1 Software for Design of Experiments

*Design Expert* is a piece of software designed to help with the design and interpretation of multi-factor experiments. In polymer processing, we might use the software to help us design an experiment to see how a property such as tensile strength varies with changes in the processing conditions - e.g. changes in rotor speed or ram pressure.

The software offers a wide range of designs, including factorials, fractional factorials and composite designs. It can handle both process variables, such as rotor speed, and also mixture variables, such as the proportion of resin in a plastic compound. *Design Expert* offers computer generated D-optimal designs for cases where standard designs are not applicable, or where we wish to augment an existing design - for example, to fit a more flexible model.

The aim of this document is to help you get started with *Design Expert*. After a brief review of statistical terms and concepts, Section 3 gives some advice on selecting an appropriate class of designs. Section 4 gives an overview of the main steps involved in running *Design Expert*, while Sections 5, 6 and 7 give some more detailed guidance.

If you’re new to the statistical approach to design, you may find it useful to consult some of the books listed in the reference section at the end of the document.

**Warning!** *Design Expert* is not suitable for designing and analysing *repeated measures* designs of the kind that are often used in the Human Sciences.

2 Statistical terms and concepts

This section reviews some statistical terms and concepts that are used in the *Design Expert* software.

2.1 Data

The factors that we vary in experiment can be divided into *Process* variables, such as the speed of an engine or the thickness of an adhesive layer, and *Mixture* variables, such as the proportion of resin in a plastic compound, or the proportion of fat in a chicken feed. With a mixture variable, the effect depends on the *proportion* of a constituent in the mixture, rather than on the absolute amount.
Process variables can be split into Continuous and Categorical.

- Continuous - can be varied freely over a range
  - Engine speed, with speed varying from 1000 to 5000rpm
- Categorical - restricted to a few distinct values
  - Filler, with a choice between pulverised fuel ash and glass beads

Categorical variables are sometimes divided into Nominal and Ordinal. An Ordinal variable is a categorical variable in which the categories have a natural order - e.g. Small, Medium, Large. A Nominal variable is one where no order is implied - e.g. a set of categories like colour or make of car.

**Note:** Design Expert uses the term ‘factor’ to refer to both continuous and categorical variables - this contrasts with some statistical texts and software that reserve the term ‘factor’ for a categorical variable. In Design Expert, continuous and categorical variables are described as ‘Numeric’ and ‘Categoric’ respectively.

### 2.2 Model

In analysing an experiment, we fit models relating a *response* or *quality characteristic* to a set of controllable variables. For continuous control variables, we often use a linear, factorial or quadratic model - for example...

- **Linear model** \( Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon \)
- **Factorial model** \( Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_{12} X_1 X_2 + \epsilon \)
- **Quadratic model** \( Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_{12} X_1 X_2 + \beta_{11} X_1^2 + \beta_{22} X_2^2 + \epsilon \)

Apart from the intercept, the terms in these models fall into one of three categories.

- Linear terms (Main effects) of the form \( \beta_i X_i \)
  - model the average effect of varying a control
- Two-factor interactions of the form \( \beta_{ij} X_i X_j \)
  - allow the effect of changing a control to vary with the setting of another control
- Quadratic terms of the form \( \beta_{ii} X_i^2 \)
  - allow for curvature in the effect of a control on the response

Models for categorical controls often involve a *set* of terms to represent a single main effect or two-factor interaction, but the interpretation of the effects is similar.
2.3 Resolution

A full factorial design is one where the experiment uses all combinations of the levels of factors. Many designs involve running only a small fraction of a full factorial. This makes our experiments more economical, but results in what is known as aliasing between different effects. If two effects are aliased together, we can estimate their combined effect, but cannot separate out the size of each individual effect. For example, if A and BC are aliased, we’ll be able to estimate the combined effect of A and BC, but we won’t be able to obtain a separate estimate of A, or of BC.

The resolution of a design gives an indication of the degree to which we’re going to be able to separate out individual effects.

- Resolution III In a resolution III design, main effects are aliased with two-factor interactions. Unless the two-factor interactions are negligible, our estimates of the main effects will be biased.
- Resolution IV Two-factor interactions will be aliased in pairs, but we’ll be able to estimate the main effects clear of any other main effects or two-factor interactions.
- Resolution V All main effects and two-factor interactions will be clear of other main effects or two-factor interactions. Unless the higher order interactions are sizeable, a Resolution V will often be almost as good as a full factorial.

3 Selecting a Design

*Design Expert* offers a large number of different classes of design. If you’re new to the software, you may well need some help in selecting a class of designs that’s appropriate for your particular situation. The following are some suggestions, based on the type of control variables that you’re dealing with and on the type of model that you wish to fit.

In *Design Expert*, the design classes are arranged in tabs on the left hand side of the screen. In the recommendations below, I give the tab first and then the class within the tab, for example ‘Factorial/2-Level Factorial’. In some cases, I have suggested more than one class of design.

3.1 Process variables only

- All continuous
  - Linear or Factorial model
    Factorial/2-Level Factorial
  - Quadratic model
    Response Surface/Central Composite
• All categorical
  – All factors at two levels
    Factorial/2-Level Factorial
  – Some factors at more than two levels
    Factorial/General Factorial
    Factorial/D-Optimal
• Mix of continuous and categorical
  – Linear or factorial model for continuous controls
    * All categorical factors restricted to two levels
      Factorial/2-Level Factorial
    * Some categorical factors have 3 or more levels
      Factorial/General Factorial
      Factorial/D-Optimal
  – Quadratic model for continuous controls
    Response Surface/Central Composite
    Response Surface/D-optimal

3.2 Mixture variables only

• All components have same range and no constraints on design space
  Mixture/Simplex Lattice
  Mixture/Simplex Centroid
• Above conditions not satisfied
  Mixture/D-optimal

3.3 Mixture and process variables

If you have a combination of mixture and process variables, you’ll need to use the Combined/D-optimal class.

4 Running Design Expert

Once you’ve decided on the type of design that you’re going to use, the Design Expert software is quite easy to run. There are three main steps...

1. Constructing the design
   Design Expert takes you through a series of screens in which you specify the information needed to construct the design - e.g. names and ranges of your variables and
degree of replication. At the end of this step, Design Expert gives the design layout. This is a list of the experimental settings to be used for each of the experimental runs. The order of the runs is randomised and this is the order in which they should be carried out.

2. Evaluating the design

Design Expert offers two types of information to help you check whether a design will meet your requirements.

- Alias pattern
  - This shows whether you’ll be able to estimate the effects that you’re interested in.

- Precision of the fitted model
  - The precision of predictions from a fitted model will depend partly on the background process variation and partly on the experimental design. Provided you’ve got some idea of the likely size of the background variation, Design Expert can help you to estimate the kind of precision that you’re likely to achieve. If it looks as though you’re not going to be able to achieve the required precision, you may need to consider carrying out a larger experiment.

3. Modelling and interpreting the experimental data

Design Expert offers a wide range of analytical and graphical techniques for model fitting and interpretation.

In the analysis of 2-level Factorial designs, extensive use is made of Normal probability plots to highlight any active factors - i.e. factors that affect the response. If you’re not familiar with this approach, see Montgomery(2005), section 6.5. The idea of this approach is that if none of the factors is active, the variation in the estimates of effects will be purely due to random variation, so that a Normal plot of the estimates will be roughly linear. Active factors will show up as points that are separated from the underlying linear pattern.

Design Expert provides an extensive help system. You can access this from any screen by clicking on the Help or Screen Tips buttons on the toolbar - these are indicated by a question mark and light bulb. You can also obtain help by selecting Help...Contents from the main menu.

In addition to the help system, there is a set of tutorials, which take you through the design and analysis of particular types of experiment. You can access these as follows.

1. Select Help...Contents

2. Click on the Contents tab

3. Select Web-based Tutorials...User Tutorials

4. Select the tutorial that you require
5 Specifying the features of a design

This section offers some help with the information that you’ll need to supply during the design stage.

5.1 Lower and Upper limits for variables

For each numeric variable, you’ll be asked for lower and upper limits. In specifying the limits, you should aim to make the range of variation large enough to produce effects that will show up against the background process variation, while avoiding limits that are so extreme as to prevent the process from operating properly.

5.2 Replication

We say that we are replicating a run, when we include the same set of processing conditions more than once during the course of an experiment. There are two reasons for replication.

1. Increases the precision of estimates of effects
2. Gives additional information on background process variation

Replication is particularly important with small designs, such as a $2^2$ Factorial, where there are very few runs at each setting of a factor.

Note: If the initial design is a fractional Factorial, it is generally better to move to a full Factorial (or a larger fraction of the full Factorial), rather than replicating the original fractional design. Moving to a less fractionated design will reduce the amount of aliasing, while giving the same improvement in precision that we’d obtain from pure replication.

5.3 Replication vs Repeated measurements

One common mistake is to confuse genuine replicates with repeated measurements on the same experimental unit.

Suppose we are producing rubber sealing strips for use with car doors and wish to assess the effect of varying the processing conditions used in mixing the raw materials - e.g. rotor speed or ram pressure. In our experiment, we’ll try a range of different combinations of processing conditions. Each batch of material will pass through a series of processes, such as extrusion, and we’ll then measure the properties of the finished product. To perform a genuine replicate, we’ll need to mix up a new batch of material (using the same rotor speed, ram pressure, etc) and pass it through the intermediate processes such as extrusion, to give the final door seal. The idea is that the variation from one replicate to another should reflect all sources of background variation that arise when we go from one set of processing conditions to another.

If we simply take several measurements on the output produced from a single batch of material, the variation that we observe will reflect only the measurement error and not
the variation between different runs of the mixer or extruder. As a result, the variation
between different measurements will seriously underestimate the total process variation
and will probably lead to us highlight far too many factors as active.

**Note:** Although repeated measurements will not usually give a realistic picture of the
total background variation, it’s often a good idea to take repeated measurements in order
to reduce the measurement error. If you do this, the best way of handling the data is to
find the *mean* of the measurements for each run and to enter this value as your response
in *Design expert*. By doing this, you’ll benefit from the increase in the precision of your
measurements, while avoiding the problem of underestimating the process variation.

### 5.4 Blocking

Experiments are often subject to sources of variation that are unavoidable, but can be
predicted in advance. For example, we may have to spread the experiment over several
days, possibly with very different ambient temperature and humidity. This day to day
variation may well affect our measured response. Many of the designs offered by *Design
Expert* can be split into two or more blocks, so that we can correct for these unwanted
sources of variation. For a discussion of blocking, see Montgomery (2005).

### 5.5 Centre points

In constructing 2-level factorial designs, *Design Expert* allows you to add *centre points*,
at which all continuous controls are set in the middle of their ranges. The inclusion of
centre points allows us to check whether our fitted model is adequate, or whether we need
to include some quadratic terms to allow for curvature.

### 5.6 Randomisation

*Design Expert* automatically randomises the order of the experimental runs. There are
two reasons for randomisation.

- Reduces the risk of unanticipated sources of variation affecting the estimates of
effects
- Helps to meet the assumptions of the statistical methods used in analysing experi-
mental data

Sometimes one or more of the variables are difficult to change and it is necessary to impose
restrictions on the degree of randomisation. This results in a *split plot* design, which is
rather more difficult to analyse - see Montgomery (2005), section 14-4. If you feel that
full randomisation is not feasible, you are strongly advised to consult a statistician *before*
proceeding with your experiment.
6 Looking at the properties of a design

Once a design has been constructed, you’ll see a tree diagram on the left hand side of the Design Expert window. To examine the properties of the design, select Design(Actual)...Evaluation.

6.1 Alias pattern

To examine the alias pattern for a design, click on the Results tab. Near the top of the output, you’ll see a table giving a list of estimated terms, together with their aliases. You can use this table to check whether you’ll be able to isolate the effects that you’re interested in.

Note: If you’ve selected a full factorial design, all effects will be estimable and the table of aliases will not appear.

6.2 Precision

Design Expert offers two ways of assessing the precision that you’re likely to obtain with a given design.

- Precision of predictions at different points in the design space
  
  In the evaluation window, click on Graphs. Design Expert will give you a contour plot showing the standard error for predictions of the response at different points in the design space. Note that the figures on the plot need to be scaled by an estimate of the standard deviation of the background process variation. For example, if previous experimentation suggests that the standard deviation of the background variation, $\sigma$, is 12, a figure of 0.25 on the plot would indicate a standard error of $0.25 \times 12 = 3$.

- Power analysis
  
  In the evaluation window, click on Results. Scroll down the display until you come to a table giving information about each term in the model. The columns on the right of this table give a power analysis for effects of size $0.5\sigma$, $1\sigma$ and $2\sigma$. The figures in these columns give the chance of detecting an effect of the corresponding size.

7 Using Design Expert to analyse a design

Once you’ve carried out your experiment, you enter the response values into the appropriate columns on the Design Layout Screen. If this screen is not currently visible, you can switch to it by selecting Design(Actual) (in the tree on the left of the screen).

To analyse a response, click on the response name (in the tree on the left of the screen). You’ll now see a set of tabs that you can use to access various techniques for analysing
and interpreting the fitted models. The following are a few notes on the facilities that are available under each tab.

- **Effects**
  - Half-Normal and Normal plots for highlighting active factors
  - Pareto chart for giving a picture of the relative sizes of the different effects

- **ANOVA**
  - Analysis of variance
    - This can sometimes be used as alternative way of highlighting active factors
  - Summary statistics.
    - One useful statistic here is the one labelled ‘Adeq Precision’. This is a kind of signal-to-noise ratio that measures the ratio of the range of variation in the predicted response to an estimate of the standard error of the predictions. A high value indicates that the variation that we’re observing is large in relation to the underlying uncertainty of the fitted model.
  - Coefficients of fitted model
    - Unless the interactions are negligible, the numerical coefficients can be difficult to interpret. It is generally better to examine the model through graphical plots - see below.

- **Diagnostics**
  - Residual plots
    - *Design Expert* offers the usual range of residual plots for checking assumptions such as Normality and constant variance.
  - Box-Cox plot for power transformations
    - This can help us to decide whether we could improve the fit of the model by measuring the response on a different scale - e.g. by using the log of the response values.
  - Plots of leverage and influence statistics
    - These plots show the influence of individual data points on the fitted model. One of the aims of statistical design is to ensure that our models make good use of all observations and are not critically dependent on just a few points. So for standard designs such as Factorials, these statistics will not usually be needed.

- **Model Graphs**
  - *Design Expert* offers a wide range of different plots to show how the response varies with changes in the controls. To change the type of plot, use the View menu. Notice that contour and 3D surface plots are only appropriate for continuous control variables.
If you have 3 or more controls, you’ll obtain a plot of two of the controls with the remaining variables held at fixed settings. You can change the variables that are plotted and you can also change the settings of the fixed variables.

Available plots are . . .

- One Factor
  
  *Main effects* plot showing the average effect of shifting a single control, while holding the other controls constant.

- Interaction
  
  Plot showing how the effect of changing one control varies with changes in a second control

- Contour

- 3-D Surface
  
  Note that the surface plot can be rotated to obtain a better view

- Cube
  
  Gives the numerical response values at each combination of three of the controls. Any further controls are held at fixed settings.

8 References

For a clear *introduction* to design of experiments, see Part 3 of DeVor et al (1992) or Part 4 of Montgomery (2001).

For a more comprehensive coverage, see Montgomery (2005), Wu and Hamada (2000) or Myers and Montgomery (1995).


