Some Small Response Surface Designs for Three-Factor Experiments

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Four readily available second-order small response surface designs for three-factor experiments were examined and compared in order to find an alternative design for experiments with limited resources. In this paper, the prediction variances of Roquermore's three-factor hybrid design and Draper-Lin's small composite design are investigated over the experimental region using box plot and fraction design space (FDS) plot. For each spherical region, the replication of center and axial points were compared. The Box plot and Fraction Design Space plot shows that increasing the number of center and axial points will decrease the standard error of D311B, yield a more stable prediction variance and consequently, decrease the spread of dispersion of the prediction variance. These results suggest that D311B was more efficient and is preferred for three-factor experiments with inadequate resources.

INTRODCUTION

In scientific and engineering experiments, scientists and engineers want to investigate the relationship between the input or process variables and the response variable. This investigation includes finding the factor settings that will produce the optimum response. This could imply, for example, minimization of the cost of operation of a production process, minimization of the variability of a quality characteristics, maximization of the yield in a chemical process, or to achieve desired specifications for a response variables (del Castillo, 2007). In mathematical perspective, it will try to model a relationship between the quantitative process variables and the response variables.

In response surface methodology (RSM), finding a relationship between the quantitative process variables ($x_1, x_2, \ldots, x_k$) and the response variable (y), requires N- experimental runs to obtain the data and these are fitted into a second-order response surface model,

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i<j}\sum \beta_{ij} x_i x_j \,, \tag{1}$$

which is more widely used and more useful in finding the optimum conditions. Equation (1) can take varieties of response surfaces and the precision of plotting these surfaces are dependent on the standard error of the predicted response. The standard error of the predicted response at any point in the design space is dependent on the experimental error, the choice of experimental design, and the location of points in the design space. The experimental error is expressed as the standard deviation and the experimental design refers to the number of experimental runs and the scaled levels of the process variables. Therefore, it is necessary to choose an experimental design which will yield a prediction equation that will minimize the error of an estimated response anywhere inside the selected region of experimentation.

The Box-Behnken Designs (BBD) and Central Composite Designs (CCD) are the most popular class of second-order designs. The popularity of these two designs is based from the properties mentioned by Box and Draper (1959) and Myers and Montgomery (2002). Despite of the importance of BBD and CCD, there are instances in which the researchers, particularly from the industries, cannot afford the required number of experimental runs due to the limited resources such as time, operating costs and labor. Therefore, choosing an alternative design with fewer experimental runs that is close to, but not less than $1 + 2k + k(k\text{-}1)/2$ with excellent prediction efficiency is crucial. Designs with fewer runs that is almost close and not lesser than $1 + 2k + k(k\text{-}1)/2$ are called near saturated designs and should not be used unless cost prohibits the use of one of the standard designs (Myers and Montgomery, 2002).

Roquemore (1976) and Draper-Lin (1990) have developed a class of saturated experimental designs which resembled the central composite designs. The purpose of creating their designs is to come up with an alternative design with fewer experimental runs but still have the same characteristics with CCD. For three factors, these designs are competitive in terms of the number of experimental runs. Block and Mee (2001) recommend the comparison of the prediction performance of Roquemore's hybrid designs and Draper-Lin's small composite designs for three factor experiment. Thus, this will be the focus of the study.

RESPONSE SURFACE DESIGN EVALUATION AND COMPARISON

The Traditional alphabetic optimality criteria are often used in comparing competing designs. However, Zahran *et al.* (2003) have examined that these single-valued criteria do not reveal the true complexities of design prediction capability and can be sometimes misleading. As a result, Zahran *et al.* (2003) have developed the fraction design space (FDS) plot as an alternative method in comparing competing response surface designs. The FDS plot allows detailed information to be extracted from a single curve of the scaled prediction variance (SPV) for an assumed model and specified design region for a particular design. The reader is referred to the works of Zahran *et al.* (2003) for the details of the calculation of the FDS plot.

To interpret the FDS plot, the region having a large area relatively close to the minimum of the SPV is highly desirable (Zahran *et al.*, 2003). Therefore, a good design will have a flatter and lower curve than a poor design. "Flatter" means, the overall prediction error will be constant; lower means the overall prediction error will be smaller (Design-Expert® 8). Standard error of prediction relates to the prediction interval around a predicted response at a given combination of factor levels and/or components. In essence, the larger the standard error of prediction, the less likely the result can be repeated, and the less likely a significant effect will be detected.

Anderson-Cook *et al.*(2009), Giovannitti-Jensen *et al.*(1989) and Zahran *et al.*(2003) have investigated the effects of center points up to three replications, this paper will investigate the effects of the replication of center points up to six center points and the replication of the axial points of the hybrid and Draper-Lin designs.

Figure 1.a and Figure 1.b show that, at one center point, D311B is the most desirable design given that it has the flattest curve and has the least variability of the prediction variances among the four designs. Although, it has the largest prediction variance in the entire spherical space but the stability of its prediction variance over the design region and having the smallest variability of the prediction values makes the D311B design to be desirable.

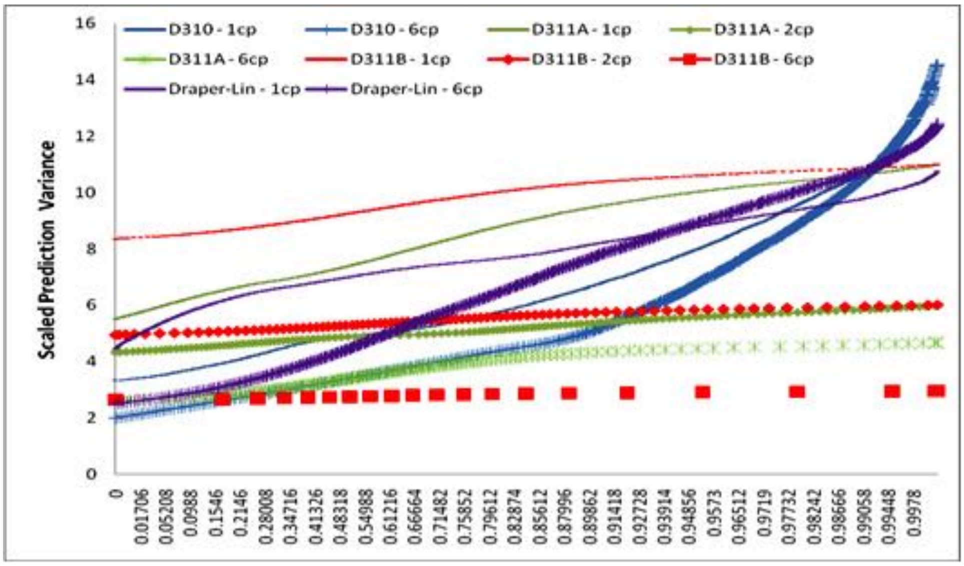

Figure 1.a. Fraction of design space plot for Hybrid and Draper-Lin designs over a spherical region.

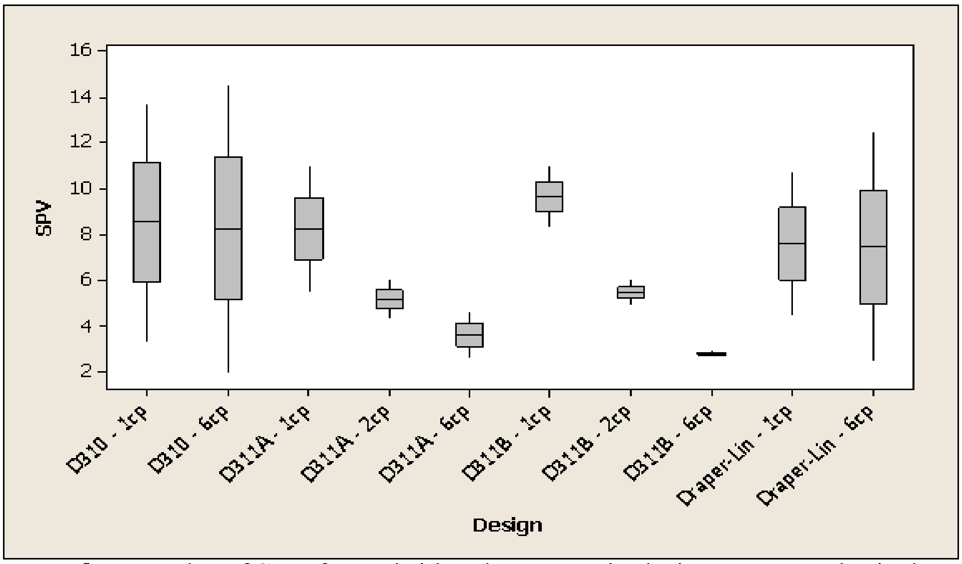

Figure 1.b. Box plot of SPV for Hybrid and Draper-Lin designs over a spherical region.

Increasing the center points will decrease the prediction variance and will also increase the stability of the scaled prediction variance throughout the spherical region of D311B. The box plot also shows that increasing the center points will also decrease the variability of the scaled prediction variance values of D311B. D311A also competes with D311B when center points are added. The stability of the prediction variance of D311A also increases and the variance dispersion of the scaled prediction variance values of D311A conversely, decreases as the center points increases. As the center point is replicated up to six times, D311B becomes more stabilized and the deviation of the scaled prediction variance decreases.

Figure 1.b also shows that increasing the center points of D310 and Draper-Lin designs will also increase the dispersion of their scaled prediction variance values as compared with D311A and D311B. Figure 1.a shows that the desirable center points for Draper-Lin design are "singular" or one since the scaled prediction variance of the design with a single replicated center point is more stable. Figure 1.b also shows that the spread of dispersion of the scaled prediction variance gradually increases as the center point increases. Increasing the center point will only minimize the minimum variance and will increase or maximize the maximum variance resulting to poor prediction efficiency in the perimeter of the Draper-Lin design.

A detailed evaluation of the replication of the center point of D311B shows that, in Figure 2.a and Figure 2.b, the minimum and maximum prediction variances of D311B are minimized. The scaled prediction variance rapidly decreases when the center point is replicated from one up to three replications and gradually decreases from four to six replications. The design will be more stable if the center point is replicated five times. The suggestion of four to five replications also confirms Myers and Montgomerey's (2002) suggested center runs from three to five center point replications. Figure 2.b also shows that the spread of dispersion becomes narrower if additional center points are added five times. The replication of six center points is less desirable since the minimum and maximum prediction variances of D311B will start to widen resulting to instability and subsequently, the dispersion of its prediction variance values will increase.

Figure 3.a shows that D311A and D311B have the highest maximum prediction variances while D310 has the lowest minimum prediction variance when the two axial and center points are replicated once. The scaled prediction variance of D311A rapidly increases up to 90% of the design space and gradually rises as it approaches the edge of the design. The Draper-Lin design rapidly increases its prediction variance up to the half of the design space and also slowly increases as it approaches to the perimeter. Draper-Lin and D310 prediction variances rapidly increase when these are very close to the edge of the design.

Even if D311B has the highest minimum and maximum prediction variances at a single replication of the axial points, it is still the most desirable design given its prediction variance is more stable in the entire region. Furthermore, Figure 3.b also suggests that D311B is more desirable since it has the smallest spread of dispersion and its minimum and maximum prediction variances are closer with each other as compared with the other designs.

Increasing the replication of the center point and axial points will minimize the maximum prediction variances of all the designs except for D310. All of the designs' minimum scaled prediction variance will decrease when the center point and the axial points are replicated. Figure 3.a illustrates that the replication of the center and axial points will stabilize the prediction variance of D311B in the entire space. This ensures that the prediction variance of D311B will be almost the same in the design region. For D311A, on the contrary, the prediction variance is partly stabilized from the midpoint to the perimeter of the design space. Additionally, Figure 3.b shows that their spread of dispersion also decreases when the center point and axial points are replicated. Draper-Lin and D310 have no changes relative to the stability and spread of dispersion of their prediction variances which resulted to the undesirable designs.

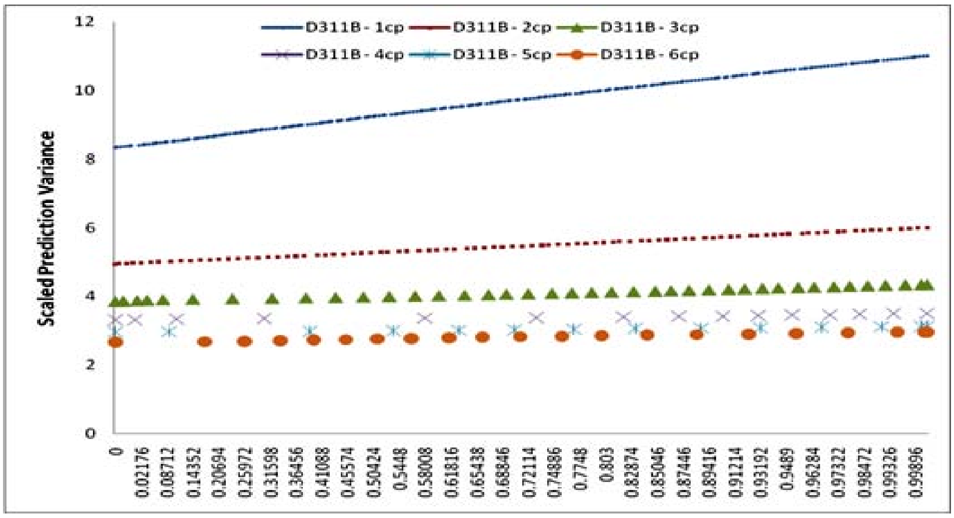

Figure 2.a. Fraction of design space plot for D311B design over a spherical region.

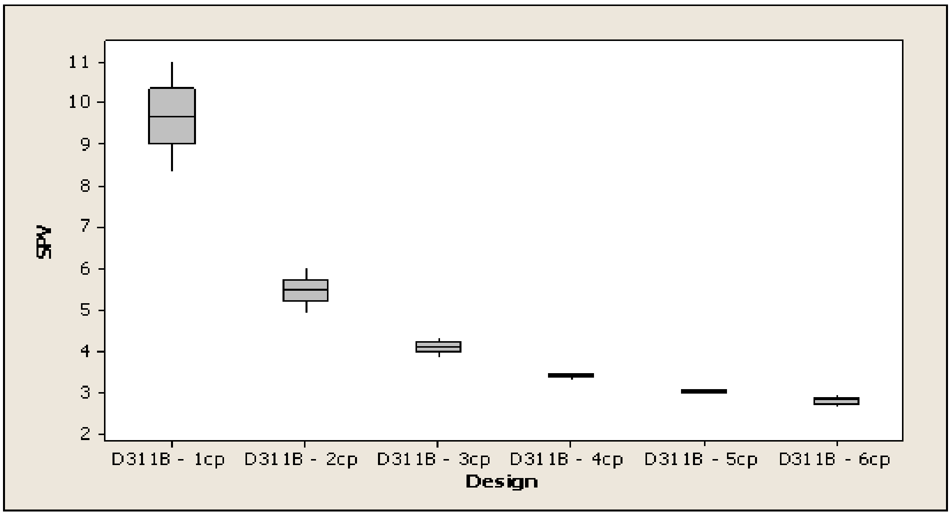

Figure 2.b. Box plot of SPV for D311B design over a spherical region.

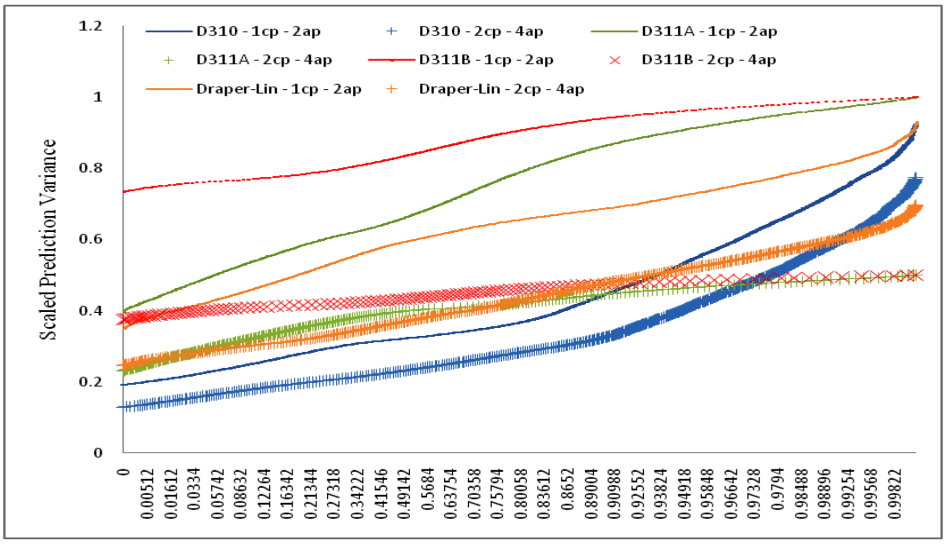

Figure 3.a. Fraction of design space plot for Hybrid and Draper-Lin designs with replicated axial and center points over a spherical region.

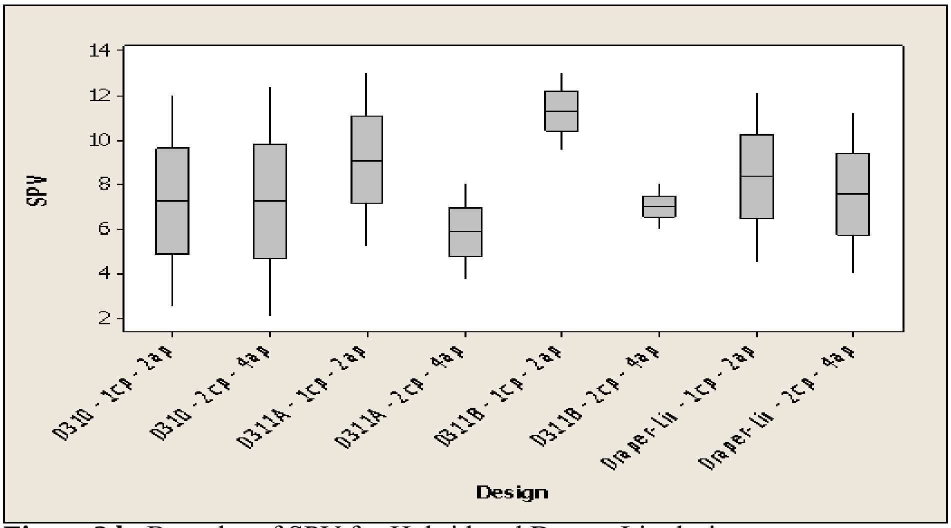

Figure 3.b. Box plot of SPV for Hybrid and Draper-Lin designs with replicated axial and center points over a spherical region.

CONCLUSIONS

Some of fraction of design space plot shows that D311B is the most desirable design for three-factor experiments since it had the most stable prediction variance and had the lowest spread of dispersion of the prediction variance values in the spherical region. A single replicate from the center point and from the axial points resulted to a large prediction variance of D311B as compared with the other designs but had the most stable and has the lowest spread of dispersion of the prediction value. Increasing the center points and axial points resulted in the decrease in the standard error of D311B; which also resulted in a more stable prediction variance and further resulted to the decrease in the spread of dispersion of the prediction variance. A competing design, D311A had similar results with D311B. Increasing the center points and axial points did not greatly affect the stability and the spread of dispersion of the prediction variances of D310 and Draper-Lin designs which resulted to the most undesirable of designs.

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