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Formulation Data Analysis in Design-Expert

Practical 13 - Software and data-analysis practical

Aim

To analyse formulation-design data and evaluate the proposed response model.

Principle

Design of experiments varies selected factors systematically so that their effects and interactions can be estimated. Factor coding, randomisation, replication and a defined response are essential to interpretation. An unreplicated saturated design cannot independently estimate experimental error.

Keep the supplied data, transformations, software version, analysis settings and complete output together. Record units explicitly and distinguish assumptions from observations.

Materials and Requirements

- Defined formulation factors and feasible ranges
- Critical response definitions and measurement methods
- Design-Expert or institution-approved design software
- Spreadsheet or institution-approved analysis software
- Raw-data dictionary and analysis worksheet

Procedure

1. Define the analysis question and the variables, units, identifiers and missing-data conventions in the dataset.
2. Import a working copy and check values against the original file. Inspect ranges, duplicates, timing and unit consistency.
3. Define the formulation question, critical quality attributes, factor types and feasible ranges.
4. Choose an appropriate factorial, response-surface or mixture design and justify the choice.
5. Add replication, centre points or other elements needed to estimate variability and assess model adequacy.
6. Randomise the practical run order where appropriate and issue controlled run sheets with coded and actual settings.
7. Check the design for infeasible combinations and specify how process deviations and missing observations will be handled.
8. Retain diagnostics, intermediate calculations and the selected analysis settings. Explain exclusions and sensitivity checks.
9. Write a conclusion that addresses the stated question and the limitations of the design rather than relying on one fitted statistic.

Observations and Record

Enter actual measurements or the supplied teaching data. Record the method, material identity, conditions and units.

Run	Coded factor X1	Coded factor X2	Measured response
1	-1	-1	Record
2	+1	-1	Record
3	-1	+1	Record
4	+1	+1	Record

Run	Coded factor X1	Coded factor X2	Measured response
Additional replicates / centre points	State	State	Record

Calculations

• Coded factor = (actual value - centre value) / half-range
• For a two-factor model, y = b0 + b1X1 + b2X2 + b12X1X2

Worked Example

Illustrative responses for the four listed factor combinations are 40, 60, 50 and 90 units.
The fitted coefficients are b0 = 60, b1 = 15, b2 = 10 and b12 = 5.
The four-point model exactly fits these four values. Additional evidence is needed for an error estimate, adequacy test and confirmation.

Analysis and confirmation

• Import the controlled run data and review deviations and missing values before fitting.
• Assess model hierarchy, residuals, uncertainty and lack of fit when the design permits its estimation. A saturated four-point fit alone does not support a meaningful residual-error F test.
• Define an optimisation objective with justified constraints, then evaluate independently prepared confirmation runs at the selected settings.

Result and Interpretation

• Present the rationale, randomised run plan and response definitions. A design is complete only when the measurement and execution plan are clear.

Precautions

• Use feasible, scientifically meaningful factor ranges.
• Plan replication before conducting the experiment.
• Avoid confusing mixture fractions, which sum to a constraint, with independent factorial factors.
• Preserve the original dataset and a reproducible record of the analysis.

Viva Questions and Answers

Why randomise run order?

It helps reduce confounding with time-related changes.

What is an interaction?

The effect of one factor depends on the level of another.

Why use replication?

It provides information on experimental variability.

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