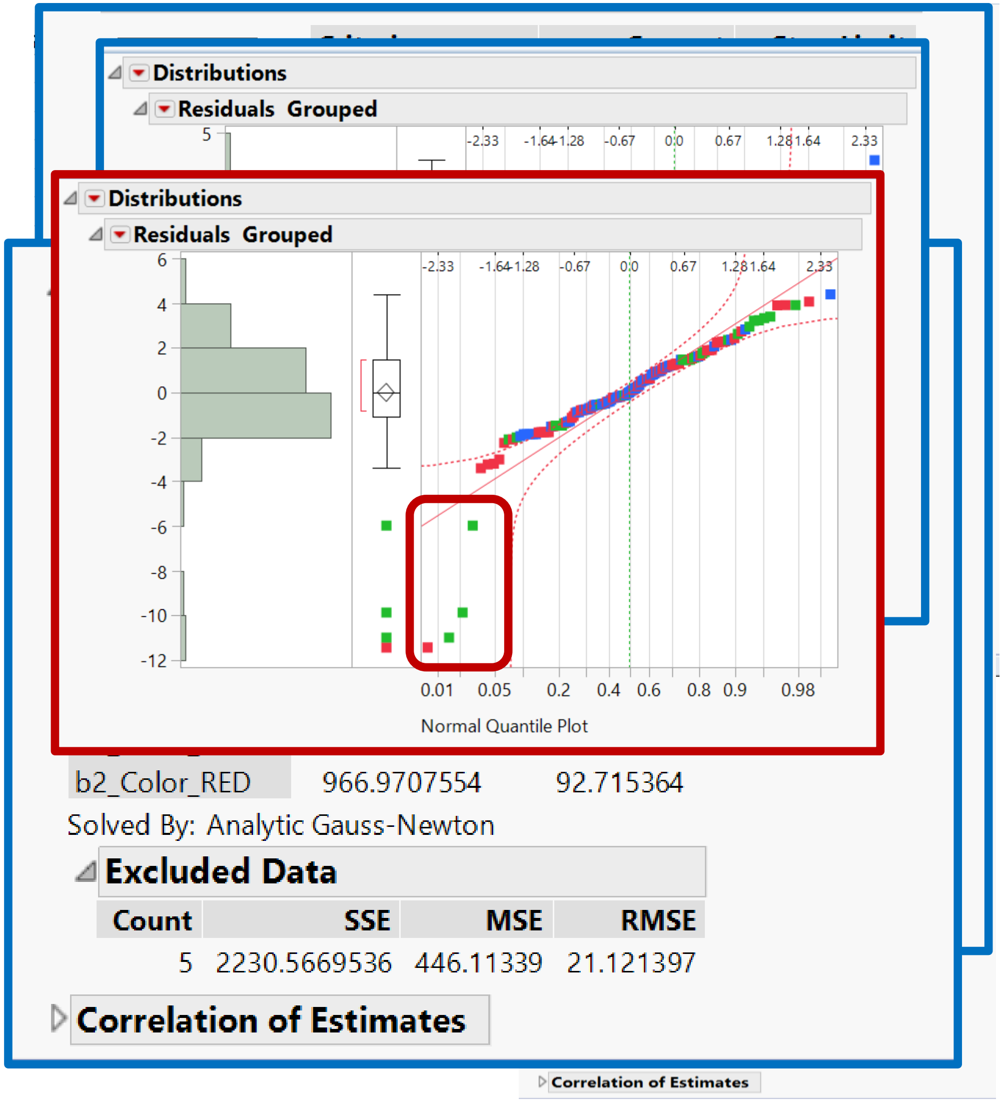
Engine oil oxidation – simultaneous fitting

- Analyze ➔
- Specialized Modeling ➔
- Nonlinear ➔
- Ox→ Y, Response
- Grouped→ X, Predictor Formula
  - “Grouped” is the new equation
- OK ➔
- Go ➔
- Output similar to before, but all nine parameters fit at once
- Check diagnostics, as before
- Compare parameters, *etc*.
  - $b0_{Blue} \approx bo_{Green} \approx b0_{Red} > 0$
  - $b1_{Blue} < b1_{Red} << b1_{Green}$



b2_Color_RED	966.9707554	92.715364

Solved By: Analytic Gauss-Newton

Excluded Data

Count	SSE	MSE	RMSE
5	2230.5669536	446.11339	21.121397

Correlation of Estimates

Correlation of Estimates

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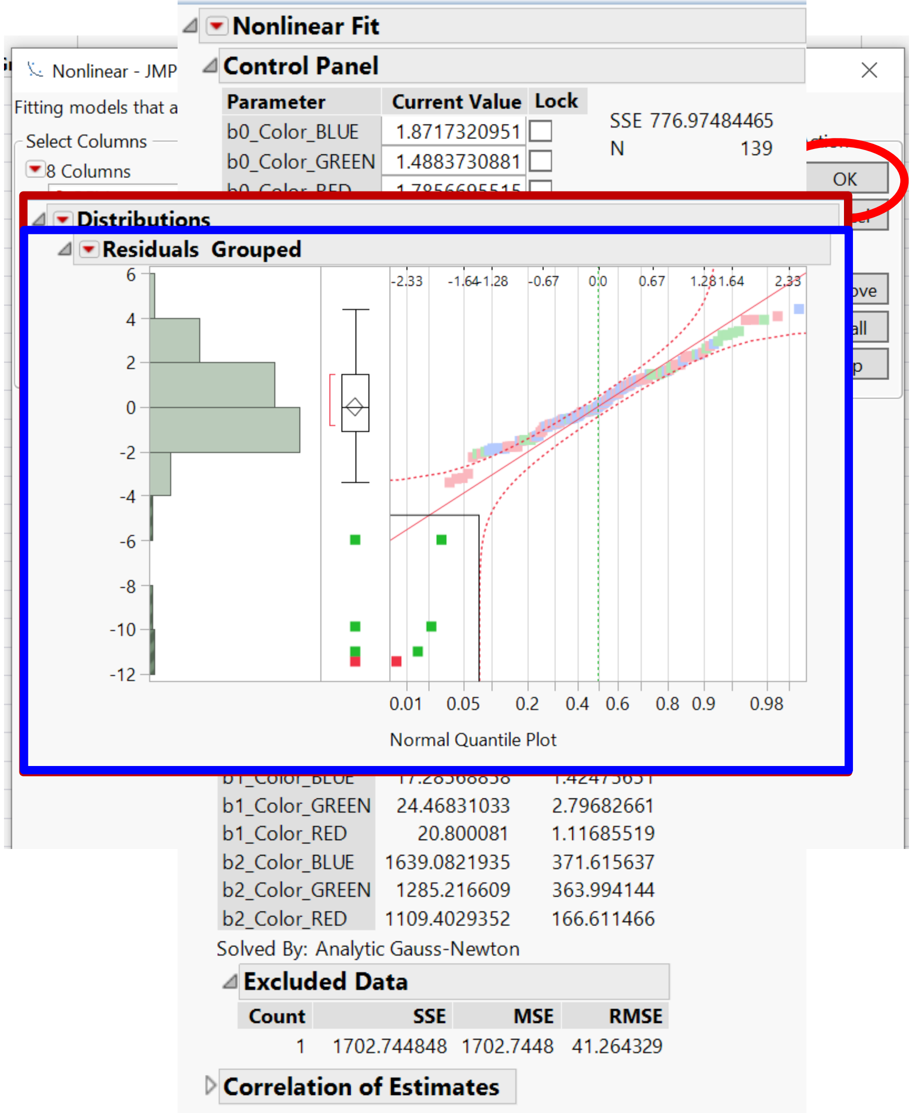
Engine oil oxidation – simultaneous fitting

- Analyze ➔
- Specialized Modeling ➔
- Nonlinear ➔
- Ox→ Y, Response
- Grouped→ X, Predictor Formula
  - "Grouped" is the new equation
- OK ➔
- Go ➔
- Output similar to before, but all nine parameters fit at once
- Check diagnostics, as before
  - Four outliers
- Using cursor, select the four points
- Go to Dataset
  - Rows, Hide and Exclude



Nonlinear Fit

Control Panel

Parameter	Current Value	Lock
b0_Color_BLUE	1.8717320951	□
b0_Color_GREEN	1.4883730881	□
b0_Color_RED	1.7856695515	□

SSE 776.97484465
N 139

b1_Color_BLUE	17.28568858	1.42475651
b1_Color_GREEN	24.46831033	2.79682661
b1_Color_RED	20.800081	1.11685519
b2_Color_BLUE	1639.0821935	371.615637
b2_Color_GREEN	1285.216609	363.994144
b2_Color_RED	1109.4029352	166.611466

Solved By: Analytic Gauss-Newton

Excluded Data

Count	SSE	MSE	RMSE
1	1702.744848	1702.7448	41.264329

Correlation of Estimates

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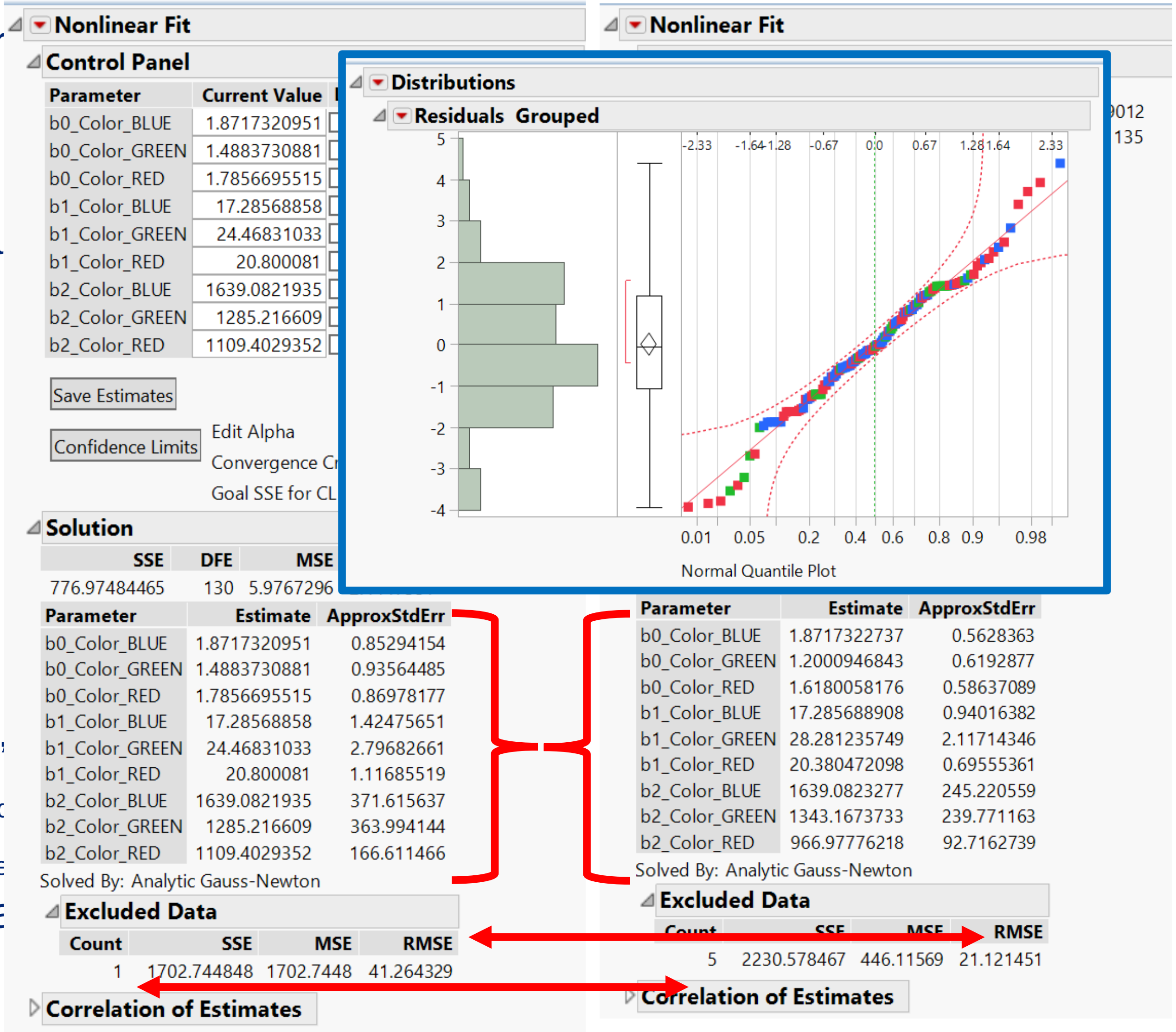
Engine oil oxidation – simultaneous fitting

- Return to ▼Nonlinear
- Go ➔
- Repeat diagnostics, a
- Compare to previous
  - N changes
  - Excluded changes
  - RMSE changes
  - Parameters change
- Compare parameters,
  - $b0_{Blue} \approx bo_{Green} \approx b0_{Red}$
  - $b1_{Blue} < b1_{Red} << b1_{Gre}$
- Export to Excel for gra
  - Save As, .xsl



Nonlinear Fit

Control Panel

Parameter	Current Value
b0_Color_BLUE	1.8717320951
b0_Color_GREEN	1.4883730881
b0_Color_RED	1.7856695515
b1_Color_BLUE	17.28568858
b1_Color_GREEN	24.46831033
b1_Color_RED	20.800081
b2_Color_BLUE	1639.0821935
b2_Color_GREEN	1285.216609
b2_Color_RED	1109.4029352

Solution

SSE	DFE	MSE
776.97484465	130	5.9767296

Parameter	Estimate	ApproxStdErr
b0_Color_BLUE	1.8717320951	0.85294154
b0_Color_GREEN	1.4883730881	0.93564485
b0_Color_RED	1.7856695515	0.86978177
b1_Color_BLUE	17.28568858	1.42475651
b1_Color_GREEN	24.46831033	2.79682661
b1_Color_RED	20.800081	1.11685519
b2_Color_BLUE	1639.0821935	371.615637
b2_Color_GREEN	1285.216609	363.994144
b2_Color_RED	1109.4029352	166.611466

Solved By: Analytic Gauss-Newton

Excluded Data

Count	SSE	MSE	RMSE
1	1702.744848	1702.7448	41.264329

Correlation of Estimates

Nonlinear Fit

Parameter	Estimate	ApproxStdErr
b0_Color_BLUE	1.8717322737	0.5628363
b0_Color_GREEN	1.2000946843	0.6192877
b0_Color_RED	1.6180058176	0.58637089
b1_Color_BLUE	17.285688908	0.94016382
b1_Color_GREEN	28.281235749	2.11714346
b1_Color_RED	20.380472098	0.69555361
b2_Color_BLUE	1639.0823277	245.220559
b2_Color_GREEN	1343.1673733	239.771163
b2_Color_RED	966.97776218	92.7162739

Solved By: Analytic Gauss-Newton

Excluded Data

Count	SSE	MSE	RMSE
5	2230.578467	446.11569	21.121451

Correlation of Estimates

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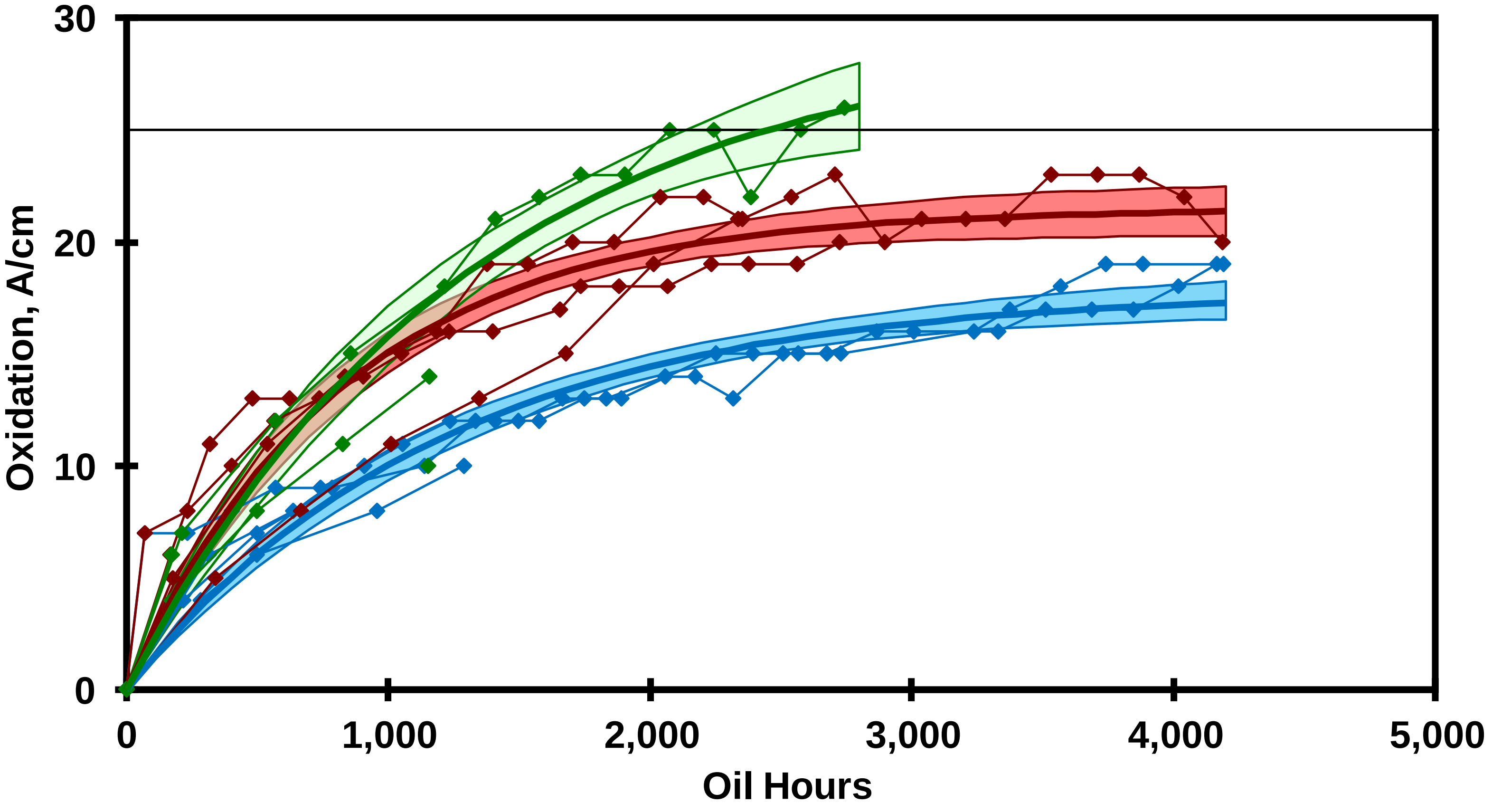
Engine oil oxidation – PowerPoint version

- **BLUE** is better than **RED** is better than **GREEN**
  - **GREEN** crosses the engine manufacturer’s limit around 2500 hours
  - **BLUE** and **RED** last over 4000 hours



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Conclusions and Future

Conclusions and future directions

- Conclusions
  - – JMP non-linear platform is a powerful tool for lubricants research
  - – Lubricant experimental results are often inherently non-linear
  - – There are differences among engine oils

- Future directions
  - – Get better at JMP!
  - – "Non-linear ANOVA"
    - Combining categorical and non-linear numerical variables
  - – Nested Non-Linear models
  - – Multivariate regression
  - – Functional regression

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