A Conceptual Approach to Determine Optimal Indoor Air Quality: A Mixture Experiment Method

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ABSTRACT

Achieving good air quality in large residential and commercial buildings continues to be a top priority for owners, designers, building managers and occupants. The challenge is even greater today. There are many new materials, furnishing, products and processes used in these buildings that are potential source of contaminations and pollutants.

A common problem to the indoor and outdoor environments is that of exposure to mixtures of air pollutants. Researchers and practitioners tend to focus on single pollutants (e.g. $CO_{2,}$ $PM_{2.5}$) ignoring the mixtures combined effect. Fashion dictates to study the pollutant most thoroughly talked about. Distinguishing the effects of such co-pollutants is difficult. The conclusions about which component of a mixture is actually producing a given effect are sometimes less soundly based than could be wished. It is especially important in considering the indoor mixture of air pollutants as this mixture may be entirely different from those found outside. Exposures to raised levels of air pollutants can damage health, for example carbon monoxide can cause death and significant lasting disability. Controlling levels of indoor air pollutants is therefore important, as good indoor air quality is essential to health.

There are three strategies for achieving acceptable indoor air quality: ventilation, source control and cleaning/filtration. Depending on the building and the specific characteristics of the location, these strategies can be used singly or in combination. However, *mixture experiment* would throw more light and understanding into indoor air composition and interaction properties and the combine effects it has on human health.

Mixture experiments have been used extensively in other industries, for example the pharmaceutical industry and the agrochemical industry, for the production of tablets and the control of plant diseases and pests. Developing a *mixture model* for the internal microclimate for a particular building type and/or location may help us in developing better indicators, standards and policy document in the near future, when the levels of pollutants concentration can be successfully predicted.

INTRODUCTION

Clean air is a basic requirement for human health and wellbeing. More work has been done to discover and control the effects of outdoor air pollution than indoor air pollution. In some ways, this is natural as great outdoor air pollution episodes claim lives. Indoor environment is also important. The indoor environment is important not only because of the amount of time spent inside buildings but also because there are some very important indoor sources of pollution; including, for example, heating and cooking appliances, open fires, building and insulation materials, furniture, glues, cleaning product, other consumer products, and various biological sources – for example, house dust mites, fungi, and bacteria. There is also the inflow of polluted outdoor air through windows, evaporation of substances from water, and, in some locations, infiltration of radon and other gases into the building from the underlying soil and bedrock.

Important chemical pollutants include combustion products such as nitrogen dioxide, fine particles, and carbon monoxide, formaldehyde from furnishing and furniture. Renovation, remodelling, and repair introduce volatile organic compounds and other toxic compounds from cleaners, paints, carpets, adhesives and flooring into the air system. Office supplies and equipment by hospital workers introduce toxic compounds into the air. Some of these pollutants pose a high risk to human health and wellbeing. Moreover, it is clear that exposure to high peak concentrations of pollutants is likely to be highly relevant for certain health end points; for nitrogen dioxide, for example, such exposure can occur where there is an indoor source – such as a gas cooker or an unflued kerosene heater. Also the drive over the past few decades to install energy efficiency in houses has tended to reduce ventilation rates and thus raise exposure to indoor pollutants (Harrison, 2002).

Seppanen et al. (2006) analysis studies on the effects of temperature on performance at work. They analyses studies that had used objective indicators of performance that are likely to be relevant in office work, such as text processing, simple calculations, length of telephone customer service time, and total handling time per customer for calling centre workers. The results show that performance increases with temperature of around 21-22^{0}C, and decreases with temperature above 23-24^{0}C. The highest productivity is at a temperature of about 22^{0}C (Seppanen, 2006).

Many other studies show that increased temperatures, reduced ventilation and poor air quality are linked to the prevalence of building-related SBS –symptoms experienced by occupants of the building (e.g. Mendell et al 2002; Seppanen et al 1999; Wargocki et al 2002; Wyon and Wargocki, 2006). SBS symptoms cause distraction from work and include such symptoms as headaches, difficulty to concentrate or think clearly. It is reasonable to expect that they also affect performance (Clements-Croome, 2005; Seppanen et al 2006). In spite of the researches that have been conducted thus far, there seems to be little data in the literature to develop quantitative relationship between SBS and any of the causative factors. The rest of the paper is as follows: characteristics of the indoor environment; mixture experiments; problem formulation; plan and analysis; worked example and finally discussion and conclusions.

CHARACTERISTICS OF INDOOR CLIMATE

Sick building syndrome (SBS) symptoms experienced by building occupants which may include irritation of eyes, nose, and skin, headache, fatigue and difficulty in breathing are related to the characteristics of the buildings and indoor environments or indoor climate. The symptoms improve when the occupant is away from the building and are not related to any known disease or exposure.

The indoor climate in the enclosed area is formed by appropriate characteristics, which can be classified into three distinct form; *condition* characteristics, *composition* characteristics and *aerodynamics* characteristics. These are shown in Table 1. A series of external and/or internal disturbances acts, having various directions and characters that will change without controlling the indoor climate characteristics. In other to keep the indoor climate characteristics within certain permissible deviation limits we need to respond by using *active* or *passive* system to condition the environment. In this paper we are concerned about conditioning the *composition* characteristics of the indoor space (i.e. the microclimate). The composition characteristics are more to do with the level of concentrations of substances in the indoor air that may be directly linked to SBS. They are in effect mixtures of various substances existing in the indoor air.

Table 1: Indoor Climate Characteristics (Anon, 2000)

Group Type	Group Characteristics	Individual Parts of the Group
1	Condition	• Air temperature • Humidity • Lighting
2	**Composition** (concentration levels)	• **Gases** • **Vapours** • **Dust** • **Odours** • **Radioactivity** • **Aerosol** • **Others**
3	Aerodynamics	• Noise • Vibrations • Air speed • Air flow through treated space flushing

Figure 1 is a schematic of a building interacting with its environment. The main emphasis of this schematic is that the volume of the indoor air is fixed in the interacting environment. We assume there is no change to the volume.

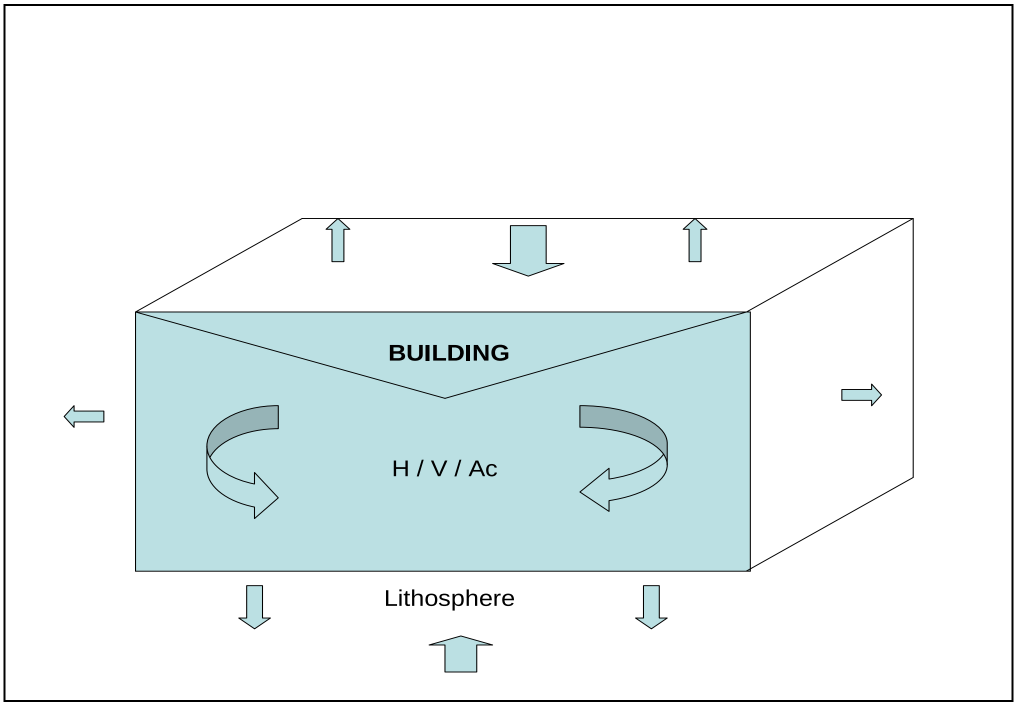

Figure 1: Interaction of building (fixed volume) with its environment

MIXTURE EXPERIMENTS

Many products are formed by mixing two or more ingredients together. Some examples are

1. *Cake formulations* using baking powder, shortening, flour, sugar, and water
2. *perfume formulation* formed by mixing different proportion of scents from varied products
3. *Building construction concrete* formed by mixing aggregates, sand, water and cement

In each case one or more properties of each product are generally of interest to the manufacturer of experimenter who is responsible for mixing the ingredients. For example, such property as the *hardness* or *compressive strength* of the concrete, where hardness is a function of the percentages of the cement, aggregates, and water in the mix. Another reason for mixing together ingredients in blending experiments is to see whether there exist blends of two or more ingredients that produce more desirable product properties than are obtainable with the single ingredients individually. Blending of a product - These are designs which involve factors, but factorial designs and analysis are inappropriate. This occurs when factors are combined to make up a whole which remains constant. These are known as mixture experiments (Cornell 2002).

Mixture experiment is an experiment in which the response (i.e. *occupants' response*) is assumed to depend only on the relative proportions of the ingredients present in the mixture and not on the amount of the mixture. In a mixture experiment then, if the total amount is held constant and the value of the response changes when changes are made in the relative proportions of those ingredients making up the mixture, then the behaviour of the response (e.g. *occupants' performance*) is said to be a measure of the joint blending property of the ingredients in the mixture.

A *factorial experiment* studies the effect of some observable quantity (the response) of varying two or more factors, such as temperature and source of raw material. A series of values or levels of each factor is chosen, and certain combinations of the levels of the factors are tested. In a complete factorial design, all combinations of the levels of all the factors are tested. The objective of a factorial experiment is to measure the change response when changing the level of each factor while holding the levels of the other factors fixed as well as when changing the levels of two or more factors simultaneously. Such changes in the response are called the main effects of the factors and interaction effects between the factors.

In the proposed *hypothetical* experiment we will model the effect of the proportions of three components (denoted by PM_{10}, CO, TVOC). Such experiments are known as mixture experiments (Cornell, 2002). In a mixture experiment, each proportion may vary between zero and one, and the components must sum to one. As a result, three components, as in our example, the experimental region is a triangle, defined by the points (0, 0, 1), (0, 1, 0) and (1, 0, 0). Traditionally, this region has been viewed in two dimensions as displayed in Figure 2 that employs a triangular simplex coordinate system. Each point lying on or in the interior of the triangle represents a possible mixture. The plot can be interpreted in the following way. Each vertex of the triangle represents a pure mixture (100% of one component and none of the rest). As one moves away from this vertex toward the opposite side, the proportion of the component gradually decreases to zero. Points interior to the triangle have some proportion of each of the three components. For example, the point shown by the black dot in Figure 2 corresponds to a mixture of xx% PM, yy% CO, and zz% TVOC. The project could be extended to include more components but that would increase complexity, especially in terms of the graphical displays (Cornell, 2002).

In this application the experimental region is further constrained because we know, before running the experiment that some combinations will not, or is not likely in the indoor environment for certain regions (i.e. location) and building types (i.e. levels of gaseous concentration).

For a mixture experiment, the standard linear first-order response model for a normally distributed response Y is

$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3$ -- (1)

Where

$X_1 + X_2 + X_3 = 1$ -- (2)

So:

$$Y = \beta_0 (X_1 + X_2 + X_{3)}) + \beta_1 X_1 + \beta_2 X2 + \beta_3 X_3 \quad \text{--------------------------------} \quad (3)$$

Y can represent any attribute of the indoor environment (e.g. excellent to bad-indoor air quality which are subjective measures) and/or the occupant response (e.g. severity of headache which are objective measures) that can be linked to the gaseous composition.

Mixture model polynomials is one way of modelling the response surface in the space of the constrained stimulus variables, so that:

- We can use the surface to predict responses for given combinations
- We can evaluate single and joint contributions of the individual components

We can then studying the effect of indoor exposure to the occupants by some of the behaviours the occupant is exhibiting, for example like SBS symptoms.

PROBLEM FORMULATION

We do not need to make the mixture as the different contaminants and pollutants as in the strict *mixture experiment*. The mixture has occurred naturally either *passively* or *actively* by conditioning of the indoor space (e.g. room) as shown in Figure 1. However, since the volume of our environment is fixed (e.g. room) we can take *samples* of the mixture to determine the different composition of the contaminants and pollutants levels within the environment.

The objective of the problem is to find the *optimal indoor quality*. *Optimum indoor air quality* is defined as the indoor air quality that will enhance an occupant's performance that will results in the occupants maximum productivity when the other conditions (e.g. temperature, humidity) are held constant. To do this we need to choose a target population, which is the conditions over which the various gases would interact with each other within the environment to give have an effect on the human response. We need to select an appropriate response variate and population attribute.

The choice of response and population attribute is tied to the definition of best or optimal indoor air quality, and has a big impact on an appropriate analysis of the subsequent experimental data. A possible extension of the basic is to use more than one response. This will lead to multiple analyses and possibly the need to compromise in some way when making recommendations. To assess this, we need to think ahead of the analysis stage. An appropriate choice depends on the analysis of the data.

PLAN OF THE EXPERIMENT

In the plan stage we must determine the details of the experiment and see how we can find the optimal solution as defined in the problem stage. More specifically, we need to select the experimental factors and levels, choose a specific building type, and then worry about what sort of measurement of the occupants response we want to measure and think about the logistics of the data collection.

A cause and effect diagram (Ishikawa, 1982) is a useful tool in the planning stage. To produce a cause and effect diagram a fishbone or Ishikawa diagram, we attempt to list possible important explanatory variates that may influence the response. This is typically done using a team of subject matter experts. An example of a possible cause and effect diagram is shown in Figure 2.

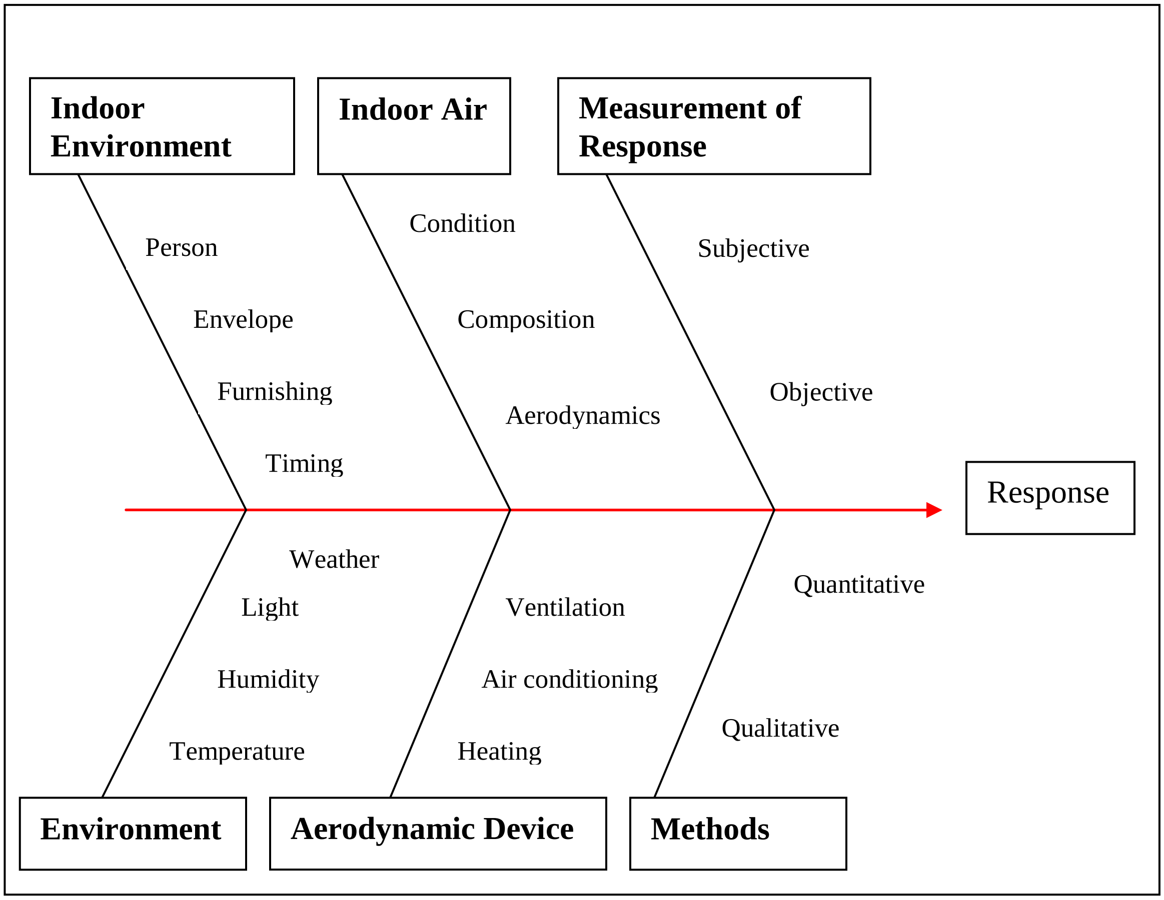

Figure 2: Indoor Air Quality Cause and Effect Diagram

In the example project (i.e. particular building type), one can deliberately vary the carpet type (i.e. particular form of furnishing) and furniture type in the experiment which emit some amount of the mixture components. By choosing different types the composition of the optimal indoor air will depend on the levels of concentration of these two noise factors.

Another option is to create blocks within which some explanatory variates are held fixed, and then replicate the design over a number of blocks. For instance, we could block by time by repeating the design over two (or more) different time frames (e.g. 1-hour measure, 8-hour measure for an office type building), if we thought there might be a large time effect. This helps achieve the goal of seeing the effect of changing the mixture components while at the same time allowing us to check that the results obtained under one set of conditions (one day) are also valid for other conditions (i.e. the second day).

WORKED EXAMPLE: HOSPITAL INDOOR AIR QUALITY

Nowadays, air pollutant from the outdoor and the import of organic synthetic material in building fabric and furniture, and the use of organic solvent in cleaning exercise) makes the indoor quality management more complex. This increases the number of indoor air quality parameters to be sampled during IAQ evaluation in buildings. As a result more instruments have to be used for a thorough investigation.

In this study the sampling exercises is chosen from three indicators described below. They are Carbon monoxide, TVOC and PM_{10} concentration. CO represents the incomplete combustion from internal and external sources and inorganic componuds; TVOC represents the emission from building materials and PM_{10} accounts on the adequacy of filtration and the degree of outdoor particulates to the building.

Carbon monoxide (CO) is a colourless, odourless gas that can be poisonous to humans. Ambient levels in the atmosphere are increased by both natural processes (volcanoes, fires) and human activities. These include incomplete combustion of fuels, especially vehicles, as well as industrial processes such as milling and foundries.

PM_{10} is a subset of the particular matter found in the air which includes both aerosols and larger particles, such as dust, ash fibre, and pollen, with particles ranging in diameter from 0.05 to 100µm. PM_{10} has been selected as the indicator of particulate contamination since this is the component which is greatest effect and is well established internationally as indicator. The adverse environmental effects of PM_{10} include acute and chronic effects on human health, nuisance effects such as deposition, and amenity effects, such as degradation of the visual clarity of air.

Total Volatile Organic Compounds (TVOC) is an indicator of the minimum response in the form of perceived unspecific stimulation of nerves caused by multi-component exposure of air pollutants at low levels. The value is calculated as the sum of concentration of all VOCs in the air measured.

Table 2: Concentration of indoor air pollutant in Hospital (Yoon Shin Kim *et al*, 2006)

Pollutants	**N**	**Mean**	**S.D.**	**Max.**	**Min.**
PM_{10} (/m^3)	40	60.135	36.06	180.9	10.600
$PM_{2.5}$(/m^3)	40	41.373	23.778	137.9	2.200
CO_2 (ppm)	40	729.121	176.865	989.000	405.00
CO (ppm)	40	.667	.612	2.900	.110
NO_2 (ppm)	40	.018	.007	.035	.003
O_3 (ppm)	40	.016	.016	.064	.001
Rn (pCi/L)	40	.428	.335	1.500	.100
TBC (CFU/ m^3)	40	142.982	121.257	452.460	2.000
Asbestos (f/cc)	40	.007	44.629	.020	.004
HCHO (/m^3)	40	63.954	44.6290	206.965	2.695
TVOCs (/m^3)	40	240.418	254.165	1078.85	21.750

Pollutants (PPM)	**Average**	**Minimum**	**Maximum**
PM_{10}	.0414	.0022	.1379
CO	.677	.1100	2.900
TVOC	.2400	.02175	1.07885
Total	**0.9584**	**.13395**	**4.11675**

Pollutants (PPM)	**Average**	**Minimum**	**Maximum**
PM_{10}	.04320	.01642	.03350
CO	.70638	.82120	.70444
TVOC	.25042	.16238	.26206
Total	**1**	**1**	**1**

Limitations

Frequently situations exist where some of the proportions xi are not allowed to vary 0 to 1.0. Instead, some, or possibly all, of the component proportions are restricted by either a lower bound and/ or an upper bound. In the case of component I, these constraints might be written as

$$0 < Li\ xi < Ui < 1.0 \qquad 1<I < q$$

Where Li, is the lower bound and Ui is the upper bound. In much of the experimental work involving multi-component mixtures, the emphasis is on studying the physical characteristics, such as the shape or the highest point, or the measured response surface.

The main considerations connected with exploration of the response surface over the simplex region are (1) the choice of a proper model to approximate the surface over the region of interest (2) the testing of the adequacy of the model in representing the response surface, and (3) a suitable design for collecting observations, fitting the model and for testing the adequate of fit.

Analysing CO_2 concentration response in a room makes it possible to assess the air exchange rate of the room. In practice two types of recording sequences can be analysed: the build-up and the decay of CO_2 concentrations. Requiring emissions testing from manufacturers study is time consuming and expensive. Numerous samples are required at several locations over an extended period of time. Numerous variables need to be considered and controlled in the building, or accounted for in the data analysis.

DISCUSSION AND CONCLUSIONS

If the objective is for optimum health; then the symptoms that are prevalent would be the response surface fit of the model which will link the attributes of the occupants to the objective function. If the objective function is for comfort/well-being of the occupant then the attribute will have to be linked to the level of comfort.

Although we have standards and regulations for each outdoor pollutant, however, they are based on the pollutant acting alone; we do not know the combined effects of these pollutants. Factorial analysis involving one or two variables was done in earlier studies, in which it was said that performance and productivity of the individual was enhanced. But now the opportunity for understanding the combine effect of the different pollutants in the environment is possible. The mixture method can actually encourage the conditioning of air coming to the enclosure to reflect those proportions of pollutant that will improve the performance of the occupants and also improve their productivity, without exceeding their recommended levels. However, what we must not forget is that such method depends on the effect of the control variables being fully understood. I believe some of these has already be done form the previous factorial methods. All what is required is to use such results as controlled variables when analysing within the mixture method.

This method can also be used in consultancy in the study of odours. In the BRE study, reported in the *2006 Healthy Building Conference* on obnoxious odour in the reception area of the hospital, more would have been done in terms of studying the interaction effects of the different odour contributing to the indoor environment. In the analysis of the data an experiment would have been carried out to determine the right proportion the different gases that are contributing to this smell. After all this is no different from the manufacturing of perfume that uses mixture experiment to come up with a blend that is a winner in the market, accept that instead of sweet smelling fragrance we are talking about sweet odour that is an irritant to occupants in the A&E reception area. The recommendations made would have been better and of more academic credentials.

Nobody knows exactly if MRSA prevalent in hospitals and other such diseases are due to the right conditions of the mixture of the different substances present. Simultaneous ventilation rate measurements are required to normalise chemical concentration measurements to the area/materials in the buildings. Besides the limited number of chemicals with unique sources, it is extremely difficult to pinpoint the source of the majority of chemicals. This can also be the first step in developing software tools for modelling air quality. Such tools can add to the suite of materials that the facilities management sections would be applying.

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Appendix A

X =

0.0615	0.6929	0.2456	0.0426	0.0151	0.1702
0.0432	0.7064	0.2504	0.0299	0.0108	0.1769
0.0335	0.7044	0.2621	0.0236	0.0088	0.1846
0.0525	0.7417	0.2058	0.0389	0.0108	0.1526
0.0482	0.6835	0.2683	0.0329	0.0129	0.1834
0.0395	0.7296	0.2309	0.0288	0.0091	0.1685

Y =

3
3
4
3
4
4

β =

1.0e+003 *

$$\left.\begin{array}{l} \beta_1 = -1.7963 \\ \beta_2 = 0.0238 \\ \beta_3 = 0.0198 \\ \beta_{12} = 1.5591 \\ \beta_{13} = 2.9622 \\ \beta_{23} = -0.1118 \end{array}\right\}$$

Equation of is $Y = -1.7963X_1 + 0.0238\ X_2 + 0.0198\ X_3 + 1.5591\ X_1X_2 + 0.0238\ X_1X_3 + 0.0238\ X_2X_3$