

# A SCREENING METHOD FOR CUSTOMIZING DESIGNS AROUND NON-CONVERGENT REGIONS OF DESIGN SPACES

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## **ABSTRACT**

In engineering design, Response Surface Methodology is often used to explore a design space and to generate a meta-model of the space. Designs of Experiments are used in this process to obtain the most behavioral information from the space with the fewest number of runs. Often, the designer discovers that the analysis program cannot converge to an answer for one or more regions of the design space. Traditionally, the designer gets around this problem by shrinking the variable ranges so that there are no regions of non-convergence. Instead of this process, this paper suggests that it is better to treat the non-convergent points as a region of infeasibility. Extra runs can be made to determine the border of this infeasible region, and then a custom Design of Experiments can be constructed to explore the design space while excluding the non-convergent region. This process still generates a valid meta-model yet retains more of the design space than the simple reduction of variable ranges.

## **INTRODUCTION**

Response Surface Methodology is a common practice in engineering design. This methodology consists of using statistical Designs of Experiments (DoE) to create an accurate approximation, or meta-model, of a more complex system. This meta-model, which runs in a fraction of the time of the complex analysis, can then be used for fast system analysis or optimization. The Design of Experiments is key to this process, as it is a statistical method that generates the maximum amount of model information for the fewest number of computer runs. A key element in the generation of this information is the fact that the Designs of Experiments are orthogonal; each variable can be independently examined from the DoE runs.

The general approach to response surface methodology is well laid out. First, a set of variables of interest and variable ranges are chosen. Next, a screening test, which is a Design of Experiments that is designed to capture only first order effects, is run on the complex system. With the results of the screening test, the decision-maker can determine which variables contribute most of the variability to the response. Variables that do not contribute greatly to the response can be eliminated. Next, a larger Design of Experiments is generated to test for higher order effects. Typically the user wants to capture second order effects as well as cross-terms. Many of these Designs of Experiments are predefined, such as Central Composite Designs (CCD) or face-centered Central Composite Designs. Once the complex system has been exercised around the Design of Experiments, a meta-model can be created by doing a least-squares regression. “Goodness of fit” statistics exist to examine the meta-model, and finally, random verification runs of the complex analysis code can be made to compare against the meta-model.

## **Current Approach**

Sometimes, while evaluating the screening test, the computer analysis cannot converge to a solution in some regions of the design space. This lack of convergence can be for a number of reasons, the program may have hit a “bug”, it may have run into a region where the convergence scheme fails, or the computer program may be failing because it cannot meet some physical constraint. For instance, common aircraft sizing programs often crash when there is not sufficient thrust for the aircraft to climb. Thus, often the programs’ lack of convergence signifies that an implicit physical constraint is being violated within the set of design parameters. Therefore, the lack of convergence of a computer program should not be ignored, but instead treated as a potential region of design infeasibility.

There are two common ways to handle non-convergent regions of design spaces. The first method is to simply reduce the variable ranges until the entire space can be run. This is often done during the screening test. The

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screening test is re-run, each time shrinking variable ranges, until the computer program no longer crashes. Unfortunately, this method is poor because it can lead to the elimination of design space that is feasible, just to remove some infeasible space. This is illustrated in Figure 1, which shows a small region of non-convergence in the corner of a design space, and the large area of feasible space that is lost by simply reducing the variable ranges.

Another approach to this problem is taken when the number of failed cases is small compared to the total number of runs (if only 4 or 5 cases fail out of 273 runs). In this situation, the failed cases are just thrown out, with a meta-model built around the remaining cases. This approach has two drawbacks. For one, the orthogonality of the design can be compromised by the random exclusion of points in the DoE (the failed points are excluded). In addition, the fact that the cases failed is significant, signifying that perhaps an implicit constraint is being violated in this region. For this reason, it is inadvisable to throw out failed computer runs, as it is also important to know in what regions of the design space the system fails.

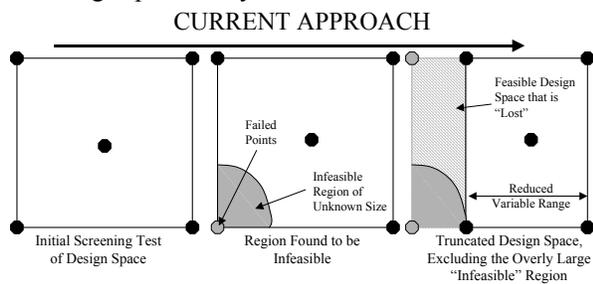


Figure 1: Current Approach for Non-Convergent Regions of the Design Space

Proposed Alternative

Instead of simply reducing the variable ranges, it may be advisable to spend some extra resources to more fully “explore” the region of non-convergence. Once this region has been explored, the actual size and shape of the region of non-convergence can be understood. With this understanding, in lieu of decreasing the variable ranges, the user can simply build a custom Design of Experiments that includes the full ranges and excludes only the non-convergent reasons. In this case, the custom DoE should still consist of a minimum number of runs to build a second order model and remain orthogonal. Fortunately, software already exists, specifically JMP, which can build custom DoEs of this type, with a constraint added to remove a specific non-convergent region in the design space. Once this custom DoE is built, the full DoE can be run and a meta-model generated.

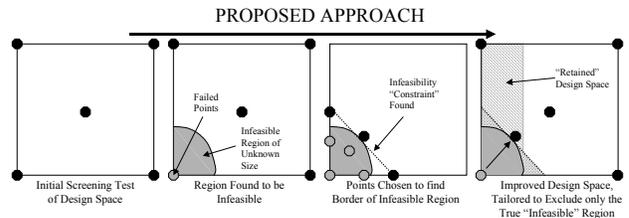


Figure 2: Proposed Approach for Non-Convergent Regions of the Design Space

This new approach can easily be integrated into the screening step in the RSM process. It is at this screening step that decision-makers would commonly reduce the variable ranges to ensure that all points in the design space converge. Instead of reducing ranges, the user could add additional runs to specify the boundary of the non-convergent region. Then, with the additional data generated from these runs, the user can still build a first order model to look at primary effects for the purposes of reducing the number of variables. Once this is done, the user may continue, building a custom Design of Experiments around the non-convergent region to build the final meta-model. The proposed alterations to the traditional Response Surface Methodology are given in Figure 3.

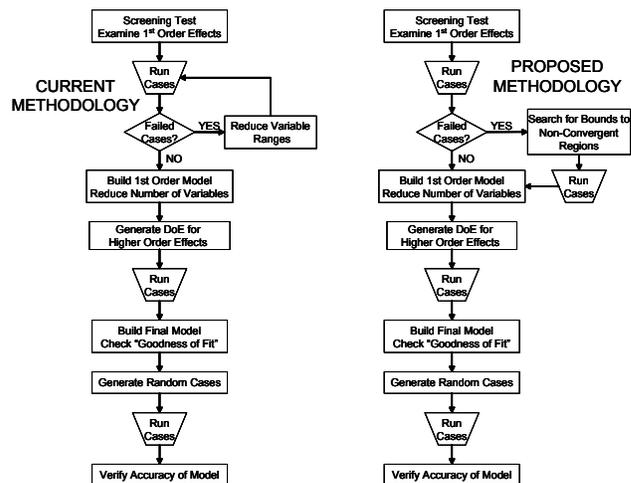


Figure 3: Comparison of Current RSM Methodology and Proposed Methodology

**METHOD FOR EXPLORATION OF NON-CONVERGENT REGION**

Design of Experiments constraints in JMP and other programs are generally treated as linear constraints, with no second order or cross-product terms used. Therefore, in order to generate the appropriate custom-made DoE, a set of linear constraints must be established around the non-convergent region of the design space. The following example illustrates the process for finding the constraints.

Begin with two variables,  $X_1$  and  $X_2$ . Run a screening test around the variables, which consists of five points: the four corner points and the center point. Assume that the computer analysis of one of the corner points fails (is non-convergent). This occurs at (1,1), and is illustrated in Figure 4. It is now known that there is a non-convergent region in the corner; therefore the user must discover the size of the non-convergent region. First, find how far the non-convergent region extends toward the center of the Design Space (0,0). The bisection method is used to determine the location of the point of failure on this line. The bisection method works by testing the midpoint of the line, excluding the region that is not under consideration, then testing the midpoint of the smaller line. This method continues until the desired fidelity is reached. The advantage of the bisection method is that it is very robust and handles discontinuous spaces well, a requirement for this type of application. There is also the advantage that the number of function calls to reach the specified fidelity is fixed. Unfortunately, the bisection method does not converge as quickly as other line-search techniques.

The bisection method takes three additional runs to find the edge of the constraint towards the center, occurring in the example at (.625,.625), see Figure 5. Now the constraint must be found in another direction, so the bisection method is again used along the line  $X_2 = 1$  (Figure 5). Once this edge of feasibility is found (.375,1.0), a constraint line in  $X_1$  and  $X_2$  can be drawn. However, the region of non-convergence is not yet completely specified. One must also verify that the constraint line crosses  $X_1 = 1$  at a feasible region, otherwise some region of non-convergence may not be appropriately excluded from the design space. This can be verified by the addition of a single point at the location where the constraint line crosses the  $X_1=1.0$  axis (1.0,0.06). If the point is valid (Figure 6-Left), the constraint is good and the remaining space can be examined. If the point is not valid (Figure 6-Right), then the edge of the constraint along  $X_1=1$  needs to be found, and a new constraint line drawn. At this point a custom Design of Experiments can be calculated using JMP, by selecting an RSM-based Design of Experiments and adding the line of the constraint:  $1.5X_1 + X_2 < 1.56$ , in example 1, and  $1.6X_1 + X_2 < 1.6$  for example 2.

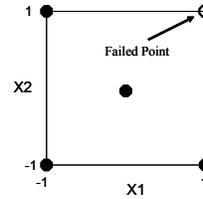


Figure 4: Failed Point in Screening Test

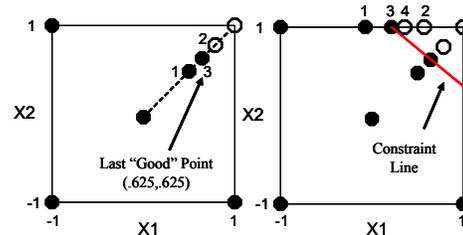


Figure 5: Use Method of Bisections to Find Constraint Line

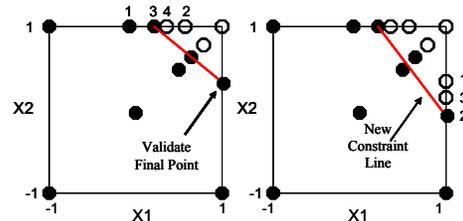
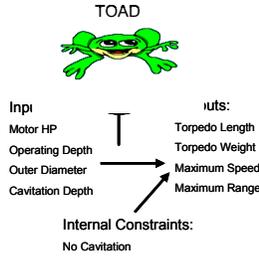


Figure 6: Check to Verify Constraint covers all Infeasible Regions

## RESULTS

This method was tested using a torpedo sizing and synthesis code as the application test-bed. The code, called Torpedo Optimization, Analysis, and Design (TOAD) is used to size electric torpedo systems. It takes inputs such as motor horsepower, operating depth, outer diameter, minimum cavitation depth, etc., to size a torpedo. Key outputs of the program include torpedo length, weight, maximum range, and maximum velocity. The program also has several internal convergence criteria, one of which is to determine if a torpedo can be sized to meet the operating conditions without failing one key criterion: cavitation. Cavitation is the creation of bubbles in the water around the propulsor. It occurs when the static pressure at the propulsor drops below the vapor pressure of the fluid. If TOAD cannot converge to a design that does not have a cavitation problem, it returns an error and gives non-physical outputs. Thus, a response for the design space must be generated that excludes the regions in which non-cavitating designs cannot be generated.



**Figure 7: Inputs and Outputs for TOAD**

Test Case 1 – Two Dimensions

The first test case was a 2-Dimensional problem. It involved the variables outer diameter and motor horsepower. A five point screening test was run. Similar to the previous example, one point in the design space failed. Using the methodology previously described and seven additional points, the constraint for the non-convergent region was quickly identified. The original DoE and additional points are shown in Figure 8. The equation of the constraint was determined to be:

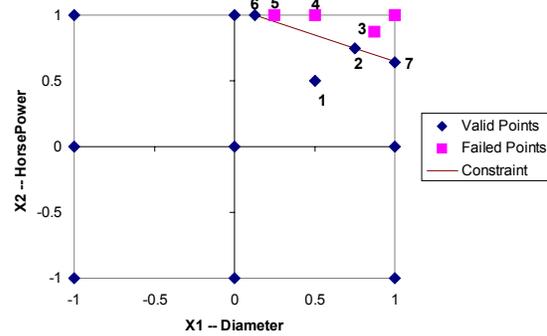
$$0.4 X1 + X2 < 1.05 \quad \text{EQ 1}$$

Once the constraint line was found, a new Design of Experiments was generated that excluded the non-convergent region. This Design of Experiments is shown compared to the original DoE in Figure 9. Note that the new DoE includes points on the constraint line, has no points in the infeasible region, and has shifted some of the remaining points. These remaining points were shifted in order to maintain orthogonality in the DoE. The standard model error, which is the expected error for each term in the RSE model shown in Equation 2, is given in Table I. This table includes the model error for both the original face-centered Central Composite Design DoE and the custom-made DoE, along with the error for a face-centered Central Composite Design with the original failing point removed.

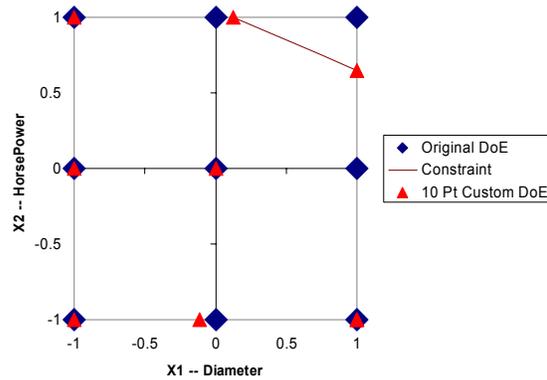
$$Y = A \cdot X1 + A2 \cdot X1^2 + \dots \\ B \cdot X2 + B2 \cdot X2^2 + AB \cdot X1 \cdot X2 \quad \text{EQ 2}$$

The custom DoE had only slight increases in the standard error from the baseline face-centered Central Composite Design. The truncated CCD had even more error than the custom design, indicating that building custom designs is superior to simply eliminating failed points from the model. If the other traditional approach of simply reducing the variable ranges was followed, then the variable X2 would have been reduced from 1.0 to 0.65. This reduction excludes feasible space that is included in the proposed approach. By reducing the range of X2, 17.5% of the design space is being removed. But, by excluding only the non-convergent region, only 3.8% of the design space is being

discarded. Thus, using the historical approach, almost 15% of the design space would have been inappropriately discarded.



**Figure 8: Exploration of Non-Convergent Region in 2-Dimensions**



**Figure 9: Comparison of Central Composite Design to Custom Design**

**Table I: Comparison of Error between Designs of Experiments**

Term	CCD 9 Runs		Truncated CCD 8 Runs		Custom DoE 9 Runs	
	Std Error	Rel. Error	Std Error	Rel. Error	Std Error	Rel. Error
A	0.408	0.00	0.556	0.15	0.430	0.02
B	0.408	0.00	0.556	0.15	0.422	0.01
A2	0.707	0.00	0.802	0.09	0.738	0.03
B2	0.707	0.00	0.802	0.09	0.845	0.14
AB	0.500	0.00	0.756	0.26	0.526	0.03

Test Case 2 – Three Dimensions

The next test case involved the addition of a third dimension. Instead of only using motor horsepower and outer diameter as the design variables, operating depth was also used as a criterion. This case had the same problem as the first test case; the computer analysis program, TOAD, could not converge to a non-cavitating torpedo for all combinations of the design parameters. This problem was setup by first doing a

screening test. In a higher dimension problem, this screening test would be used to eliminate unnecessary variables. However, in the case of only three dimensions, elimination of variables is not necessary, so the screening test just served to test the convergence of the analysis code throughout the design space. The screening test consisted of nine points. Only one of the nine points failed, see Figure 10. Using the same method as before, starting with a line towards the center of the design space, then searching along each edge of the design space, the constraints around the non-convergent region were found. Ten extra points were required to find the region of non-convergence. A plot of the valid and failed points ran in determining this region is given in Figure 11. The equation of the constraint region is:

$$.875 X_1 - X_2 + X_3 < -1 \quad \text{EQ 3}$$

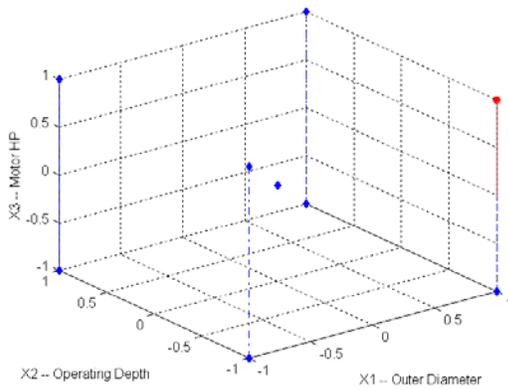


Figure 10: Non-Convergent Points in Screening Test (Red Circle == Failed Case)

A custom-made DoE was then generated that excluded these constraints. The DoE is shown, along with the original face-centered Central Composite Design, in Figure 12. Note that the custom design has only one more point than the original. A comparison of the standard error of the three DoE designs is given in

Table II. These designs include the original face-centered CCD as a baseline, a truncated CCD with the single failed corner point removed, and the custom design. Again, the custom design has slightly worse error than the unaltered Central Composite Design, but the error is not very significant. The custom design has approximately the same error as the simple, truncated CCD.

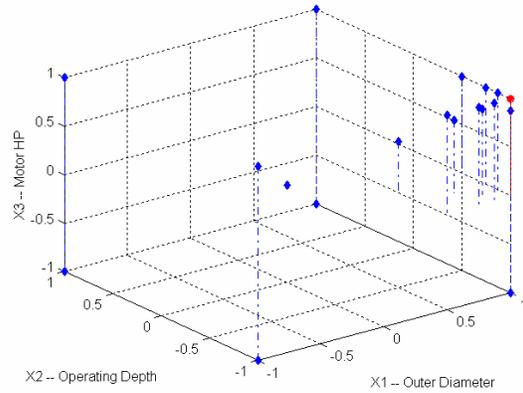
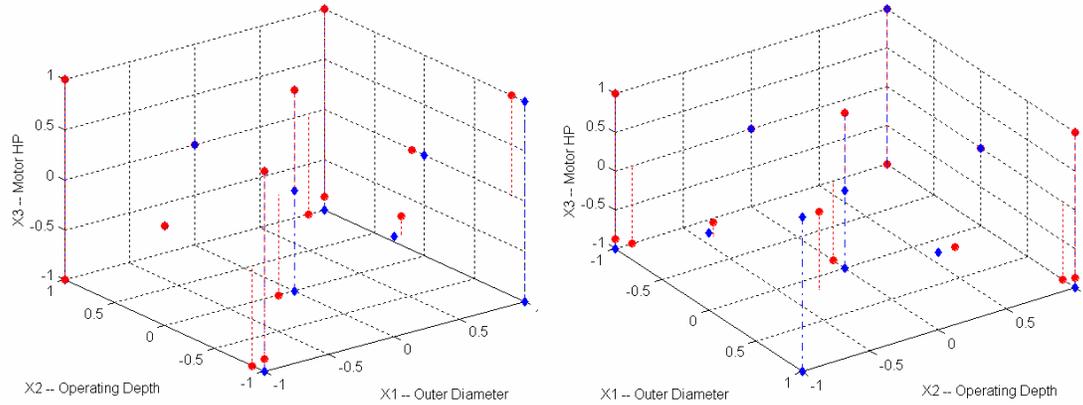


Figure 11: Additional Test Points (Red Circle == Failed Case)

Table II: Comparison of Error between Designs of Experiments

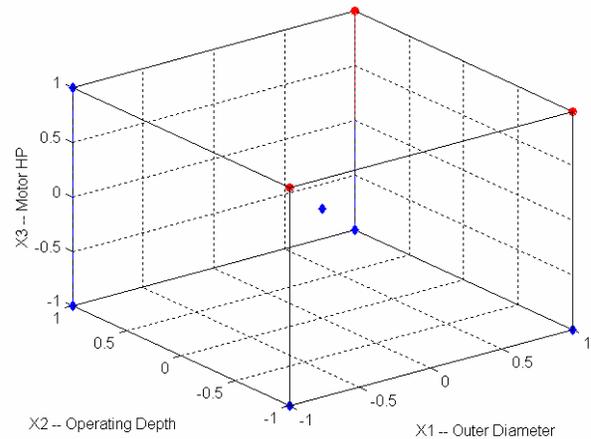
Term	CCD 15 Runs		Truncated CCD 14 Runs		Custom DoE 16 Runs	
	Std Error	Rel. Error	Std Error	Rel. Error	Std Error	Rel. Error
A	0.32	0.00	0.386	0.07	0.392	0.08
B	0.32	0.00	0.386	0.07	0.397	0.08
C	0.32	0.00	0.386	0.07	0.376	0.06
A2	0.62	0.00	0.636	0.01	0.637	0.01
B2	0.62	0.00	0.636	0.01	0.651	0.03
C2	0.62	0.00	0.636	0.01	0.643	0.02
AB	0.35	0.00	0.450	0.10	0.430	0.08
AC	0.35	0.00	0.450	0.10	0.407	0.05
BC	0.35	0.00	0.450	0.10	0.409	0.06



**Figure 12: Comparison of Central Composite Design (Blue Diamond) to Custom Design (Red Circle)**

### Test Case 3 – Three Dimensions

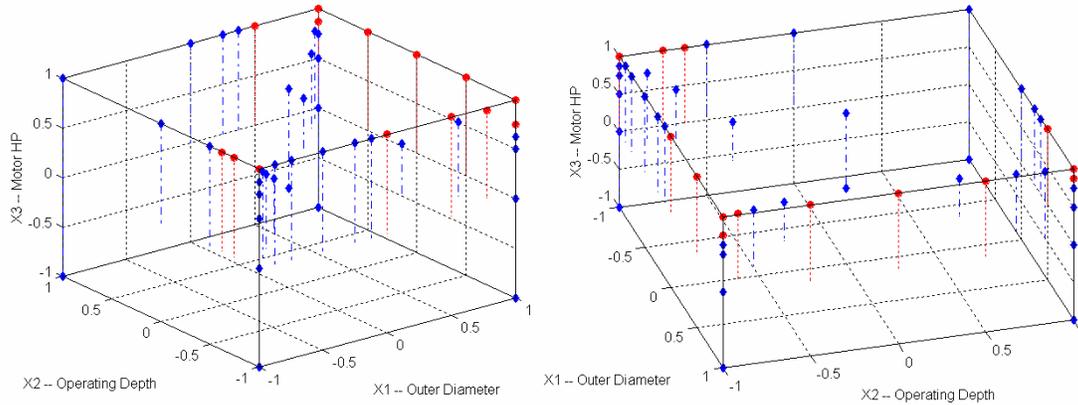
The next sample case involved the same three design variables as the previous case: motor horsepower, outer diameter, and operation depth. However, another design parameter, cavitation depth, was changed to make it more difficult for the analysis code to converge to a valid torpedo design. Hence, for this case there were larger non-convergent regions than the previous case. During the initial screening of nine runs, three corner points were non-convergent. These points are shown in Figure 13. Having three non-convergent points instead of one requires a slightly different approach than before. For this problem, it was decided that it would be easiest to develop a separate constraint for each of the failed corner points. Thus the final Design of Experiments would be generated with three constraint sets. This method was the most straightforward way to include the entire non-feasible region within a series of linear constraints. As was expected, many of the constraint regions ended up overlapping.



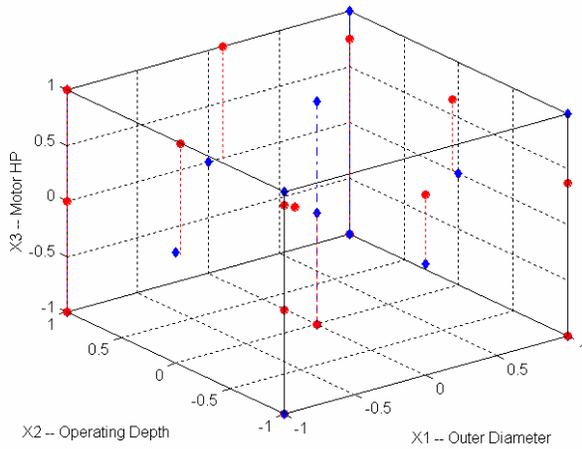
**Figure 13: Non-Convergent Points in Original Screening Test (Red Circle == failed)**

$0.25 X_1 - 0.25 X_2 + X_3 < 0.875$	EQ 4
$0.333 X_1 - 0.1875 X_2 + X_3 < 1.1458$	EQ 5
$0.4 X_1 + 0.125 X_2 + X_3 < 1.275$	EQ 6

Forty additional points were required to generate the three constraints. The points, which help the user to visualize the non-feasible regions, are given in Figure 14. The three constraint equations are also given as Equation 4 through Equation 6.



**Figure 14: Additional Points to Determine Non-Convergent Region (Blue Diamond == Valid, Red Circle == Failed)**



**Figure 15: Comparison of Central Composite Design (Blue Diamond) to Custom Design (Red Circle)**

Once the constraints were found, a new Design of Experiments could be generated. This DoE consisted of 16 points, and is shown in Figure 15. Also shown in the figure are the DoE points for a traditional Central Composite Design. Note that there are DoE points along all three constraints and many of the other points have been offset to maintain orthogonality. Comparisons between the model error for three Design of Experiments are given in Table III. The first DoE is a traditional face-centered, Central Composite Design. This design has 15 runs. A truncated Central Composite Design with the non-convergent corner points removed is also shown in the table. This truncated design has only 12 runs (three having been removed) and has significantly higher model error than the pure CCD. Finally, the model error of the custom made DoE is shown. Note that the model error for the incomplete CCD has been greatly increased, while the

error for the custom made design is on the same order as the error for the original CCD.

**Table III: Comparison of Error between Designs of Experiments**

Term	CCD 15 Runs		Truncated CCD 12 Runs		Custom DoE 16 Runs	
	Std Error	Rel. Error	Std Error	Rel. Error	Std Error	Rel. Error
A	0.32	0.00	0.61	0.29	0.30	-0.02
B	0.32	0.00	0.61	0.29	0.31	-0.01
C	0.32	0.00	0.60	0.28	0.35	0.03
A2	0.62	0.00	0.68	0.06	0.62	-0.01
B2	0.62	0.00	0.68	0.06	0.62	0.00
C2	0.62	0.00	0.68	0.06	0.72	0.10
AB	0.35	0.00	0.49	0.14	0.33	-0.03
AC	0.35	0.00	0.74	0.39	0.40	0.04
BC	0.35	0.00	0.74	0.39	0.38	0.03

## MODEL ACCURACY

Response surface equations were generated for test case 3. Response surface equations were constructed for two system responses, torpedo length and maximum velocity. Responses were made from three types of models. The first model used was the simple, truncated face-centered Central Composite Design, i.e., the original design with the failed points removed. The second model is the custom designed DoE that excludes the non-convergent regions. The third model, included for comparison, is a model that was generated by including only random points. Since the custom DoE had 16 points with 40 additional points used to determine the size of the non-convergent regions, it was decided to make a comparison against a completely randomized system with the same total number of runs, i.e., 56 runs.

Several statistics are given in Table IV to compare the RSEs. The first statistics are given to show how well the model compares to the points used to generate the model. These statistics include the  $R^2$  and  $R^2$ -adjusted,

along with the average percent error and maximum percent error for the model points. Next, a validation set of 50 runs was made and compared to the RSE. Again, the average and maximum percent error for the test cases is shown.

In all the cases, the response surface equations had excellent  $R^2$  and  $R^2$ -adjusted. In addition, all of the models performed nearly the same with respect to percent error and the error in the validation runs. Thus, for a three dimensional problem, the same accuracy is achieved from simply truncating the CCD, excluding the non-convergent region, or taking a large random sampling. However, even though the final models are equivalent, the proposed method of exploring constraints does have benefit, because unlike the other models, only the custom designed DoE includes information as to the size and shape of the non-convergent, or infeasible, region of the design space. Both the truncated CCD and the random sampling provide no way to distinguish between the convergent and non-convergent regions of the design space.

**Table IV: Response Surface Equation Statistics**

Length Response	Model Fit				Validation Runs		
	MODEL	$R^2$	$R^2$ Adj	Avg % Error	Max % Error	Avg % Error	Max % Error
Truncated CCD		0.994	0.968	0.41%	0.69%	0.42%	1.54%
Custom Design		0.996	0.989	0.38%	1.06%	0.52%	1.42%
Random		0.998	0.998	0.16%	0.61%	0.18%	0.53%
Velocity Response	Model Fit				Validation Runs		
	MODEL	$R^2$	$R^2$ Adj	Avg % Error	Max % Error	Avg % Error	Max % Error
Truncated CCD		1.000	1.000	0.15%	0.35%	0.81%	1.81%
Custom Design		0.998	1.000	0.23%	0.79%	0.70%	2.22%
Random		0.999	0.999	0.35%	1.61%	0.55%	1.76%

### CONCLUSIONS

The proposed method is a good alternative to traditional Response Surface Methodology approaches. With the addition of extra analysis runs during the screening test, a boundary to the non-convergent regions can be found.

A custom generated Design of Experiments can be built around this border that maintains the same model accuracy yet excludes the non-convergent regions. Response Surface Equations generated with this technique compare well against actual data. The RSE's for both the current and the proposed approach have similar performance; however the proposed approach has a key advantage because it develops information about the size and the shape of the non-convergent, or infeasible, regions.

The user must be careful when using the Response Surface Equations made from the custom-built DoEs. The newly generated RSEs are not valid in the non-convergent region, so care must be taken whenever using the RSEs in later analyses so that these non-convergent regions are excluded.

As the number of dimensions increases, so does the number of additional runs required to define the borders of the non-convergent regions. Since so many more runs are required for larger dimensions, it may be more efficient to use a simple random scattering of points, which may be sufficient to both build a good meta-model and define the regions of non-convergence. More investigation is needed in this area. In addition, more investigation is needed to generate less computationally intensive methods to define the constraints, including looking at building a single hyperplane constraint instead of multiple planar constraints.

### ACKNOWLEDGEMENTS

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