Science-driven software solutions

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- Why augment a Definitive Screening Design?
- What do you get from Scoping Designs?
- Do you routinely perform Stability Analyses?
- How do you analyse complex plate-based assay data?

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Why augment a Definitive Screening Design?

Background

- DSDs are extremely efficient and effective, but rely on sparsity – e.g. for a 6-factor design, a full RSM model can be fitted if up to 3 factors are active!
- However, what happens if you suspect or discover that 4 factors are active?

Approach

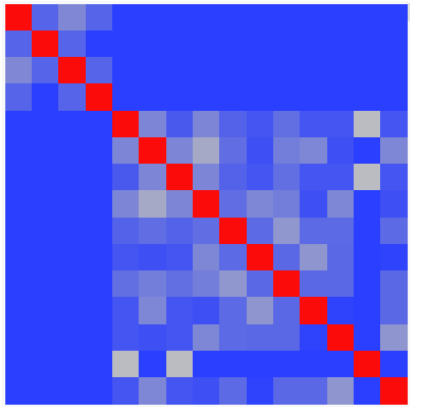
- Method identified to augment DSDs – proactively or reactively – to fit the full 4-factor RSM model
- Method maintains desirable DSD properties, but addresses common real-world problem of many active factors
- **Attend Paul Nelson & Phil Kay's talk to learn more!**

Solution

- DSD structure lends itself to a sequential strategy, in cases where DSDs are unable to resolve all ambiguity
- New add-in available upon request

Design

Run	Block	Volume vols	Catalyst %	Temperature deg C	Time hours
1	1	6.5	5	120	24
2	1	6.5	0.5	80	8
3	1	10	2.75	80	24
4	1	3	2.75	120	8
5	1	10	0.5	100	8
6	1	3	5	100	24
7	1	10	5	80	16
8	1	3	0.5	120	16
9	1	10	5	120	8
10	1	3	0.5	80	24
11	1	10	0.5	120	24
12	1	3	5	80	8
13	1	6.5	2.75	100	16
14	2	10	5	100	24
15	2	3	0.5	100	8
16	2	10	5	80	8
17	2	3	0.5	120	24
18	2	10	0.5	80	24
19	2	3	5	120	8
20	2	6.5	5	80	24
21	2	6.5	0.5	120	8
22	2	6.5	2.75	100	16

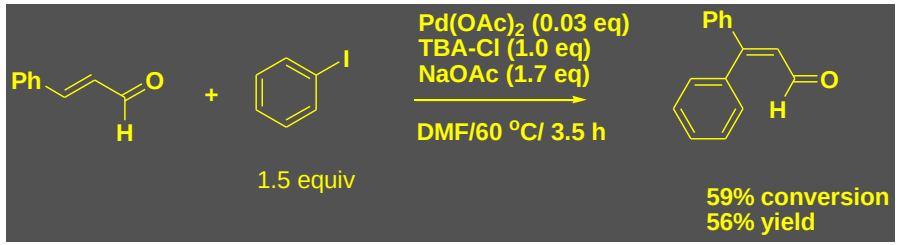


What do you get from Scoping Designs?

Background

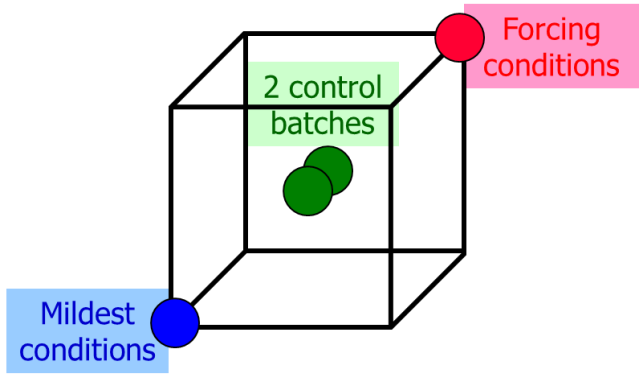
- Prior to performing a screening study, why not check:
  1. Have you chosen appropriate factor ranges?
  2. Are your response goals achievable?
  3. Are your effects likely to be greater than the background noise?

Example: Improve yield of a Heck reaction



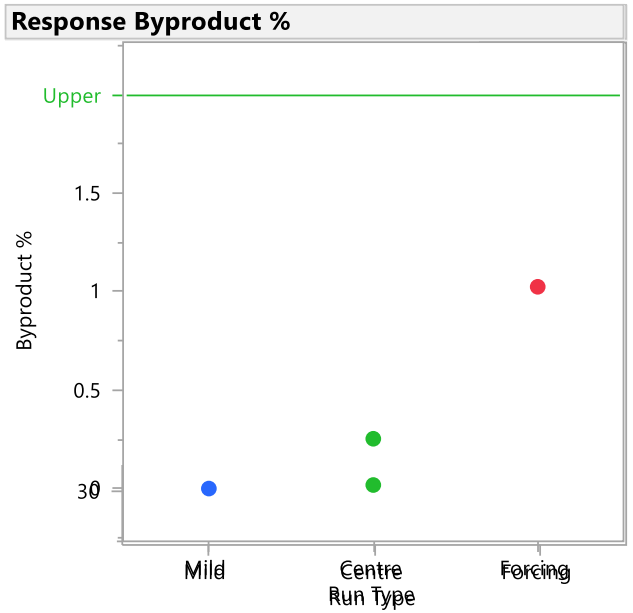
Approach

- Identify Mild and Forcing conditions around your ideal setting for each factor
- Perform:
  - Run(s) with all factors at Mild conditions
  - Run(s) with all at Forcing
  - Replicated Centre Points



Solution

- New version of add-in available upon request



1. Nonlinear trend => optimal factor ranges ✓
2. Specification achievable! ✓
3. Signal appears > Noise ✓

Do you routinely perform Stability Analyses?

Background

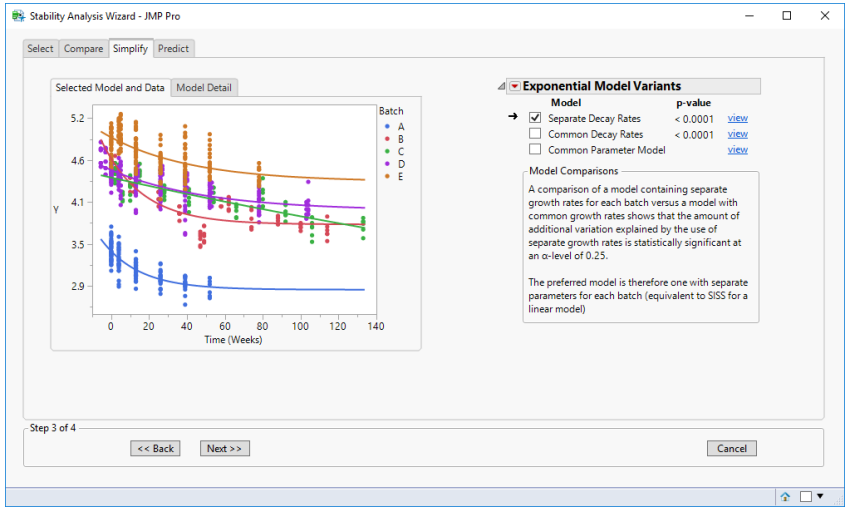
- Stability and Shelf Life Prediction is available using JMP's *Degradation* platform. However, it only applies to straight line model fits & single factor analysis, and doesn't always correctly apply the ICH guidance
- *Fit Model* and *Nonlinear* platforms can perform required analysis, but are not straightforward!

Approach

- Create workflow add-in to guide user through ICH-compliant analysis
- Extend poolability tests (recommended by ICH) to nonlinear models
- Use existing JMP functionality wherever possible
- Allow drill-down from add-in to native JMP platforms to explore results further

Solution

- Bespoke add-in developed for clients requiring both linear & nonlinear stability analysis in line with ICH guidance



How do you analyse complex plate-based assay data?

Background

- Using a complex, multi-step process, a client generates a large amount of plate-based data to evaluate, qualify & develop a vital potency assay

Approach

- Manage, import & process raw plate data
- Subset & analyse available Control data to establish LoD/LoQ and endpoint titre
- Fit multiple curves accounting for complex data structure
- Extract and compare curve parameters to discriminate between treatment groups

Solution

- Bespoke add-in developed to easily guide user through the process steps. This reduces user error, and provides additional options & flags