



BSI Standards Publication

Selected illustrations of response surface method — Central composite design

National foreword

This Published Document is the UK implementation of ISO/TR 13195:2015.

The UK participation in its preparation was entrusted to Technical Committee MS/6, Methodologies for business process improvement using statistical methods.

A list of organizations represented on this committee can be obtained on request to its secretary.

This publication does not purport to include all the necessary provisions of a contract. Users are responsible for its correct application.

© The British Standards Institution 2015. Published by BSI Standards Limited 2015

ISBN 978 0 580 74473 0

ICS 03.120.30

Compliance with a British Standard cannot confer immunity from legal obligations.

This Published Document was published under the authority of the Standards Policy and Strategy Committee on 31 December 2015.

Amendments issued since publication

Date	Text affected
------	---------------

Selected illustrations of response surface method — Central composite design

*Illustrations choisies de méthodologie à surface de réponse — Plans
composites centrés*





COPYRIGHT PROTECTED DOCUMENT

© ISO 2015, Published in Switzerland

All rights reserved. Unless otherwise specified, no part of this publication may be reproduced or utilized otherwise in any form or by any means, electronic or mechanical, including photocopying, or posting on the internet or an intranet, without prior written permission. Permission can be requested from either ISO at the address below or ISO's member body in the country of the requester.

ISO copyright office
Ch. de Blandonnet 8 • CP 401
CH-1214 Vernier, Geneva, Switzerland
Tel. +41 22 749 01 11
Fax +41 22 749 09 47
copyright@iso.org
www.iso.org

Contents

Page

Foreword	iv
Introduction	v
1 Scope	1
2 Terms and definitions	1
3 Symbols and abbreviated terms	6
3.1 Symbols	6
3.2 Abbreviated terms	6
4 Generic descriptions of central composite designs	7
4.1 Overview of the structure of the examples in Annexes A to D	7
4.2 Overall objective(s) of a response surface experiment.....	7
4.3 Description of the response variable(s).....	8
4.4 Identification of measurement systems.....	8
4.5 Identification of factors affecting the response(s).....	8
4.6 Selection of levels for each factor.....	8
4.6.1 Factorial runs.....	9
4.6.2 Star runs.....	9
4.6.3 Centre run.....	9
4.7 Layout plan of the CCD with randomization principle	10
4.8 Analyse the results — Numerical summaries and graphical displays	10
4.9 Present the results.....	11
4.10 Perform confirmation run.....	12
5 Description of Annexes A through D	12
5.1 Comparing and contrasting the examples.....	12
5.2 Experiment summaries	13
Annex A (informative) Effects of fertilizer ingredients on the yield of a crop	14
Annex B (informative) Optimization of the button tactility using central composite design	28
Annex C (informative) Semiconductor die deposition process optimization	41
Annex D (informative) Process yield-optimization of a palladium-copper catalysed C-C-bond formation	52
Annex E (informative) Background on response surface designs	70
Bibliography	80

Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights. Details of any patent rights identified during the development of the document will be in the Introduction and/or on the ISO list of patent declarations received (see www.iso.org/patents).

Any trade name used in this document is information given for the convenience of users and does not constitute an endorsement.

For an explanation on the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the WTO principles in the Technical Barriers to Trade (TBT) see the following URL: [Foreword - Supplementary information](#)

The committee responsible for this document is ISO/TC 69, *Applications of statistical methods*, Subcommittee SC 7, *Applications of statistical and related techniques for the implementation of Six Sigma*.

Introduction

The present Technical Report takes one specific statistical tool (Central Composite Designs in Response Surface Methodology) and develops the topic somewhat generically (in the spirit of International Standards) but then illustrates it through the use of four detailed and distinct applications. The generic description focuses on the Central Composite Designs.

The annexes containing the four illustrations follow the basic framework but also identify the nuances and peculiarities in the specific applications. Each example offers at least one “wrinkle” to the problem, which is generally the case for real applications. It is hoped that practitioners can identify with at least one of the four examples, if only to remind them of the basic material on response surface method that was encountered during their training.

Each of the four examples is developed and analysed using statistical software of current vintage. The explanations throughout are devoid of mathematical detail—such material can be readily obtained from the many design and analysis of experiments textbooks (such as those given in References [1] to [7]).

Selected illustrations of response surface method — Central composite design

1 Scope

This Technical Report describes the steps necessary to understand the scope of Response Surface Methodology (RSM) and the method to analyse data collected using Central Composite Designs (CCD) through illustration with four distinct applications of this methodology.

Response surface methodology (RSM) is used in order to investigate a relation between the response and the set of quantitative predictor variables or factors. Especially after specifying the vital few controllable factors, RSM is used in order to find the factor setting which optimizes the response.

2 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

2.1

experiment

purposive investigation of a system through selective adjustment of controllable conditions and allocation of resources

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.1. (The notes are not reproduced here.)

2.2

response variable

variable representing the outcome of an *experiment* ([2.1](#))

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.3. (Except for NOTE 3 the notes are not reproduced here.)

Note 2 to entry: A common synonym is “output variable”.

Note 3 to entry: The response variable is likely to be influenced by one or more *predictor variables* ([2.3](#)), the nature of which can be useful in controlling or optimizing the response variable.

2.3

predictor variable

variable that can contribute to the explanation of the outcome of an *experiment* ([2.1](#))

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.4. (The notes are not reproduced here.)

Note 2 to entry: Natural predictor variables are expressed in natural units of measurement such as degrees Celsius (°C) or grams per liter, for example. In RSM work, it is convenient to transform the natural variables to coded variables which are dimensionless variables, symmetric around zero and all with the same spread.

2.4

model

<experiment> formalized representation of outcomes of an *experiment* ([2.1](#))

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.2. (The notes and examples are not reproduced here except for NOTE 2 which is NOTE 1 in ISO 3534-3.)

Note 2 to entry: The model consists of three parts. The first part is the *response variable* (2.2) that is being modelled. The second part is the deterministic or the systematic part of the model that includes *predictor variable(s)* (2.3). Finally, the third part is the *residual error* (2.12) that can involve *pure random error* (2.13) and *misspecification error* (2.14). The model applies for the experiment as a whole and for separate outcomes denoted with subscripts. The model is a mathematical description that relates the response variable to predictor variables and includes associated assumptions. Outcomes refer to recorded or measured observations of the response variable.

Note 3 to entry: In some areas the term transfer function is used for the systematic part of the model.

EXAMPLE In the models considered in response surface methodology the deterministic or systematic part are polynomials in the predictor variables. A second order model with two predictor variables is written as

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \varepsilon$$

where ε is the random error. The associated assumptions on the random error could be either that individual random errors are uncorrelated with constant variance or independent and normally distributed. The deterministic part of the model is the second degree polynomial in the predictor variables x_1 and x_2

$$E_y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2$$

which explains the mean (E_y) of the response variable as a function of the predictor variables.

2.5 factor

<design of experiments> feature under examination as a potential cause of variation

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.5. (The notes are not reproduced here.)

Note 2 to entry: Generally the symbol k is used to indicate the number of factors in the experiment.

2.6 factor level

setting, value or assignment of a *factor* (2.5)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition (3.1.12). (The notes are not reproduced here.)

2.7 coding of factor levels

<design of experiments> one-to-one relabelling of factor levels

Note 1 to entry: The coding of factor levels facilitates the identification of the design and the properties of the design.

Note 2 to entry: In response surface experiments the actual (or natural or operational) levels are relabelled such that the coded levels are numeric and symmetric around 0.

Note 3 to entry: A two-level factor is usually coded to have coded levels -1 and $+1$. A factorial design where all factors are two-level factors can be coded such that all runs are represented as *factorial runs* (2.9).

Note 4 to entry: In central composite designs numeric (or continuous) factors with five levels are considered, except for the face-centred central composite designs, where only three levels are needed, see note 6 to 2.7. If the actual (or natural or operational) levels are $l_1 < l_2 < l_3 < l_4 < l_5$ then the middle level l_3 shall be the average of the lowest level l_1 and the highest level l_5 , and, furthermore, l_3 shall be the average of the intermediate levels l_2 and l_4 . The form of the coding operation can be expressed as

$$\text{coded value} = \frac{\text{actual value} - l_3}{C}$$

where C is half the distance from l_2 to l_4 . With this coding of the factors each *run* (2.8) of a central composite design can be identified as either a *factorial point* (2.9), a *centre point* (2.10), or an *star point* (2.11). This is the coding used in textbooks for discussing central composite designs.

Note 5 to entry: An alternative coding is sometimes applied in the computations in software programs. The form of the coding operation can be expressed as

$$\text{coded value} = \frac{\text{actual value} - l_3}{M}$$

where M is half the distance from the lowest level l_1 to the highest level l_5 . This coding will be referred to as *software coding* in this Technical Report.

Note 6 to entry: In the face-centred CCD, only three levels of each factor are needed, so $l_1 = l_2 < l_3 < l_4 = l_5$, and l_3 shall be the average of the lowest level l_1 and the highest level l_5 . This design could be of interest if it is difficult to select five levels of the factors. For the face-centred CCD, the possible coded values of a factor are only -1, 0, 1. The face-centred CCD is not rotatable, see [2.18](#).

Note 7 to entry: A class of designs that can be used to fit second order models and only require three equidistant levels of each factor are Box-Behnken designs. Box-Behnken designs are not central composite designs and are therefore not treated in this Technical Report. But they may be a useful alternative, if only three equidistant levels of each factor can be used, see References [\[5\]](#), [\[2\]](#) and [\[7\]](#).

2.8

run

experimental treatment

<design of experiments> specific settings of every *factor* ([2.5](#)) used on a particular *experimental unit* ([2.15](#))

Note 1 to entry: Ultimately, the impact of the factors will be captured through their representation in the *predictor variables* ([2.3](#)) and the extent to which the model matches the outcome of the *experiment* ([2.1](#)).

EXAMPLE Consider a chemical process *experiment* ([2.1](#)) in which a high yield is the objective and the predictor variables are temperature, duration, and concentration of a catalyst. A run could be a setting of temperature of 350 °C, 30 min duration and 10 % concentration of the catalyst, assuming that all of these settings are possible and permissible.

Note 2 to entry: Adapted from ISO 3534-3:2013, definition 3.1.13.

2.9

factorial point

factorial run

cube point

cube run

vector of factor level settings of the form $(a_1, a_2, \dots, a_k)$, where each a_i equals -1 or +1 as a notation for the coded levels of the factors

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.37. (The notes are not reproduced here.)

2.10

centre point

centre run

vector of factor level settings of the form $(a_1, a_2, \dots, a_k)$, where all a_i equal 0, as notation for the coded levels of the factors

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.38. (The notes are not reproduced here.)

2.11
star point
axial point
star run
axial run

vector of *factor level* (2.7) settings of the form $(a_1, a_2, \dots, a_k)$, where one a_i equals α or $-\alpha$ and the other a_i 's equal 0, as notation for the coded levels of the *factors* (2.6)

Note 1 to entry: For a k factor experiment, this process yields $2k$ -star points of the form: $(\pm\alpha, 0, \dots, 0)$, $(0, \pm\alpha, 0, \dots, 0)$, ..., $(0, 0, \dots, \pm\alpha)$.

Note 2 to entry: Star points are added to the design in order to estimate a quadratic response surface.

Note 3 to entry: Special values of α give a nice geometric structure. For a k factor experiment, if $\alpha = \sqrt{k}$ then the factorial points and the star points are all on the sphere with radius $\sqrt{k}$. This design is therefore called a spherical CCD. If $\alpha = 1$, the star points are on the faces of the unit cube and the design is a face-centred CCD.

2.12
residual error
error term

random variable representing the difference between the *response variable* (2.3) and its prediction based on an assumed *model* (2.4)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.6. (The notes are not reproduced here.)

2.13
pure random error
pure error

part of the residual error (2.12) associated with replicated observations

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.9. (The notes are not reproduced here.)

2.14
misspecification error

part of the *residual error* (2.12) not accounted for by *pure random error* (2.13)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.9. (The notes are not reproduced here.)

2.15
experimental unit

<design of experiments> basic unit of the experimental material

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.24. (The notes are not reproduced here.)

2.16
designed experiment

experiment (2.1) with an explicit objective and structure of implementation

Note 1 to entry: The purpose of a properly designed experiment is to provide the most efficient and economical method of reaching valid and relevant conclusions from the experiment.

Note 2 to entry: Associated with a designed experiment is an *experimental design* (2.17) that includes the *response variable* (2.2) or variables and the *experimental treatments* (2.8) with prescribed *factor levels* (2.6). A class of models that relates the response variable to the predictor variables could also be envisaged.

Note 3 to entry: Adapted from ISO 3534-3:2013, definition 3.1.27.

2.17
experimental design

assignment of *experimental treatments* (2.7) to each *experimental unit* (2.15)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.28. (The notes are not reproduced here.)

2.18

rotatability

characteristic of a *designed experiment* (2.16) for which the *response variable* (2.2) that is predicted from a fitted *model* (2.4) has the same variance at all equal distances from the centre of the design

Note 1 to entry: A design is rotatable if the variance of the predicted response at any point $\mathbf{x}$ depends only on the distance of $\mathbf{x}$ from the *centre point* (2.10). A design with this property can be rotated around its centre point without changing the prediction variance at $\mathbf{x}$.

Note 2 to entry: Rotatability is a desirable property for *response surface designs* (2.25).

Note 3 to entry: Rotatability of a central composite design is obtained setting α equal to the fourth root of the number of factorial points, i.e

$$\alpha = (n_F)^{1/4}$$

where n_F denotes the number of factorial points in a CCD.

Note 4 to entry: The definition and notes 1 and 2 are adapted from ISO 3534-3:2013, definition 3.1.40.

2.19

interaction

influence of one *factor* (2.6) on one or more other factors' impact on the *response variable* (2.2)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.17. (The notes are not reproduced here.)

2.20

factorial experiment

designed experiment (2.16) with one or more *factors* (2.5) and with at least two levels applied for one of the factors

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.2.1. (The notes are not reproduced here.)

2.21

full factorial experiment

factorial experiment (2.12) consisting of all possible combinations of the levels of the *factors* (2.6)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.2.2. (The notes are not reproduced here.)

2.22

fractional factorial experiment

factorial experiment (2.12) consisting of a subset of the *full factorial experiment* (2.21)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.2.3. (The notes are not reproduced here.)

2.23

randomization

process used to assign treatments to experimental units so that each experimental unit has an equal chance of being assigned a particular treatment

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.26. (The notes are not reproduced here.)

2.24

replication

performance of an experiment more than once for a given set of predictor variables

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.35. (The notes are not reproduced here.)

2.25

response surface design

designed experiment (2.16) that identifies a subset of *factors* (2.5) to be optimized

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.2.19. (The notes are not reproduced here.)

2.26

analysis of variance

ANOVA

technique which subdivides the total variation of a *response variable* (2.2) into components associated with defined sources of variation

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.3.8. (The notes are not reproduced here.)

3 Symbols and abbreviated terms

3.1 Symbols

y	Response variable
$\hat{y}$	Predicted response variable
$\hat{y}_S$	Predicted response variable at the stationary point
$\mathbf{x}_S$	Stationary point of fitted response surface
D_S	Distance of stationary point to the design centre
A, B, C, D	Factors
k	Number of factors
2^k	Number of runs in a full factorial experiment with k factors all having two levels
2^{k-p}	Number of runs in a fractional factorial experiment with k factors and fraction 2^{-p}
n_F	Number of factorial points in a CCD
n_S	Number of star points in a CCD
n_0	Number of centre points in a CCD
a_i, b_i, l_i	Levels of factors
+1, -1	High and low coded factorial levels
$-\alpha, \alpha$	Axial levels of coded factors
σ	Standard deviation

3.2 Abbreviated terms

ANOVA	analysis of variance
CCD	central composite design
DOE	design of experiments

RSM response surface methodology
R&R repeatability and reproducibility

4 Generic descriptions of central composite designs

4.1 Overview of the structure of the examples in [Annexes A to D](#)

This Technical Report provides general guidelines on the design, conduct and analysis of central composite designs consisting of a specified number of two-level factors, and illustrates the steps with four distinct applications given in the annexes. Each of the four examples in [Annexes A through D](#) follows the basic structure as given in [Table 1](#).

Table 1 — Basic steps in CCD design

1	Overall objective(s) of experiment
2	Description of the response variable(s)
3	Identification of factors affecting the response(s)
4	Selection of levels for each factor
5	Identification of measurement systems
6	Layout plan of the CCD (depending upon which main effects and two factor interactions are to be studied) with “randomization” principle (if these are physical runs)
7	Analyse the results – numerical summaries and graphical displays
8	Present the results
9	Perform confirmation run

4.2 Overall objective(s) of a response surface experiment

Experiments may be conducted for a variety of reasons. Therefore, the primary objective(s) for the experiment should be clearly stated and agreed to by all parties involved in the design, conduct, analysis and implications of the experimental effort.

The main goal of response surface experiments is to create a model of the relationship between the factors and the response in order to explore optimum operating conditions. This involves choosing a design which allows the fitting of a quadratic function as the systematic part of the model. The Central Composite Design (CCD) can achieve this and this design has been popular since its introduction in the first paper on response surface methods in 1951.^[1]

Although the fundamental method for fitting first order (linear) or second order (quadratic) function of the predictor variables to the response is regression, the focus is not on the individual regression coefficients but on the regression function, the response surface, as a whole. This emphasis is reflected in the name Response Surface Methodology. Strong arguments in favour of this approach are given on pages 508-509 of Reference [\[2\]](#).

Typically, the primary goal for the experiment is to find optimal operating conditions based on the estimated response surface, this could involve doing several experiments, using the results of one experiment to provide direction for what to do next. This next action could be to focus the experiment around a different set of conditions, or to collect more data in the current experimental region in order to fit a higher-order model or confirm what seemed to be the conclusion.

The CCD is an appropriate name because three types of design points can be identified after a coding of the factor levels: centre points ([2.10](#)), factorial points ([2.9](#)) and star points ([2.11](#)), and those design points are indeed centred at the origin of the design space after the coding of the factor levels ([2.7](#)).

Response surface experiments traditionally involve a small number of continuous factors. Some software packages have an upper limit of 8 factors. Response surface experiments are typically used when the investigators already know which factors are important. One way to obtain this knowledge is to apply a screening experiment, for example a fractional factorial experiment as explained in ISO/TR 12845.^[11]

4.3 Description of the response variable(s)

Associated with the objective of an experiment is a continuous outcome or performance measure. A response of interest could involve maximization (larger is better), minimization (smaller is better) or meet a target value (be close to a specified value), but, in all cases, that task is one of optimization.

The response variable (denoted by the variable y) should be closely related to the objective of the experiment. For some situations, there are more than one variable of interest to be considered, although, typically, only a primary response variable will be associated with the experiment. In other cases, multiple responses should be considered. In case of multiple responses, the approach taken in response surface methodology is to analyse and optimize each response separately. The fitted response surfaces will then be studied to find settings that meet the requirements of all the responses. The example in [Annex C](#) has three responses.

4.4 Identification of measurement systems

Assessment of repeatability and reproducibility of the measurement systems for factors and responses should be done prior to designing the experiment.

4.5 Identification of factors affecting the response(s)

Response surface experiments are usually not done in isolation. They rely on prior knowledge concerning important influential variables on the selected response. If this knowledge is not available, it is necessary to conduct a different type of experiment to identify the factors affecting the response.

During the final selection of factors, attention shall be paid to the ability to set the levels of each individual factor independently of the other factors.

4.6 Selection of levels for each factor

There are two aspects to the selection of factors. One is selecting the *experimental region* which is the multidimensional range of interest for the factors selected. The other is the exact selection of the factor levels in such a way that the design has desirable properties. The first one requires subject matter knowledge as to the impact of factors on the response. The second one is more straightforward once the factors and the type of design to be used are known. The second one is further discussed in this Clause.

The response surface methods considered in this Technical Report are about the second order centre models using the CCD. The CCD is an augmentation of 2^k factorial experiments (or 2^{k-p} fractional factorial experiments). In addition to the two factorial levels that are used in the (fractional) factorial experiments, the user selects three additional levels, one centre level which is the average of the two factorial levels, and two extreme levels which are chosen symmetrically around the centre level and typically outside the range of the two factorial levels.

When the experimenter selects the levels of each factor he will be thinking in terms of the operational levels of a factor, the exact setting of a temperature, for example. But when studying the properties of the design and also when analysing the data from the design coded levels of the design are used.

If the actual (or operational) levels are $l_1 < l_2 < l_3 < l_4 < l_5$ then the middle level l_3 shall be the average of the lowest level l_1 and the highest level l_5 , and, furthermore, l_3 shall be the average of the intermediate levels l_2 and l_4 . The form of the coding operation can be expressed as Formula (1):

$$\text{coded value} = \frac{\text{actual value} - l_3}{C} \quad (1)$$

where C is half the distance from l_2 to l_4 . The coded value of the upper extreme level, l_5 , will be denoted by α , and the coded value of the lower extreme level, l_1 , will be denoted by $-\alpha$. It is very important to note that the value of α is the same for all the factors of the design. Thus, the coded levels of all the factors are $(-\alpha, -1, 0, 1, +\alpha)$.

An alternative coding is sometimes applied in the computations in software programs. The form of the coding operation can be expressed as Formula (2):

$$\text{coded value} = \frac{\text{original value} - l_3}{M} \quad (2)$$

where M is half the distance from the lowest level l_1 to the highest level l_5 , or, equivalently, the distance from l_3 to l_5 . This coding will be referred to as *software coding* in this Technical Report.

When the levels of the factors have been chosen, the levels of the individual factors have to be combined to define the runs of the experiment. A CCD has three types of experimental runs: factorial, centre and axial ones.

4.6.1 Factorial runs

A factorial run is a setting of all k factors to coded levels either -1 or $+1$. The factorial runs are the runs used in 2^{k-p} fractional factorial experiments or 2^k factorial experiments.

Written as a k -dimensional vector in coded levels, the factorial run has the form $(\pm 1, \pm 1, \dots, \pm 1, \dots, \pm 1)$. Considered as points in k -dimensional space, the factorial runs are the vertices of a cube and the factorial runs are for this reason also called cube points.

There are 2^k different factorial runs with k factors.

4.6.2 Star runs

The star runs are those where one of the factors has its coded levels either $-\alpha$ or α and the remaining factors are at their coded level 0.

Written as a k -dimensional vector in coded levels, the star run has the form $(0, 0, \dots, \pm\alpha, \dots, 0)$, having $-\alpha$ or α on the i^{th} position and 0 on all other positions.

Viewed as points in k -dimensional space, the star runs are located on the coordinate axes, and for this reason, the star runs are also called axial runs.

There are 2^k different star runs with k factors.

4.6.3 Centre run

The centre run is the one where all the factors are on their coded level 0. Written as a k -dimensional vector, it is the point $(0, 0, \dots, 0)$.

There is only one centre run but the centre run may be replicated in a CCD. One reason for replicating the centre point is to get an estimate of pure error which can be used to check the fit of the model.

4.7 Layout plan of the CCD with randomization principle

In a report, the full description of the design and the observed responses should be given. In addition to reporting the levels of the factors, as described in 4.6, this includes reporting the following:

- the number of replications of the three types of design points;
- the number of blocks;
- the randomization.

If the design has only a few factors, a table where each run is represented as a row is useful for this purpose. It is easier to grasp the design if coded levels are used. The randomization can be explained by including a column giving the order in which the runs have been performed. If blocking is applied, a column can similarly be added to explain the allocation of runs to blocks.

As an illustration, Table 3 provides a basic layout of a CCD for 2 factors with full factorial design in *serial order*. While there is a standard order for factorial designs there is no such thing for a CCD, so the term *serial order* is used for a way to write the runs in a CCD in such a way that the design is easily recognized. The serial order used in Table 3 and throughout this Technical Report lists the factorial runs in standard order, first, followed by the star runs and, finally, the centre runs. Each row of the table represents one set of experimental conditions that when run will produce a value of the response variable y . The two factors are designated as A and B. In this case, only one response variable is shown, but more columns should be added if more than one response variable is studied. In this case, it is readily seen that the design has five centre runs replicated. The last column shows the *run order*, i.e. the order in which the experimental conditions have been applied. This experiment has been performed in one block.

Table 3 — Layout of a generic Central Composite Design

Serial order	A	B	y	Run order
1	-1	-1	y_1	6
2	1	-1	y_2	4
3	-1	1	y_3	13
4	1	1	y_4	7
5	-1,41	0	y_5	12
6	1,41	0	y_6	8
7	0	-1,41	y_7	9
8	0	1,41	y_8	5
9	0	0	y_9	2
10	0	0	y_{10}	10
11	0	0	y_{11}	1
12	0	0	y_{12}	11
13	0	0	y_{13}	3

4.8 Analyse the results — Numerical summaries and graphical displays

The second order model that can be fitted with the data from a CCD is a regression model and the usual output and graphs from a regression analysis are reported. This includes the table of estimated regression coefficients and associated t-statistics and p -values. A special feature of RSM regression is ANOVA tables that exploit the structure of the model.

For the design in Table 3, one such ANOVA table is shown in Table 4.

Table 4 — ANOVA table for Central Composite Design

Response: y					
	Df	Sum Sq	Mean Sq	F-value	Pr(>F)
FO(x1, x2)	2	ddd,dd	ddd,dd	ddd,dd	d,dd
TWI(x1, x2)	1	ddd,dd	ddd,dd	ddd,dd	d,dd
PQ(x1, x2)	2	ddd,dd	ddd,dd	ddd,dd	d,dd
Residuals	7	ddd,dd	ddd,dd		
Lack of fit	3	ddd,dd	ddd,dd	ddd,dd	d,dd
Pure error	4	ddd,dd	ddd,dd		

[Table 4](#) is given by most, if not all, statistical packages for RSM analysis. The names of the rows and the columns may differ between statistical packages, but they are easily understood. Here, FO, TWI and PQ are short for First Order, Two Way Interaction and Pure Quadratic. Examples are given in [Tables A.5](#), [B.6](#) to [B.7](#), and [D.5](#).

In this case, there is no data, so the table is filled in with ddd,dd or d,dd except for the degrees of freedom which are the correct ones for the design in [Table 3](#). The four F-tests are of interest. Read from the bottom of the table, the first one is the ratio of the mean squares for Lack of fit and Pure error and is a check of the fit of the model. The second F-test is in the PQ line and it tests the need for pure quadratic terms in the model; in this case the hypothesis that $\beta_{11} = \beta_{22} = 0$. It is the ratio of the mean square in the PQ line to the mean square in the Residuals line of the table.

Another ANOVA table of potential interest tests for each predictor variable, the hypotheses that it is not needed in the model. For the example with two predictor variables in [Table 3](#), this ANOVA table has two F-tests: One for the hypothesis that $\beta_1 = \beta_{12} = \beta_{11} = 0$, and one for the hypothesis that $\beta_2 = \beta_{12} = \beta_{22} = 0$. Note that β_1 , β_{12} , and β_{11} , for example, are the coefficients of all the terms in the model that involve x_1 . Examples can be found in [Tables B.5](#) and [C.7](#).

When looking at analyses of response surface experiments using different software, it is possible to identify two different approaches. One approach uses all the tools of regression analysis to find a model where only significant terms are included in the estimated systematic part of the model. The other approach focuses on the response surface and only tests the hypotheses described in the two clauses above, i.e. tests whether a linear model can be used instead of a quadratic model or tests whether a factor can be considered to be essentially inert. In this Technical Report, the second approach is taken and therefore individual non-significant terms are not removed from the model. Strong arguments in favour of the second approach are given on pages 508-509 in Reference [2].

4.9 Present the results

Of course, one presentation of the result of the analysis is to give the estimated systematic part of the model. Although the systematic part of the model is indispensable for calculating the predicted response for various settings, it is not very useful for understanding the nature of the response surface. In [Annex E](#), four second order polynomials in two variables are given in Formulae (E.3), (E.4), (E.5) and (E.6). The four polynomials look very similar. They have the same distribution of signs among the coefficients and the coefficients are very similar. But the perspective and contour plots in [Figures E.1](#) to [E.4](#) show that the polynomials represent four very different response surfaces.

For two and three predictor variables, it is possible to get an understanding of the response surface from contour plots, but a more formal analysis called *canonical analysis* is always useful, because it gives a precise characterization of the surface that gives an understanding of the response surface even when the number of predictor variables is larger than 3.

Canonical analysis is a method of rewriting a fitted quadratic function of the predictor variables in a form which can be more easily understood. This is achieved by a rotation of the coordinate axes which removes all cross-product terms. This may be followed by a change of origin to remove first order terms as well. Details are given in [E.3](#).

Software packages for response surface methodology report the result of the canonical analysis. The result has the following parts:

- stationary point and predicted value at stationary point of the response surface;
- eigenvalues;
- eigenvectors.

The stationary point is the point where the fitted response surface has a maximum, a minimum or a saddle point, and the eigenvalues tell exactly which one is the case. Associated with each eigenvalue is an eigenvector. Moving away from the stationary point in the positive or negative direction of the eigenvector the response will decrease if the eigenvalue is negative, and it will increase if the eigenvalue is positive, so

- if all the eigenvalues are negative, the stationary point is a maximum,
- if all the eigenvalues are positive, the stationary point is a minimum, and
- if some eigenvalues are negative and some are positive, the stationary point is a saddle point or a minimax.

The situation is further complicated by the fact that one can only hope to approximate the response by the fitted second order model in the experimental region, so it should also be considered whether the stationary point is inside or outside the experimental region.

The situation is only simple, if the object is to maximize the response and if the stationary point is a maximum located inside the experimental region, or, alternatively, if the object is to minimize the response and if the stationary point is a minimum located inside the experimental region, and then the optimal settings is the stationary point. In all other cases, the optimal settings need to be found towards the boundary of the experimental region. The proprietary software packages provide a variety of tool for this purpose.

4.10 Perform confirmation run

After determining the optimal combination of levels of the factors and predicting the value of response variable for these factor levels, it is recommended that the user performs confirmation runs at the chosen setting to check whether the new observations confirm the predictions of the experiment.

If the computer output gives the standard deviation (std.dev) of a single observation and the standard error (std.err) of the predicted value at the optimum, then the following formulas apply for

- a 95% confidence interval for the mean at the optimum: $\hat{y} \pm t_{0,975}(v) \cdot \text{std.err}$ and
- a 95% prediction interval for a new observation at the optimum: $\hat{y} \pm t_{0,975}(v) \cdot \sqrt{\text{std.dev}^2 + \text{std.err}^2}$.

Here, v denotes the degrees of freedom for error.

The 95 % prediction interval is particularly useful for it explains what can be expected from future observations; if the model is good, 95 % of the observations will fall inside the 95 % prediction interval.

5 Description of [Annexes A through D](#)

5.1 Comparing and contrasting the examples

Four distinct examples of response surface designs are illustrated in [Annexes A to D](#). Each of these examples follows the same general template as given in [Table 1](#).

5.2 Experiment summaries

[Table 5](#) summarizes the four examples detailed in the annexes and indicates aspects of the analyses which were unique to each experiment.

Table 5 — Experiment summaries

Annex	Experiment	Problem-specific aspects	Software used for analysis
A	Yield of a crop	Repetitions; important 2-factor interaction; con- tour plots	Minitab® 17 ^a
B	Button tactility	Centre points; curvature in response	SAS® 9.4 ^a
C	Semiconductor die deposition	Curvature in response; face-centred central composite design; three re- sponses need to be optimized; trade- off between three responses	JMP® 10 ^a
D	Palladium-copper catalysed C-C- bond formation	Replication; central composite design	destra®V11 ^a
^a This information is given for the convenience of users of this document and does not constitute and endorsement by ISO of these products. Equivalent products may be used if they can be shown to lead to the same results.			

Annex A (informative)

Effects of fertilizer ingredients on the yield of a crop¹⁾

A.1 Purpose of the experiment

An experiment was conducted to investigate the effects of three fertilizer ingredients on the yield of beans under field conditions. The fertilizer ingredients applied were nitrogen (N), phosphoric acid (P₂O₅) and potash (K₂O). The response of interest was the yield in kg per plot.

Response surface methodology is often thought of as a sequential experimentation process which begins with a screening to determine the active factors. However, in this case, the active ingredients in the composition of the fertilizer were well understood and the purpose of the experiment was simply to find an optimal combination of the three ingredients. For this purpose, and because the surface was expected to be quadratic, a central composite design (CCD) was chosen.

A.2 Response variable

Only one response variable was considered in this experiment: Yield of beans measured in kg per plot.

A.3 Predictor variables

The three fertilizer ingredients were the predictor variables in the experiment. It was decided that the feasible amounts of the three fertilizer ingredients were within the ranges:

- **N:** Nitrogen: 0,425 kg/plot to 2,833 kg/plot
- **P₂O₅:** Phosphoric Acid: 0,266 kg/plot to 1,326 kg/plot
- **K₂O:** Potash: 0,278 kg/plot to 1,900 kg/plot

Special attention was given to the extreme settings and the scientist was confident that all combinations of extreme settings of the variables were within the region of operability.

All variables were continuous in the sense that all values within the chosen ranges were possible settings of the variables.

A.4 Identification and estimation of measurement systems

The repeatability and reproducibility of the measurement system for the associated response and predictor variables was deemed adequate for the objectives of this experiment, so no further work was initiated.

A.5 Selection of the settings of the predictor variables in the design

A.5.1 General considerations

To decide on the settings of the predictor variables in this experiment the following considerations were made. First, it was decided that the extreme levels of all variables should be the endpoints of the

1) Source: Renu Gupta, Bureau of Indian Standards, India.

ranges above. Taking nitrogen as an example and using the notation of 4.6 where the actual levels are denoted by $l_1 < l_2 < l_3 < l_4 < l_5$ implies that the lowest level is $l_1 = 0,425$, the highest level is $l_5 = 2,833$, and the middle level is $l_3 = (l_1 + l_5) / 2 = 1,629$. In order to find the values of l_2 and l_4 , the value of α needs to be known. It was decided to use a rotatable design with $k = 3$ factors and 8 factorial points. By the formula in 2.18, Note 3, α is the fourth root of the number of factorial points, so $\alpha = 8^{1/4} = 1,682$. This means that $\alpha = 1,682$ is the distance in coded units from the middle level to the highest level,

$$\frac{l_5 - l_3}{C} = 1,682 \text{ or } C = \frac{l_5 - l_3}{1,682} = 0,716 \quad (\text{A.1})$$

Now, the actual cube levels l_2 and l_4 are found as

$$l_2 = l_3 - C = 1,629 - 0,716 = 0,913 \text{ and } l_4 = l_3 + C = 1,629 + 0,716 = 2,345 \quad (\text{A.2})$$

Similar calculations were used on phosphoric acid and potash with the results given in Table A.1.

Table A.1 — Coded and actual levels of the experimental factors. Coded levels are in the top row and actual levels are in the following rows. The actual levels of all variables are kg/plot.

Coded levels	-1,682	-1,000	0,000	+1,000	+1,682
N	0,425	0,913	1,629	2,345	2,833
P ₂ O ₅	0,266	0,481	0,796	1,111	1,326
K ₂ O	0,278	0,607	1,089	1,571	1,900

Coded values of N, P₂O₅ and K₂O are denoted by x_1 , x_2 and x_3 respectively, and the conversions from the actual levels given in Table A.1 to the coded levels are given as

$$\begin{aligned} x_1 &= \frac{N - 1,629}{0,716}, \\ x_2 &= \frac{P_2O_5 - 0,796}{0,315}, \\ x_3 &= \frac{K_2O - 1,089}{0,482}. \end{aligned} \quad (\text{A.3})$$

In a CCD, the settings or levels of the predictor variables are of three types to be considered next.

A.5.2 Factorial levels

The factorial levels are coded as -1 and +1, so the factorial levels in actual or natural units are given in the two columns labelled -1,000 and +1,000, in Table A.1. Factorial levels of the predictor variables in this experiment are the following:

- N: 0,913 and 2,345 (coded as -1 and 1 respectively);
- P₂O₅: 0,481 and 1,111 (coded as -1 and 1 respectively);
- K₂O: 0,607 and 1,571 (coded as -1 and 1 respectively).

The factorial levels have been given their name because those levels are used to define a factorial design, which is an important building block in a CCD. The factorial design is typically a full two-level factorial design or a fractional two-level design if the number of factors is large.

A.5.3 Axial levels

These are the extreme values for the predictor variables, so the axial levels in actual or natural units are given in the two columns labelled -1,682 and +1,682, in [Table A.1](#). In this experiment, the axial levels are the following:

- **N**: 0,425 and 2,833 (coded as -1,682 and 1,682 respectively);
- **P_{2O₅}**: 0,266 and 1,326 (coded as -1,682 and 1,682 respectively);
- **K_{2O}**: 0,278 and 1,900 (coded as -1,682 and 1,682 respectively).

A.5.4 Centre levels

The centre levels are the average of the two factorial levels, or the average of the two axial levels. Its coded value is 0. In this experiment, the centre levels were the nominal values of the predictor variables. But this is not a requirement. The experimenter is free to choose the region of experimentation where the response surface is being investigated. In this experiment, the centre levels are the following:

- **N**: 1,629 (coded as 0);
- **P_{2O₅}**: 0,796 (coded as 0);
- **K_{2O}**: 1,089 (coded as 0).

A.6 Experimental design

A.6.1 General

The levels of the individual predictor variables defined in [A.5](#) are combined to define the runs of the experiment. The three types of runs in the CCD are the factorial, the star (or axial) and the centre runs.

A.6.2 Factorial runs

In the factorial runs, all predictor variables are at their factorial levels. The factorial runs usually constitute a full factorial or a fractional factorial design. In this experiment, a full factorial design was chosen, so the number of factorial runs was $2^k = 2^3 = 8$. The factorial runs are given as serial numbers 1 to 8 in coded levels in [Table A.2](#).

A.6.3 Axial runs

In the axial runs, one of the predictor variables is at its upper or lower extreme level and the rest of the predictor variables are at their centre value. The total number of axial runs in the experiment was $2k = 2 \times 3 = 6$. The axial runs are given as serial number 9 to 14 in coded levels in [Table A.2](#).

A.6.4 Centre runs

In the centre runs, all of the predictor variables are at their centre level. The centre runs were replicated six times in this experiment. The six centre runs are given as numbers 15 to 20 in the serial order in [Table A.2](#). This is an agricultural experiment where the experimental units are plots of land. The time order of the recording of the yields is not relevant in this case, and for this reason there is no run order given in [Table A.2](#). It is important to randomize allocation of treatments to plots, but the information of the randomization has not been made available.

Table A.2 — Experiment layout in coded levels

Serial order	x_1	x_2	x_3
1	-1	-1	-1
2	1	-1	-1
3	-1	1	-1
4	1	1	-1
5	-1	-1	1
6	1	-1	1
7	-1	1	1
8	1	1	1
9	-1,682	0	0
10	1,682	0	0
11	0	-1,682	0
12	0	1,682	0
13	0	0	-1,682
14	0	0	1,682
15	0	0	0
16	0	0	0
17	0	0	0
18	0	0	0
19	0	0	0
20	0	0	0

A.7 Data generated by the experiment

The response variable from the experiment is given in the last column in [Table A.3](#). The runs are given in coded levels in the first three columns and in actual levels in columns 4 to 6. The total amount of fertilizer applied is given in the seventh column and the yield is given in the last column.

Table A.3 — Data collected during the experiment. The Total Amount of Fertilizer is the row sum of N, P₂O₅ and K₂O columns.

x_1	x_2	x_3	N	P ₂ O ₅	K ₂ O	Total amount of fertilizer	Yield
-1	-1	-1	0,913	0,481	0,607	2,001	5,076
1	-1	-1	2,345	0,481	0,607	3,433	3,798
-1	1	-1	0,913	1,111	0,607	2,631	3,798
1	1	-1	2,345	1,111	0,607	4,063	3,469
-1	-1	1	0,913	0,481	1,571	2,965	4,023
1	-1	1	2,345	0,481	1,571	4,397	4,905
-1	1	1	0,913	1,111	1,571	3,595	5,287
1	1	1	2,345	1,111	1,571	5,027	4,963
-1,682	0	0	0,425	0,796	1,089	2,310	3,541
1,682	0	0	2,833	0,796	1,089	4,718	3,541
0	-1,682	0	1,629	0,266	1,089	2,984	5,436

Table A.3 (continued)

x_1	x_2	x_3	N	P ₂ O ₅	K ₂ O	Total amount of fertilizer	Yield
0	1,682	0	1,629	1,326	1,089	4,044	4,977
0	0	-1,682	1,629	0,796	0,278	2,703	3,591
0	0	1,682	1,629	0,796	1,900	4,325	4,693
0	0	0	1,629	0,796	1,089	3,514	4,563
0	0	0	1,629	0,796	1,089	3,514	4,599
0	0	0	1,629	0,796	1,089	3,514	4,599
0	0	0	1,629	0,796	1,089	3,514	4,275
0	0	0	1,629	0,796	1,089	3,514	5,188
0	0	0	1,629	0,796	1,089	3,514	4,959

A.8 Analysis of results

A.8.1 Software used for the analysis

Data acquired through the experiment are analysed using Minitab® 17.²⁾

A.8.2 Transfer function

The analysis was performed using the software coded versions of the predictor variables, but the estimated transfer function (the estimated systematic part of the model) for Yield of a crop (in kg) is more useful when expressed in the actual or natural units. The estimated transfer function in natural units in [Table A.4](#) is taken from the Minitab® 17²⁾ output.

Table A.4 — Estimated transfer function in actual units

Yield = 6,08 + 1,559 N - 6,01 P ₂ O ₅ - 0,90 K ₂ O - 0,739 N*N + 2,116 P ₂ O ₅ *P ₂ O ₅ - 0,715 K ₂ O*K ₂ O - 0,142 N*P ₂ O ₅ + 0,784 N*K ₂ O + 2,411 P ₂ O ₅ *K ₂ O
--

A.8.3 Estimation of coefficients

The result of the estimation is displayed in [Table A.5](#) using software coded units.

As explained in the last paragraph of [4.8](#), the approach to analysis adopted in this Technical Report is the one recommended by Box et al. on pages 508-509 in Reference [2]. Thus, it is not recommended to inspect the individual regression coefficients and trying to interpret whether some of the coefficients might fail to be significantly different from 0. The point is that a second order surface is being fitted and the least squares estimate of the fitted surface has the coefficients in the “Estimated Regression Coefficients for Yield” part of [Table A.4](#) or [Table A.5](#) depending on the coding of the predictor variables used.

Table A.5 — Estimated regressions coefficients and CCD ANOVA table using software coded levels

Estimated regression coefficients for yield				
Term	Coef	SE Coef	T	P
Constant	4,692 60	0,145 4	32,282	0,000
N	-0,129 18	0,162 2	-0,796	0,444

2) This information is given for the convenience of users of this document and does not constitute an endorsement by ISO of these products. Equivalent products may be used if they can be shown to lead to the same results.

Table A.5 (continued)

P205	-0,130 21	0,162 2	-0,803	0,441		
K20	0,602 38	0,162 2	3,713	0,004		
N*N	-1,070 92	0,265 5	-4,033	0,002		
P205*P205	0,594 49	0,265 6	2,238	0,049		
K20*K20	-0,470 01	0,265 6	-1,770	0,107		
N*P205	-0,090 89	0,356 5	-0,255	0,804		
N*K20	0,765 69	0,356 5	2,148	0,057		
P205*K20	1,036 50	0,356 7	2,906	0,016		
S = 0,356 408 PRESS = 7,324 51						
R-Sq = 84,40 % R-Sq(pred) = 10,07 % R-Sq(adj) = 70,37 %						
Analysis of variance for yield						
Source	DF	Seq SS	Adj SS	Adj MS	F	P
Regression	9	6,874 26	6,874 26	0,763 81	6,01	0,005
Linear	3	1,913 51	1,913 51	0,637 84	5,02	0,022
Square	3	3,294 20	3,294 20	1,098 07	8,64	0,004
Interaction	3	1,666 54	1,666 54	0,555 51	4,37	0,033
Residual error	10	1,270 27	1,270 27	0,127 03		
Lack-of-Fit	5	0,745 30	0,745 30	0,149 06	1,42	0,355
Pure error	5	0,524 97	0,524 97	0,104 99		
Total	19	8,144 53				

While it is inappropriate to change the values of individual estimated regression coefficients, it does make sense to look for model simplification where one answers questions like the following:

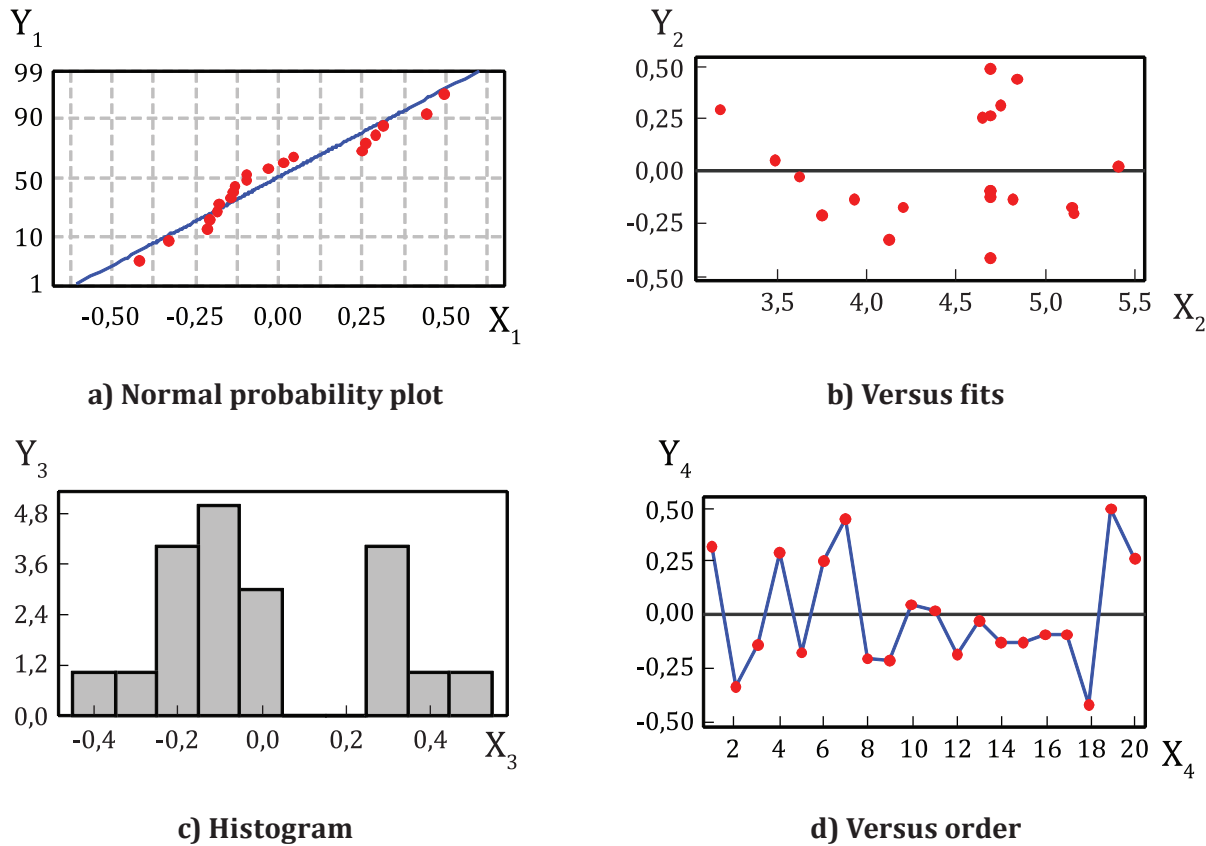
- Are the pure quadratic terms needed in the model?
- Is a first order model satisfactory?

This is where the “Analysis of Variance for Yield” part of [Table A.5](#) is useful. Read from the bottom of the table, the first F-test of interest is the ratio of the mean squares for Lack-of-Fit and Pure Error which comes from the replication of the centre points and is a check of the fit of the model. In this case, the p -value is 0,355 and the model is not questioned. The second F-test is in the Square line and it tests the need for pure quadratic terms in the model; in this case, the hypothesis that $\beta_{11} = \beta_{22} = \beta_{33} = 0$. It is the ratio of the mean square in the Square line to the mean square in the Residual Error line of the table. The p -value is 0,004 and the hypothesis is strongly rejected, so quadratic terms are needed in the model. The F-test in the Interaction line tests the hypothesis $\beta_{12} = \beta_{13} = \beta_{23} = 0$ and this hypothesis is also rejected and so is the hypothesis $\beta_1 = \beta_2 = \beta_3 = 0$ which is tested by the F-test in the Linear line.

A.8.4 Graph of residuals

[Figure A.1](#) shows some standard model checking plots based on the residuals that are produced by Minitab®. The observation order that is used in the plot of residuals against observation order is the serial order in [Table A.2](#). There is a strange pattern in this plot: large residuals in the factorial runs, small residuals in the axial runs and the first three centre runs, and finally large residuals in the final three centre runs. A plot of residuals against observation order is most useful if observations are made in a natural order, for example a time sequence. As mentioned in [A.6.4](#), the experiment is a field experiment so, no single one-dimensional plotting order is relevant. In this case the information about

how the plots were laid out in the field is not available, so the plot is not particularly relevant here but is kept as an illustration of a potentially useful plot.



Key	
X_1	residual
X_2	fitted value
X_3	residual
X_4	observation order
Y_1	percent
Y_2	residual
Y_3	frequency
Y_4	residual

Figure A.1 — Residual plots

A.9 Presentation of results — Optimization

A.9.1 General

Just looking at the transfer function (the estimated systematic part of the model), whether it is shown in actual units as in [A.8.2](#) or in coded units, does not reveal the properties of the response surface. It is important to realize that the second order polynomial in two or more variables can represent a variety of surfaces. The stationary point can be a maximum, a minimum or a saddle point. Furthermore, the stationary point can be located outside as well as inside the experimental region. The situation is only simple, if the object is to maximize the response and if the stationary point is a maximum located inside the experimental region, or, alternatively, if the object is to minimize the response and if the stationary point is a minimum located inside the experimental region, and then the optimal settings is the stationary point. In all other cases, the optimal settings need to be found towards the boundary of the experimental region. If the number of predictor variables is two or three, then, contour plots can be of help as illustrated in [A.8.3](#). Alternatively, numerical methods, such as the desirability function, can be used. An application of the desirability function is given in [A.9.2](#).