Comparison of Prediction Accuracy of Surrogate Models Developed Using Nested Latin Hypercube Designs

"How Many Simulation Experiments Do I Need to Run?"

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Projects Using DOE at U.S. Army ECBC CY05-08

- JPM Nuclear Biological Chemical Contamination Avoidance (NBCCA) - Whole Systems Live Agent Test (WSLAT) Team support to the Joint Biological Point Detection System (JBPDS)
- Agent Fate wind tunnel experiments
- Decontamination Sciences Team
  - Contact Hazard Residual Hazard Efficacy Agent T&E Integrated Variable Environment (CREATIVE) - real and simulation data
  - Modified vaporous hydrogen peroxide (mVHP) decontamination – real data
- Smoke and Target Defeat Team
  - Pepper spray characterization – real data
  - Obscurant material evaluation (with OptiMetrics, Inc.) – simulation data
- U.S. Army Independent Laboratory In-house Research (ILIR) on novel experimental designs used with simulations
  - Re-analysis of U.S. Air Force Kunsan Focused Effort BWA simulation data
  - CB Sim Suite used for sensitivity analysis of atmospheric stability
- U.S. Marine Corps Expeditionary Biological Detection (EBD) Advanced Technology Demonstration (ATD)
  - Chamber testing of detectors – real data
  - CB Sim Suite sensor deployment studies – simulation data
- U.S. Navy lead on Joint Expeditionary Collective Protection (JECP)
  - Swatch and chamber testing – real data
  - Computational Fluid Dynamics (CFD) – simulation data

Goal

Evaluate potential use of sequential Nested Latin Hypercube Designs (NLHD) with long-running Computational Fluid Dynamics (CFD) simulations

In lieu of CFD model a transcendental function known to exhibit “rapid change” in corners of 2-factor space was used to stress extrapolation of Gaussian Process metamodel.

- Accuracy evaluated by comparing Actual vs. Predicted (i.e. simulation vs. metamodel) checkpoint response values
- Three sets of checkpoints over different ranges were used
- Relative sizes of regions of extrapolation at each succeeding stage – with & w/o inclusion of checkpoints – compared by looking at slices through convex hull
- Augmentation of first block of NLHD with moderate order polynomial evaluated as alternate strategy

What is a metamodel?

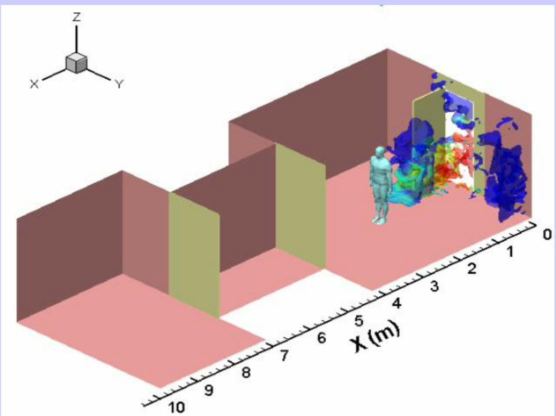
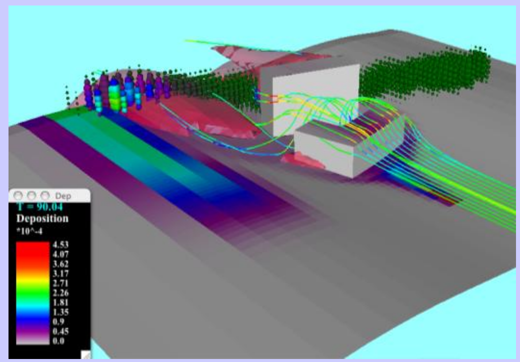
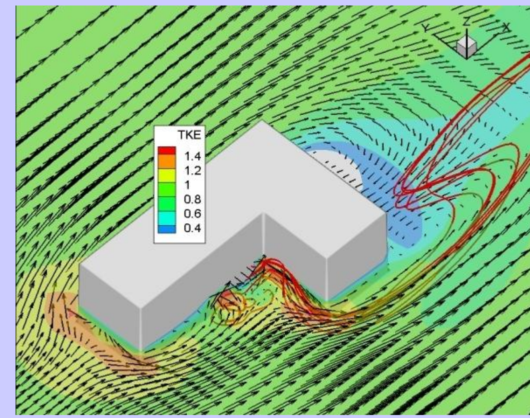
- A metamodel is a “model of a model”
  - Also called a *surrogate* model, it can be a fast approximation of a longer running simulation
    - Metamodel is less accurate – the tradeoff to be evaluated is the gain in speed versus the loss in accuracy
    - Metamodel is generally valid over smaller volume of factor-space than the full computer simulation model – invariably it is better for interpolation than it is for extrapolation

Why would I want to create a metamodel?

- Some computer simulations take a long time to run
  - This makes it difficult to extract useful information about factor sensitivity or to be used by an operational test analyst seeking quick answers to “what if?” questions

Some Long Running Simulations

Detailed Physics Models can require a great deal of runtime to generate a short period of simulation time.

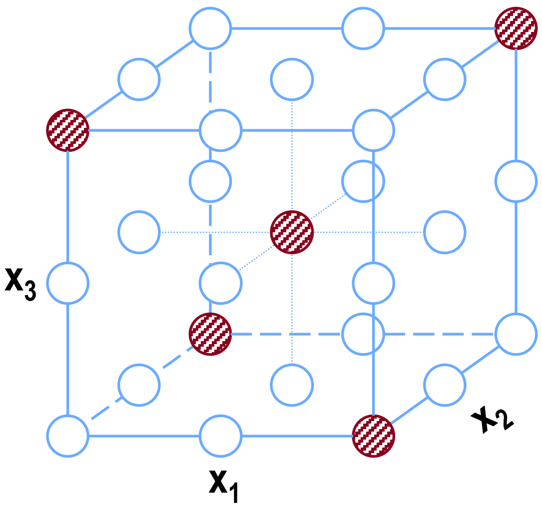
Computational Fluid Dynamics (CFD) Models		Lagrangian-Particle
		
Developed for Interior Moving Man in Simulation 8M cells 10 Seconds of Simulation 50 CPUs – 4K slower 12 Hours of Runtime	Developed for Exterior Stationary Grids 1.5M Cells 30 Seconds of Simulation Single CPU – 20K slower 7 Days of Runtime	Developed for Exterior Stationary Grids TBD Cells Min-Hours of Simulation Single CPU Minutes-Days of Runtime
Detailed Ingress/Egress, Internal Airflow and Convection	**External CW Deposition/ Evaporation, Vegetation, Solar Heating**	**Speed, Flexibility, More User Friendly, V&V**

What is a Design of Experiments (DOE)?

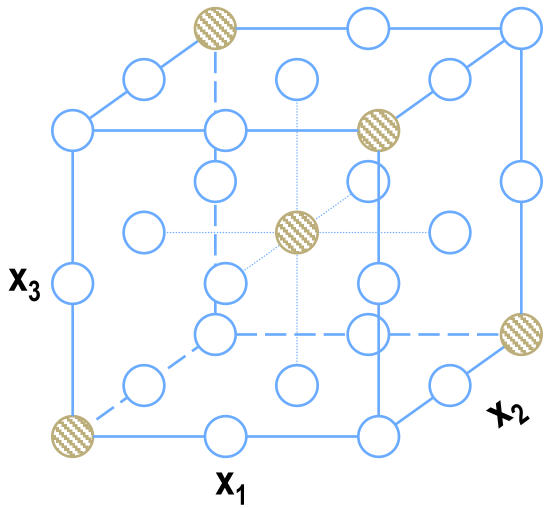
- It's the specific collection of trials run to support a proposed model.
  - If proposed model is simple, e.g. just 1st order or main effects, the design is called a *screening* DOE
    - Goals include rank factor importance or find a "winner" quickly
    - Often used with many (> 6?) factors at start of process characterization
  - If the proposed model is more complex and includes 2nd order effects - particularly if the control variables are continuous and the model includes interaction and squared terms, the design is called a *response-surface* DOE
    - Goal is generally to develop a predictive model of the process
    - Often used with a few (< 6?) factors after a screening DOE

Response Surface DOE in a Nutshell

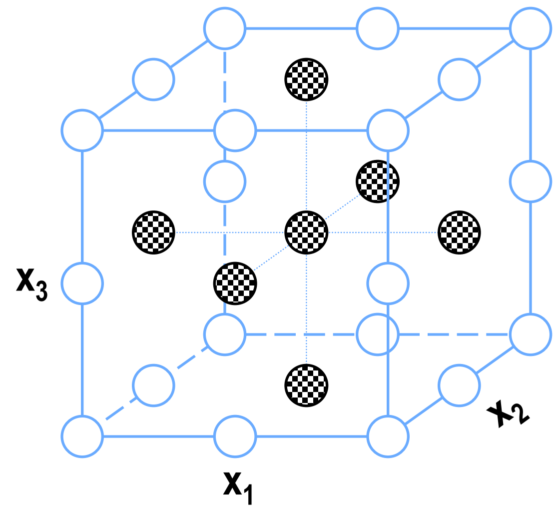
Block 1



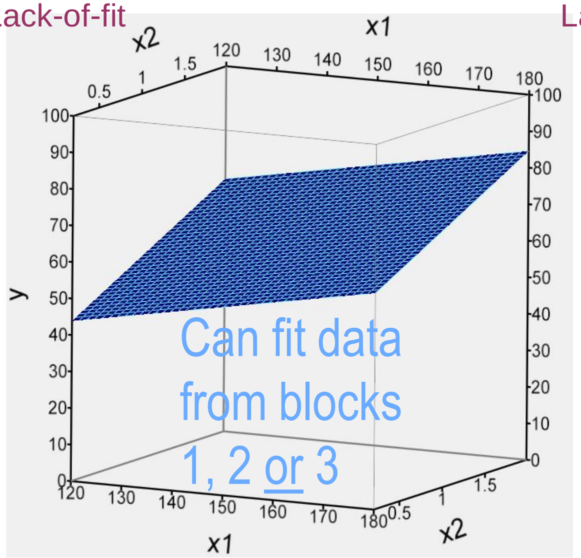
Block 2



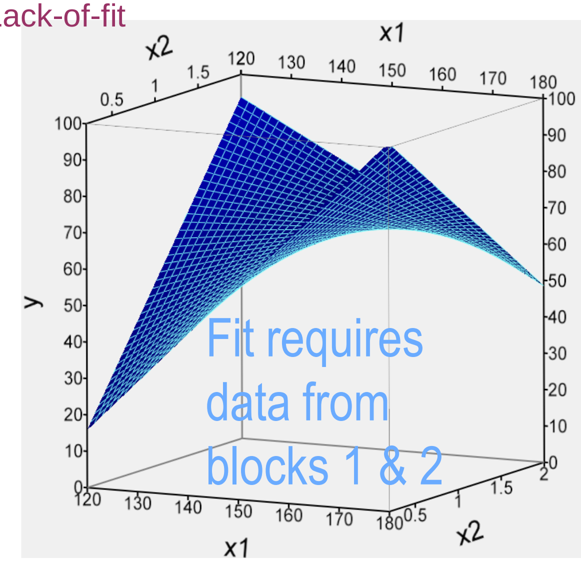
Block 3

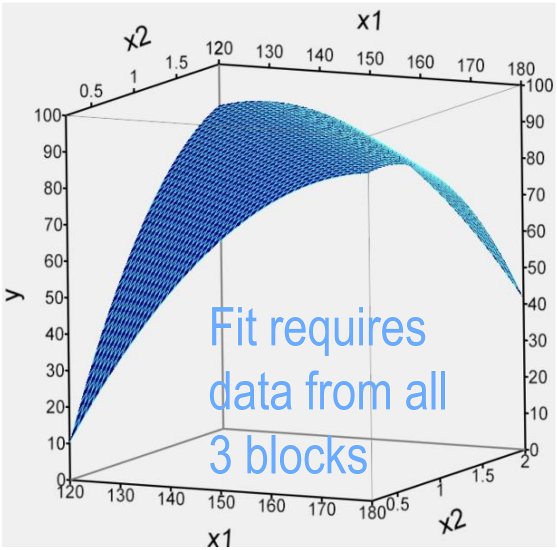


Lack-of-fit



Lack-of-fit





Why Use Design of Experiments Methods with Simulation Experiments?

Quicker answers, lower costs, solve bigger problems

- Obtain a fast surrogate *metamodel* of the simulation
  - Individual simulations can run for hours, days, a week!
    - Computational Fluid Dynamics (CFD)
    - Simulation runs in real-time
  - Numbers of factors can be very large (40+)
  - Numbers of simulations needed can be large (thousands in many cases)
  - Simulations can be stochastic requiring many replications
- Metamodel yields a fast approximation of the simulation
  - more rapidly answer “what if?” questions
  - do sensitivity analysis of the control factors
  - optimize multiple responses and make trade-offs
- By running efficient subsets of all possible combinations, one can – for the same resources and constraints – *solve bigger problems*
- By running sequences of designs one can be as *cost effective as possible* & run *no more trials than are needed* to get a useful answer

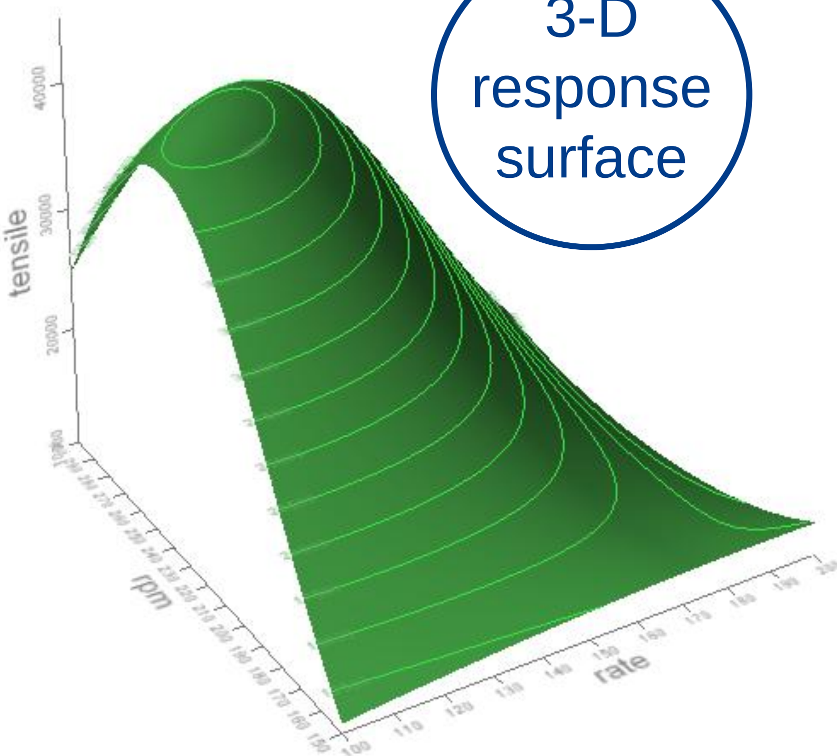
Why is Using DOE Important?

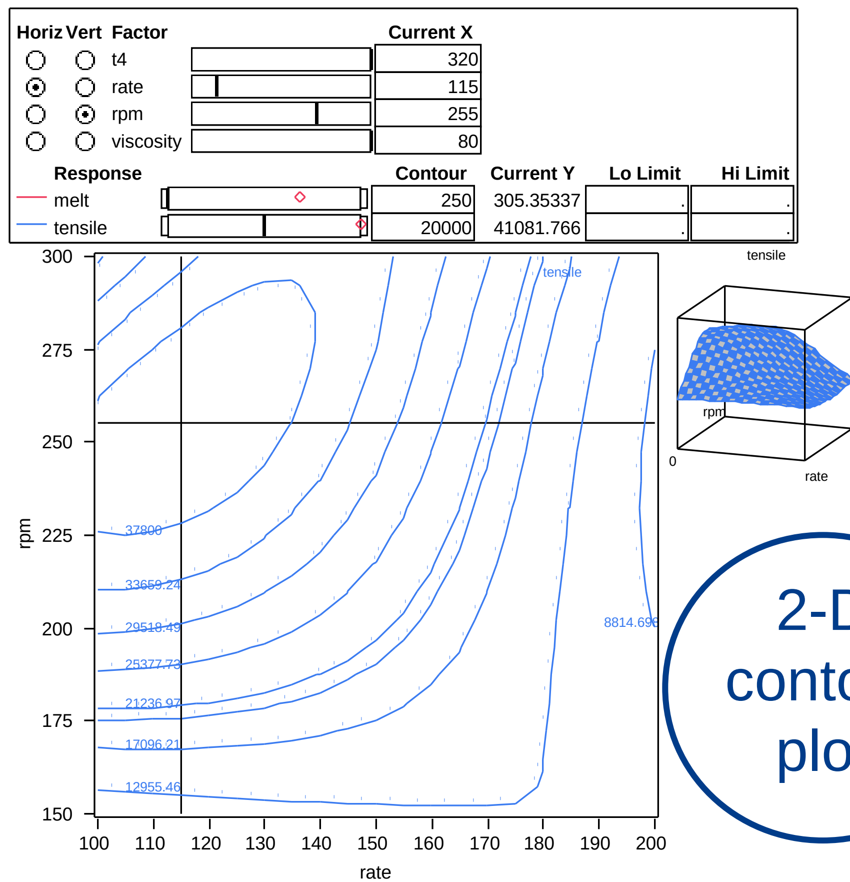
- *“One thing we have known for many months is that the spigot of defense funding opened by 9/11 is closing.”*
- *“In the past, modernization programs have sought a 99 percent solution over a period of years, rather than a 75 percent solution over a period of weeks or months.”*
  - Two quotes from the January 27, 2009 submitted statement of Secretary of Defense Robert M. Gates to the Senate Armed Services Committee.
- DOE is one of the more powerful tools we can use to efficiently accomplish our goals.
  - DOE yields the maximum information from the fewest experiments.
  - DOE often yields an 80% solution in less than 20% of the work.

Response Surface & Contour Plot

(four control variables)

3-D response surface

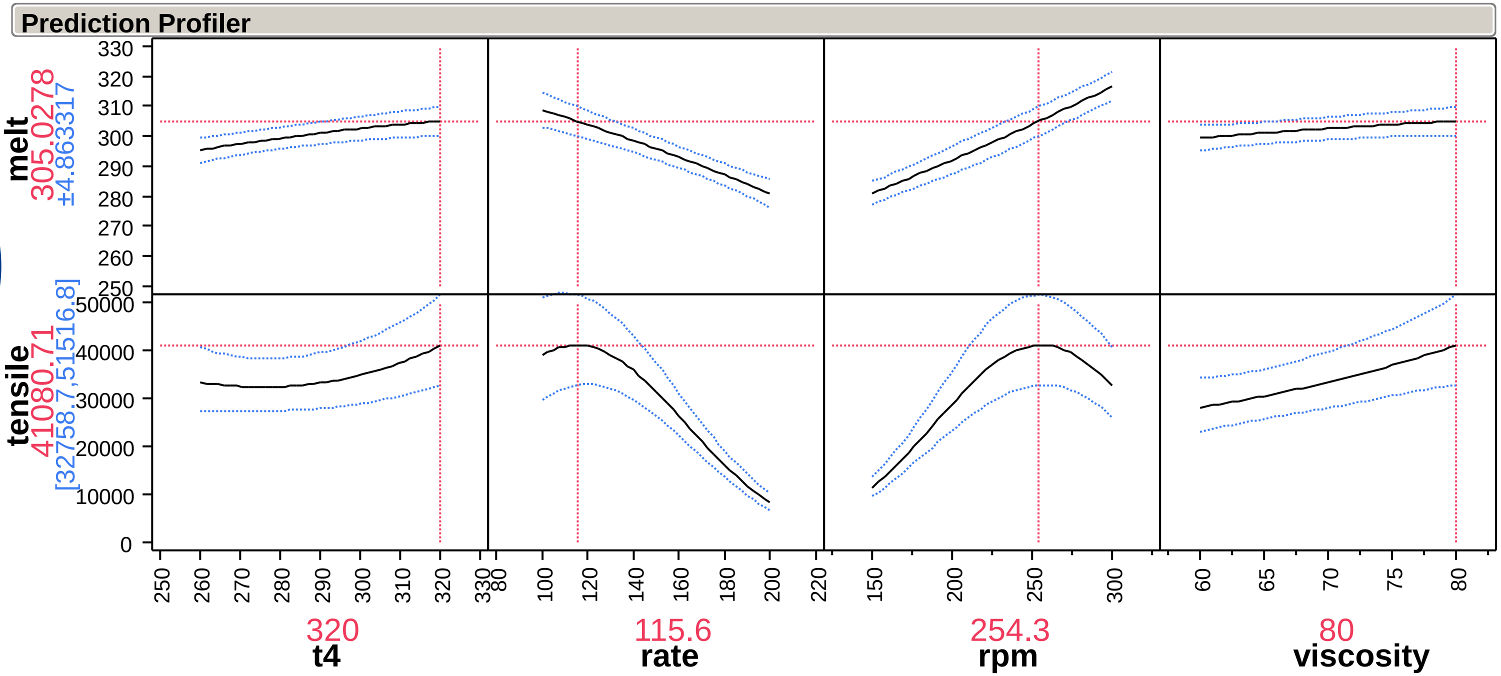




2-D contour plot

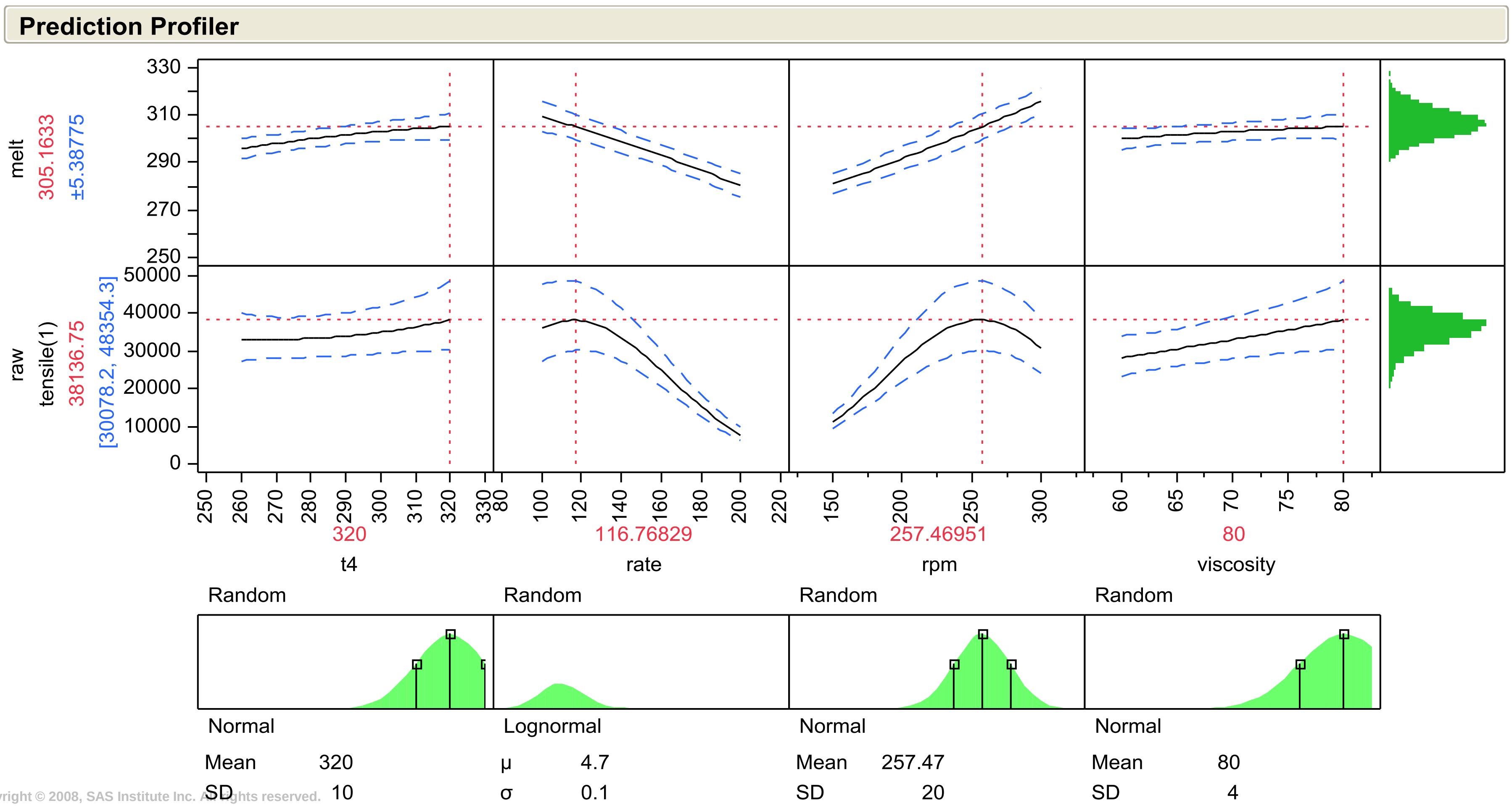
1-D Prediction Profiles are a Way to View Higher Dimensionality as "Interactive Small Multiples" - Here 4 Controls & 2 Responses

1-D profiler plots



Assess Uncertainty in Metamodel Predictions Even for a Non-Stochastic Simulation with No Replications

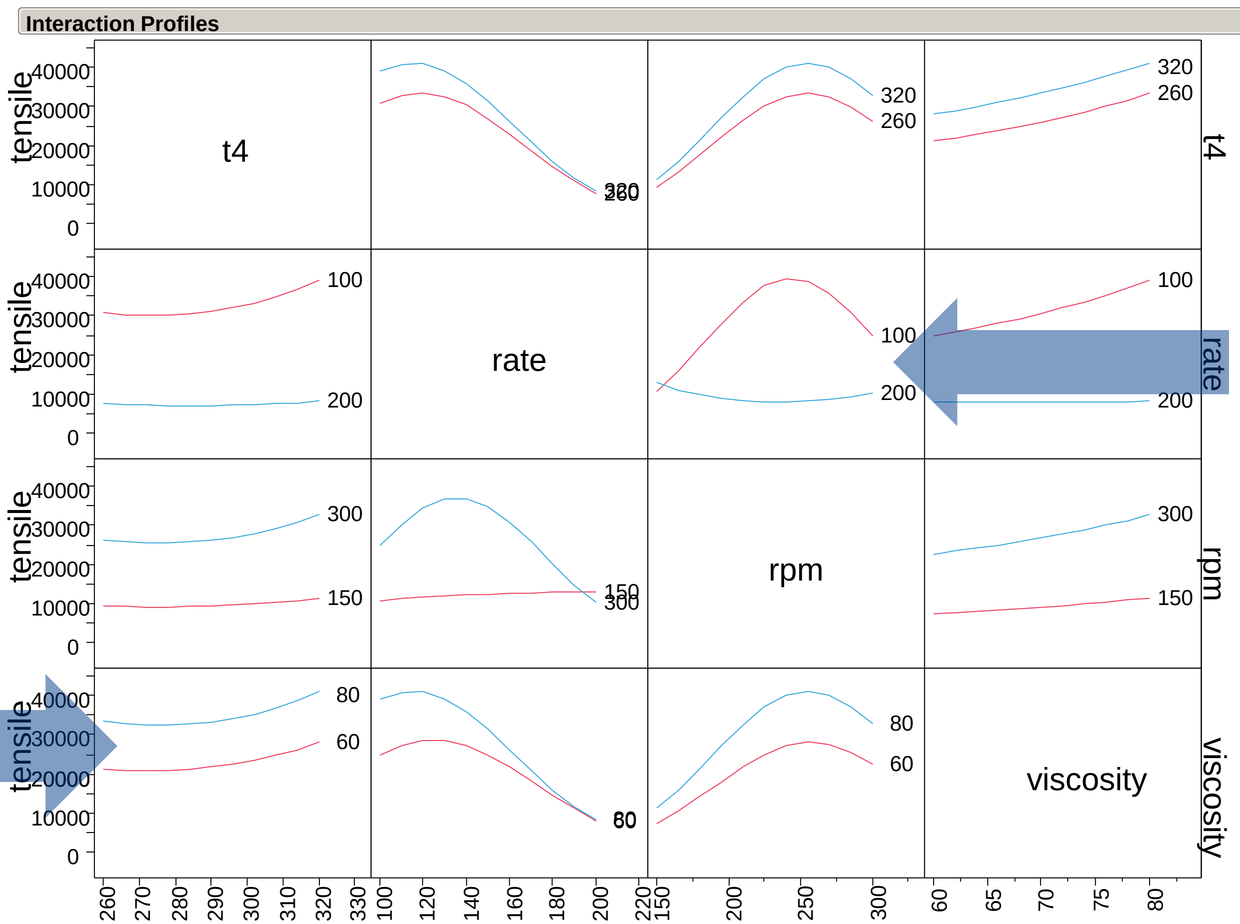
For non-stochastic simulations for which a metamodel has been created, Monte Carlo simulations can be run using assumed distributions for inputs to better assess transmitted variation about the model point estimate.



1-D Prediction Profiles are a Way to View Higher Dimensionality as "Interactive Small Multiples" - Here 4 Controls & 2 Responses

1-D profiler plots

Interaction Profiles are Another Way to View Higher Dimensionality - Here 4 Controls and 1 Response



1-D plots at high & low of other factors

NOT Parallel indicates interaction

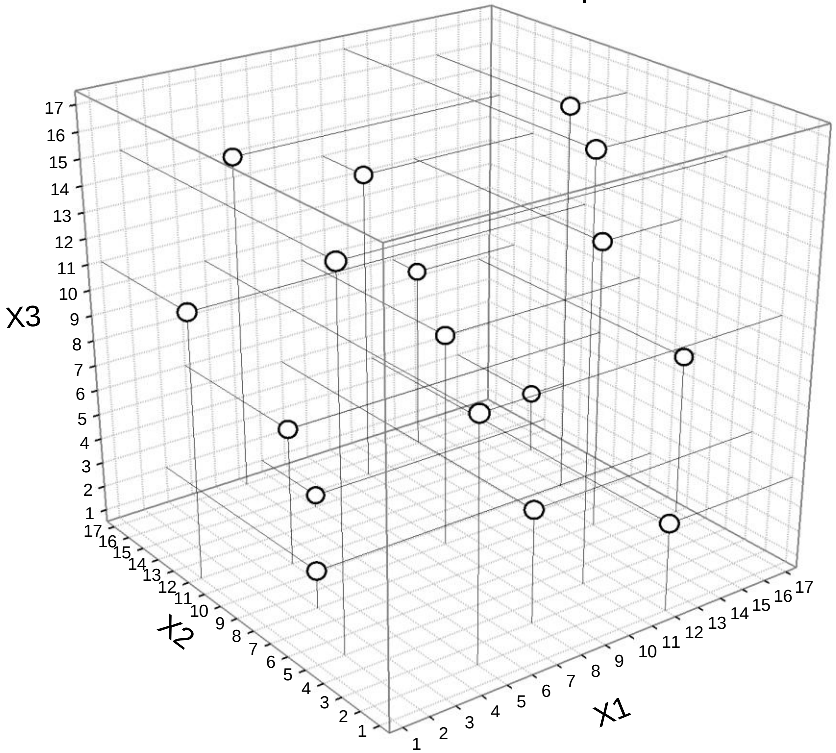
Parallel indicates NO interaction

Two Classes of Designs for Two Types of Metamodeling of Simulations

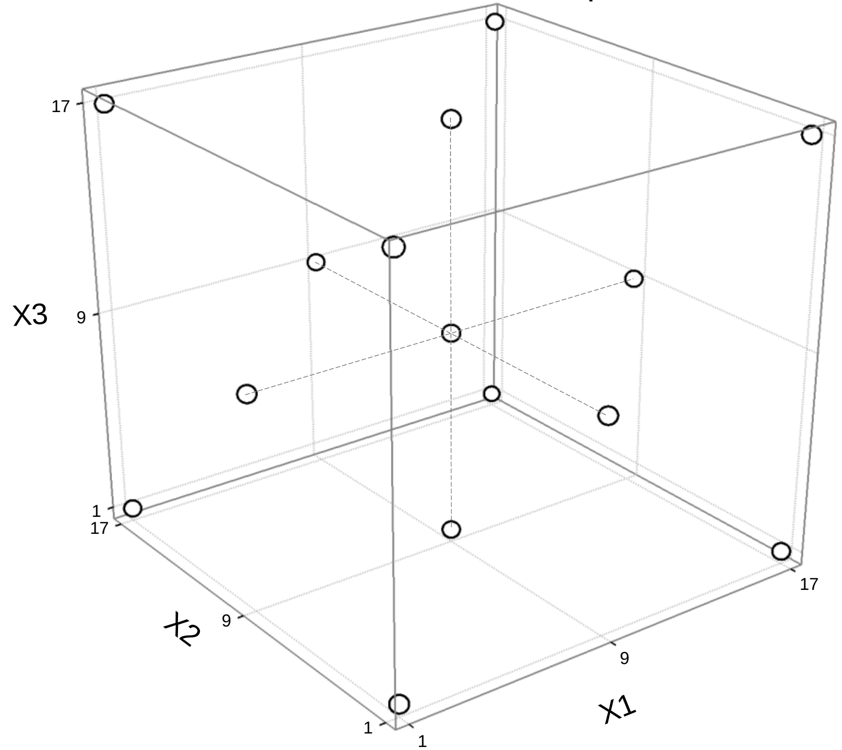
- “Traditional factorial/response surface” designs for polynomial modeling with categorical (qualitative) and continuous (quantitative) variables
  - Designs can be sequentially constructed to support increasingly complex models
  - Whitepaper example reanalyzes a simulation case matrix in which all 648 = 6X3X3X3X2X2 combinations of 6 variable settings were originally run
  - References on Resolution V, Fractional-Factorial Designs for many (40+) factors
    - Mee, R. W. (2004), **Efficient Two-Level Designs for Estimating Main Effects and Two-Factor Interactions**, *Journal of Quality Technology*, 36, 400-412.
    - Sanchez, S.M. and Sanchez, P.J. (2005), **Very Large Fractional Factorial and Central Composite Designs**, *ACM Transactions on Modeling and Computer Simulation*, Vol. 15, No. 4, October 2005, Pages 362–377.
    - Xu, H. (2009), **Algorithmic Construction of Efficient Fractional Factorial Designs with Large Run Sizes**, *Technometrics*, (in press) http://www.stat.ucla.edu/~hqxu/pub/ffd2r3.pdf
- “Space-filling” designs primarily for use with continuous variables AND non-stochastic/deterministic responses
  - These designs can support “Gaussian Process” or “Kriging” spatial regression analysis – an interpolation technique, as well as linear regression – an approximation method

How are Space-Filling Designs Different from Traditional Designs?

Space-Filling Design
for 3 Variables with 17 Unique Trials



Response-Surface Design
for 3-Variables with 15 Unique Trials



Rather than emphasizing high leverage trials ("corners") for a simple polynomial model, space-filling designs "spread" their trials more uniformly through the space to better capture the local complexities of the simulation model.

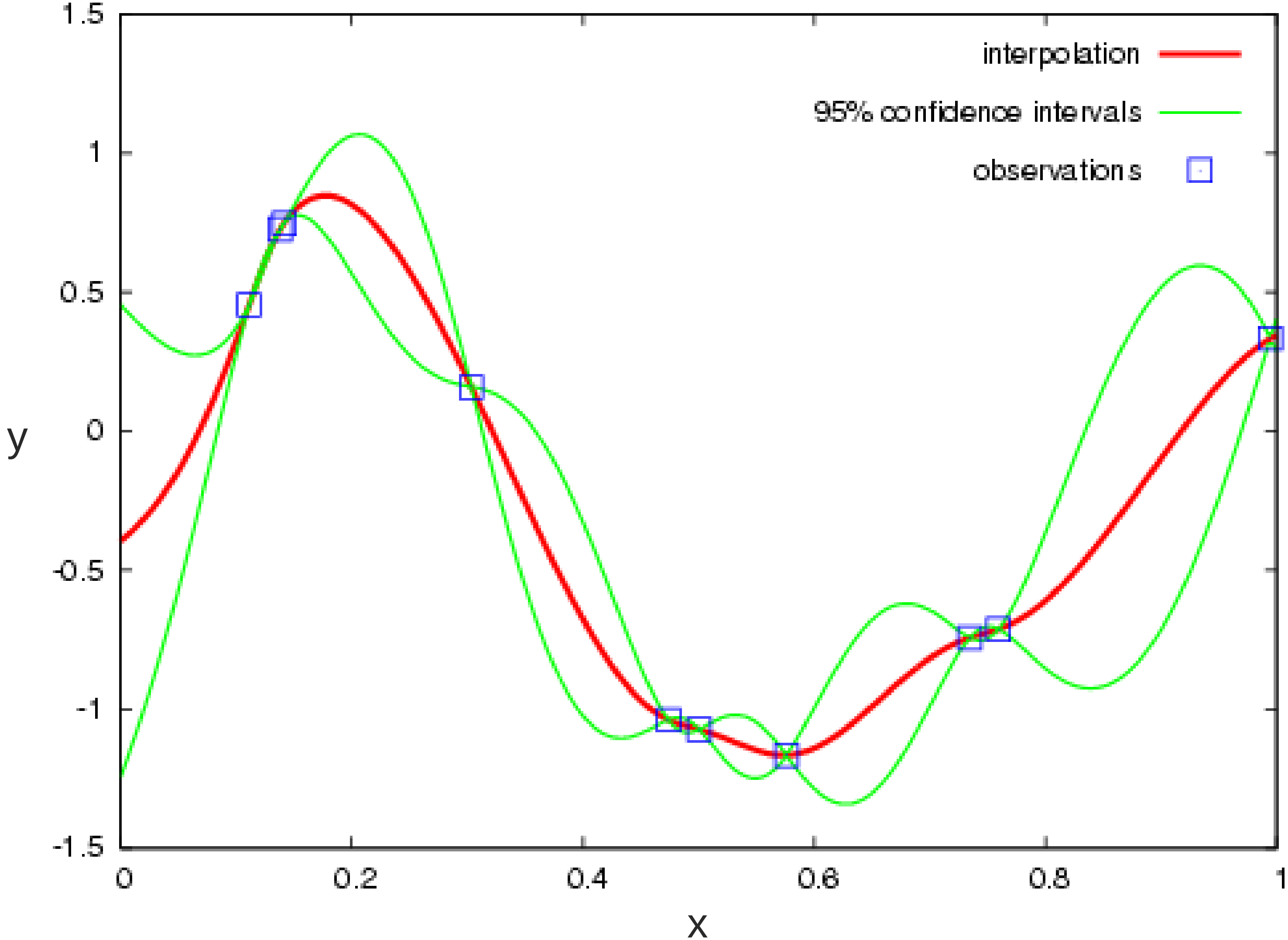
29 CFD Simulations Run – 17 Used to Metamodel & 12 Used as Checkpoints

17-trial Orthogonal Latin Hypercube (OLH) space-filling design settings used for creating the metamodel

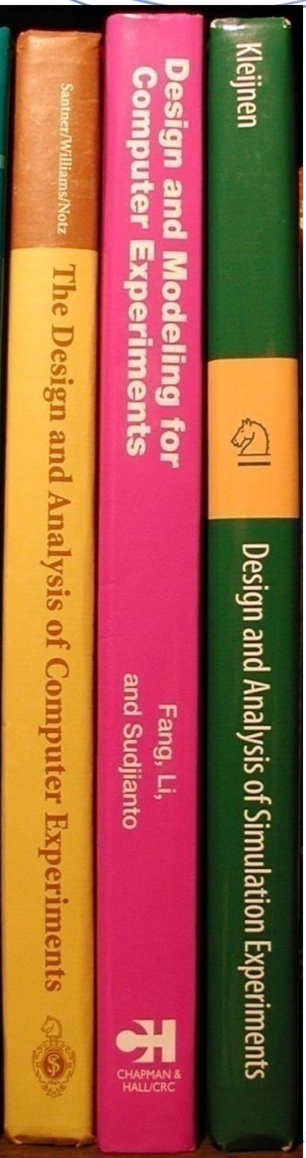
12-trial Plackett-Burman screening design settings used as checkpoints – half just inside and half just outside design boundary (convex hull)

Trial	Time of Day	Temperature	Wind Speed	Wind Direction	Relative Humidity	Cloud Cover	
1	505	37	5.3	247.5	30	0.92	
2	165	13	5.6	281.25	10	0.32	
3	250	19	1.7	225	60	0.8	
4	335	25	2.9	360	55	0.14	
5	1100	35	3.5	202.5	35	0.02	- Min
6	1440	15	3.2	326.25	15	0.74	
7	930	11	6.2	236.25	80	0.44	
8	845	33	5	348.75	75	0.62	
9	760	21	3.8	270	50	0.5	- Mid
10	1015	5	2.3	292.5	70	0.08	
11	1355	29	2	258.75	90	0.68	
12	1270	23	5.9	315	40	0.2	
13	1185	17	4.7	180	45	0.86	
14	420	7	4.1	337.5	65	0.98	- Max
15	80	27	4.4	213.75	85	0.26	
16	590	31	1.4	303.75	20	0.56	
17	675	9	2.6	191.25	25	0.38	
18	972.5	26	3.05	298.125	62.5	0.65	Inside
19	547.5	16	4.55	241.875	62.5	0.65	Outside
20	972.5	26	3.05	241.875	37.5	0.65	Outside
21	547.5	26	4.55	298.125	37.5	0.35	Outside
22	972.5	16	4.55	298.125	62.5	0.35	Inside
23	547.5	16	3.05	241.875	37.5	0.35	Inside
24	547.5	26	4.55	241.875	62.5	0.65	Outside
25	972.5	16	4.55	298.125	37.5	0.65	Inside
26	547.5	26	3.05	298.125	62.5	0.35	Inside
27	547.5	16	3.05	298.125	37.5	0.65	Outside
28	972.5	16	3.05	241.875	62.5	0.35	Outside
29	972.5	26	4.55	241.875	37.5	0.35	Inside

Kriging Fit in 1-D Showing Interpolation and Confidence Intervals on Prediction



Seminal Paper on "Space-Filling" DOE for Computer Experiments



- **Design and Analysis of Computer Experiments**
  Sacks, J., Welch, W.J., Mitchell, T.J. and Wynn, H.P.
  Statistical Science 4. 409-423, 1989

- Textbooks on this topic include:
  - Santner, T. J., Williams, B. J., and Notz, W. I. (2003), *The Design and Analysis of Computer Experiments*, Springer, New York
  - Fang, K. T., Li, R. Z., and Sudjianto, A. (2005), *Design and Modeling for Computer Experiments*, Chapman & Hall/CRC Press, New York
  - Kleijnen, J. P. C. (2008), *DASE: design and analysis of simulation experiments*. Springer, New York.

Software Tools for Kriging Analysis
(that I know about…)

- JMP® (called Gaussian Process modeling)
- ECHIP® (called Smoothing analysis)
- SYSTAT® (called Kriging analysis)
- Matlab® Toolbox Modules
  - Design and Analysis of Computer Experiments (DACE)
  - SUrrogate MOdeling (SUMO)
    - Contains DACE as well as another Kriging tool and many other surrogate modeling methods
- PErK (code available from authors of 2003 text by Santner, et. al.)
- “Blind” Kriging – R code potentially available from GA Tech
- The Gaussian Processes Website: http://www.gaussianprocess.org
- Code to do Bayesian Hierarchical Gaussian Process (BHGP) modeling by combining simulation and real experimental data is available from Prof. Peter Qian of the University of Wisconsin

Websites for Designs, Software & Publications

- http://harvest.nps.edu/
  The Simulation Experiments & Efficient Design (SEED) Center for Data Farming at Naval Postgraduate School
  - Designs
    - Nearly Orthogonal Latin Hypercubes (NOLH) and
    - Resolution V, Fractional Factorials for many factors
  - Agent-Based Simulation Software
    - Pythagoras
    - MANA (Map Aware Non-uniform Automata)
  - Many Papers for Download and Links to INFORMS and WSC
- http://www.research.att.com/~njas/oadir/index.html
  Library of Orthogonal Arrays maintained by Neil J.A. Sloane
- http://support.sas.com/techsup/technote/ts723.html
  Library of Orthogonal Arrays maintained by Warren F. Kuhfield

Publications Discussing Recent Advances in Metamodeling Simulations

- **Blind Kriging: A New Method for Developing Metamodels**,
  Joseph, V.R., Hung, Y., and Sudjianto, A.,
  ASME Journal of Mechanical Design, 130, 031102-1-8, 2008
- **Gaussian Process Models for Computer Experiments With Qualitative and Quantitative Factors**,
  Qian, P.Z.G., Wu, H., and Wu, C.F.J.,
  Technometrics, 50 (4), 383-396, 2008
- **Bayesian Hierarchical Modeling for Integrating Low-Accuracy and High-Accuracy Experiments,**
  Qian, P. Z. G. and Wu, C. F. J.,
  Technometrics, 50 (2), 192-204, 2008
- **Regression-Based Inverse Distance Weighting for Multivariate Interpolation,**
  Joseph, V.R., and Kang, L.,
  (submitted) Preprint May 2009
- **Nested Latin Hypecube Designs,**
  Qian, P. Z. G.
  Biometrika (to appear) Preprint September 2008

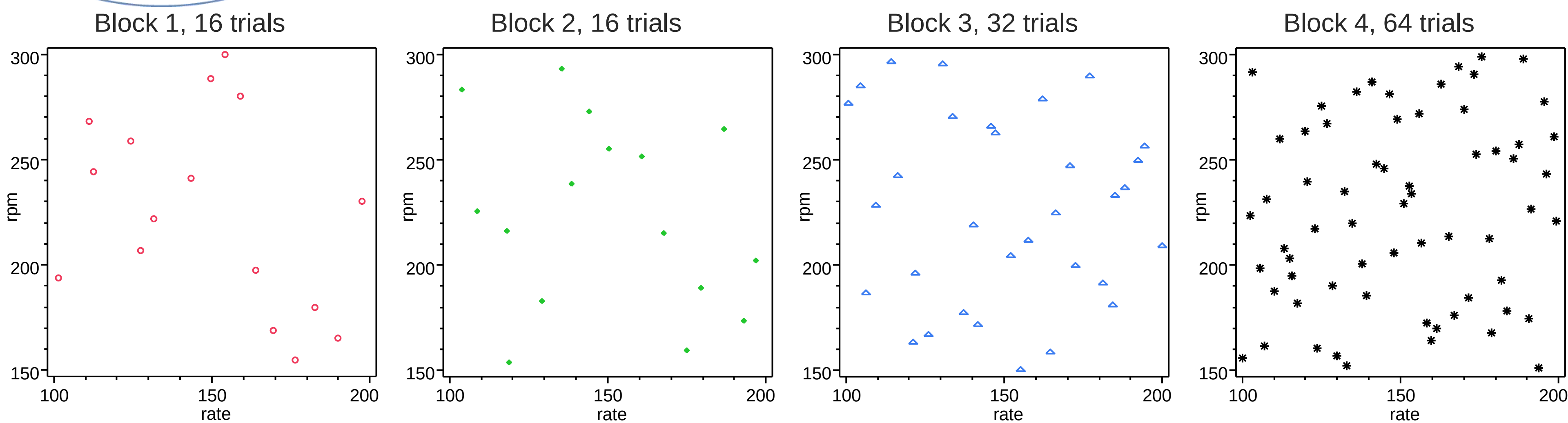
Why Is a Sequential Approach So Useful?

We wanted to run the fewest simulations that would allow us to extract useful information about the simulated process. We wanted to not just do sensitivity analysis of the factors, but **provide an interactive surrogate** model of the long-running simulation so that analysts could evaluate “what if?” scenarios.

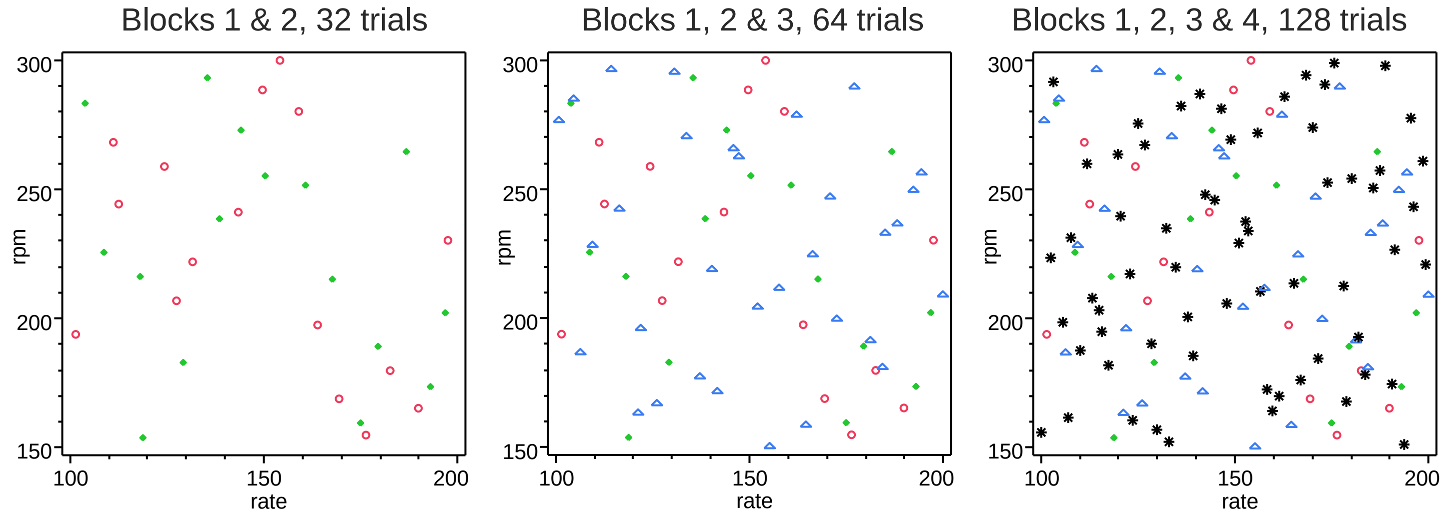
The problem was that the Computational Fluid Dynamics models we were looking to run could take a week on a single CPU or 12 hours on 50 CPU cluster. With on the order of 10 factors we expected to need to run on the order of 100 simulations. **This meant it could be weeks or months before we could start our analysis.**

Nested Latin Hypercube Designs gave us a way to start analyzing data after about the first 20% of the simulations were run. We also wanted to be able to run just enough simulations to achieve a surrogate model accuracy of 90%. We measured the accuracy using checkpoints and report the **% Off Target** for individual points as well as the RMS of the group and visualize the error using plots of Actual (from simulation) vs. Predicted (from surrogate model) values.

Projections of Trial Locations in 2 factors for a 10-factor, 128-trial, Nested Latin Hypercube Design* (NLHD) with 4 Blocks

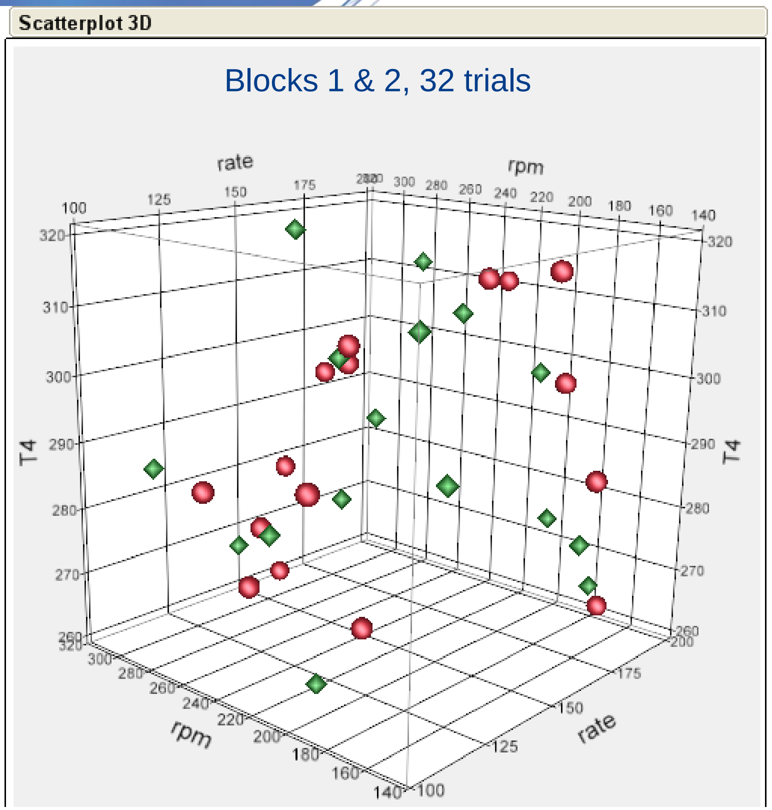


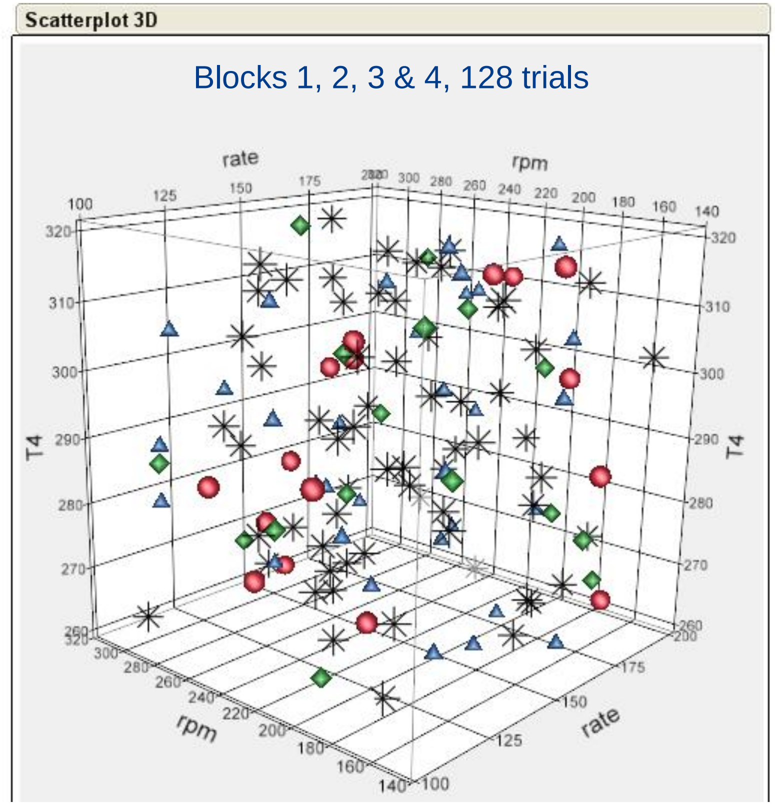
Running totals of blocks are also Latin Hypercube Designs

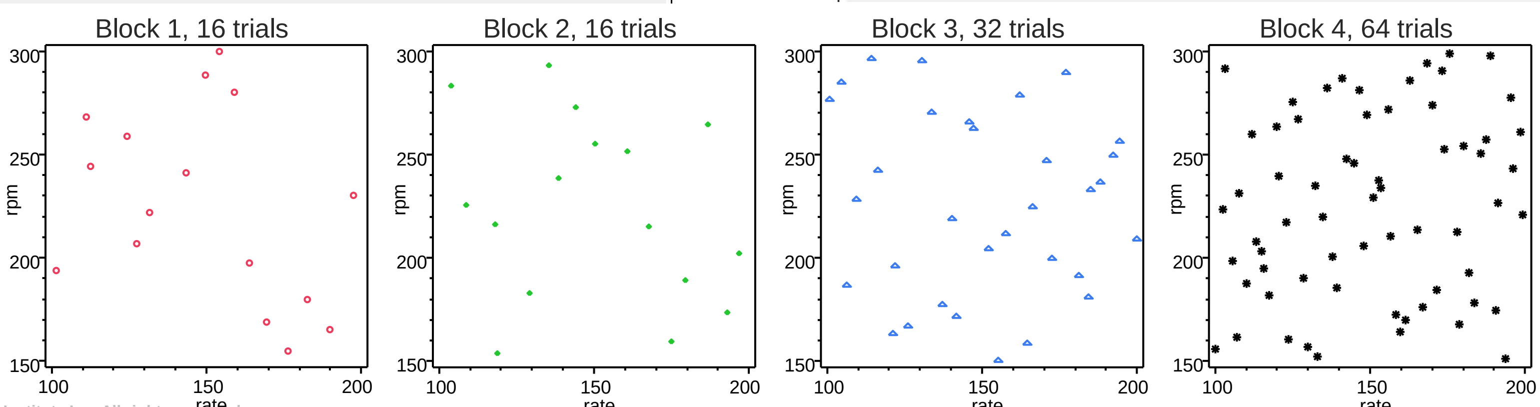


*Generated with Matlab Code Received from Prof. Peter Qian of U of Wi.

Projections of Trial Locations in 3 factors for a 10-factor. 128-trial, Nested Latin Hypercube Design (NLHD) in 4 Blocks



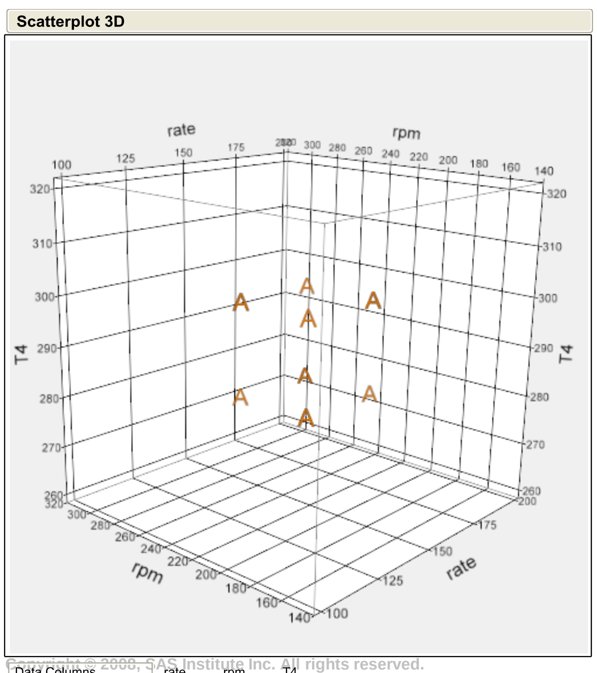


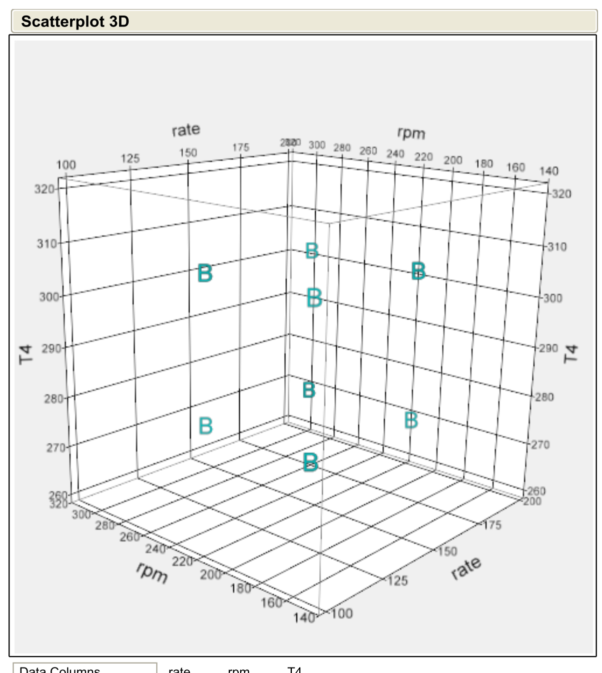


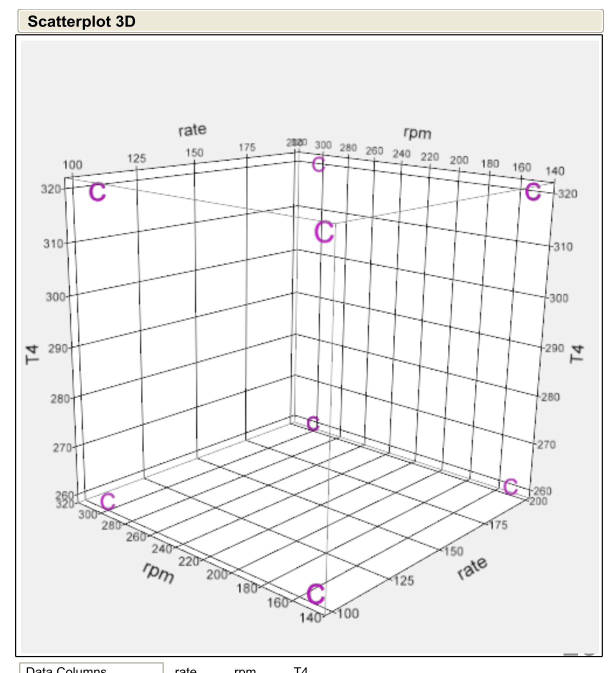
Why Run Simulations in Sequential Blocks?

The point of running this sequence of blocks is to be able to evaluate the metamodel after each stage to see how accurately it is predicting observed values of 3 sets of checkpoint trials. If it proves to be sufficiently accurate, then subsequent blocks of simulation trials need not be run.

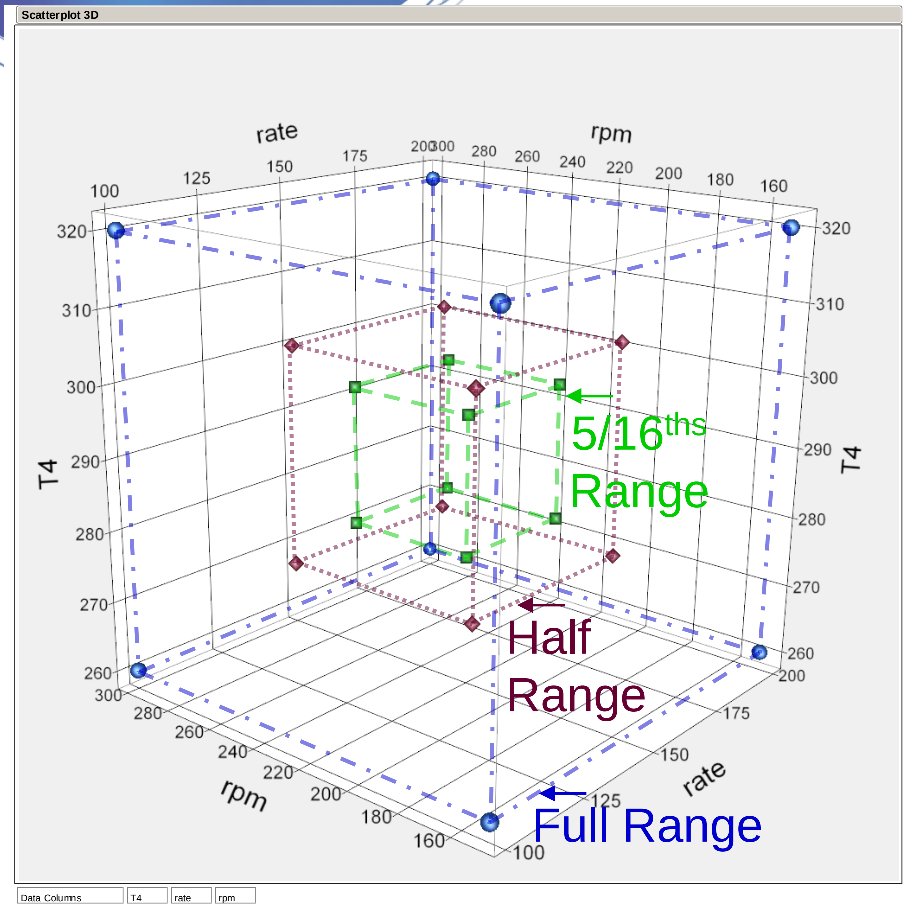
Without the NLHD approach one has to choose the “right” size space-filling design in order to get useful results. If you choose too small a design, one has to start over with a larger design.

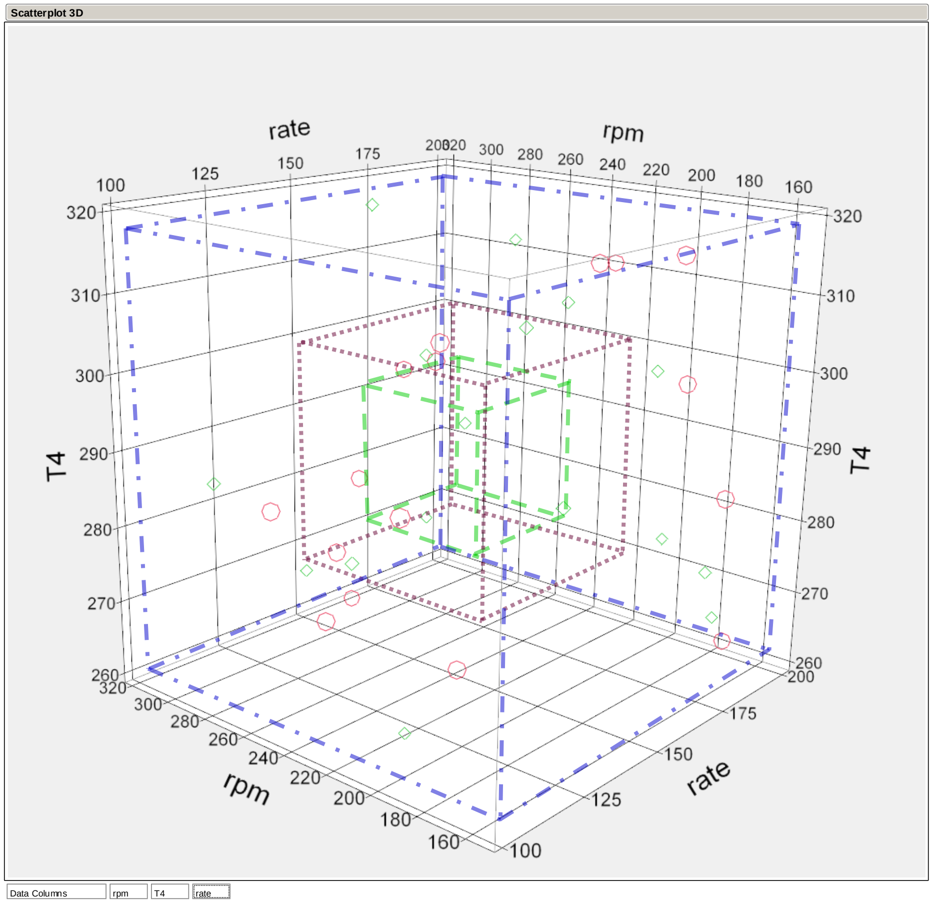






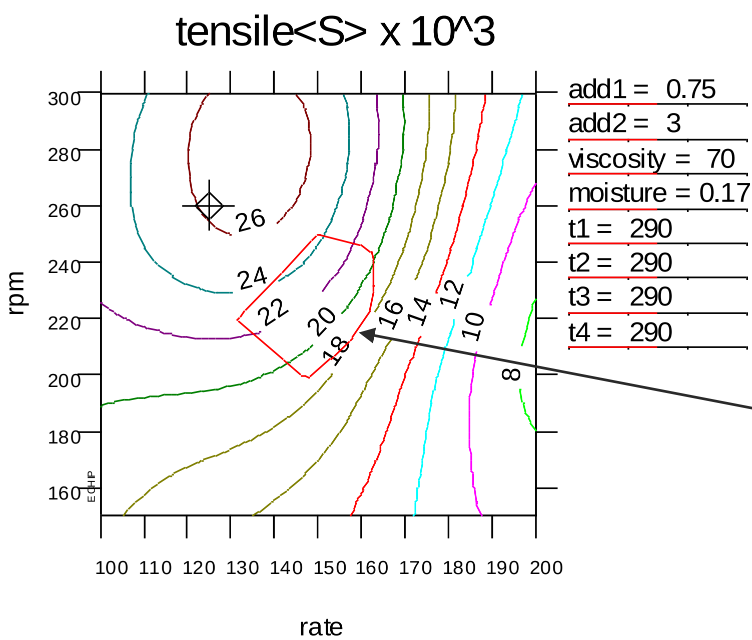
Relative Ranges for 3 Sets of 12 Checkpoints Shown in a 3-factor Space and Superimposed on Block 1 & 2 trials





In the full design space over 10 factors there are 10 dimensions and 1024 corners. The 12 trials in a Plackett-Burman design populate only about 0.1% of these combinations of settings.

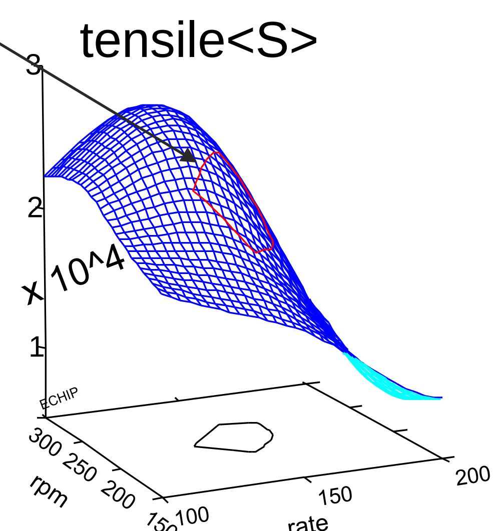
Used 10-factor Process Based on a Transcendental Function as the “Simulation” to Evaluate Improvement in Accuracy



rate=125.00		rpm=260.00	
Value	Low Limit	High Limit	
26259.40	-1.#J	1.#J	

The 10-dimensional design space is only sparsely covered by the initial 16-trial NLHD Block. As a result only a small fraction of the full design region is valid for interpolation with the Kriging analysis.

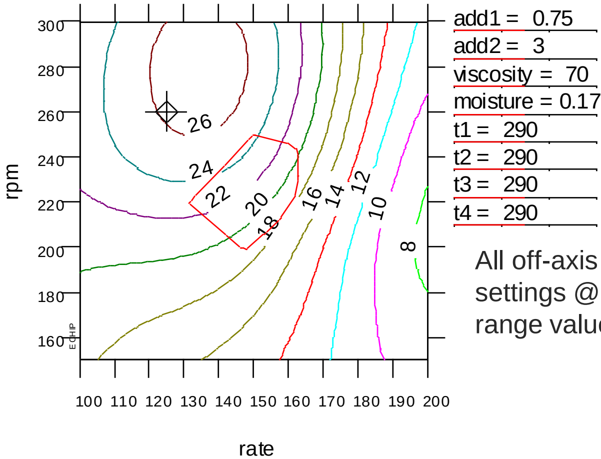
Red polygon marks boundary between regions of interpolation (inside) and extrapolation (outside). Statistical name for the design boundary is the “Convex Hull.”



NLHD, 16 trials Block 1 only

Outside Design ← Note that this entire plot is extrapolation.

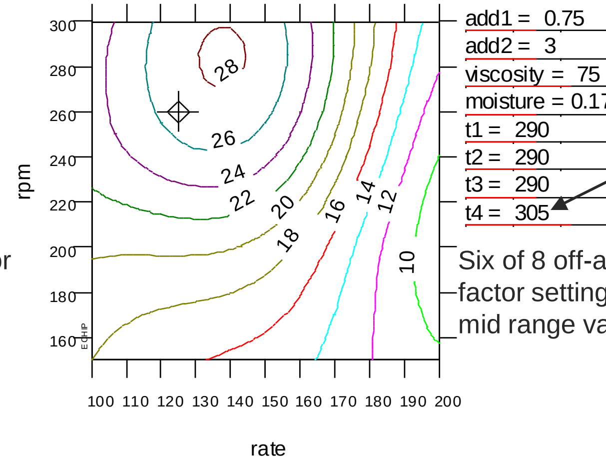
tensile<S> x 10^3



All off-axis factor settings @ mid range value

rate=125.00		rpm=260.00
Value	Low Limit	High Limit
26259.40	-1.#J	1.#J

tensile<S> x 10^3



viscosity and *t4* factor settings @ 75% of range

Six of 8 off-axis factor settings @ mid range value

rate=125.00		rpm=260.00
Value	Low Limit	High Limit
26826.46	-1.#J	1.#J

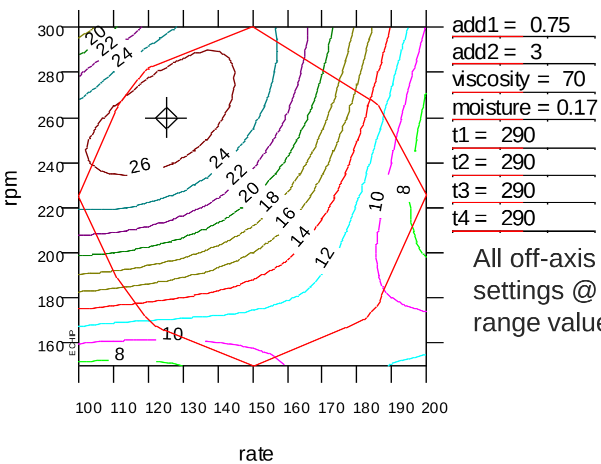
COEFFICIENTS	SD	P	CONDITION	TERM
18903.8				0 CONSTANT
-6319.34	8425.11	0.4870-	0.559	1 add1
-882.924	1658.5	0.6173-	0.703	2 add2
139.372	143.796	0.3769-	0.820	3 viscosity
-25974.4	19170.6	0.2334	0.813	4 moisture
32.8283	74.8572	0.6793-	0.515	5 t1
21.6944	79.5117	0.7959-	0.488	6 t2
61.0479	88.6668	0.5218-	0.432	7 t3
44.7973	81.6762	0.6070-	0.477	8 t4
-128.299	42.7544	0.0301	0.550	9 rate
96.4185	27.5245	0.0172	0.546	10 rpm

N trials = 16

Closer to 1.000 the CONDITION is, the closer the term is to being orthogonal

NLHD, 16 + 12PB = 28

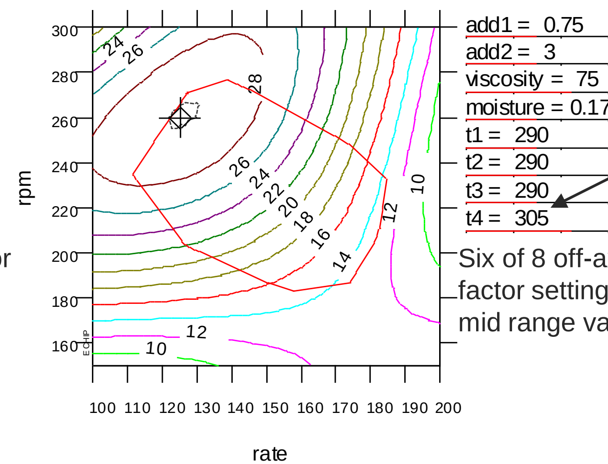
tensile<S> x 10^3



All off-axis factor settings @ mid range value

rate=125.00		rpm=260.00
Value	Low Limit	High Limit
27257.18	-1.#J	1.#J

tensile<S> x 10^3



viscosity and *t4* factor settings @ 75% of range

Six of 8 off-axis factor settings @ mid range value

rate=125.00		rpm=260.00
Value	Low Limit	High Limit
30078.62	-1.#J	1.#J

COEFFICIENTS	SD	P	CONDITION	TERM
15760.2				0 CONSTANT
-721.328	6720.15	0.9158-	0.958	1 add1
966.423	1647.02	0.5651-	0.974	2 add2
65.0763	163.369	0.6953-	0.986	3 viscosity
4164.81	21651	0.8497-	0.989	4 moisture
-7.23148	54.8311	0.8966-	0.973	5 t1
1.39981	54.9105	0.9800-	0.973	6 t2
-38.7242	56.0048	0.4986-	0.951	7 t3
47.8879	54.5957	0.3926-	0.981	8 t4
-49.521	32.9741	0.1515	0.976	9 rate
43.0792	21.8001	0.0646	0.971	10 rpm

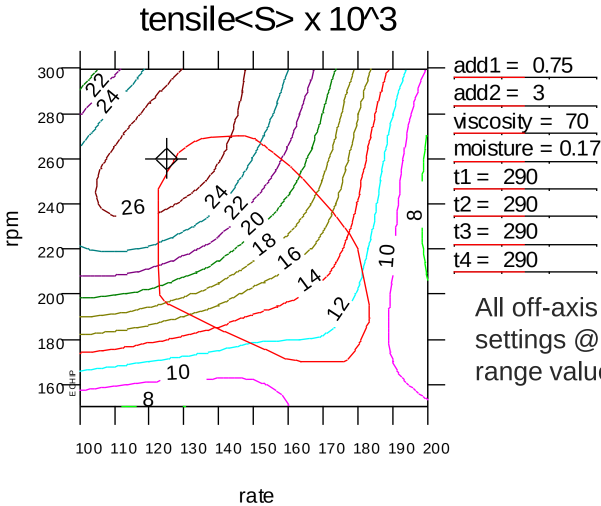
N trials = 28

Closer to 1.000 the CONDITION is, the closer the term is to being orthogonal

Inclusion of checkpoints – here the 12 over the full range of the factors – increases the size of the design boundary and the volume of interpolation region.

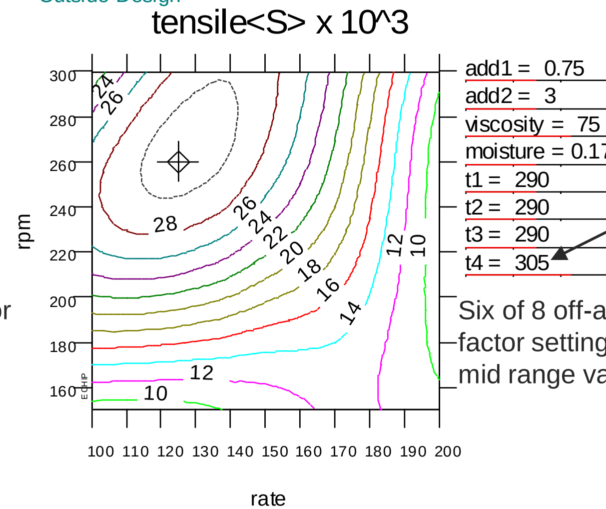
Note that this entire plot is extrapolation.

NLHD, 16+16=32
Blocks 1 & 2



All off-axis factor settings @ mid range value

rate=125.00		rpm=260.00
Value	Low Limit	High Limit
27472.20	-1.#J	1.#J



Six of 8 off-axis factor settings @ mid range value

viscosity and *t4* factor settings @ 75% of range

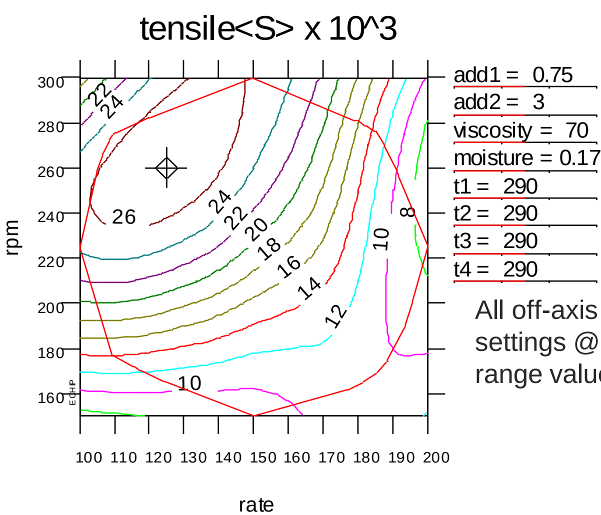
rate=125.00		rpm=260.00
Value	Low Limit	High Limit
30883.50	-1.#J	1.#J

COEFFICIENTS	SD	P	CONDITION	TERM
18531.7				0 CONSTANT
1212.93	4539.39	0.7919-	0.726	1 add1
135.003	958.231	0.8893-	0.851	2 add2
221.529	90.1658	0.0228	0.912	3 viscosity
-30145.8	11927.6	0.0196	0.927	4 moisture
-14.2204	29.1939	0.6312-	0.934	5 t1
49.8103	32.4395	0.1396	0.845	6 t2
48.3131	38.6135	0.2246	0.714	7 t3
15.6962	29.8311	0.6043-	0.918	8 t4
-112.799	19.747	0.0000	0.834	9 rate
92.325	11.7728	0.0000	0.926	10 rpm

N trials = 32

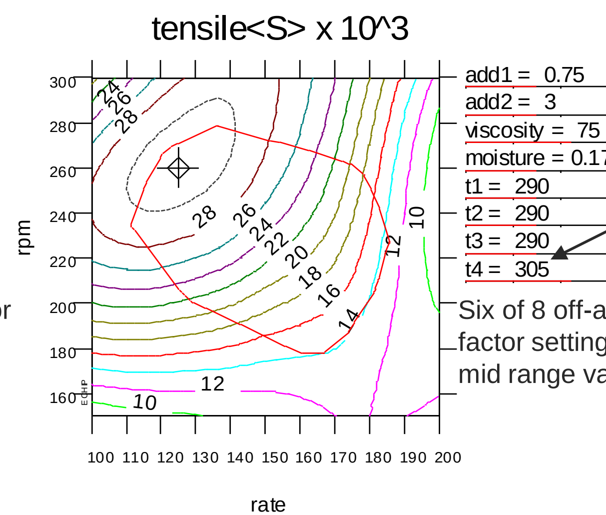
Closer to 1.000 the CONDITION is, the closer the term is to being orthogonal

NLHD, 16+16+12PB=44



All off-axis factor settings @ mid range value

rate=125.00		rpm=260.00
Value	Low Limit	High Limit
27563.82	-1.#J	1.#J



Six of 8 off-axis factor settings @ mid range value

viscosity and *t4* factor settings @ 75% of range

rate=125.00		rpm=260.00
Value	Low Limit	High Limit
30968.80	-1.#J	1.#J

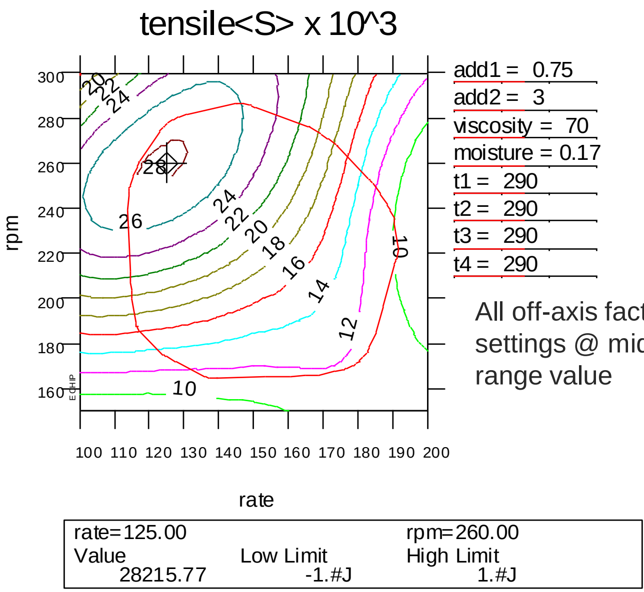
COEFFICIENTS	SD	P	CONDITION	TERM
16643.5				0 CONSTANT
-2070.44	5151.64	0.6903-	0.949	1 add1
366.611	1259.06	0.7727-	0.965	2 add2
155.971	123.529	0.2156-	0.988	3 viscosity
-7017.98	16560.7	0.6745-	0.987	4 moisture
-1.97997	41.1751	0.9619-	0.986	5 t1
-2.08728	41.927	0.9606-	0.970	6 t2
-11.9864	43.2157	0.7832-	0.944	7 t3
50.5763	41.4962	0.2316-	0.980	8 t4
-64.4773	25.1173	0.0150	0.972	9 rate
57.4236	16.5153	0.0014	0.983	10 rpm

N trials = 44

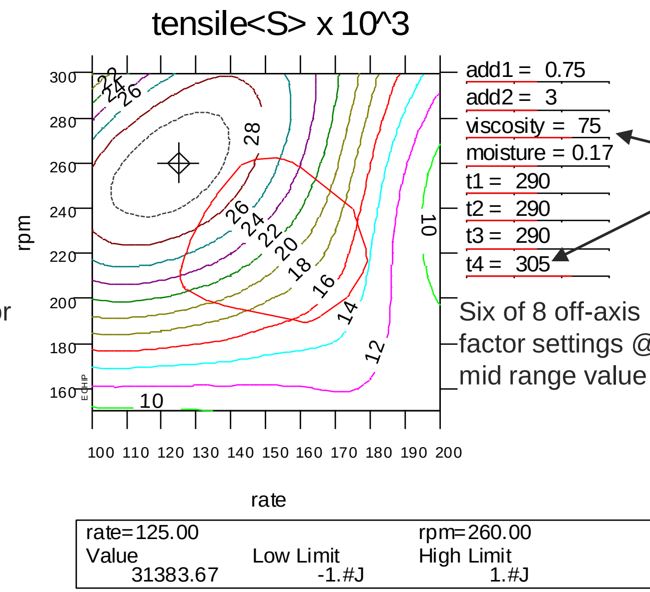
Closer to 1.000 the CONDITION is, the closer the term is to being orthogonal

Inclusion of checkpoints – here the 12 over the full range of the factors – increases the size of the design boundary and the volume of interpolation region.

NLHD, 16+16+32=64
Blocks 1, 2 & 3



All off-axis factor settings @ mid range value



viscosity and *t4* factor settings @ 75% of range

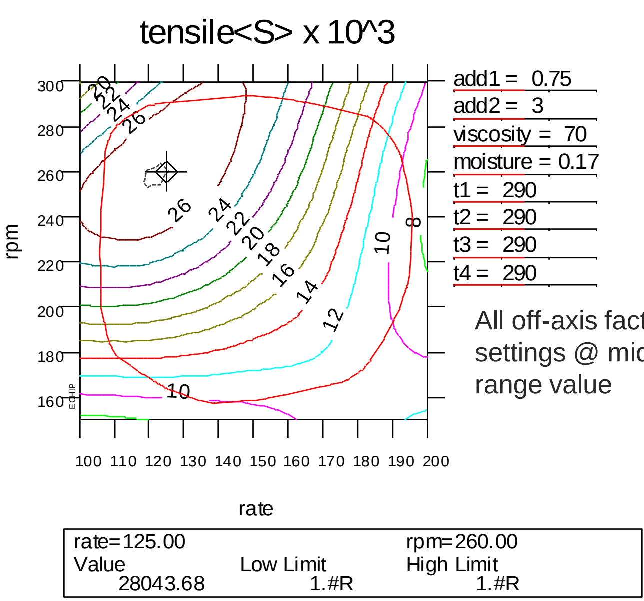
Six of 8 off-axis factor settings @ mid range value

COEFFICIENTS	SD	P	CONDITION	TERM
17650.5				0 CONSTANT
-386.323	3428.92	0.9107-	0.849	1 add1
325.397	760.293	0.6704-	0.954	2 add2
236.131	75.8927	0.0030	0.959	3 viscosity
-22930.2	10466.1	0.0329	0.931	4 moisture
-1.37838	25.5501	0.9572-	0.948	5 t1
22.6743	26.9106	0.4033-	0.898	6 t2
30.8245	28.3946	0.2826-	0.855	7 t3
44.6689	25.6003	0.0868	0.948	8 t4
-122.812	15.6562	0.0000	0.930	9 rate
84.9426	10.4351	0.0000	0.929	10 rpm

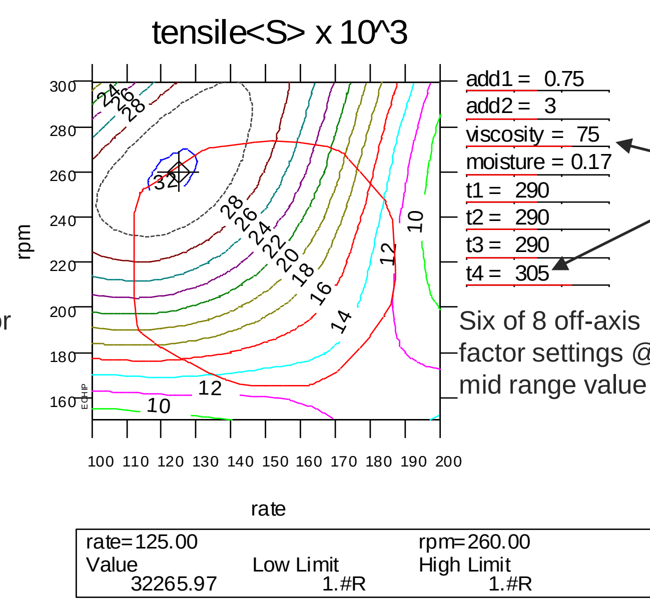
N trials = 64

Closer to 1.000 the CONDITION is, the closer the term is to being orthogonal

NLHD, 16+16+32+64=128
Blocks 1, 2, 3 & 4



All off-axis factor settings @ mid range value



viscosity and *t4* factor settings @ 75% of range

Six of 8 off-axis factor settings @ mid range value

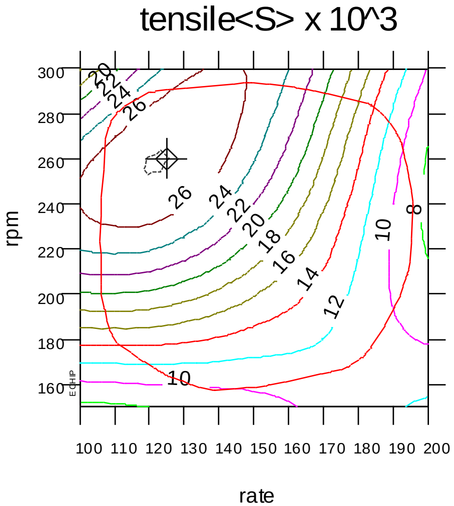
COEFFICIENTS	SD	P	CONDITION	TERM
17631.9				0 CONSTANT
-682.306	2233.14	0.7605-	0.945	1 add1
884.808	540.923	0.1046	0.975	2 add2
300.046	54.081	0.0000	0.976	3 viscosity
-3680.05	7202.41	0.6104-	0.977	4 moisture
5.82534	18.0142	0.7470-	0.976	5 t1
-11.1487	18.0473	0.5379-	0.975	6 t2
31.8328	18.7587	0.0924	0.938	7 t3
86.4875	17.8697	0.0000	0.984	8 t4
-130.079	10.864	0.0000	0.971	9 rate
90.3335	7.22455	0.0000	0.974	10 rpm

N trials = 128

Closer to 1.000 the CONDITION is, the closer the term is to being orthogonal

With the addition of each successive block of trials the size of the design boundary and the volume of interpolation region increases.

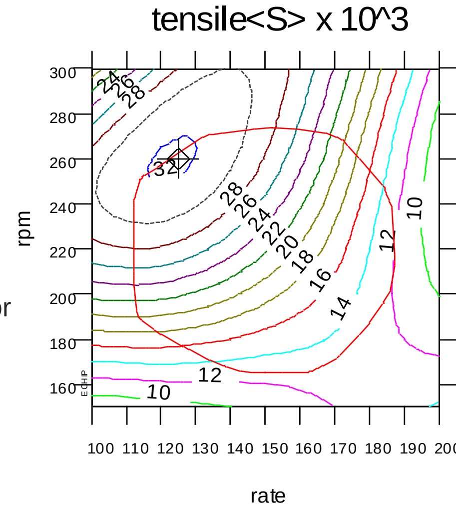
NLHD, 16+16+32+64=128
Blocks 1, 2, 3 & 4



add1 = 0.75
add2 = 3
viscosity = 70
moisture = 0.17
t1 = 290
t2 = 290
t3 = 290
t4 = 290

All off-axis factor settings @ mid range value

rate=125.00 rpm=260.00
Value Low Limit High Limit
28043.68 1.#R 1.#R



add1 = 0.75
add2 = 3
viscosity = 75
moisture = 0.17
t1 = 290
t2 = 290
t3 = 290
t4 = 305

viscosity and *t4* factor settings @ 75% of range

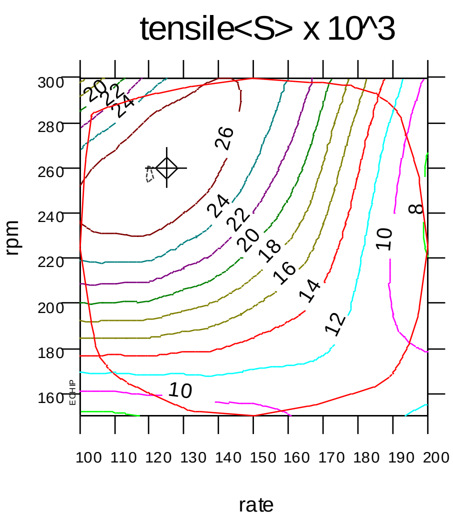
Six of 8 off-axis factor settings @ mid range value

rate=125.00 rpm=260.00
Value Low Limit High Limit
32265.97 1.#R 1.#R

COEFFICIENTS	SD	P	CONDITION	TERM
17631.9				0 CONSTANT
-682.306	2233.14	0.7605-	0.945	1 add1
884.808	540.923	0.1046	0.975	2 add2
300.046	54.081	0.0000	0.976	3 viscosity
-3680.05	7202.41	0.6104-	0.977	4 moisture
5.82534	18.0142	0.7470-	0.976	5 t1
-11.1487	18.0473	0.5379-	0.975	6 t2
31.8328	18.7587	0.0924	0.938	7 t3
86.4875	17.8697	0.0000	0.984	8 t4
-130.079	10.864	0.0000	0.971	9 rate
90.3335	7.22455	0.0000	0.974	10 rpm

N trials = 128

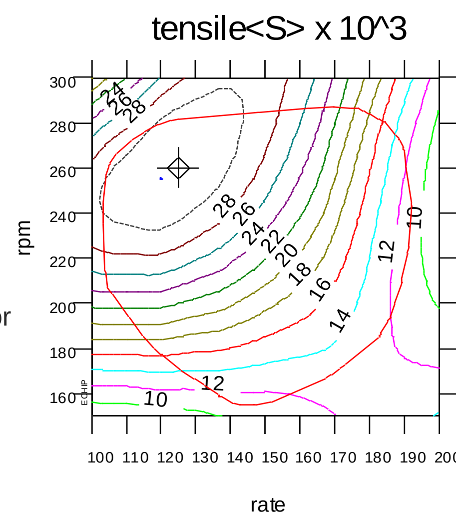
NLHD, 16+16+32+64+36ckps=164
Blocks 1- 4, & 3 sets of checkpoints



add1 = 0.75
add2 = 3
viscosity = 70
moisture = 0.17
t1 = 290
t2 = 290
t3 = 290
t4 = 290

All off-axis factor settings @ mid range value

rate=125.00 rpm=260.00
Value Low Limit High Limit
27892.11 1.#R 1.#R



add1 = 0.75
add2 = 3
viscosity = 75
moisture = 0.17
t1 = 290
t2 = 290
t3 = 290
t4 = 305

viscosity and *t4* factor settings @ 75% of range

Six of 8 off-axis factor settings @ mid range value

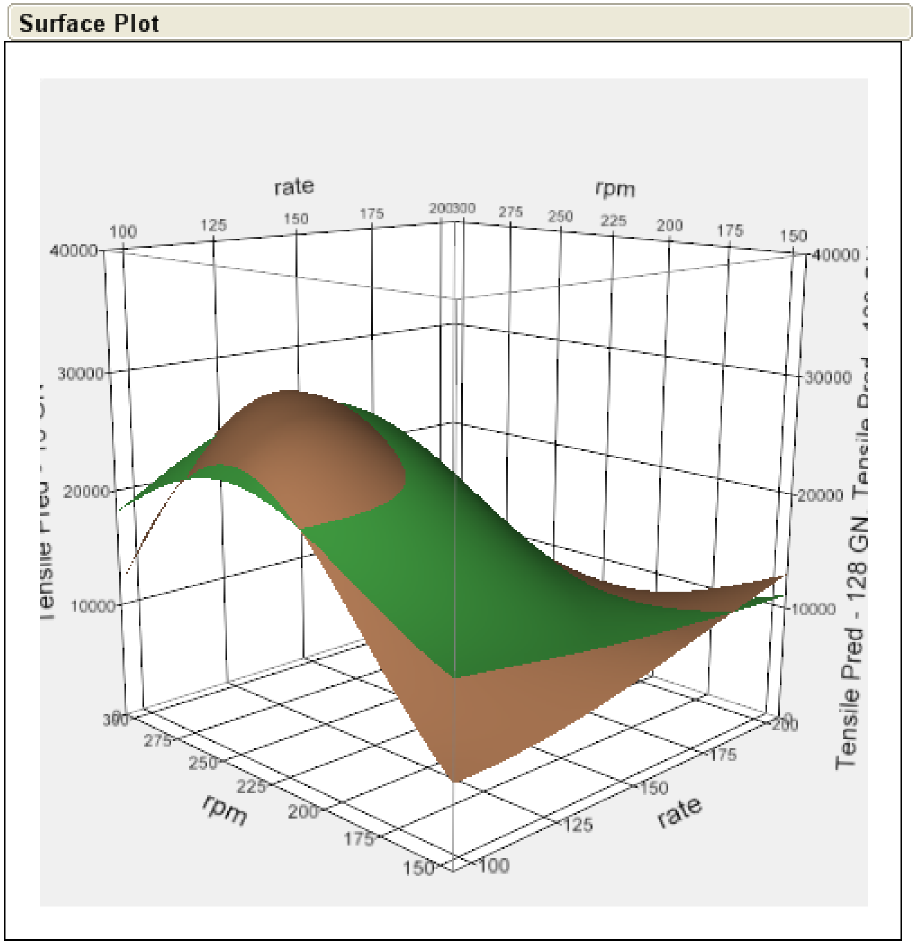
rate=125.00 rpm=260.00
Value Low Limit High Limit
31901.21 1.#R 1.#R

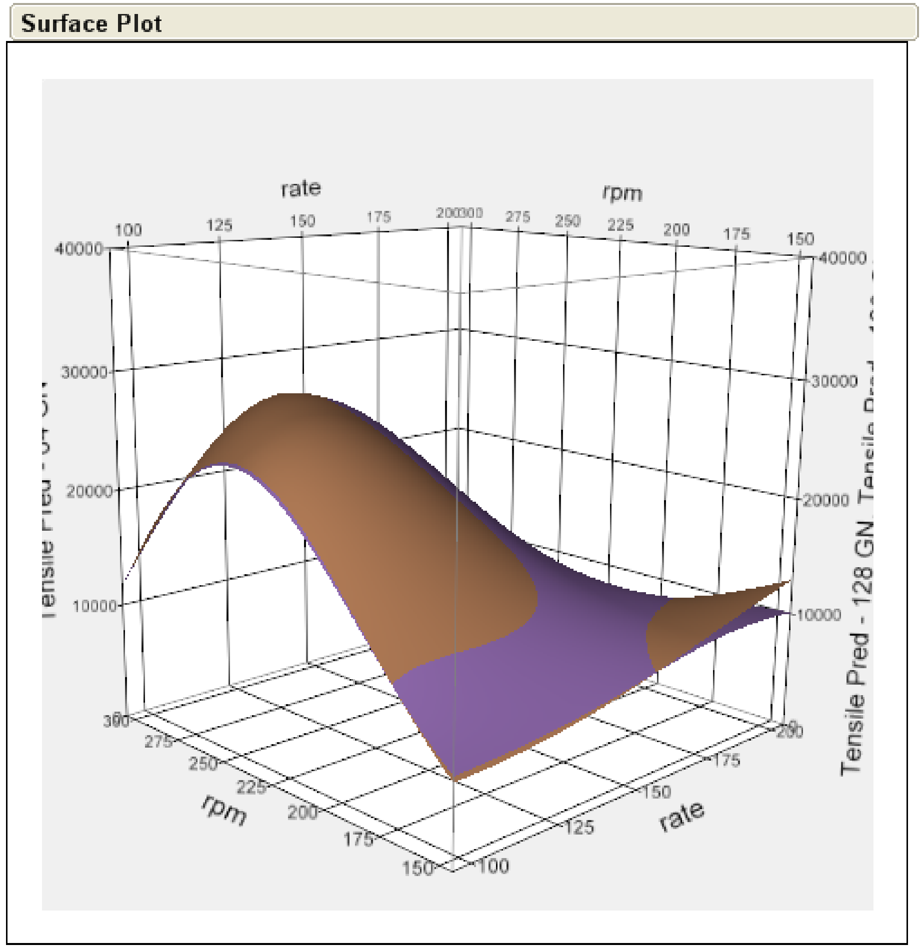
COEFFICIENTS	SD	P	CONDITION	TERM
17357				0 CONSTANT
-843.041	2246.05	0.7079-	0.973	1 add1
1016.04	553.662	0.0684	0.987	2 add2
226.532	55.3433	0.0001	0.987	3 viscosity
2098.09	7370.9	0.7763-	0.988	4 moisture
8.98137	18.4363	0.6268-	0.988	5 t1
-16.0393	18.4583	0.3862-	0.987	6 t2
5.38914	18.7981	0.7747-	0.969	7 t3
88.5134	18.3523	0.0000	0.992	8 t4
-106.215	11.086	0.0000	0.986	9 rate
76.3942	7.37976	0.0000	0.987	10 rpm

N trials = 164

Compare Response Surfaces for fit of 16 vs. fit of 128 trials (left) and for fit of 64 vs. fit of 128 trials (right)

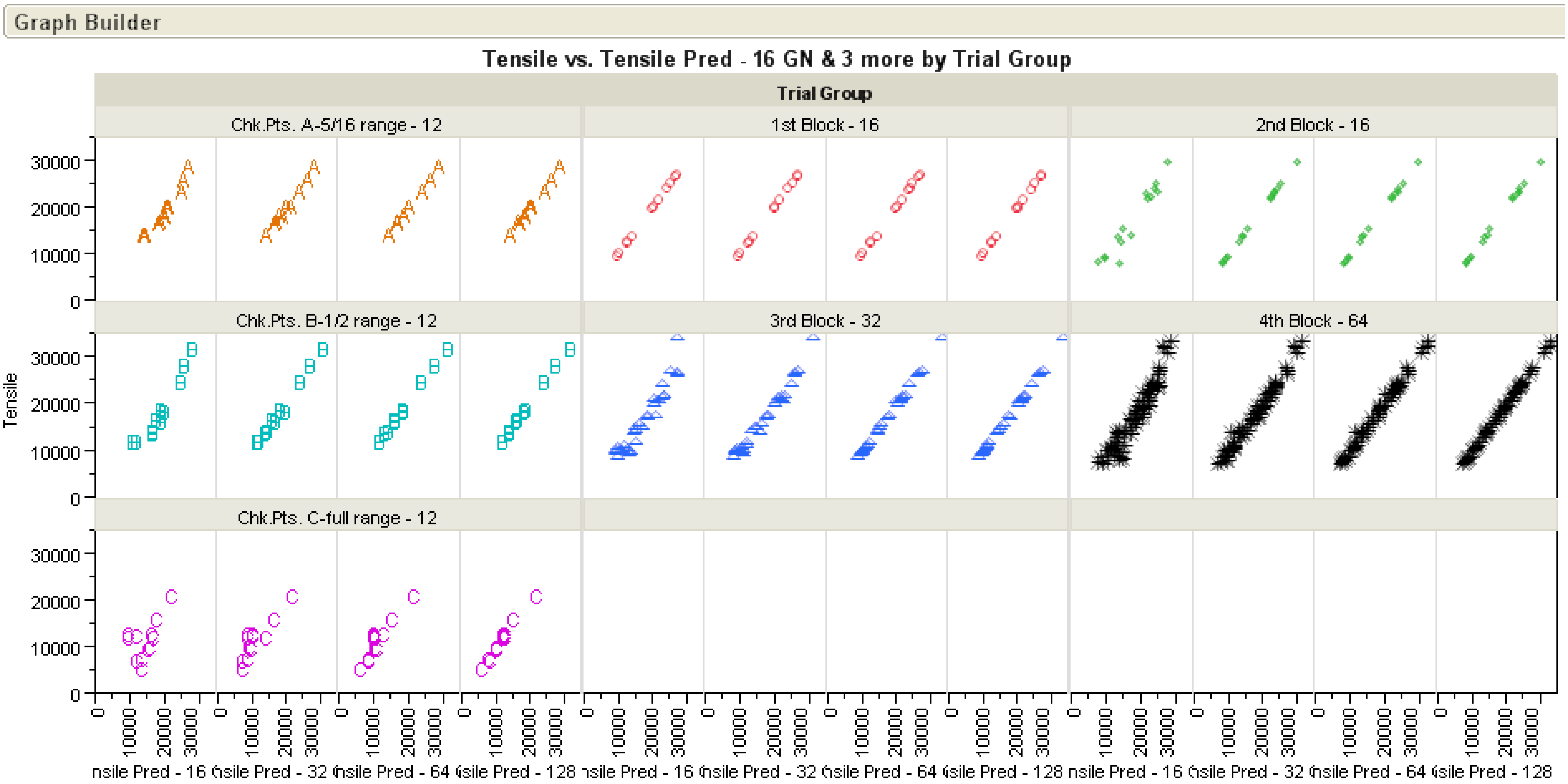
Stage 1 fit of16 trials colored green
Stage 4 fit 128 trials colored brown
Stage 3 fit 64 trials colored purple



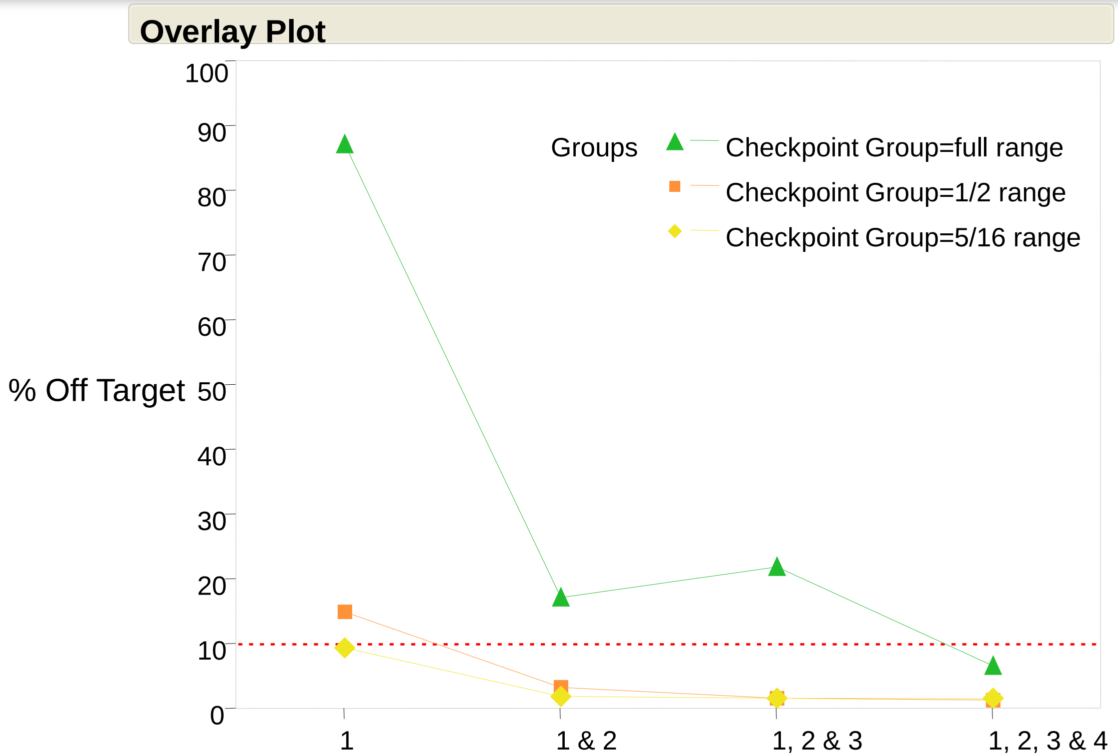


Plots of Actual vs. Predicted (Simulation vs. Metamodel) by Trial Group for Four Stages of Analysis of NLHD

Stage 1 fit just 16 trials, stage 2 fit 32 trials, stage 3 fit 64 trials and stage 4 fit 128 trials



Accuracy of Metamodel Predictions for 3 Groups of Check-points Yielding Marginal, Moderate and Extreme Extrapolation

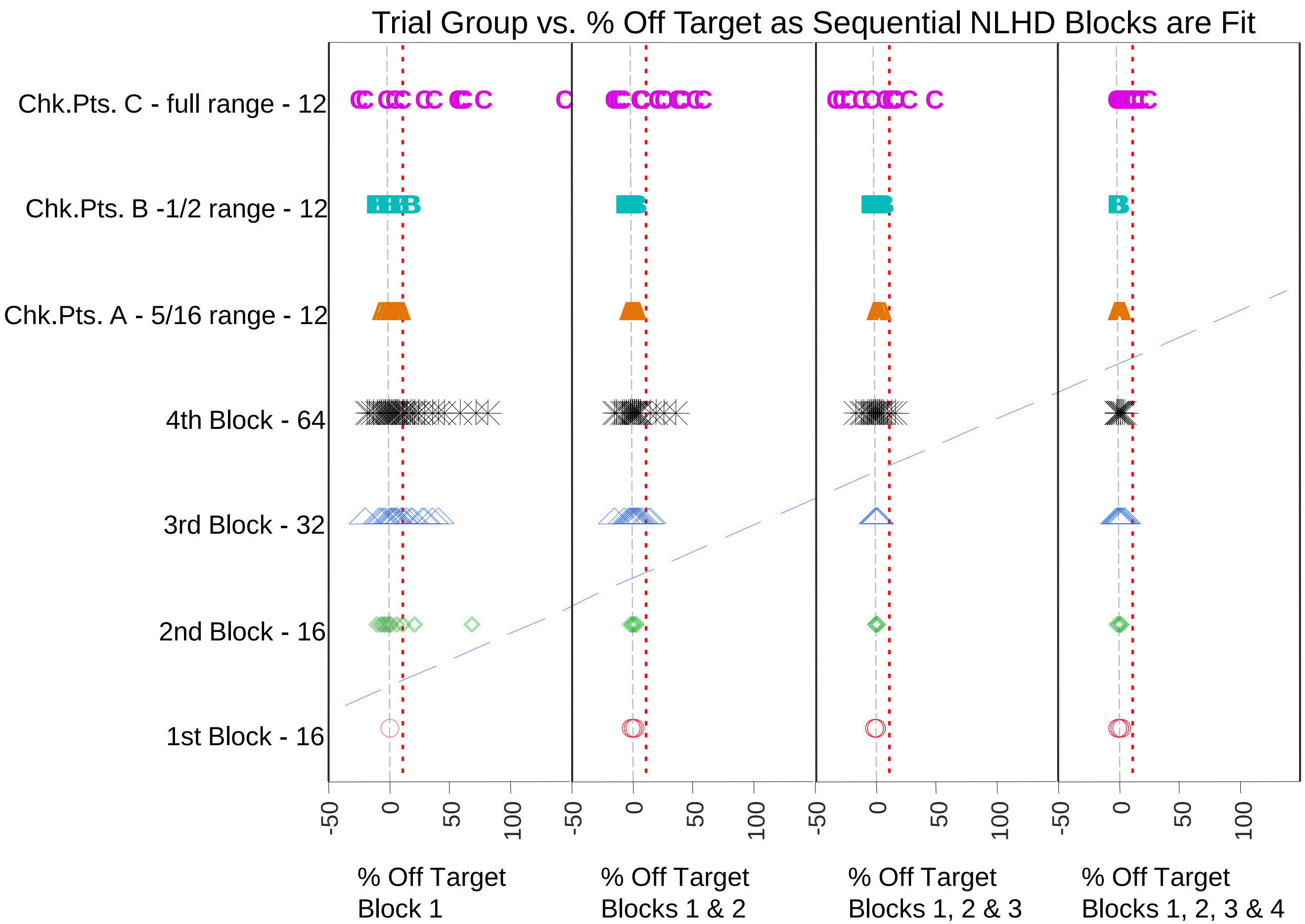


Percent Off Target - Root Mean Square of 12 Checkpoints				
Blocks	1	1 & 2	1, 2 & 3	1, 2, 3 & 4
5/16 range	9.39	2.08	1.72	1.53
1/2 range	14.94	3.33	1.79	1.27
full range	87.16	17.17	21.96	6.72

Percent Off Target - Worst Case of 12 Checkpoints				
Blocks	1	1 & 2	1, 2 & 3	1, 2, 3 & 4
5/16 range	17.13	4.52	3.48	2.74
1/2 range	33.74	7.11	-3.38	2.31
full range	225.70	34.69	46.98	16.66

Each checkpoint group consisted of a 12-trial Plackett-Burman DOE. The ranges of the factors relative to the ranges used for the NLHD were 5/16ths (marginal extrapolation), half (moderate extrapolation) and full (extreme extrapolation).

Accuracy of Metamodel Predictions for 3 Groups of Check-points Yielding Marginal, Moderate and Extreme Extrapolation

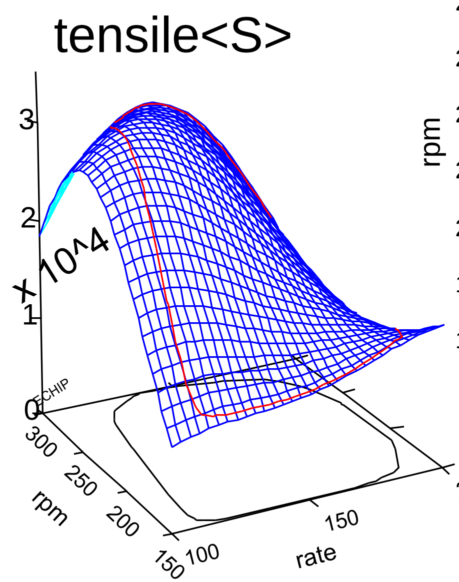


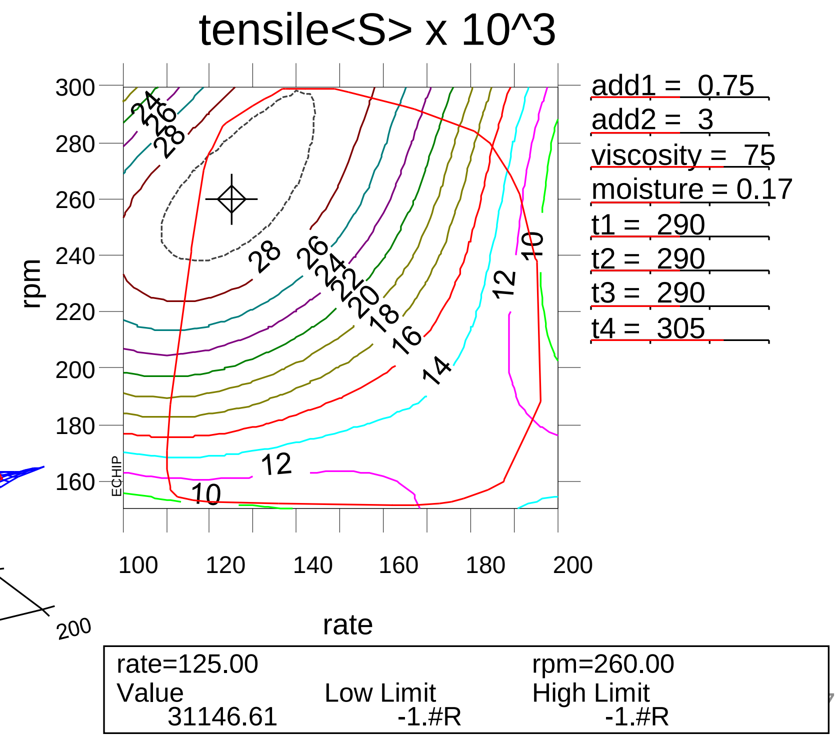
% Off Target for Checkpoints NOT Included in Model Fit

% Off Target for Points Fit with Gaussian Process Modeling

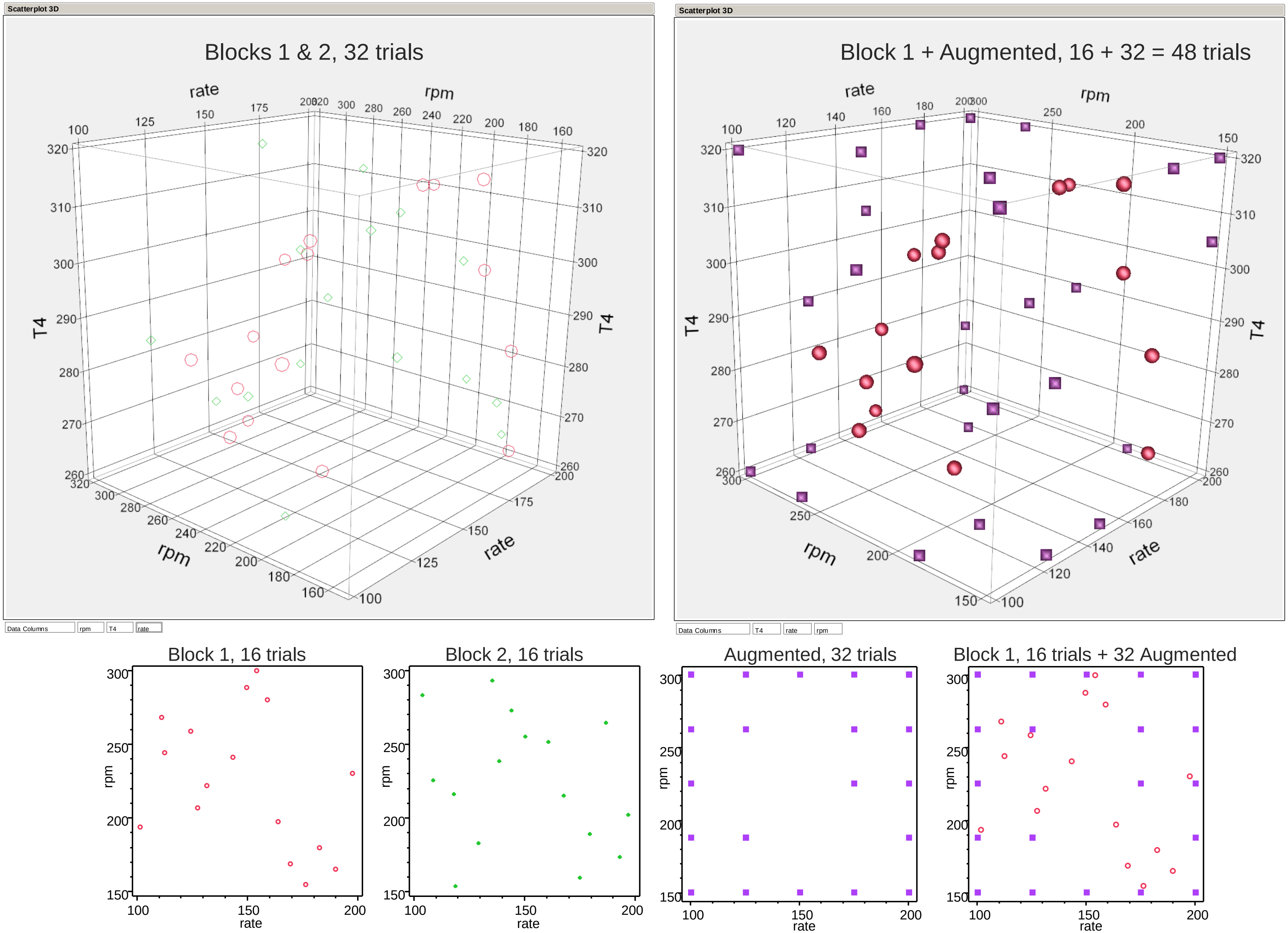
Algorithmic Augmentation Using a Stepwise Determined High-Order Polynomial Model

1. Run Block 1 of NLHD
2. Perform stepwise regression using high order polynomial model
3. Augment (D-optimal) Block 1 NLHD trials over full range of factors to expand volume of design space and to add trials to support indicated polynomial structure
   a. Use additional trials as checkpoints
   b. Use them to support polynomial analysis
   c. Use them for Kriging analysis to enlarge interpolation domain

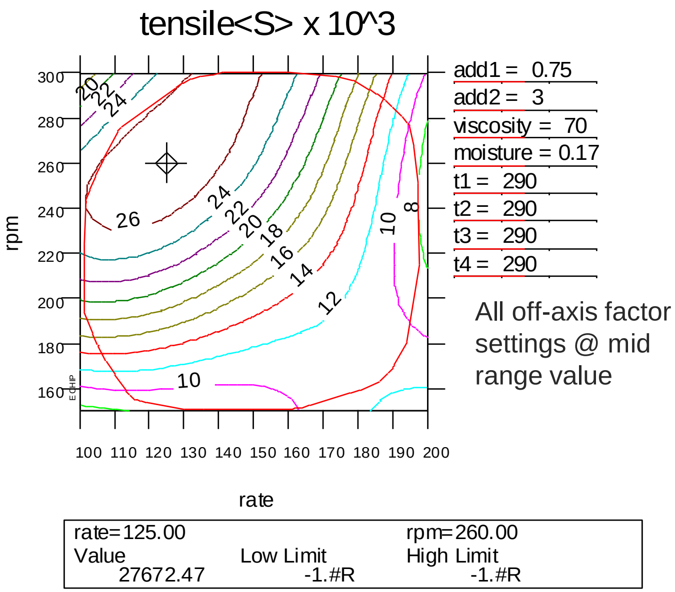




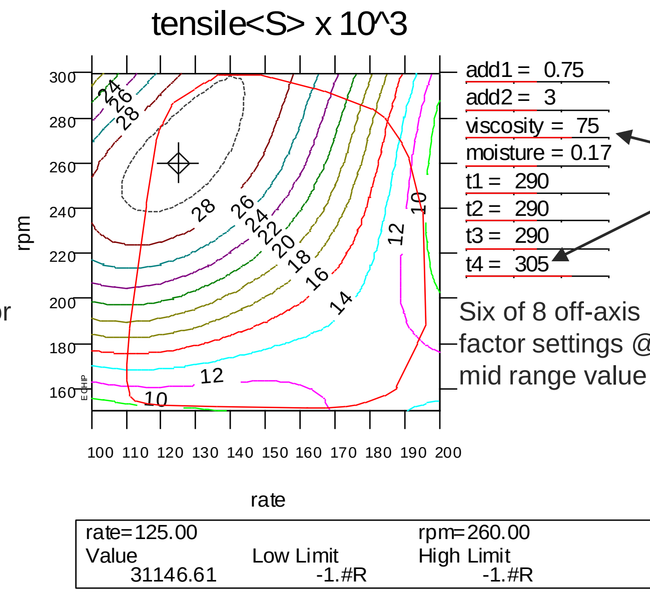
Projections of Trial Locations in 3 of 10 Factors for the First 2 of 4 Blocks in an NLHD, and 32 Trials Augmented on to the First NLHD Block for a High Order Polynomial



NLHD, 16+aug32=48
Block 1 + D-opt trials



All off-axis factor settings @ mid range value



viscosity and *t4* factor settings @ 75% of range

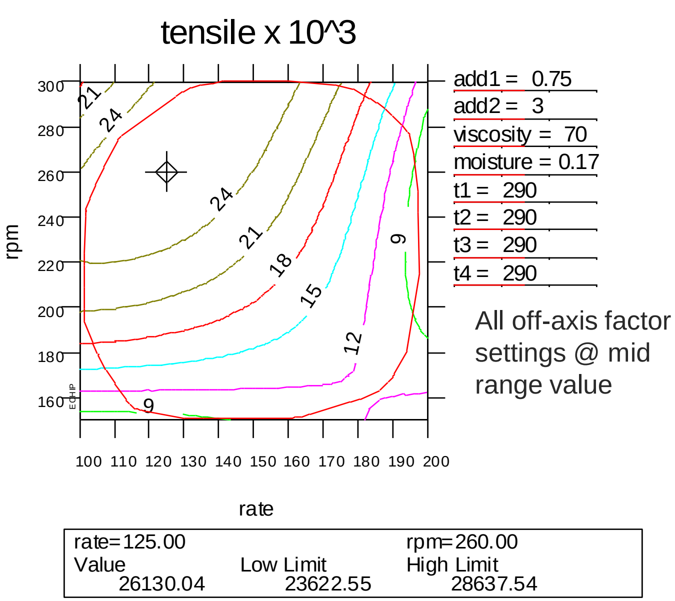
Six of 8 off-axis factor settings @ mid range value

COEFFICIENTS	SD	P	CONDITION	TERM
4.15884				0 CONSTANT
0.0408638	0.126505	0.7485-	0.983	1 add1
-0.00169897	0.0317164	0.9576-	0.992	2 add2
0.00621768	0.00300901	0.0458	0.977	3 viscosit
-0.0254722	0.41543	0.9514-	0.994	4 moisture
-0.000116459	0.0010538	0.9126-	0.984	5 t1
7.18297e-005	0.00104881	0.9458-	0.987	6 t2
-0.000164508	0.00108118	0.8799-	0.972	7 t3
0.0016304	0.0010261	0.1206	0.974	8 t4
-0.00203836	0.000666902	0.0041	0.966	9 rate
0.00179856	0.00042531	0.0001	0.975	10 rpm

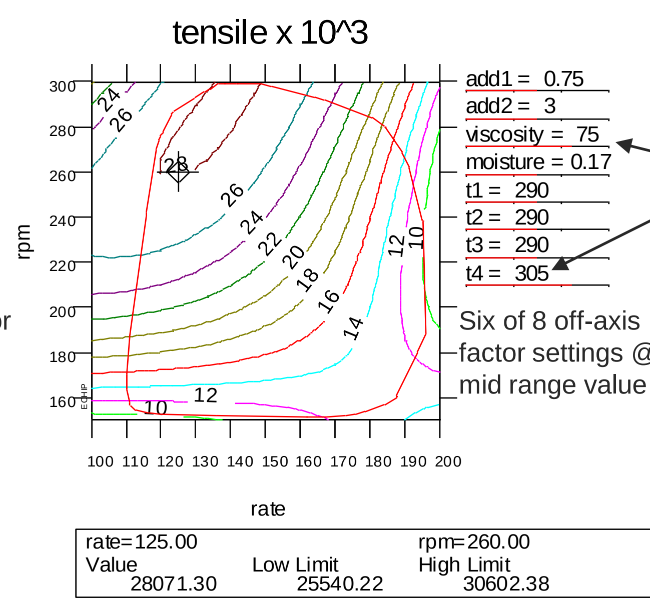
N trials = 48

Top two plots use Kriging model

NLHD, 16+aug32=48
Block 1 + D-opt trials



All off-axis factor settings @ mid range value



viscosity and *t4* factor settings @ 75% of range

Six of 8 off-axis factor settings @ mid range value

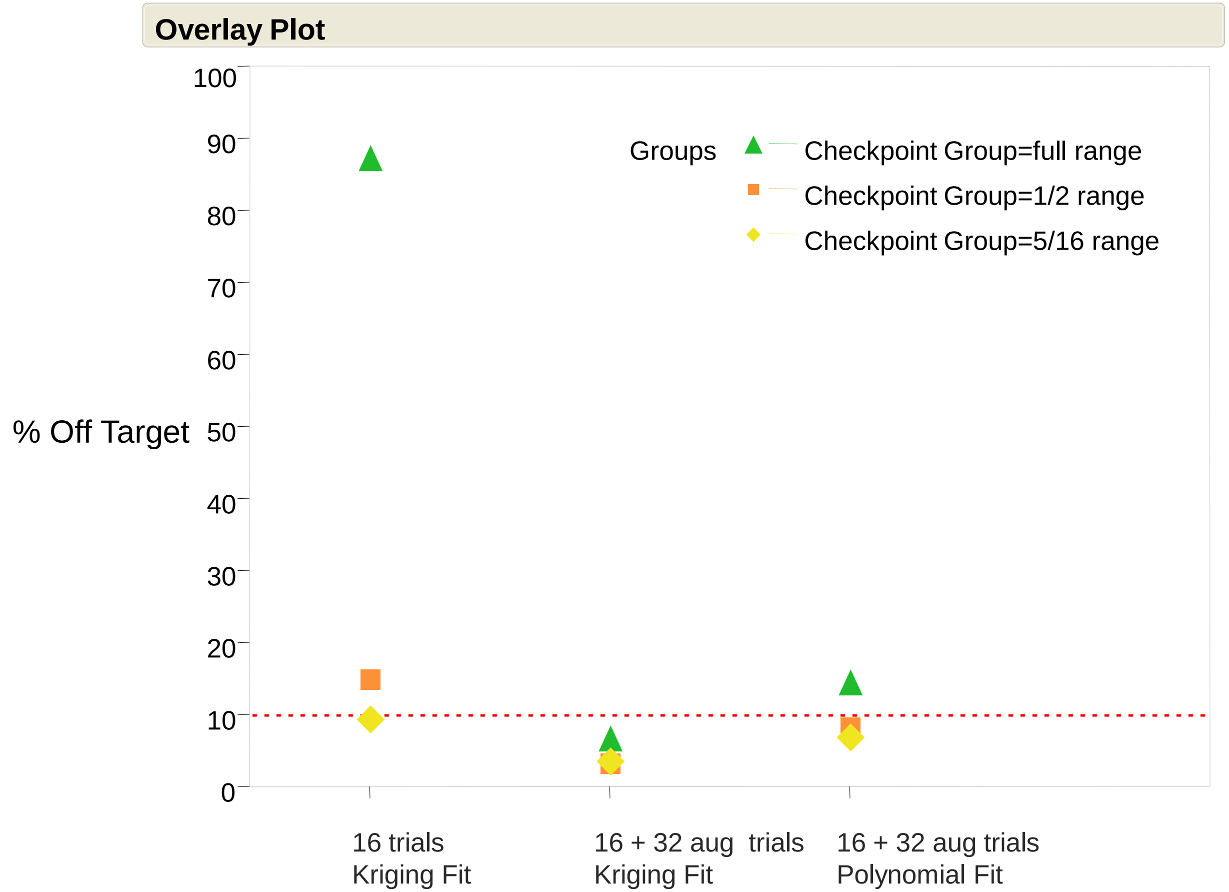
COEFFICIENTS	SD	P	CONDITION	TERM
				0 CONSTANT
		0.3944-	0.944	1 add1
		0.5643-	0.961	2 add2
		0.0000	0.954	3 viscosity
		0.3778-	0.971	4 moisture
		0.8422-	0.960	5 t1
		0.2409-	0.956	6 t2
		0.0650	0.938	7 t3
		0.0000	0.951	8 t4
		0.0000	0.553	9 rate
		0.0000	0.546	10 rpm
		0.6486-	0.916	32 viscosity*t4
		0.8245-	0.953	33 viscosity*rate
		0.3275-	0.930	34 viscosity*rpm
		0.2894-	0.904	53 t4*rate
		0.0627	0.910	54 t4*rpm
		0.0000	0.924	55 rate*rpm
		0.0698	0.905	56 add1^2
		0.4343-	0.901	57 add2^2
		0.3089-	0.899	58 viscosity^2
		0.8166-	0.915	59 moisture^2
		0.5428-	0.917	60 t1^2
		0.0399	0.918	61 t2^2
		0.4097-	0.947	62 t3^2
		0.3766-	0.876	63 t4^2
[illegible]	[illegible]	0.0000	0.917	64 rate^2
-0.565495	0.0789502	0.0000	0.873	65 rpm^2
0.0308524	0.00194633	0.0000	0.539	154 rate*rpm^2
-0.0353589	0.00302797	0.0000	0.526	155 rate^2*rpm

N trials = 48

Bottom two plots use stepped polynomial

Comparison of Accuracy of Metamodel Predictions for 3 Groups of Checkpoints for NLHD Block 1 (left)

NLHD Block 1 augmented with 32 trials and analyzed with Kriging spatial regression(middle) and Polynomial Model (right)



Percent Off Target - Root Mean Square of 12 Checkpoints			
Blocks	1	1 + aug Krig	1 + aug Poly
5/16 range	9.39	3.55	6.86
1/2 range	14.94	3.43	8.37
full range	87.16	6.53	14.49

Conclusions

- NLHD designs can be run sequentially so that metamodel accuracy can be evaluated after each block and decision made as to whether or not to move forward with the next block
- Generally as more NLHD blocks are run, the metamodel accuracy increases
- Inclusion of extreme (full range) extrapolation checkpoints will expand interpolation volume of Kriging analysis – assuming Kriging analysis remains stable
- Augmentation of early NLHD stages with trials chosen to support indicated high-order polynomial behavior may expand the interpolation volume of Kriging analysis (again assuming Kriging analysis remains stable) as well as support alternative polynomial metamodel analysis

- Caveat: These conclusions were reached using a moderately complex transcendental function in lieu of a CFD simulation model that is believed to do a good job of stressing extrapolation with the metamodel.

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