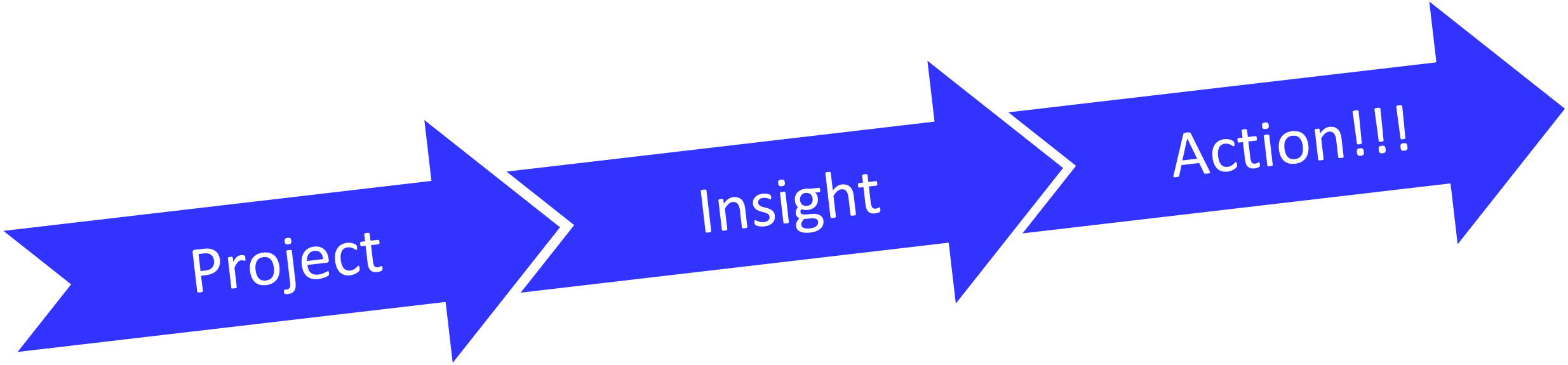


Insight by Design

Martin Owen, Director, Insight by Design & Part-time Lecturer, De Montfort University
Walkiria Schlindwein, Associate Professor of Pharmaceutics, De Montfort University

DE MONTFORT UNIVERSITY LEICESTER

(1) What are we wanting to do?

Organisational Memory Challenges

- Data derived information needs to be accessible, useable and assessible.
- Scientists in Industry and Academia need better tools to manage information effectively and efficiently.

Case Study

- De Montfort University, MSc. Quality by Design.

Assignment 1: Laboratory of Life

- How can we gain show how information builds over a series of experimental design work packages?
- How can we access, retain and communicate the knowledge using tabbed and dashboard layouts?
- How can we create a workflow of sequential operations, from designing experiments to analysing and documenting key information and actions?

Assignment 2: Suspensions

- What is the impact of team to team variation?

Target

- The aim of this presentation is to show how JMP14 Projects can accelerate learning and help teams or organizations adopt new workflows, retain insights from prior studies, make better decisions and take action.

(2) Introducing Project Zones

Bookmarks

"One stop shop"

- Including a folder in a project will include all current and future files from that folder in the project.
  - Related work packages can be grouped in sub-folders.
- Virtual groups: reconfigure order.

Conserves "One version of the truth"

- Folders or files can include associated PowerPoint and Word documents.

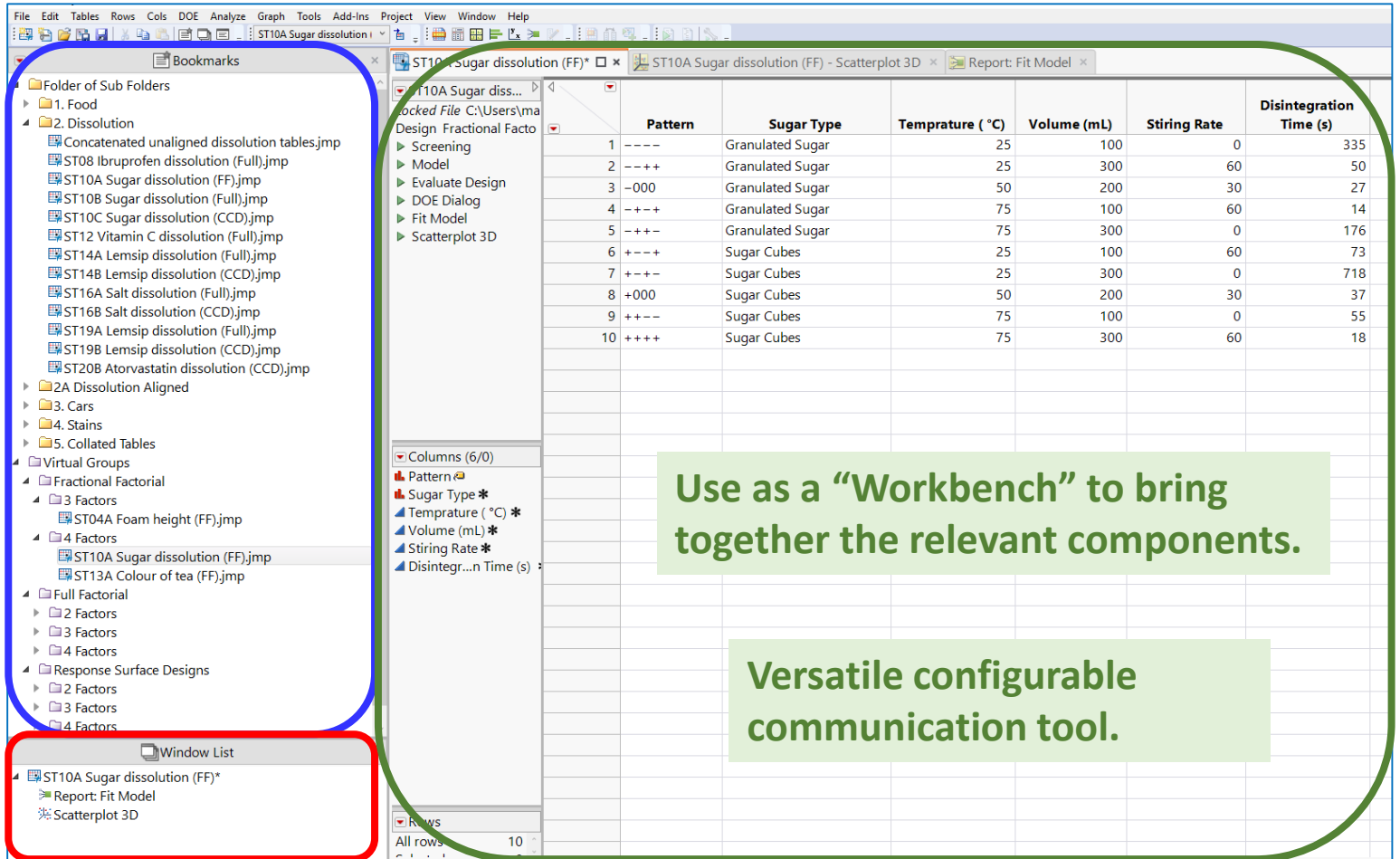
Window List

- Shows open tables and reports.
- Updated tables have asterisks- can be saved or discarded.

Facilitates "save and close as you go".

Workspace

- Tabbed view for step by step.
- Flexible configurable layout for dashboard overview.
- Zoom in on full screen view and drill down into details on demand.



(3) Assignment 1 Laboratory of Life

What datasets does it make sense to investigate cross-study insights?

- Folder of Sub Folders
  - 1. Food
    - ST01A Dunking biscuit (Full).jmp
    - ST01B Dunking biscuits (CCD).jmp
    - ST03 Crispy onions (Full).jmp
    - ST04A Foam height (FF).jmp
    - ST04B Foam height (Full).jmp
    - ST04C Foam height (CCD).jmp
    - ST05A Colour of tea (Full) .jmp
    - ST05B Colour of tea (CCD).jmp
    - ST06 Microwave popcorn (Full).jmp
    - ST09A Weetabix (Full).jmp
    - ST09B Weetabix (CCD).jmp
    - ST13A Colour of tea (FF).jmp
    - ST13B Colour of tea (CCD).jmp
    - ST15 Cup cakes (Full).jmp
    - ST17A Boiling eggs (Full) .jmp
    - ST17B Boiling eggs (CCD).jmp
    - ST21 Pizza (Full).jmp
  - 2. Dissolution
    - Concatenated unaligned dissolution tables.jmp
    - ST08 Ibruprofen dissolution (Full).jmp
    - ST10A Sugar dissolution (FF).jmp
    - ST10B Sugar dissolution (Full).jmp
    - ST10C Sugar dissolution (CCD).jmp
    - ST12 Vitamin C dissolution (Full).jmp
    - ST14A Lemsip dissolution (Full).jmp
    - ST14B Lemsip dissolution (CCD).jmp
    - ST16A Salt dissolution (Full).jmp
    - ST16B Salt dissolution (CCD).jmp
    - ST19A Lemsip dissolution (Full).jmp
    - ST19B Lemsip dissolution (CCD).jmp
    - ST20B Atorvastatin dissolution (CCD).jmp
  - 3. Cars
    - ST11 Fuel efficiency (Full).jmp
    - ST18 K'nex model (Full).jmp
  - 4. Stains
    - ST02A Henna stain (Full).jmp
    - ST02B Henna stain (CCD).jmp
    - ST07 Laundry (Full).jmp

Crispy onions

Colour of tea

Dunking biscuits

Colour of cupcakes

Lemsip dissolution

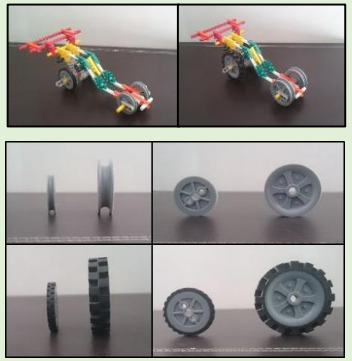
Vitamin C dissolution

Salt dissolution

Dissolution datasets share similar factors and responses

Henna stains

K'Nex models



Fuel Efficiency

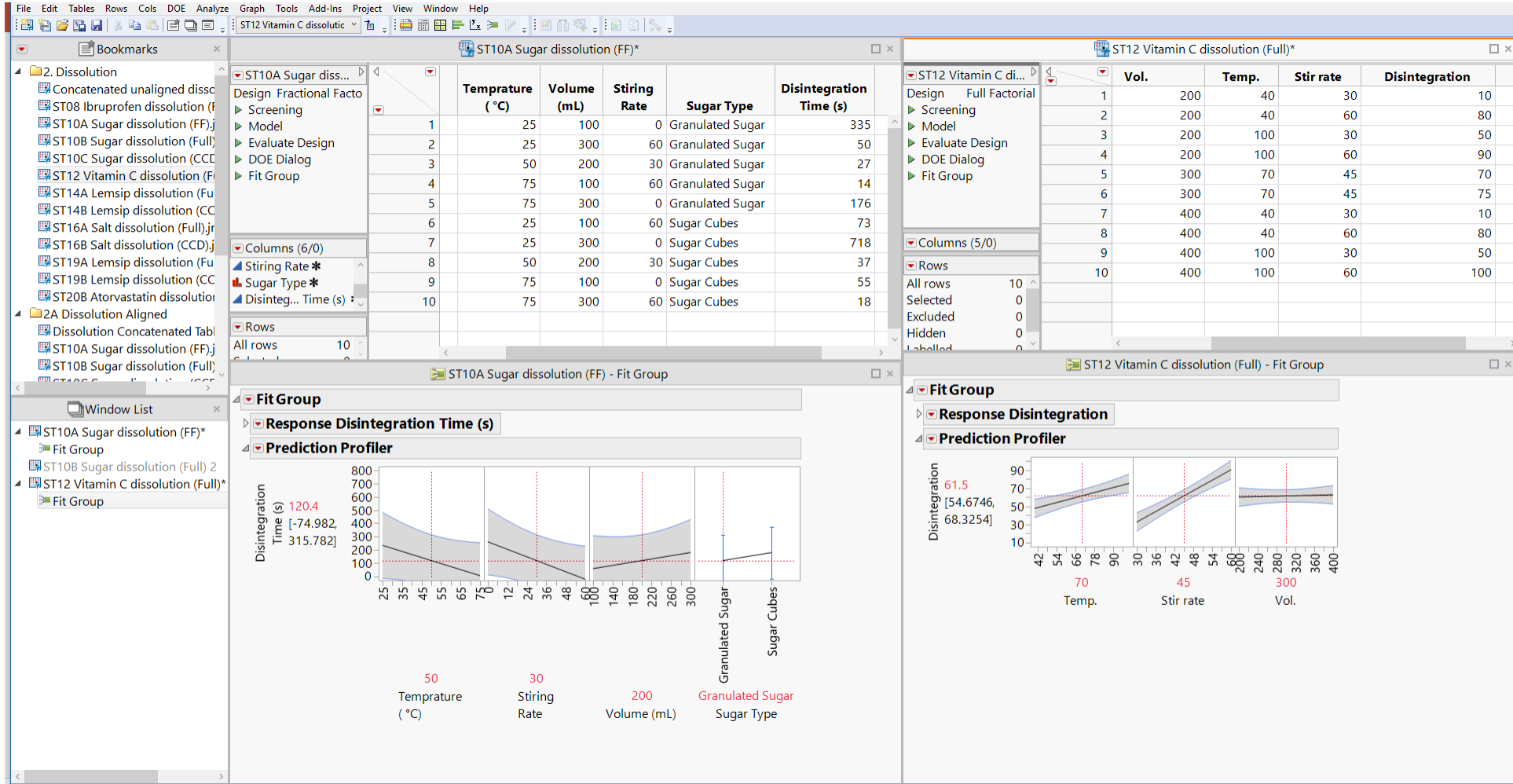
(4a) Compare individual dissolution models

Analysis

- Analyse models and save scripts to data tables.
- Check individual models look credible.

Compare models

- Rearrange tabs in workspace to display desired “dashboard configuration”.



(4b) Compare individual dissolution models

Typical inconsistencies

- Spelling mistakes.
- Full name/abbreviations.
- Capitals/lower case.
- Units/no units
- Data types (numerical/categorical)
- ...and so on

Column headings

Temprature (ºC) = Temp. ?

Stirring Rate = Stir rate ?

Volume (mL) = Vol. ?

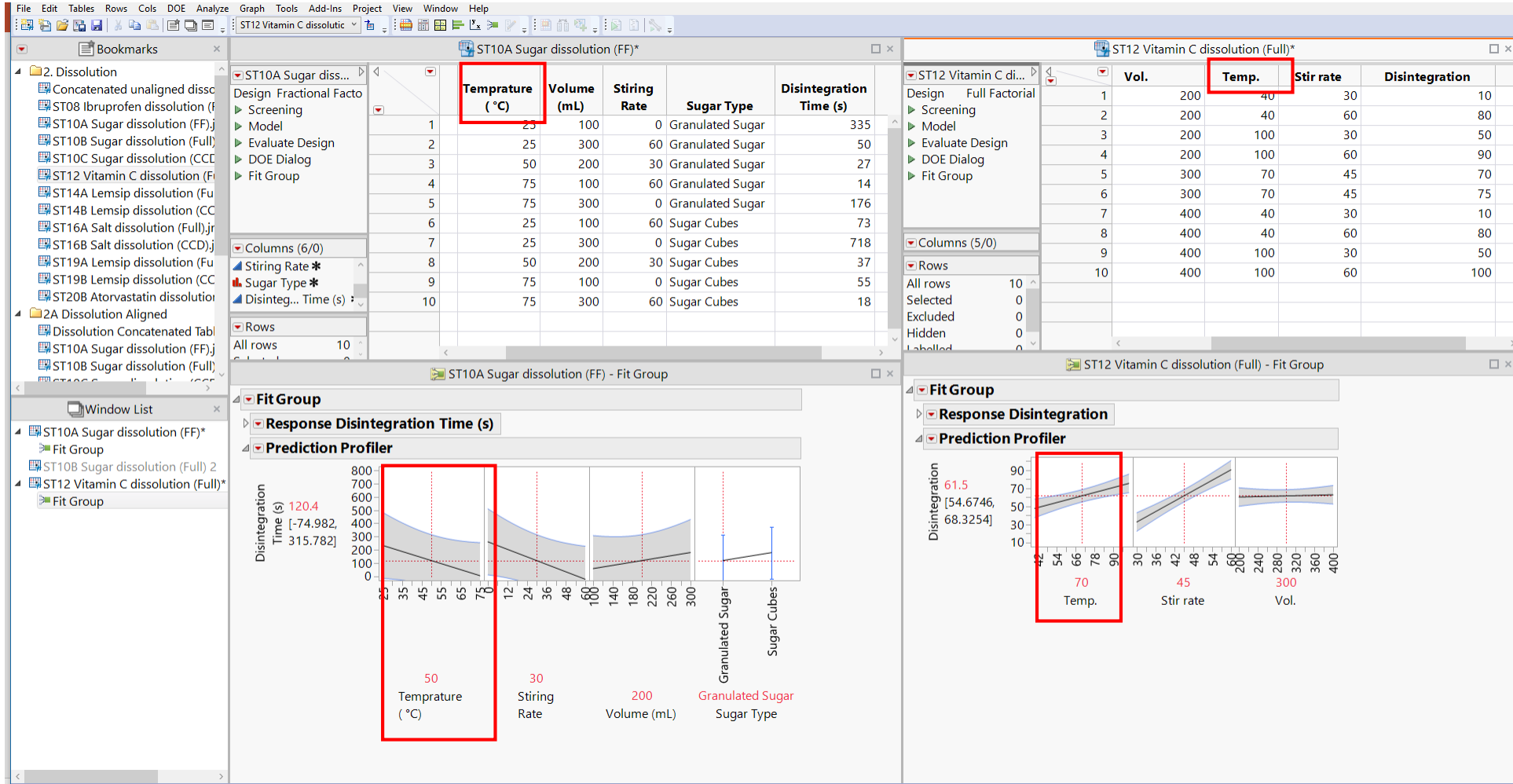
Disintegration time (s) = Disintegration ?

Impact on audience

- potentially lower trust.
- adds unnecessary complexity in interpretation.

Visualisations

- Seeing models in close proximity highlights odd behaviour.
- Are these the same or different factors/responses?



(5a) Aligning Datasets

Cross-study insights

- Often need to join or concatenate tables to see the bigger picture.

The challenge

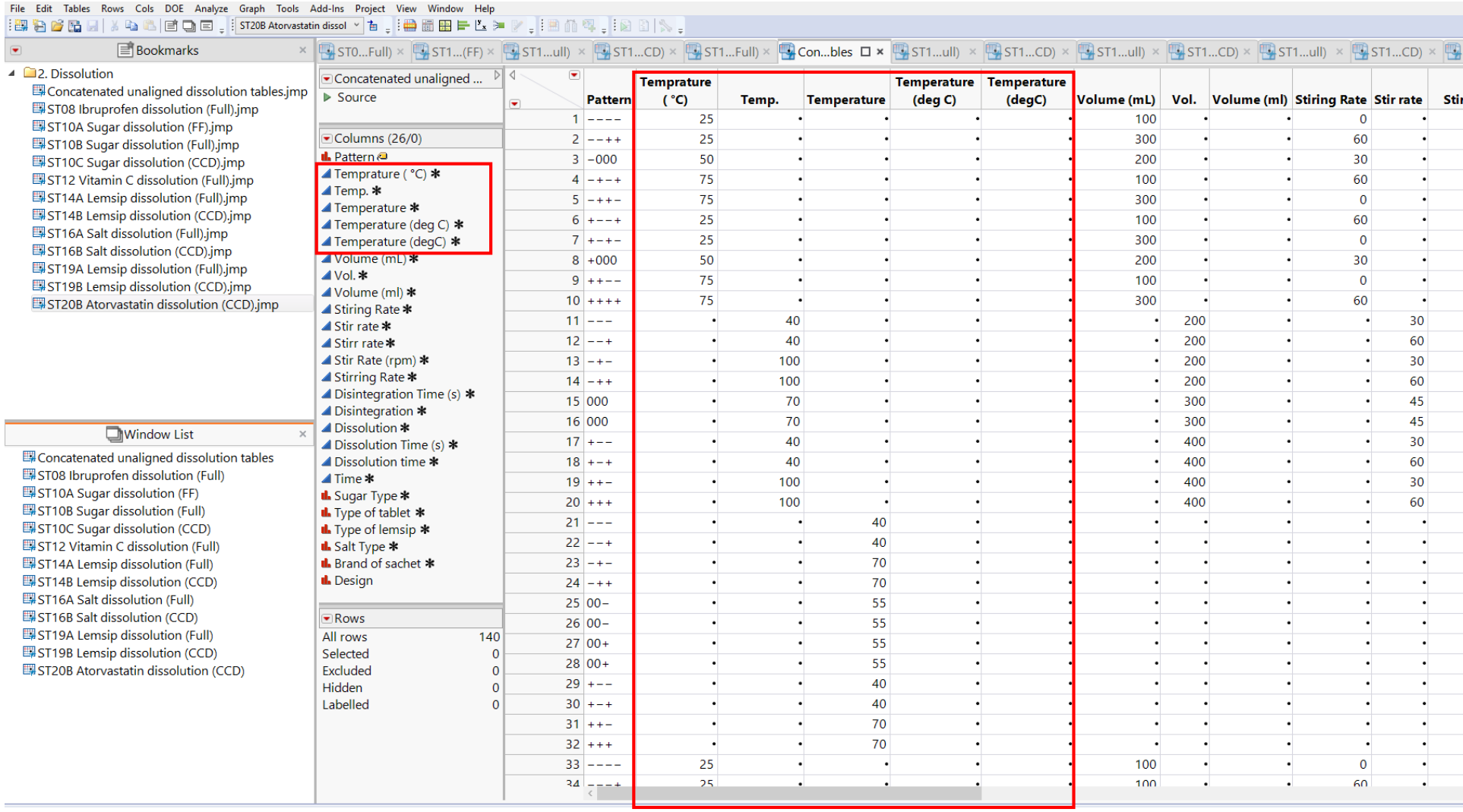
- Inconsistency of column headings adds complexity in joining or concatenating tables.

Typical early “R & D”

- No data standards in place.
- Unintended column heading creativity across and within individuals.

Unnecessary variations

- Five different “Temperatures”
- Three different “Volumes”.
- Four different “Stir rates”.
- Five different “Dissolution times”.



	Pattern	Temprature (°C)	Temp.	Temperature	Temperature (deg C)	Temperature (degC)	Volume (mL)	Vol.	Volume (ml)	Stiring Rate	Stir rate
1	−−−−	25	•	•	•	•	100	•	•	0	•
2	−−++	25	•	•	•	•	300	•	•	60	•
3	−000	50	•	•	•	•	200	•	•	30	•
4	−+−+	75	•	•	•	•	100	•	•	60	•
5	−++−	75	•	•	•	•	300	•	•	0	•
6	+−−+	25	•	•	•	•	100	•	•	60	•
7	+−+−	25	•	•	•	•	300	•	•	0	•
8	+000	50	•	•	•	•	200	•	•	30	•
9	++−−	75	•	•	•	•	100	•	•	0	•
10	++++	75	•	•	•	•	300	•	•	60	•
11	−−−	•	40	•	•	•	•	200	•	•	30
12	−−+	•	40	•	•	•	•	200	•	•	60
13	−+−	•	100	•	•	•	•	200	•	•	30
14	−++	•	100	•	•	•	•	200	•	•	60
15	000	•	70	•	•	•	•	300	•	•	45
16	000	•	70	•	•	•	•	300	•	•	45
17	+−−	•	40	•	•	•	•	400	•	•	30
18	+−+	•	40	•	•	•	•	400	•	•	60
19	++−	•	100	•	•	•	•	400	•	•	30
20	+++	•	100	•	•	•	•	400	•	•	60
21	−−−	•	•	40	•	•	•	•	•	•	•
22	−−+	•	•	40	•	•	•	•	•	•	•
23	−+−	•	•	70	•	•	•	•	•	•	•
24	−++	•	•	70	•	•	•	•	•	•	•
25	00−	•	•	55	•	•	•	•	•	•	•
26	00−	•	•	55	•	•	•	•	•	•	•
27	00+	•	•	55	•	•	•	•	•	•	•
28	00+	•	•	55	•	•	•	•	•	•	•
29	+−−	•	•	40	•	•	•	•	•	•	•
30	+−+	•	•	40	•	•	•	•	•	•	•
31	++−	•	•	70	•	•	•	•	•	•	•
32	+++	•	•	70	•	•	•	•	•	•	•
33	−−−−	25	•	•	•	•	100	•	•	0	•
34	−−−+	25	•	•	•	•	100	•	•	60	•

(5b) Aligning Datasets

A possible next step

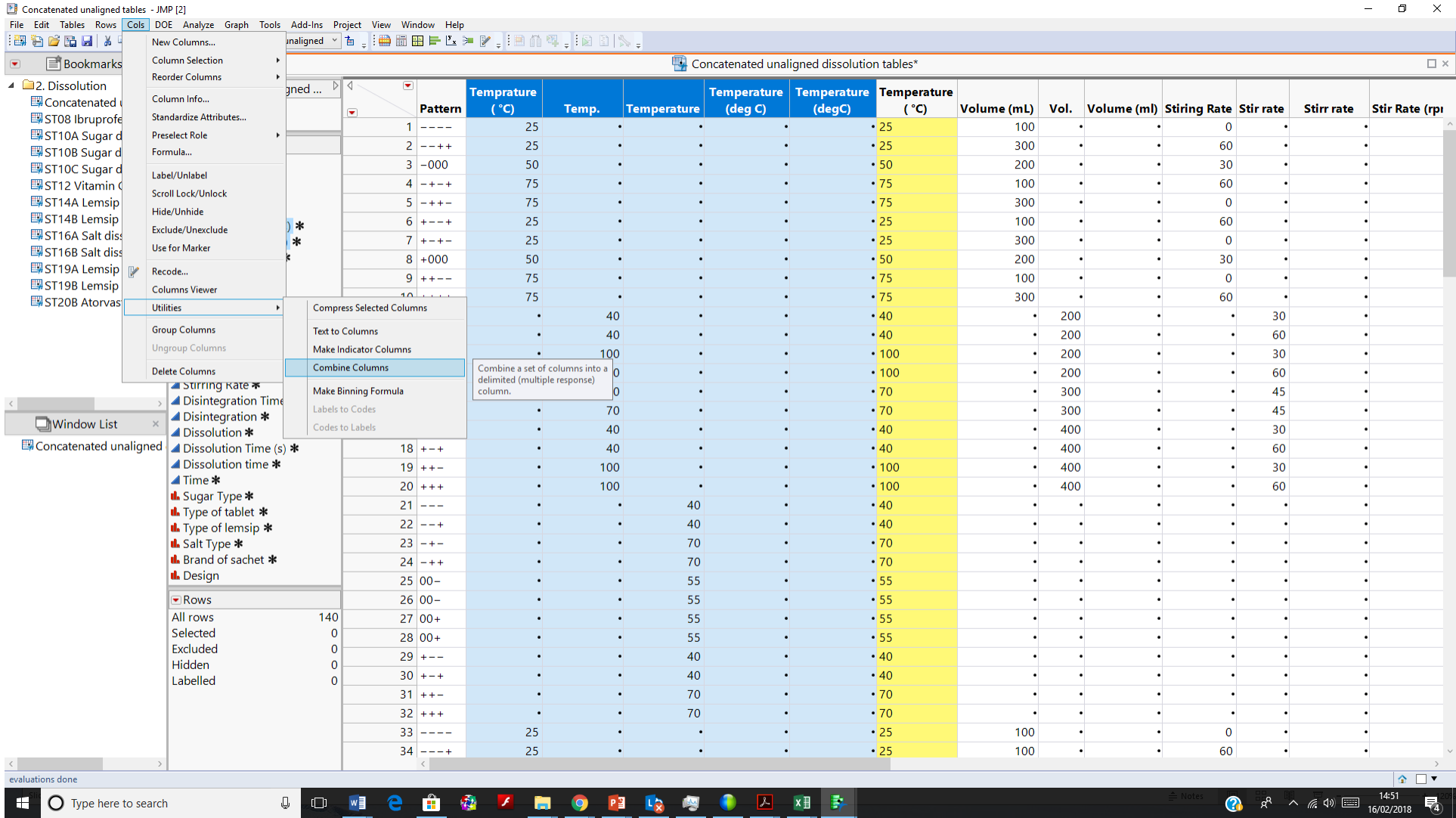
- Use Cols> Utilise>Combine columns feature to create single column

The challenge

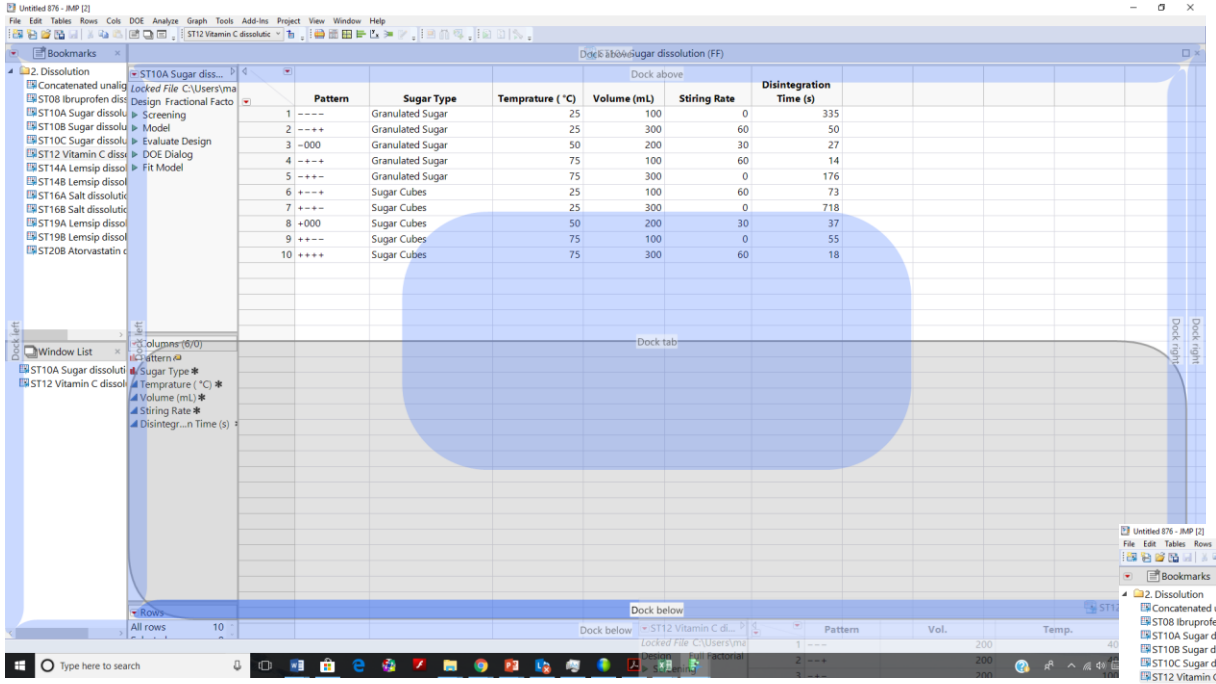
- N.b. Fixing the problem post concatenation means additional rework in the future

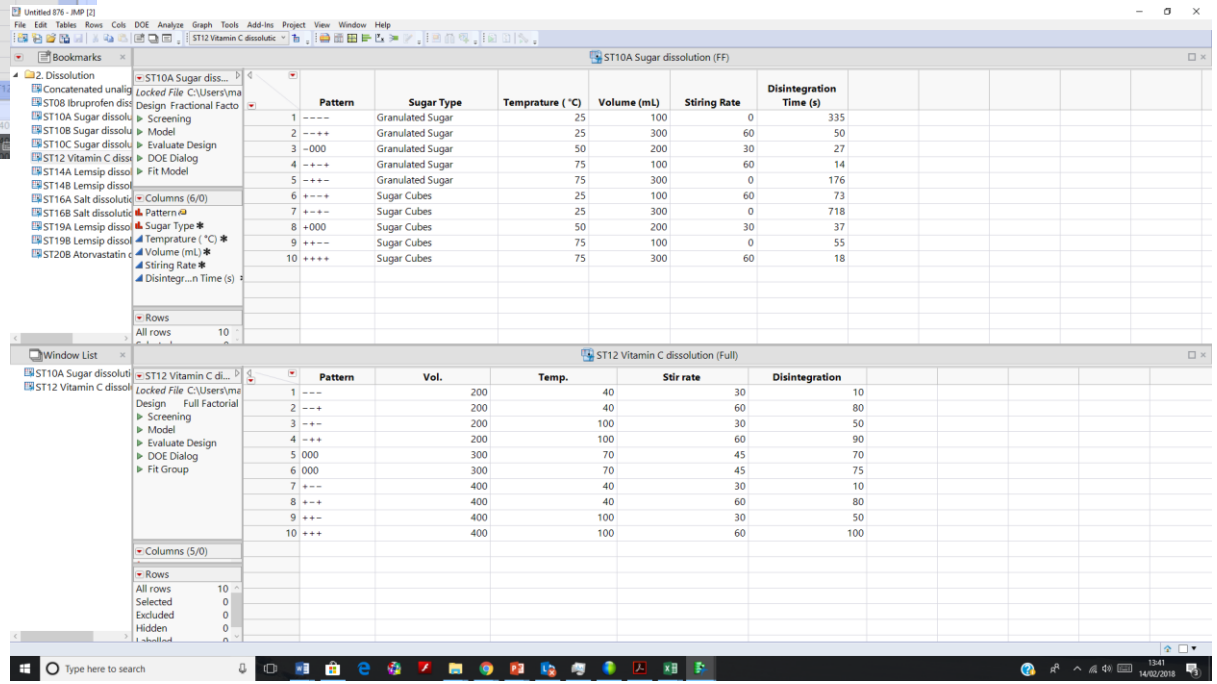
Requirement

- Is there an equivalent of a “recode” function for column headings *prior* to concatenating?



(5c) Aligning Datasets





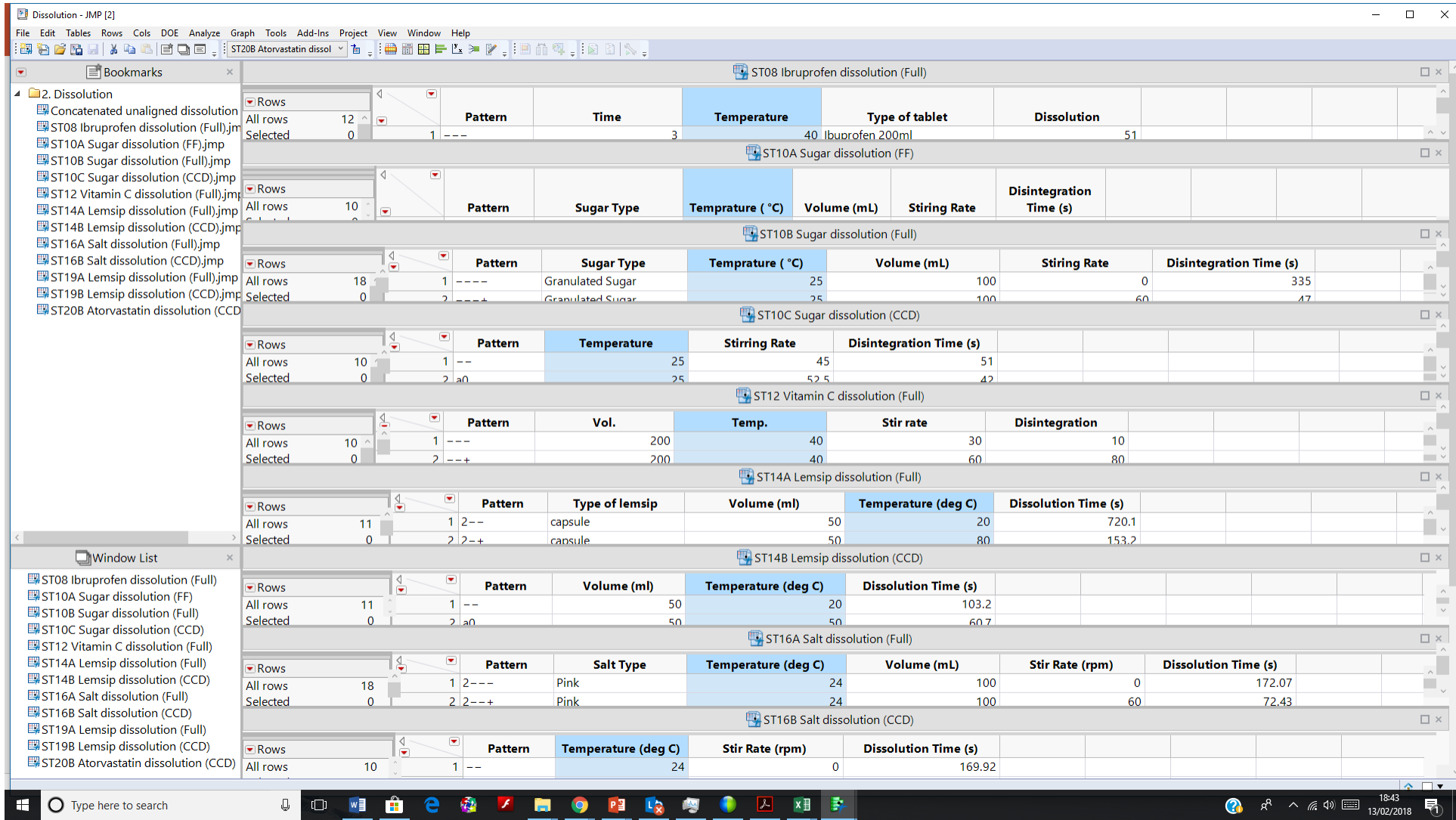
Project provides an alternative workflow

- Open up two or more tables.
- Dock the tables below one another.
- Repeat for all tables.

(5d) Aligning Datasets

Consistency

- Identify similar columns and align column names (provides a basis for future data naming standards).
- Check unit consistency.
- Check same data types.



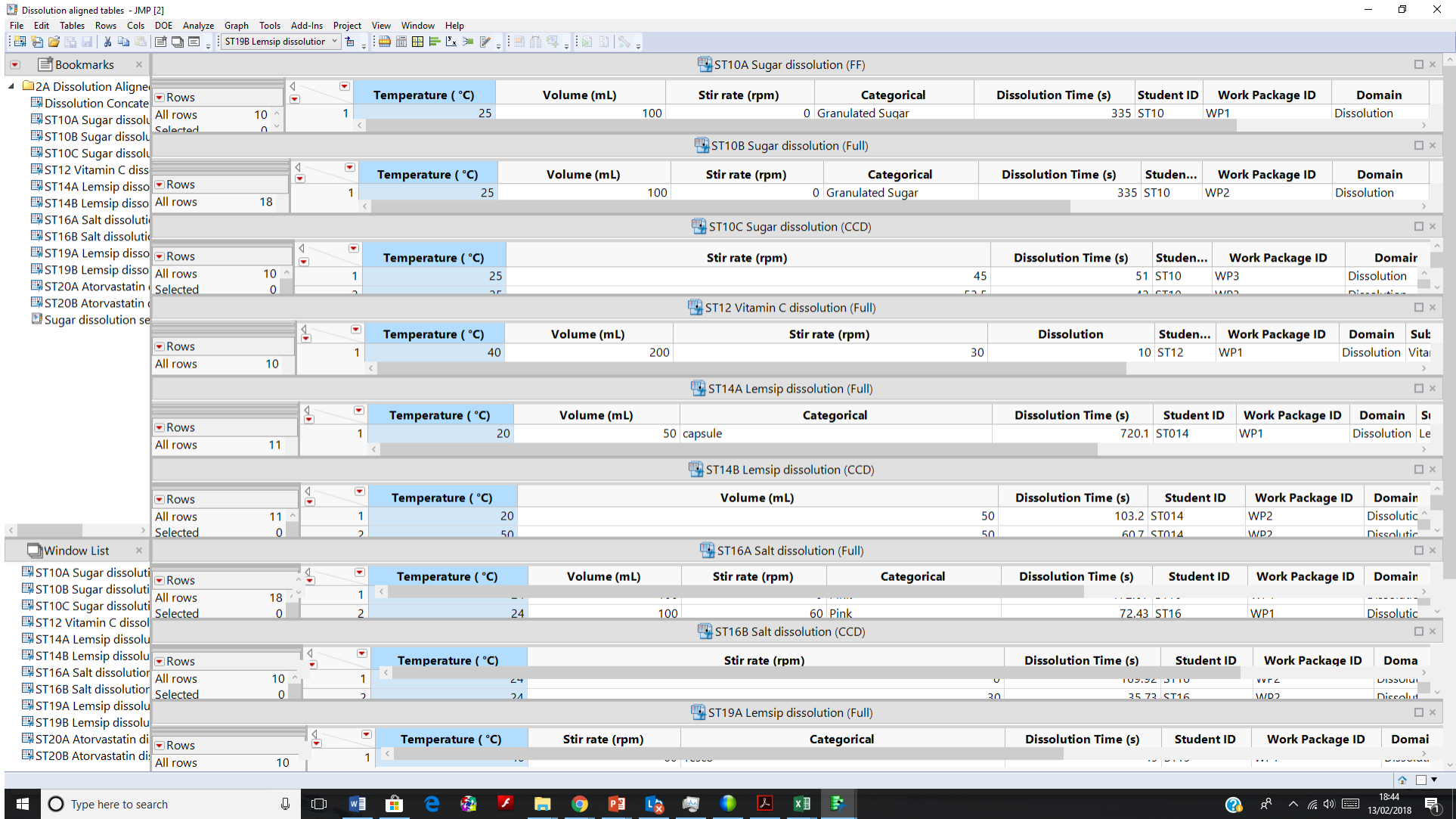
(5e) Aligning Datasets

Aligned tables

- Consistency changes preserved in the individual data tables.
- Scripts automatically updated.
- No future repeated rework.

Add metadata

- Metadata (data about data) provides additional context.



(5f) Aligning Datasets

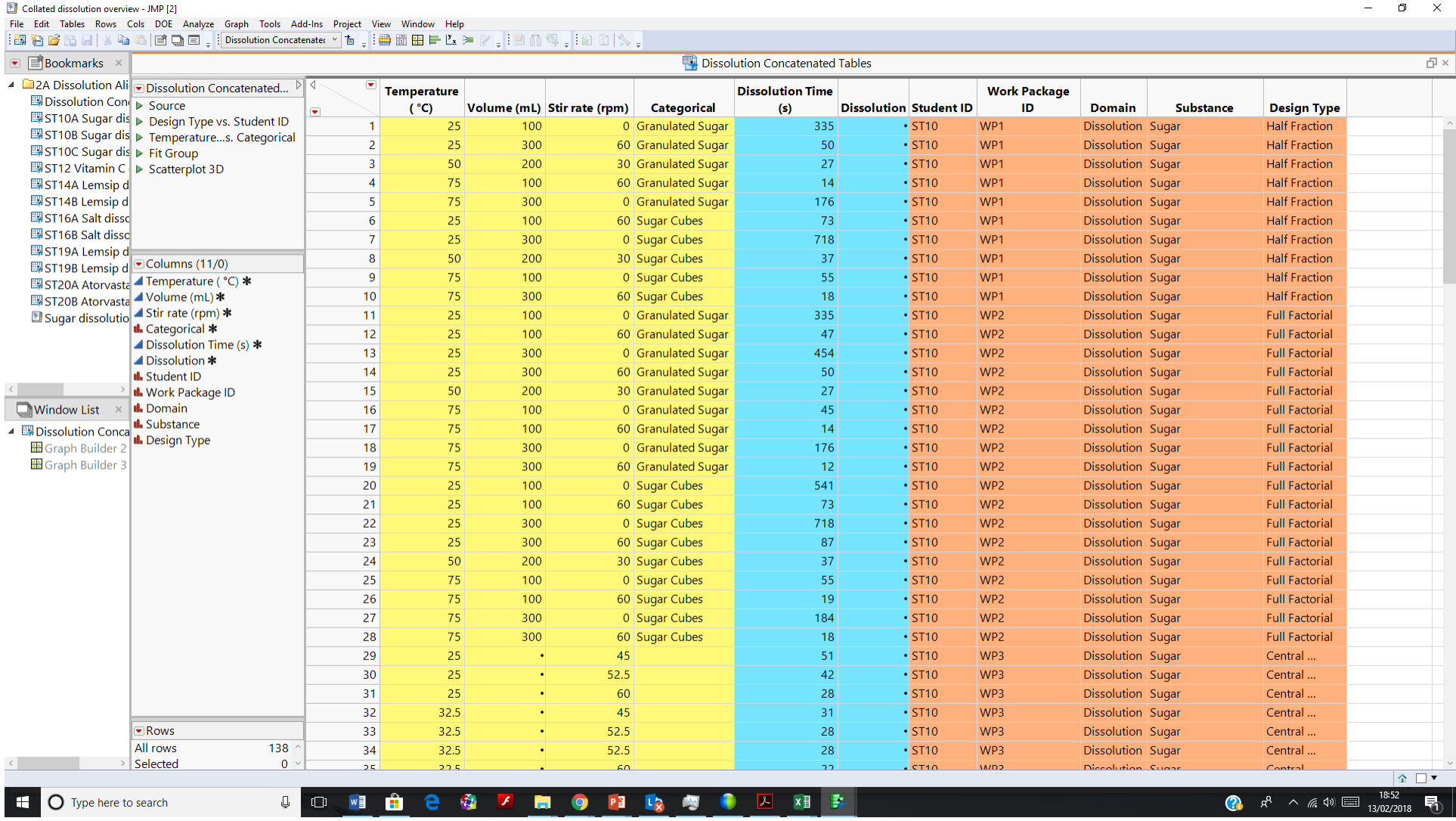
Factors | Responses | Metadata

Concatenate

- With the individual table now aligned, concatenation produces the desired concatenated table.

Roles

- Note the three different data roles:
  - Factors
  - Responses
  - Metadata



	Temperature (°C)	Volume (mL)	Stir rate (rpm)	Categorical	Dissolution Time (s)	Dissolution	Student ID	Work Package ID	Domain	Substance	Design Type
1	25	100	0	Granulated Sugar	335	•	ST10	WP1	Dissolution	Sugar	Half Fraction
2	25	300	60	Granulated Sugar	50	•	ST10	WP1	Dissolution	Sugar	Half Fraction
3	50	200	30	Granulated Sugar	27	•	ST10	WP1	Dissolution	Sugar	Half Fraction
4	75	100	60	Granulated Sugar	14	•	ST10	WP1	Dissolution	Sugar	Half Fraction
5	75	300	0	Granulated Sugar	176	•	ST10	WP1	Dissolution	Sugar	Half Fraction
6	25	100	60	Sugar Cubes	73	•	ST10	WP1	Dissolution	Sugar	Half Fraction
7	25	300	0	Sugar Cubes	718	•	ST10	WP1	Dissolution	Sugar	Half Fraction
8	50	200	30	Sugar Cubes	37	•	ST10	WP1	Dissolution	Sugar	Half Fraction
9	75	100	0	Sugar Cubes	55	•	ST10	WP1	Dissolution	Sugar	Half Fraction
10	75	300	60	Sugar Cubes	18	•	ST10	WP1	Dissolution	Sugar	Half Fraction
11	25	100	0	Granulated Sugar	335	•	ST10	WP2	Dissolution	Sugar	Full Factorial
12	25	100	60	Granulated Sugar	47	•	ST10	WP2	Dissolution	Sugar	Full Factorial
13	25	300	0	Granulated Sugar	454	•	ST10	WP2	Dissolution	Sugar	Full Factorial
14	25	300	60	Granulated Sugar	50	•	ST10	WP2	Dissolution	Sugar	Full Factorial
15	50	200	30	Granulated Sugar	27	•	ST10	WP2	Dissolution	Sugar	Full Factorial
16	75	100	0	Granulated Sugar	45	•	ST10	WP2	Dissolution	Sugar	Full Factorial
17	75	100	60	Granulated Sugar	14	•	ST10	WP2	Dissolution	Sugar	Full Factorial
18	75	300	0	Granulated Sugar	176	•	ST10	WP2	Dissolution	Sugar	Full Factorial
19	75	300	60	Granulated Sugar	12	•	ST10	WP2	Dissolution	Sugar	Full Factorial
20	25	100	0	Sugar Cubes	541	•	ST10	WP2	Dissolution	Sugar	Full Factorial
21	25	100	60	Sugar Cubes	73	•	ST10	WP2	Dissolution	Sugar	Full Factorial
22	25	300	0	Sugar Cubes	718	•	ST10	WP2	Dissolution	Sugar	Full Factorial
23	25	300	60	Sugar Cubes	87	•	ST10	WP2	Dissolution	Sugar	Full Factorial
24	50	200	30	Sugar Cubes	37	•	ST10	WP2	Dissolution	Sugar	Full Factorial
25	75	100	0	Sugar Cubes	55	•	ST10	WP2	Dissolution	Sugar	Full Factorial
26	75	100	60	Sugar Cubes	19	•	ST10	WP2	Dissolution	Sugar	Full Factorial
27	75	300	0	Sugar Cubes	184	•	ST10	WP2	Dissolution	Sugar	Full Factorial
28	75	300	60	Sugar Cubes	18	•	ST10	WP2	Dissolution	Sugar	Full Factorial
29	25	•	45		51	•	ST10	WP3	Dissolution	Sugar	Central ...
30	25	•	52.5		42	•	ST10	WP3	Dissolution	Sugar	Central ...
31	25	•	60		28	•	ST10	WP3	Dissolution	Sugar	Central ...
32	32.5	•	45		31	•	ST10	WP3	Dissolution	Sugar	Central ...
33	32.5	•	52.5		28	•	ST10	WP3	Dissolution	Sugar	Central ...
34	32.5	•	52.5		28	•	ST10	WP3	Dissolution	Sugar	Central ...

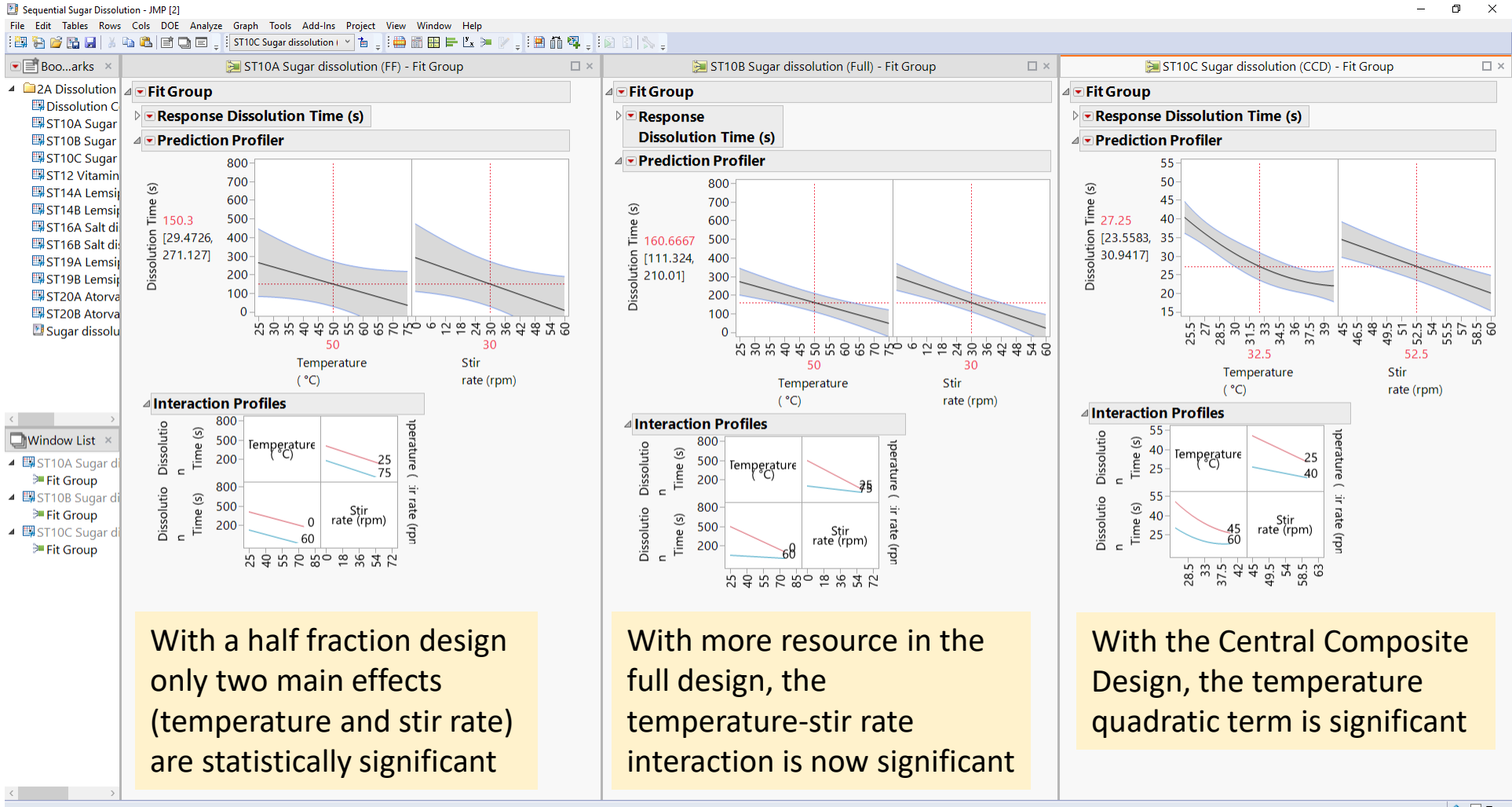
(6a) Comparing models: Sequential design example

Analysis

- Open data tables.
- Run scripts to create models.
- Hide data tables.

Sequential Designs

- Compare studies.
- Note insight gained as further resource is spent.



With a half fraction design only two main effects (temperature and stir rate) are statistically significant

With more resource in the full design, the temperature-stir rate interaction is now significant

With the Central Composite Design, the temperature quadratic term is significant

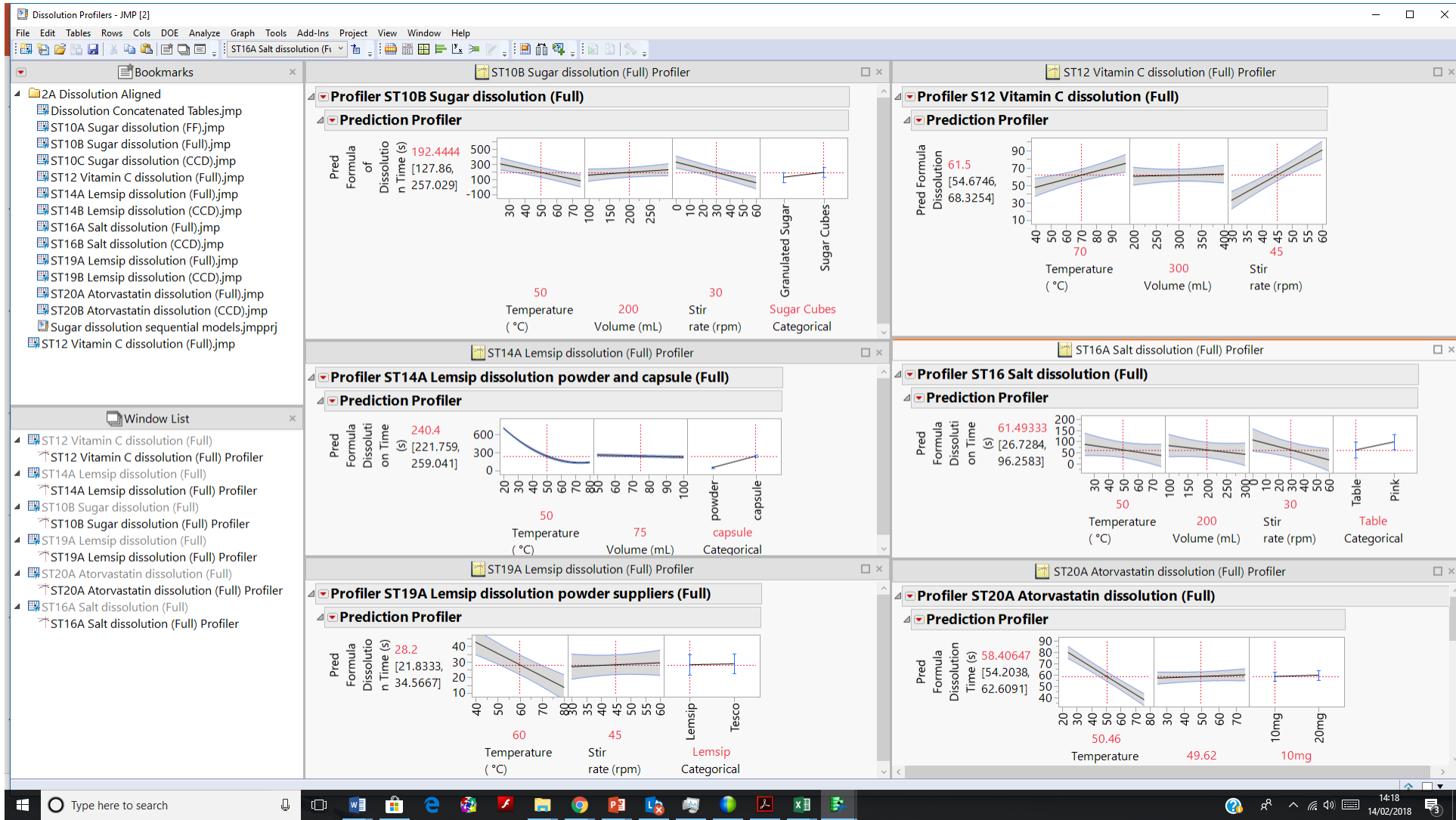
(6b) Comparing models across substances

Comparison of Dissolution Full Factorials

- Analyse models and save scripts to data tables.
- Hide data tables.

Dashboard view

- Compare studies.
- What are the key insights from the full factorial dissolution designs?



(6c) Comparing models across substances

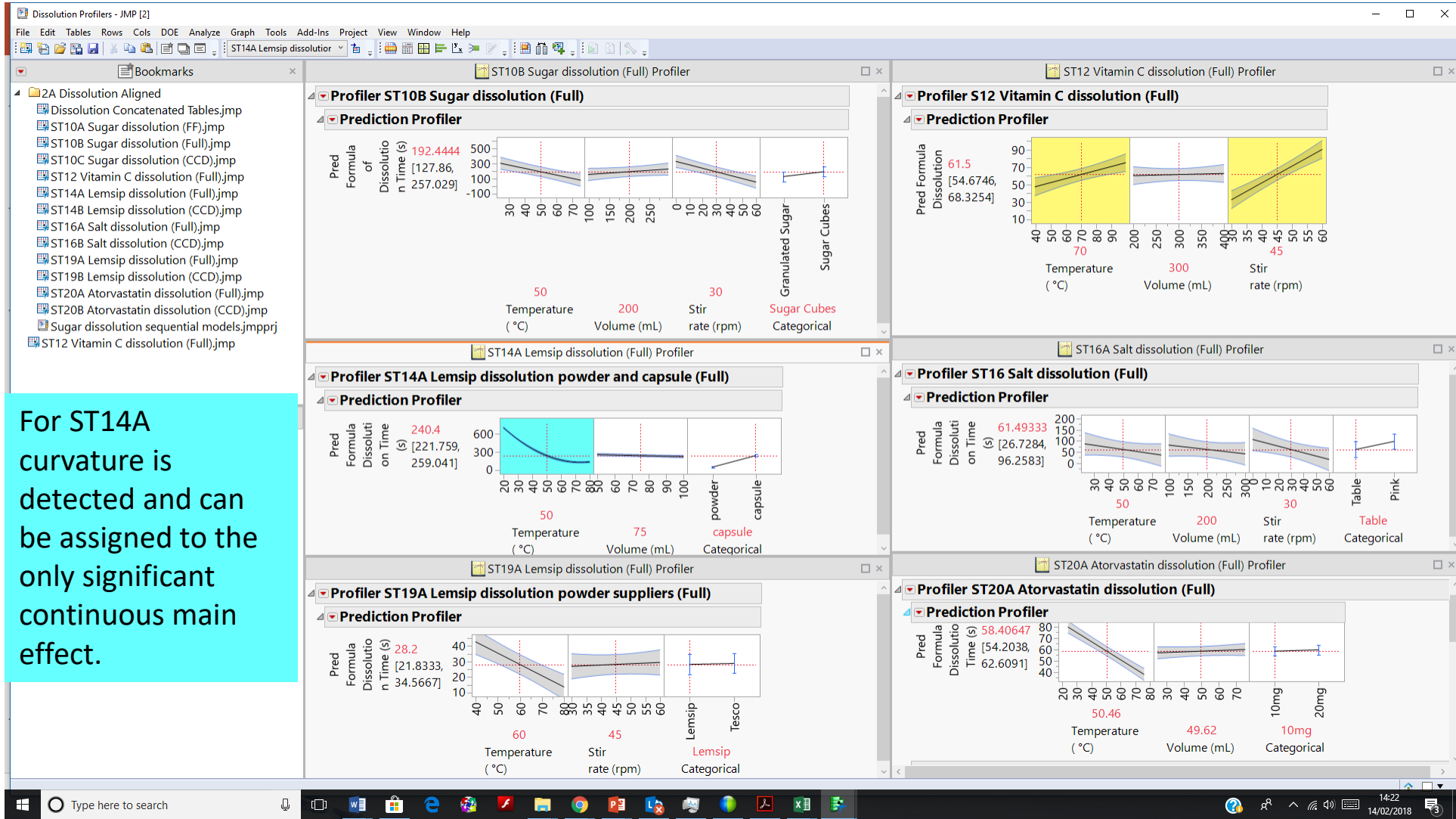
For S12 note that there are positive correlations for time and temperature in contrast with all the other models.
This is due to the response being measured in a different way (% dissolved after a given time rather than disintegration time).

Factor ranges

- Note that factor ranges are different for each study.
- For most studies there are negative correlations of dissolution time with temperature and stir rate.
- Volume has little impact.
- Can see which factors and ranges were studied in each work package.

Response ranges

- Note these are different for each work package.



For ST14A curvature is detected and can be assigned to the only significant continuous main effect.

Dissolution Profilers CCD - JMP [2]

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

ST14B Lemsip dissolutior

Bookmarks

- 2A Dissolution Aligned
  - Dissolution Concatenated Tables.jmp
  - ST10A Sugar dissolution (FF).jmp
  - ST10B Sugar dissolution (Full).jmp
  - ST10C Sugar dissolution (CCD).jmp
  - ST12 Vitamin C dissolution (Full).jmp
  - ST14A Lemsip dissolution (Full).jmp
  - ST14B Lemsip dissolution (CCD).jmp
  - ST16A Salt dissolution (Full).jmp
  - ST16B Salt dissolution (CCD).jmp
  - ST19A Lemsip dissolution (Full).jmp
  - ST19B Lemsip dissolution (CCD).jmp
  - ST20A Atorvastatin dissolution (Full).jmp
  - ST20B Atorvastatin dissolution (CCD).jmp
  - Sugar dissolution sequential models.jmpprj

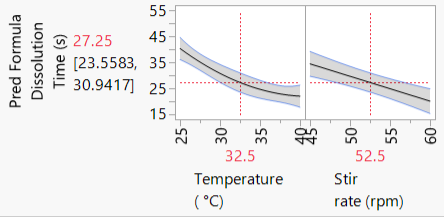
Window List

- ST10C Sugar dissolution (CCD)
- ST14B Lemsip dissolution (CCD)
- ST16B Salt dissolution (CCD)
  - ST16B Salt dissolution (CCD) Profiler
- ST19B Lemsip dissolution (CCD)
  - ST19B Lemsip dissolution (CCD) Profiler
- ST20B Atorvastatin dissolution (CCD)
  - Profiler

ST10C Sugar dissolution (CCD) Profiler

Profiler

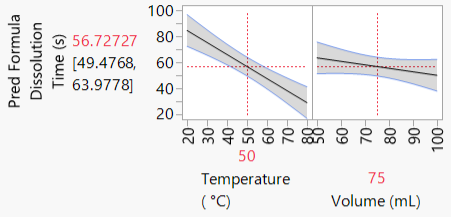
Prediction Profiler



ST14B Lemsip dissolution (CCD) Profiler

Profiler

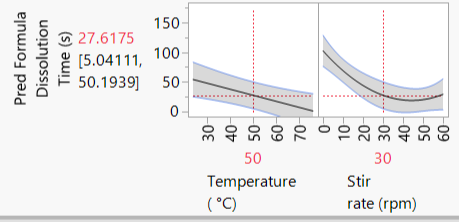
Prediction Profiler



ST16B Salt dissolution (CCD) Profiler

Profiler

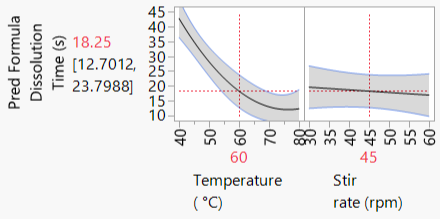
Prediction Profiler



ST19B Lemsip dissolution (CCD) Profiler

Profiler

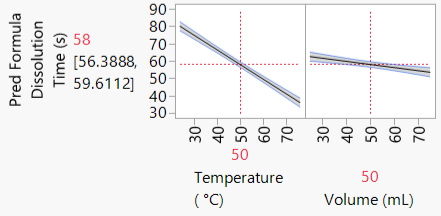
Prediction Profiler



ST20B Atorvastatin dissolution (CCD) - Profiler

Profiler

Prediction Profiler



evaluations done

Type here to search

02:20
16/02/2018

(7a) Insights from visualisation of the collated table

Overview

- The combination of Graph builder and metadata enables rapid comparison of dissolution studies.

Designs

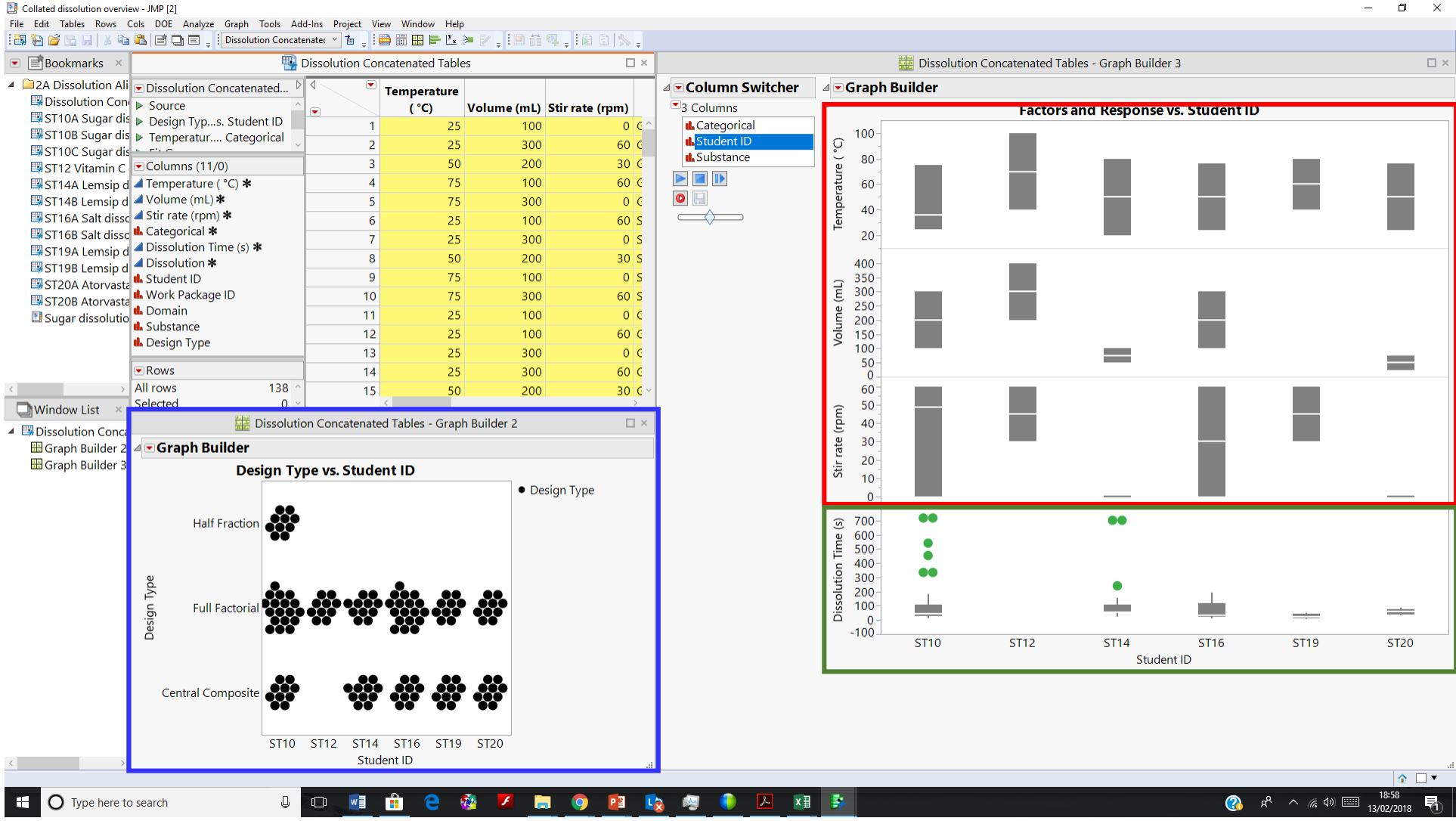
- What designs have been applied by which student?

Factors

- What ranges have been investigated?

Responses

- What are the ranges of responses achieved?



(7b) Combined dissolution models

“Big data” model

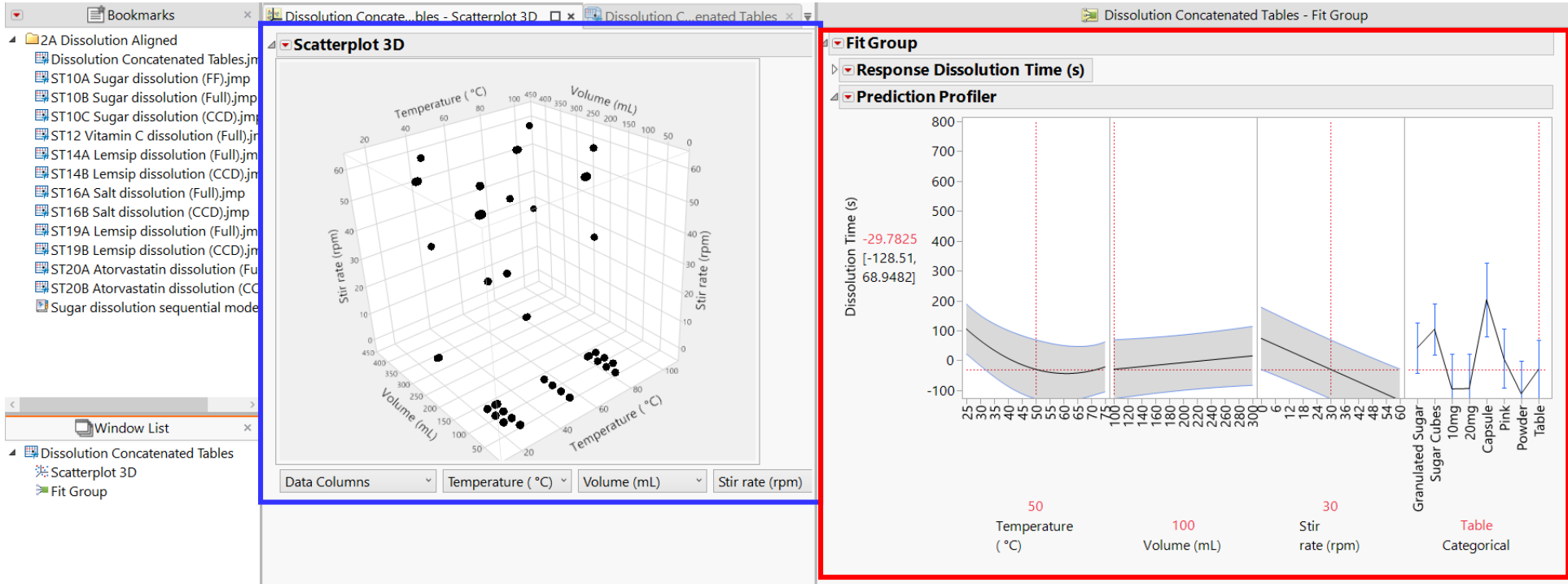
- Does it make sense to create a model from the concatenated data table?

Scatterplot 3D

- This view shows how much of the investigation space is filled.

Fit Model

- The overall model confirms the general observation that temperature and stir rate are negatively. correlated with dissolution time across a variety of materials.



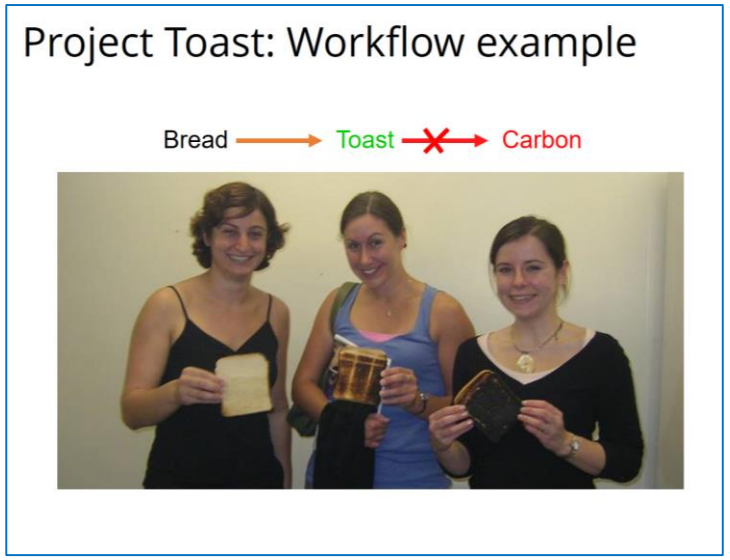
(8a) Workflow teaching tool

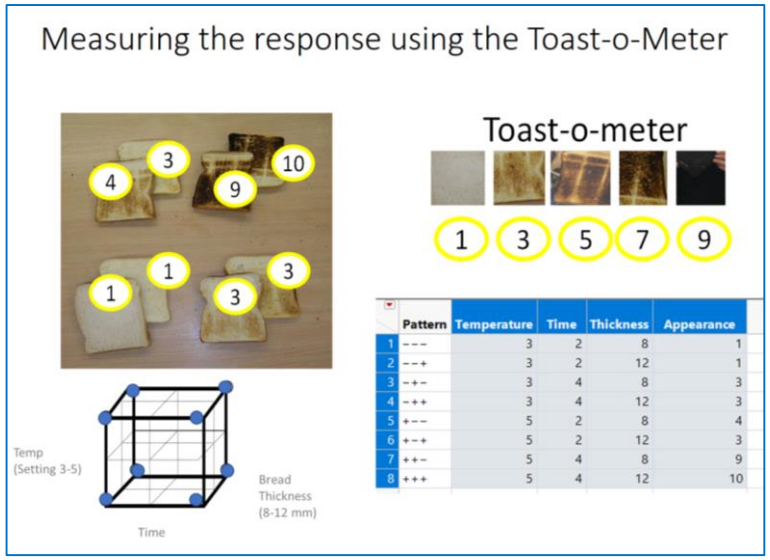
Project as a training tool

- The tabbed workspace view fits naturally with step by step instructions.
- The dashboard workspace view lends itself to comparison of methods.

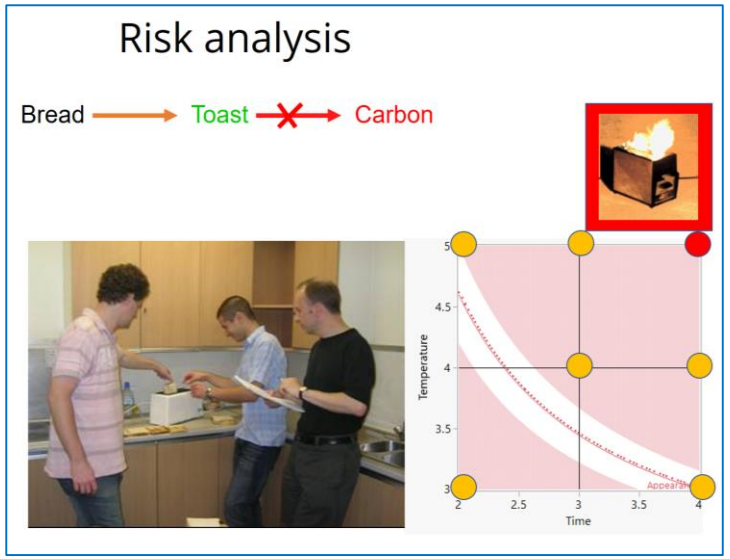
Case study

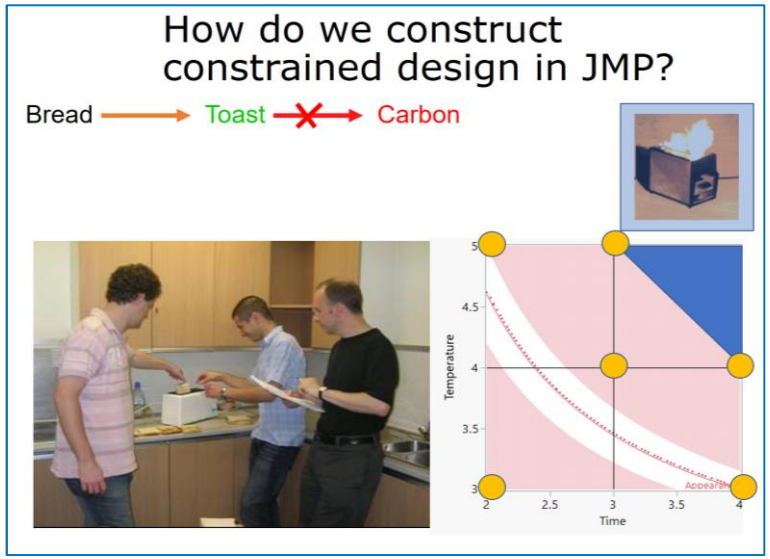
- In the Laboratory of Life assignments, students observed some combination of factor settings (e.g. high temperature, high cooking times) led to high risk situations.
- It is possible to Define Factor Constraints feature in DoE Custom design to avoid unwanted combinations.
- Save steps to tabs in Project.





	Pattern	Temperature	Time	Thickness	Appearance
1	---	3	2	8	1
2	--+	3	2	12	1
3	-+-	3	4	8	3
4	-++	3	4	12	3
5	+--	5	2	8	4
6	+-+	5	2	12	3
7	++-	5	4	8	9
8	+++	5	4	12	10





(8b) Workflow teaching tool

Launch script from Bookmarks

- This brings up a populated Custom Design page.

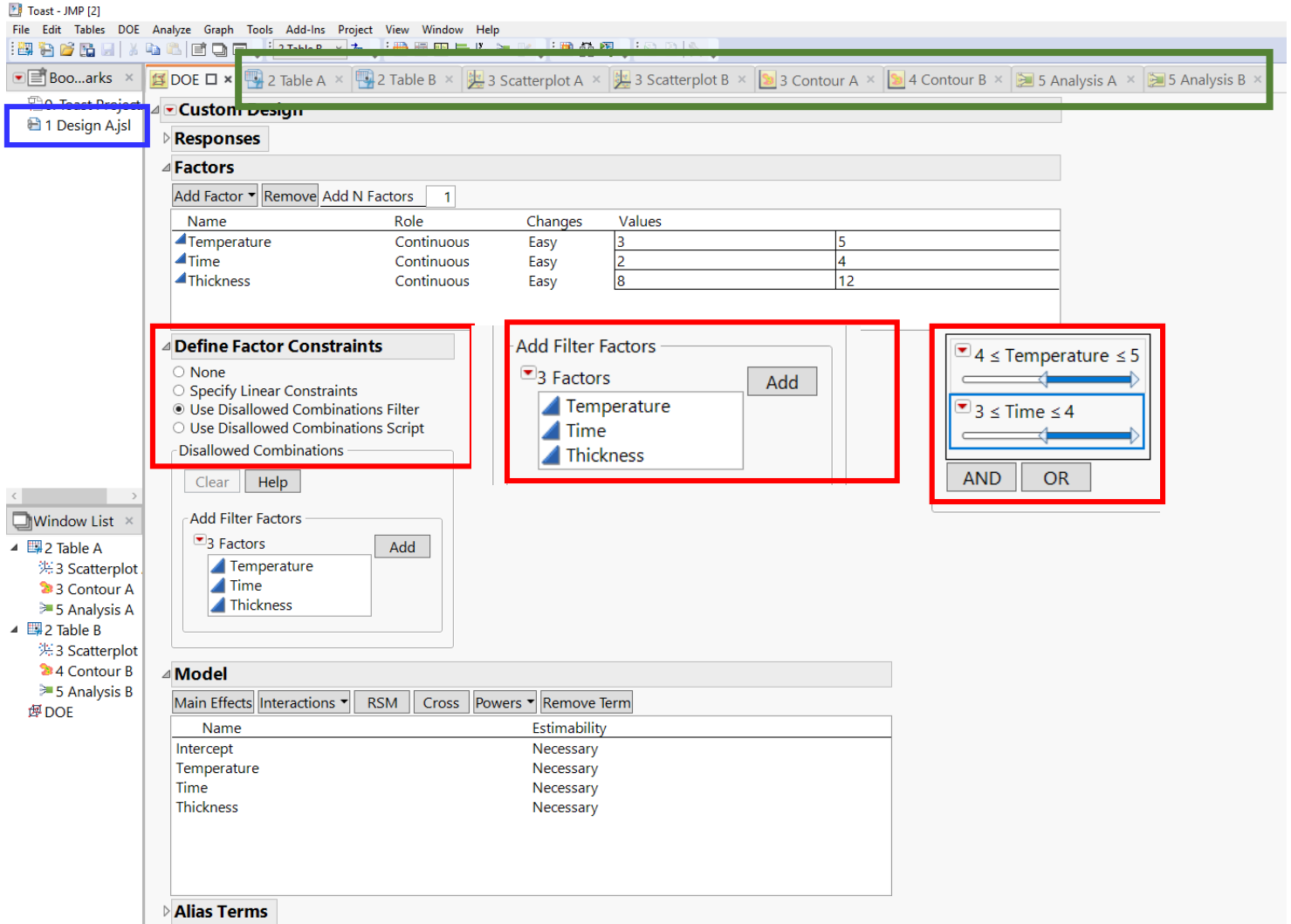
Define Factor Constraints

- Use the Disallowed Combinations Filter.
- Demo the sequence.

Show the impact

- Step through the tabs *or*
- Open up a new Project with tabs rearranged in Dashboard view.

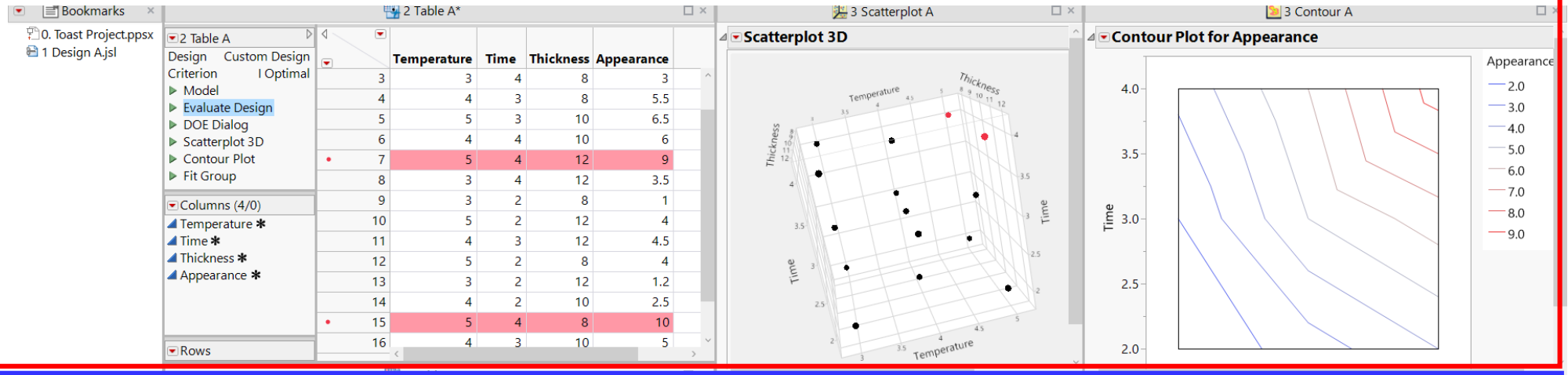
(see next slide)



(8c) Workflow comparison dashboard output

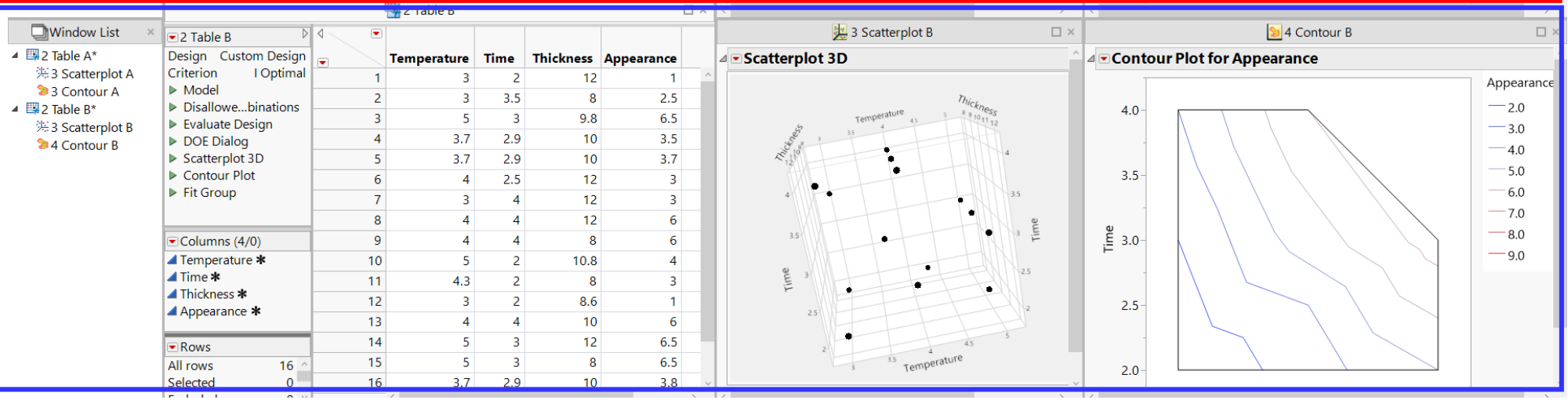
Unconstrained design

- Two rows produce high risk results.
- Scatterplot 3D view shows undesired design space.
- Contour plot shows the combination of temperature and time.



Constrained design

- No high risk results.
- Contour plot show investigation space coverage.

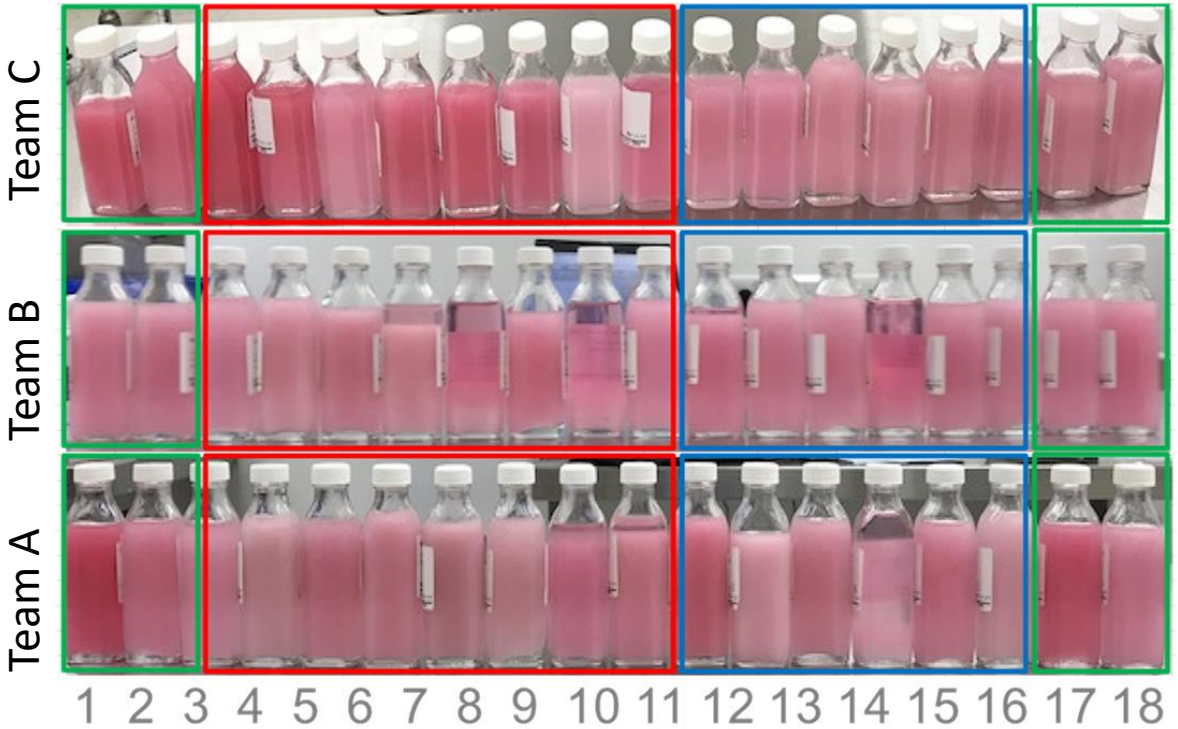


(9a) Assignment 2: Suspensions

The Teams

Assignment 2

The students are split into three groups of 7 students.
Each group is tasked with performing the same Central Composite design using the same run order.



The output

- It is easy to see that there is team to team variation in the suspensions produced in terms of colour and fill volume.
  - Suspensions outlined in green (runs 1,2. 17 &18) are supposed to be identical centre-point runs.

The challenge

- How do we visualise the variation of the Viscosity measurement?
- What is the impact of variation on models?

(9b) Assignment 2: Suspensions

Variability Gauge

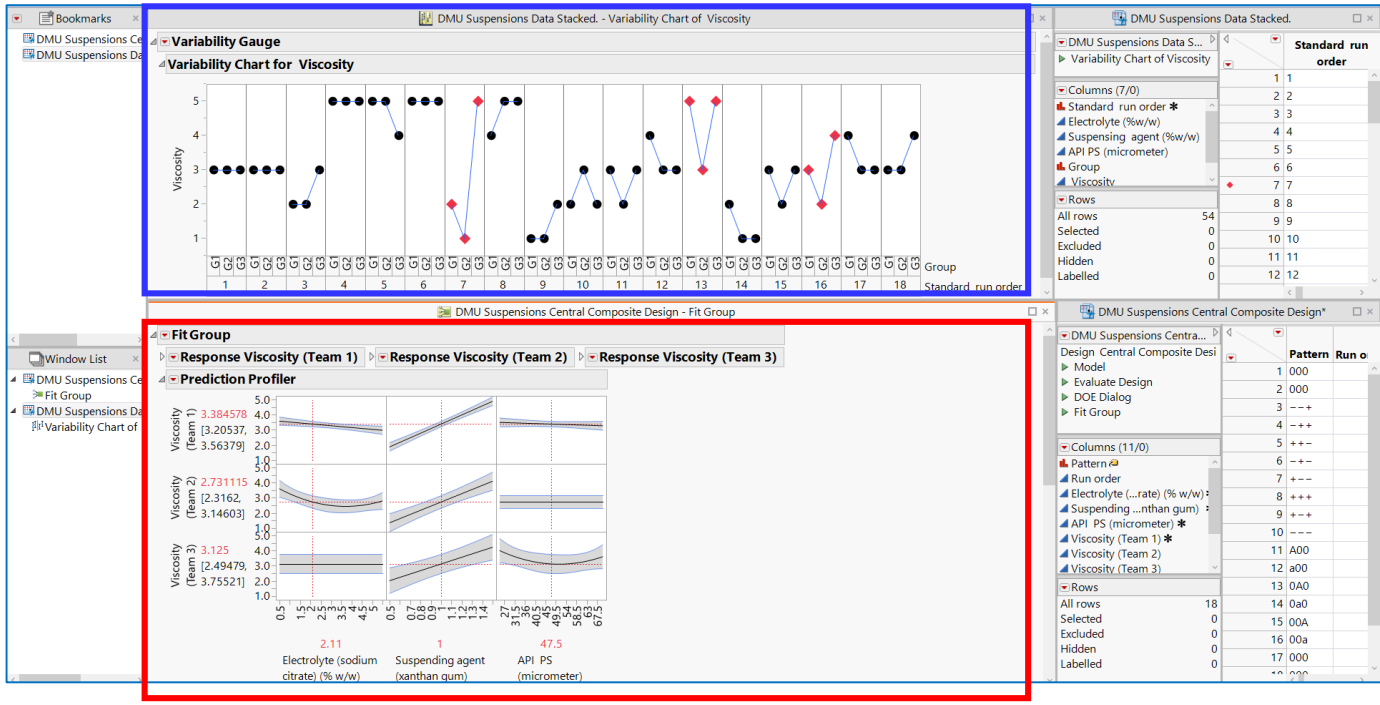
Use this platform to distinguish between team to team and run to run variation.

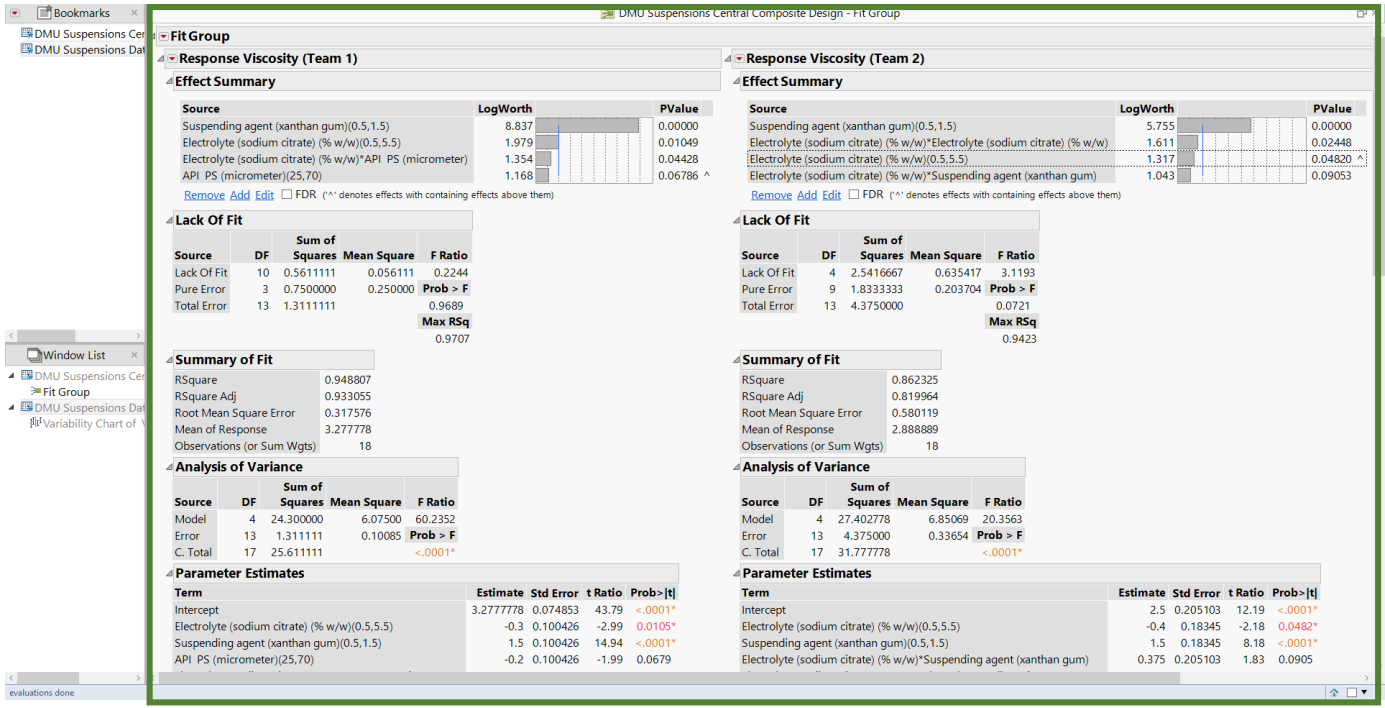
Fit Group

Even though the teams display different signal to noise ratios (as evidenced by the confidence intervals), all models broadly show the same effects.

Details on demand

- Using the same project the detailed statistical view can be inspected to compare signal to noise ratios, Adj. R^2 numerical values.





(10a) Benefits of JMP14 Project functionality

Creates new organisational structures

- Map onto existing file structures and create a new organizational structure via a single document interface.

Save and close as you go

- In the maximised screen it is possible to see what data sets and models are open in the Window List which is displayed at all times.
- If new models are created and the script saved to data tables (or if the table itself is altered), the data-tables are asterisked. When the Project is saved, the user is asked whether to save the updated tables.
- The ability to tab through or rearrange the Workspace Layout enables data tables and visualisations to be easily checked for consistency (or lack of).
- A bonus is that it is now easier to manage and curate data as one works – closing a current session ready to regenerate the next day couldn't be simpler.

Correcting inconsistencies at source

- Updating the source data tables removes complexity of future manipulations (e.g. concatenation, query builder)
- Correcting data tables and model scripts at source means that a Project which has bookmarked files or folders will always pull the most up to date "version of the truth".
- Correcting inconsistencies of data visualisations facilitates cross-comparisons across studies in reporting and presentations. This makes it easier for the audience to assimilate the learnings faster.

Transparent and traceable

- The archive feature will allow comparison of historical data tables with the current data tables. Using the compare data tables feature allows any changes to be identified.

(10b) Benefits of JMP14 Project functionality

Great tool for insight communication and workflow training

- The flexible Projects workspace brings to life compelling stories.
  - Step by step using tabs.
  - Dashboard view using the Workspace Layout.
- Dashboard view enables the benefit of dynamic links.
- Windows can be maximised to focus attention.
- Having all the components (tables, data visualisation, statistical detail) on hand facilitates construction of the story.

Drives data standards

- For observational data (e.g. manufacturing batches), use Project to create and archive standard reports that update when new data is entered.

Integrates well with other JMP functionality

- Use links from Journals to open up Projects with curated folders designed to convey a message or insight.
- Use with Dashboard Builder to quickly explore possible Dashboard layouts.
- Use with Query Builder to create standard reports and output.

(10c) Acknowledgements

- Dr Walkiria Schleinwein and the students from De Montfort University Quality by Design MSc 2017-2018 cohort.
- Industrial clients who face similar challenges in building Organisational memory.
- Associate consultants and JMP Summit delegates who inspire and help push the boundaries of learning

….and importantly

- The JMP Developers who made JMP14 Projects happen.

martin.owen.insight@gmail.com