CPID
CHEMICAL AND PROCESS INDUSTRIES DIVISION
OF THE AMERICAN SOCIETY FOR QUALITY

CPID NEWSLETTER

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CHAIR'S MESSAGE

By Kevin White
(kwhite@eastman.com)

Greetings! It's hard to believe my term as Chair of CPID is almost complete. I'm excited about what we've been able to accomplish, but at the same time realize there is much more to do. None of what CPID does would be possible without the outstanding support of numerous other volunteer leaders.

Springtime means it's nearly time for ASQ's World Conference on Quality Improvement (WCQI). This year's WCQI is in St. Louis, May 24-26. CPID was successful in getting a multi-session proposal accepted in the conference program dealing with capability and measurement system metrics (see this newsletter for more detail about CPID events at the WCQI). CPID will also continue to have our booth in the exhibit hall. Please stop by and say hello.

At the 2009 FTC, I gave a "State of the Division" address at our open council meeting. It began with a little history of CPID. CPID was formed in 1952 and was known as the Chemical Division. The Statistics Division spun out of the Chemical Division in 1979 and just finished celebrating 30 years. The name change to CPID occurred in 1982-83. And in 2012, CPID will be celebrating 60 years of existence.

The membership drop being experienced by ASQ and most Divisions, including CPID, is concerning. ASQ is working on many items to address membership recruitment and retention. CPID currently lists 1300-1400 members, with roughly 92% of these members residing in the US and Canada. Over 55% of CPID members are Senior Members of ASQ and 3.6% are Fellows of ASQ (the highest percentage of Fellows of any Division). By far, the two most common titles of CPID members were Manager and Engineer and over half of CPID's members claim to be in manufacturing. Many of CPID's members are also members of other Divisions, the most common being Quality Management Division and Statistics Division.

As for Education and Training efforts, we are getting ever closer to having some webinars available on our CPID website. Dotty Sempolinski, our Education and Training sub-team leader, has been working with ASQ and content providers to make this happen. Expect to be hearing more from us on this topic in the near future. CPID also continues to sponsor FTC short courses and tries to get relevant content to CPID members included in the WCQI program each year. We are also currently working to capture the CPID Body of Knowledge and make it available to members in various forms. Current opportunities for the CPID include special publications and revisions to some of our existing publications.

CPID continues to play a strong role in the Fall Technical Conference and I'm happy to say that I believe the conference is in sound shape to continue for many years to come. The 53rd Fall Technical Conference was held in October 2009 in Indianapolis. Paula Reardon, the General Conference Chair, did an outstanding job in organizing this conference. Marc Perry is currently working hard on the planning of the 54th Fall Technical Conference to be held October 7-8, 2010 in Birmingham. The conference website is http://cba.ua.edu/ftc2010. Check the link frequently for updates to the conference program and short courses. It's looking like the CPID sponsored short course will be on Data Mining. The FTC continues to be one of the best value conferences around. Hope to see you in Birmingham this fall.

Also of note is CPID's effort to communicate with members. We currently have a fall and spring newsletter. We also try to maintain our website with key information of interest to members. On the ASQ website, there is also a CPID discussion board for members to use to engage other members for ideas to problems unique to our industries. Email communication is

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CHAIR'S MESSAGE

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another area we try to use judiciously. We've recently started a CPID group on LinkedIn (www.linkedin.com), a professional networking site.

As the ASQ year comes to an end, I will transition out of the executive committee but do plan to stay involved with CPID in some lesser roles. The experience has been incredible and is something that I will always cherish. I've made many friends and grown my professional network that will serve me well for years to come. The future of CPID is in good hands. In July, Paula Reardon will be assuming the role of Chair, Marc Perry will become the Chair-Elect, and Wayne Wesley will be the new Secretary. I look for great things from CPID over the next several years.

Thank you for the opportunity to serve ASQ and CPID.

Congratulations to Connie Borror!

Connie has been elected a Fellow of the Society in recognition of her significant contributions to quality. Her citation reads as follows:

"For outstanding contribution in the field of quality and applied statistics as an educator and researcher; and for exemplary leadership in ASQ and continuing activity as a section representative."

An ASQ Fellow is an individual who has an established record of contributions, both to the quality profession and to the Society. The grade of Fellow is an earned distinction. Connie's achievement of this status is a symbol of respect from her colleagues that has been accepted by the highest officers of our organization. CPID is proud to have Connie as our newest ASQ Fellow!

2008 Award Winners

These prizes were awarded at the 2009 FTC for papers published in Technometrics in 2008:

The Frank Wilcoxon Prize (Best practical application paper): Xuemei Shan and Daniel W. Apley, "Blind Identification of Manufacturing Variation Patterns by Combining Source Separation Criteria," (Aug. 2008, 332-343)

The Jack Youden Prize (Best expository paper): Leland Wilkinson, "The Future of Statistical Computing," (Nov. 2008, 418-435, with discussion)

The Shewell Award for the best paper at the 2008 FTC was also presented:

Shewell Award: "Data Mining in Vaccine Manufacturing" by Julia O'Neill, Merck & Company, Inc.

ARE YOU A POTENTIAL ASQ FELLOW?

The Chemical & Process Industries Division wants high achieving members to receive the recognition due them by nominating qualified candidates to be ASQ Fellows. Our CPID membership currently has 46 or 3.6% Fellow members. We know that we other qualified members out there; we just need help in finding them. In order to determine if you or a colleague may be qualified, see ASQ Policy G-02-02.

Please notify the CPID Examining Chair, Arved Harding, aharding@eastman.com if you are a candidate or you know of a possible candidate, so that the complete Fellow nomination form can be provided. Ideally, we need to begin to process nomination forms in January to have them completed by the 1st Monday in May deadline each year. It's never too early to start working on this.

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CPID Schedule of Events at the 2010 ASQ World Conference

DAY	TIME	EVENT
Sunday		
May 23	1:00pm - 3:00pm	CPID Strategic Planning Meeting
	3:00pm - 5:00pm	CPID Division Council Meeting
	6:30pm - 8:30pm	WCQI Opening Reception (Exhibit Hall) *Stop by the CPID booth for hospitality suite location and to sign up for Monday night CPID dinner*
	9:00pm - Midnight	CPID/STAT Hospitality Suite
Monday		
May 24	5:00pm - 6:00pm	Open Council Meeting
	6:00pm - 8:00pm	CPID Dinner
	8:00pm - Midnight	CPID/STAT Hospitality Suite
Tuesday		
May 25	9:15am - 10:00am	CPID Sponsored Multi-session (1 of 3) Capability Metrics - Evaluation and Recommendations (T10)
	10:30am - 11:15am	CPID Sponsored Multi-session (2 of 3) Gauge R&R Metrics - Evaluation and Recommendations (T20)
	11:30am - 12:15pm	CPID Sponsored Multi-session (3 of 3) Effective Use of Capability and Gauge R&R Metrics (T30)

2010 Fall Technical Conference – Mark Your Calendars!

Mark Your Calendars! Please join us for the 54th Annual Fall Technical Conference, which will be held on Oct 7-8, 2010 in Birmingham, AL at The Wynfrey Hotel at Riverchase Galleria. The theme of this year's conference is *Quality and Statistics: The Engines of Success,* which reflects the importance of quality engineering concepts and statistical thinking in a highly competitive global market. The official conference website is http://cba.ua.edu/ftc2010. Four course offerings will be available at this year's event: 1) *Data Mining using JMP* and 2) *Acceptance Sampling,* offered on Wednesday, Oct 6, and 3) *Logistic Regression* and 4) *Survival Analysis,* offered on Saturday, Oct 9. We look forward to seeing everyone in Birmingham!

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CPID Sponsored Multi-Session at the WCQI

Tuesday May 25, 2010

Capability Metrics - Evaluation and Recommendations (Multi-session 1 of 3)

Session T10 (9:15am - 10:15am)
Speaker: Kevin White, Eastman Chemical Company

Process capability indices (Cp and Cpk) and process performance indices (Pp and Ppk) are commonly used to summarize processes and their ability to meet specifications. Understanding these indices and how they relate is an excellent way to evaluate processes for improvement opportunities. In addition, it will be shown how to determine the type of improvement effort that might be required. Key issues such as normality, data editing, sample size, and one-sided specifications will be addressed.

Gauge R&R Metrics - Evaluation and Recommendations (Multi-session 2 of 3)

Session T20 (10:30am - 11:15am)
Speaker: Connie Borror, Arizona State University

Gauge repeatability and reproducibility (R&R) studies are often used to assess the capability of a measurement system. In this presentation, several common gauge R&R criteria are discussed and examined along with more objective measures such as misclassification rates. Relationships between common metrics such as precision-to-tolerance ratio, number of distinct categories, signal-to-noise ratio, and the discrimination ratio will be revisited.

Effective Use of Capability and Gauge R&R Metrics (Multi-session 3 of 3)

Session T30 (11:30am - 12:15pm)
Speakers: Connie Borror, Arizona State University and Kevin White, Eastman Chemical Company

Various capability indices and measurement system metrics are used to assess process and measurement system performance. In this presentation, the key process capability indices and measurement system metrics will be identified. In addition, a methodology for using these indices and metrics in combination to facilitate the identification of improvement opportunities towards the goal of stable, on-target, and in-specification processes will be presented.

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ASQ and STANDARDS

Rudy Kittlitz

All of us in the USA are affected daily by various standards, such as ASTM, ANSI, and ISO, whether we realize it or not. The purpose of this note is primarily informational about the ASQ participation with ANSI and ISO along with the need for additional Experts.

The ASQ Standards Committee is responsible for development and approval of generic standards and other documents. Committee membership includes representative from ASQ Divisions and General Interest members. At present I am the CPID representative to this committee.

International Standards not only affect us in the USA, but also have a major impact for the rest of the world. The International Organization for Standards (ISO) was formed in 1946 with headquarters in Geneva Switzerland. There are 250 ISO committees and others added when the need arises. In the USA, standards development is not supported by the Government, but is entirely voluntary. The USA representative to ISO is the American National Standards Institute (ANSI) headquartered in New York City. The various organizations that work with ANSI are charged fees for participation.

ASQ, through ANSI, has the secretariats for:

- IEC/TC 56 on Dependability
- ISO/TC 69 on Applications of Statistical Methods
- ISO/TC 176 on Quality Management and Quality Assurance
- ISO/TC 207 on Environmental Management
- ISO/TMB/WG on Social Responsibility

ANSI Accredited Standards Committee (ASC) Z1 Subcommittees are:

- Z1 SC on Dependability
- Z1 SC on Applications of Statistical Methods
- Z1 SC on Quality Management and Quality Assurance
- Z1 SC on Environmental Management
- Z1 SC on Auditing of Management Systems.

The Subcommittees of ASC Z1 serve as the USA consensus bodies in each respective area. Given the importance of international standards in these disciplines and important work by other nationally accredited standards development organizations, the Z1 Subcommittees collaborate with related organizations in the U.S. Standards Group on Quality, Environment, Dependability, Statistics, and Social Responsibility (QEDSS).

Work on International Standards is generally conducted at an annual week-long meeting somewhere in the world, but interim meetings may occur also. At these face-to-face meetings it is vital that the USA, through ANSI, is represented by Experts. Processing of new or revised standards takes several years, but by participating in this work the USA Expert can immediately and directly influence its content and be aware of "what's coming in the near future." The ASQ "Standards Team" provides excellent orientation and guidance to the involved individuals for this work.

I challenge you all to seriously consider joining this interesting work!

Upgrading to Become an ASQ Senior Member

Since July 2005 our membership has changed from having 24% Senior members to 56%. In fact, since Jan 2005 we have had 590 members become Senior members, furthermore 79% of all our current Senior members achieved this status after Jan 2005. This implies more and more CPID members understand the benefits to becoming a Senior member. It is a necessary step if you ever plan to become an ASQ Fellow. You must be a Senior member for a minimum of 5 years before submitting your application for Fellow. If you become a Senior member in addition to the ASQ member benefits you currently receive, as a Senior member you will also receive:

- *A Senior member certificate and card.*
- R*ecognition of your achievement through an announcement in ASQ Weekly, ASQ's member e-newsletter.*
- *Special Senior member name badge at ASQ events you attend.*
- *Your choice of one extra benefit journal, or two Forums or Divisions, or one additional Section, or choose to waive additional benefits as part of your Senior member benefit package.*

Qualifying to become a Senior member is not as difficult as some people may think but it's no cake walk either. See the information below and for more information see ASQ policy G-02-01 and the Application for Senior Membership on the website www.asq1106.org. See membership and upgrades.

Achieving Senior membership in ASQ is an indication of professional growth and accomplishments in quality or the allied arts and sciences. To be eligible for advancement, a member shall demonstrate professional growth and significant achievements in his/her profession as indicated by meeting all of the following requirements:

1. *Ten years of active professional experience. Up to four years of this vocational requirement may be satisfied by graduation from an accredited college, university, or similar institution.*
2. *ASQ Full (formerly Regular) member in good standing for at least one calendar year prior to the date of application for advancement.*
3. *Qualified in one of the following ways described below:*
   a. *Conducting quality-related engineering, inspection or audit, or statistical work, or applying the methods and principles of quality on the job for at least two years.*
   b. *Teaching quality or related arts or sciences at an accredited institution for at least two years.*
   c. *Being a Senior member or comparable type in a recognized professional organization.*
   d. *Currently holding an ASQ certification that requires recertification.*

If you have questions about becoming a Senior member or filling out the application, feel free to contact the CPID Examining Chair, Arved Harding, aharding@eastman.com.

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2009 W. J. YOUDEN MEMORIAL ADDRESS

Perspectives on Prediction Variance and Bias in Developing, Assessing, and Comparing Experimental Designs

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This is a written version of my 2009 W. J. Youden Memorial Address presented October 8, 2009 at the 53rd Annual Fall Technical Conference in Indianapolis, Indiana.

I would like to thank the Statistics Division of the American Society for Quality and the Youden Address selection committee for this extremely nice honor. This is the 37th annual Youden Address since the death of William John (Jack) Youden in 1971. I am honored to join the list of previous distinguished speakers.

I never met Jack Youden, but I have used and benefited from his work and publications in the area of experimental design, as I'm sure many of you have. He was a very practical chemist turned statistician. It is relative to the practice of developing, evaluating, and comparing experimental designs that I'd like to share some perspectives with you today.

My Perspectives in a Nutshell

The vast majority of methods used in practice to develop, evaluate, and compare experimental designs focus on the variance properties of models to be fit using the experimental data. However, because models only approximate the true, unknown relationships, they are subject to *bias errors* as well as *variance errors*. These errors are the differences between fitted and true models that result from random experimental error (variance errors) and inadequacy of the assumed model (bias errors). Considerable literature from last 50 years has developed methods that consider bias (and variance) properties of designs. There has been a noticeable resurgence in work and publications in this area in the last several years. This literature has generally concluded that optimal designs that account for bias and variance errors are generally much closer to designs that account only for bias errors (*all-bias designs*) than designs that account only for variance errors (*all-variance designs*). Still, methods that consider bias properties of designs are seldom used in practice. I feel strongly that we as a profession need to routinely use methods that consider <u>variance and bias</u> properties to develop, assess, and compare experimental designs. Recommendations for achieving this goal are discussed at the end of the article.

Common Practice Focuses on Variance Properties

Methods in wide practical use for developing, evaluating, and comparing experimental designs focus on variance properties of designs, such as the (1) variance of model coefficients, and (2) the variance of model predictions (prediction variance).

For example, common response surface designs like factorial and fractional factorial designs, and rotatable central composite designs (CCDs) are variance-focused designs. As another example, the widely-used optimal design approach generally focuses on minimizing variance criteria. In particular, D-optimality (minimize $|(\mathbf{X}'\mathbf{X})^{-1}|$) and A-optimality (minimize $\mathrm{trace}[(\mathbf{X}'\mathbf{X})^{-1}]$) focus on minimizing the variances of model coefficients. Also, G-optimality (minimize $\max[\mathbf{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}]$) and IV-optimality (minimize $\mathrm{avg}[\mathbf{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}]$) focus on minimizing the variance of model predictions. In these criteria, $\mathbf{X}$ denotes the design matrix expanded in the form of an assumed model (i.e.,

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the *model matrix*) and **x** denotes any point in the experimental region of interest. For each of these cases, a single-number criterion is used to represent the goodness of a design. Obviously, the ability of a single number to represent the properties of a design is limited.

To overcome the limitation of a single-number criterion as the basis for evaluating and comparing designs, graphical methods have been proposed. The *variance dispersion graph* (VDG) displays the minimum, average, and maximum prediction variance (PV = $\mathbf{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}$) or scaled prediction variance (SPV = N*PV, where N is the number of design points) over spheres of varying radii. The *fraction of design space graph* (FDSG) displays the fraction of design space where SPV or PV is less than or equal to a given value. VDGs and FDSGs were first discussed by Giovannitti-Jensen and Myers (1989) and Zahran et al. (2003), respectively.

VDGs and FDSGs have been extended from their original spherical experimental region applications to (1) cuboidal regions, (2) simplex mixture experiment regions, (3) constrained mixture and/or non-mixture regions, (4) mixture + process variable + noise variable regions. Other graphical methods have been proposed to evaluate and compare variance properties of designs, including trace plots, quantile plots, box plots, and others.

Model Adequacy versus Inadequacy

Methods for developing, evaluating, and comparing experimental designs based on variance properties rely on the assumed model form being "adequate". We (statisticians and practitioners) too often have a "Lake Wobegon" mindset, where: (1) men and women are all good looking, (2) children are all of above average intelligence, and (3) assumed models are always adequate! (Apologies to Garrison Keillor!)

If the assumed model is inadequate, then we have model misspecification, which means predictions with the fitted model will be subject to bias. In this case, designing an experiment to (1) have precise predictions of the response (low prediction variance) for the assumed model may be much less important than designing to (2) protect against inaccurate predictions (high bias) over unknown parts of the experimental region.

Common Approach to Address Model Inadequacy

A commonly used approach to address possible model inadequacy is to design for an assumed model

$$\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \boldsymbol{\varepsilon} \qquad (1)$$

while protecting against a larger true model

$$\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \boldsymbol{\varepsilon}\,. \qquad (2)$$

For example, $\mathbf{X}_1$ might be the model matrix for a first-order model, while $\mathbf{X}_2$ would be the columns of a model matrix corresponding to a second-order model. Nonzero assumptions about the coefficient vector $\boldsymbol{\beta}_2$ should be considered when minimizing prediction error, so that both variance and bias contributions are considered. However, the true vector $\boldsymbol{\beta}_2$ is unknown and its distribution is generally not clear to the experimenter.

Literature Review of Experimental Design Methods that Consider Bias

This year (2009) is the 50th anniversary of a seminal paper by Box and Draper (1959) that considered bias, variance, and MSE in designing experiments. Much additional research on experimental design for model mis-specification and model robustness has occurred in the ensuing 50 years. At the time of the Youden Address I had found over 60 relevant publications, and since have found additional publications bringing the total to over 100. This is not counting the sizeable literature on space-filling/uniform designs and design of computer experiments (which design for a non-parametric or flexible model form).

I now present synopses of selected approaches and examples that have appeared in the literature over the past 50 years to account for bias as well as variance properties of designs.

Early Research

Early research by Box and Draper (1959, 1963) and Draper and Lawrence (1965a) considered designs for a polynomial model of degree d_1 where the true model is a polynomial of degree $d_2 > d_1$. These authors noted that differences between fitted and true models occur due to (1) random experimental error (variance error = V), and (2) inadequacy of the assumed model (bias error = B). The approach in these papers involved

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- Choosing a class of designs that minimizes the MSE averaged (integrated) over the experimental region (IMSE = V + B)
- Selecting a design from this class that maximizes $E(SS_{Residual})$

The latter can be thought of as maximizing the ability to detect model lack-of-fit.

For the case where a first-degree polynomial is assumed but a second-degree polynomial is the true model, Box and Draper (1959) said:

> "The somewhat unexpected conclusion is reached that … the optimal design in typical situations in which both variance and bias occur is very nearly the same as would be obtained if variance were ignored completely and the experiment designed so as to minimize bias alone."

Box and Draper (1963) addressed designs for a second-degree polynomial when a third-degree polynomial is the true model. They similarly concluded that appropriate integrated mean squared error (IMSE) designs are close to minimum-bias designs. Figure 1 compares IMSE-based and variance-based rotatable CCDs for k = 2 variables over a unit circle (i.e., radius = 1) as the region of interest (R). Clearly the variance-based design is much larger, with design points located

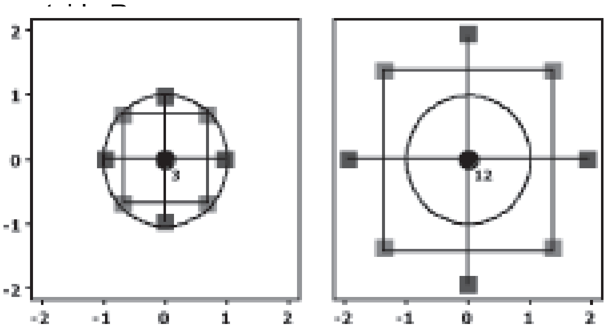

Figure 1. (a) IMSE-Based Design and (b) Variance-Based Design from Box and Draper (1963)

The work of Box, Draper, and Lawrence considered IMSE over a region of interest (R), but allowed design points in a larger operability region (O). Stigler (1971) noted that forcing designs to remain within R reduces the differences in IMSE performance of min-V, min-B, and min-IMSE designs. However, my literature review showed that there can still be substantial differences. In general, having design points on the boundary of a larger experimental region is good for reducing variance, but not for reducing bias.

Minimum-Bias Designs with Secondary Criteria

Conditions for minimum-bias designs yield a class of designs, so a secondary criterion is needed to obtain a unique design. Thompson (1973), Myers and Lahoda (1975), and Khuri and Cornell (1977) used minimum variance and other secondary criteria and developed designs on spherical and cuboidal regions. Myers and Lahoda proposed a *two-star CCD*, illustrated in Figure 2.

Donohue et al. (1992) developed minimum bias designs using minimum variance as a secondary criterion, denoted "Min V | Min-B". They maintained the same structure of standard designs

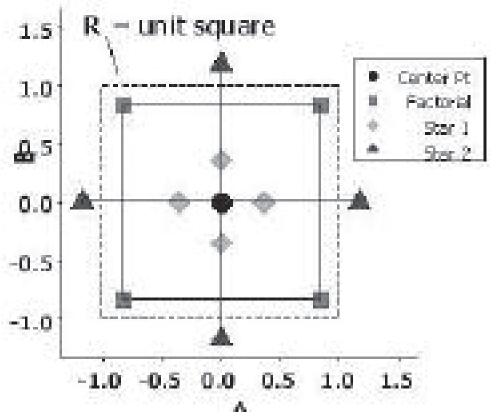

Figure 2. Two-Star CCD Consisting of Factorial Points and Two Sets of Axial (Star) Points

- 3-level factorial or fractional factorial designs (FAC)
- Box-Behnken designs (BBD)
- Central composite designs (CCD)
- Small composite designs (SCD) ,

but scaled them to support fitting second-order models while protecting against third-order models. Scaling refers to using a multiplier less than 1, so that standard design points are shrunken away from the boundary of the experimental region. Figure 1 from Donohue et al. (1992) is reproduced here as Figure 3. It shows the optimal scaling factors (denoted g) for minimum-bias FACs, CCDs, SCDs and BBDs for both spherical and cuboidal regions. The line labeled g = 1 at the top of Figure 3 represents unscaled versions of every design. There are two things I'd like to draw your attention

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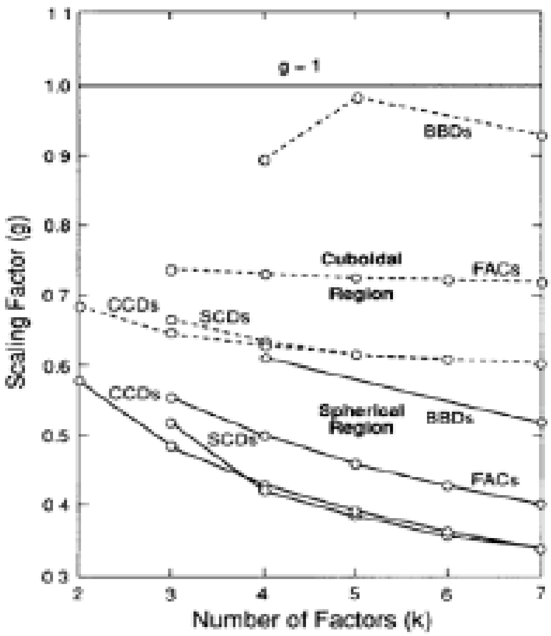

Figure 3. Optimal Scaling Factors for Minimum Bias Designs with Minimum Variance as a Secondary Criterion. Results are shown for cuboidal regions (dashed lines) and spherical regions (solid lines).

to in the figure. First, notice that designs on spherical regions require more scaling (i.e., shrinkage) than designs on cuboidal regions to achieve minimum bias. Second, notice that the BBD for a cuboidal region is fairly close to the g = 1 line. This indicates the BBD has relatively good bias properties, and thus does not require much scaling to minimize bias.

An Approach That Does Not Require Specifying the True Model Form

Welch (1983) took a more general approach that does not require specifying a true model form. Rather, a maximum relative bias (z_{max}/σ) is specified. Welch proposed a modified IMSE criterion and algorithms to develop designs robust to values of maximum relative bias. One example considered by Welch was the distribution of nine points over a 3^2 factorial design. Table 1 shows the distributions of points for designs as the maximum relative bias increases. For $z_{max}/\sigma = 0$ (all-variance design), all of the design points occur at the four corners. As z_{max}/σ increases, the replicates of the corners are replaced by mid-points of edges. Finally, when $z_{max}/\sigma = \infty$ (all-bias), a 3^2 design is

Table 1. Distribution of Points and Relative Efficiencies for 9-Point Design as the Maximum Relative Bias Increases

z_{max}/σ	9-Pt Design			Eff_V	Eff_B
	3	0	2		
0	0	0	0	100	72.3
	2	0	2		
	2	1	2		
0.4	0	0	0	98.0	77.7
	2	0	2		
	2	1	1		
0.5	0	0	1	90.5	88.9
	2	1	1		
	2	1	1		
0.75	1	0	1	85.4	96.1
	1	1	1		
	1	1	1		
∞	1	1	1	79.7	100
	1	1	1		

obtained. Welch suggested choosing designs with similar efficiencies relative to the all-variance and all-bias designs. That would be the $z_{max}/\sigma = 0.5$ design in this example. However, personally I like the symmetric 3^2 all-bias design (assuming a small number of additional points for replicates could be added in practice).

Bayesian Approaches

Several authors used a Bayesian approach of specifying a prior distribution for the $\boldsymbol{\beta}_2$ coefficients in Eq. (2). Steinberg (1985) used a modified IMSE criterion to develop model-robust scalings of 2^k and 2^{k-p} designs close to all-bias designs. Hamada et al. (2001) used a genetic algorithm to generate Bayesian near-optimal designs via the Shannon information criterion. Allen and Yu (2002), Allen, Yu, and Schmitz (2003), and Huang and Allen (2005) developed designs using a semi-Bayesian approach with an expected IMSE (EIMSE) criterion. The expectation and integration are with respect to the unknown parameters and the experimental region.

DuMouchel and Jones (1994) used a Bayesian modification of D-optimal design to reduce the dependency on a single assumed model. They used the terminology of *primary* terms (which the design must estimate), and *potential* terms (all of which may not be estimable). A simple example (involving 9-point designs for a constrained, triangular experimental region) from Figure 2 of their paper is reproduced as Figure 4. The Bayesian D-optimal design in Fig. 4(b) replaces replicated vertices in Fig. 4(a) with more edge and center points. The small number of candidate points

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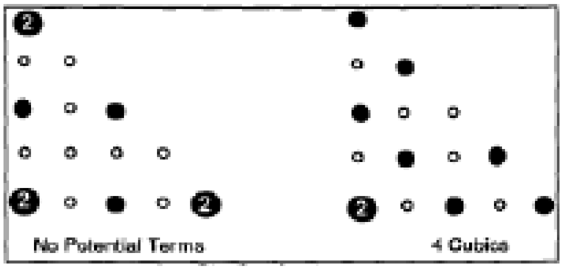

Figure 4. Designs for a Model with Quadratic Primary Terms: (a) D-optimal Design with No Potential Terms, (b) Bayesian D-Optimal Design with Four Cubic Potential Terms.

(indicated by open or closed circles in the figure) did not permit scaling (shrinking) away from the boundary of the constrained region. Still, the Bayesian D-optimal design resulted in design points closer to the center of the region than the traditional all-variance D-optimal design.

Model-Robust Experimental Design

A *model-robust design* is chosen to be relatively efficient for a set or class of models. Early work in this area was performed by Läuter (1974) and Cook and Nachtsheim (1982). Li and Nachtsheim (2000) developed model-robust fractional factorial designs that are highly efficient for all models involving main effects and "n" or fewer interactions. Heredia-Langner et al. (2004) created model-robust designs using a genetic algorithm to optimize a desirability function of D- or IV-optimality criteria for a given set of potential models.

Rotation Designs

Defoe and Myers (1992) and Bursztyn and Steinberg (2001) developed rotations of fractional factorial designs for high-bias situations. Projections of rotated first-order designs into lower-dimensional space (in the situation some variables do not affect the response) can support fitting second-order models. A simple example from Figure 1 of Defoe and Myers is reproduced as Figure 5.

Designs for Biased Estimation

The work discussed previously assumes least-squares regression will be used to fit models to the data. Karson and co-authors (1969, 1970, 1975) discussed (1) using *minimum-bias estimation* (MBE) to minimize integrated bias, and (2) selecting

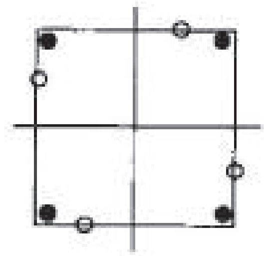

Figure 5. 2^2 Factorial Design with Two Levels per Factor (●) Rotated (○) to Have Four Levels per Factor

with least-squares estimation. Kupper and Meydrech (1973) discussed a biased, shrinkage estimator that always yields smaller IMSE than least squares for any design.

Draper and Sanders (1988) investigated minimum variance designs on the unit sphere using the MBE approach. They proposed factorial designs for an assumed first-order model protecting against a second-order model [Table 2(a)]. They also proposed two-star designs for an assumed second-order model protecting against a third-order model [Table 2(b)]. In both classes of designs, the factorial point distance decreases as the number of variables increases. This corresponds to more shrinkage (compared to all-variance designs) to achieve minimum bias via MBE.

Table 2. Minimum Variance Designs for the Minimum Biased Estimation Approach from Draper and Sanders (1988)

(a) Factorial Designs for a First-Order Model Protecting Against a Second-Order Model

# Vars.	# Center Points (n_0)	# Design Points (N)	Factorial Point Distance (a)
2	2	6	0.70
3	2	10	0.57
4	3	19	0.50
5	2	34	0.44
6	6	70	0.40

(b) 2-Star CCDs for a Second-Order Model Protecting Against a Third-Order Model

# Vars.	# Center Points (n_0)	# Design Points (N)	Factorial Point Dist. (a)	Star 1 Point Dist. (a_1)	Star 2 Point Dist. (a_2)
2	2	13	0.65	0.49	0.90
3	2	21	0.56	0.55	0.91
4	2	33	0.48	0.57	0.93

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Another Approach: Space-Filling or Uniform Designs

The goal of a space-filling or uniform design is to “uniformly cover” the experimental region with design points. This approach is often used in computer experiments, which are not subject to random error (the computer model always gives the same response value for a given set of inputs). In such situations, there is no variance error in the model, only bias error. Space-filling designs are also used in physical experiments, where a response variable may be a more complicated function of the predictor variables than can be adequately modeled by a low-order polynomial.

There is much literature for the design of computer experiments and space-filling/uniform designs that I don’t cover in this Youden Address. However, it is interesting to note that in the work of Box and Draper (1959, 1963), their all-bias design criteria were related to criteria for uniform designs.

Graphical Methods to Evaluate & Compare Bias and MSE Properties of Designs

So far I have presented synopses of several approaches to accounting for bias in developing experimental designs. Also of interest are methods for evaluating and comparing experimental designs that account for bias.

Vining and Myers (1991) used MSE dispersion graphs (similar to VDGs discussed previously) to evaluate and compare designs. Piepel et al. (1993) used VDGs and bias dispersion graphs (BDGs) to compare mixture and other designs on irregularly-shaped experimental regions. Anderson-Cook et al. (2009) used FDSGs and boxplots of

- Expected squared bias (ESB) and PV
- Expected MSE (EMSE = PV + ESB)

where ESB is based on $\beta_{2j} \sim N(0, \sigma_B)$ and typically $\sigma_B = \sigma$ (the experimental error variance).

Other numerical and graphical methods that have been used for evaluating and comparing variance properties of designs could also be used to evaluate and compare bias and MSE properties of designs.

Mixture Experiment and Irregular Region Designs Considering Bias and/or MSE

The methods summarized so far focus on considering bias and MSE when developing, evaluating, and comparing designs on spherical and cuboidal experimental regions. There has been some (limited) research on developing designs that minimize bias or MSE for (1) mixture experiments, and (2) experiments with irregular-shaped experimental regions.

Draper and Lawrence (1965b, 1965c) developed simplex designs for mixture experiments with 3 and 4 mixture components, using methods similar to Box and Draper (1959). An example showing a 13-point design on a three-component mixture simplex from Figure 1 of the (1965b) paper is reproduced as Figure 6. The design was developed assuming a quadratic mixture model, but protecting against a full cubic mixture model.

Other work to develop mixture simplex designs that minimize bias or MSE was presented by Becker (1970), Paku et al. (1971), Galil and Kiefer (1977), and Chakrabarti and Mandal (1995).

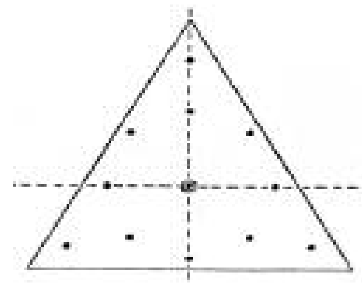

Figure 6. Draper and Lawrence (1965b) Simplex Mixture Design Developed Using the Methods of Box and Draper (1959)

Piepel et al. (1993) used VDGs and BDGs to compare mixture designs on irregular regions developed using five methods:

- Variance-optimal (D, G, IV) designs
- MSE-optimal design (Welch 1983)
- Space-filling designs
- Central-composite analogue designs (CCAD)
- Layered designs (LD)

The CCADs and LDs were new classes of designs for constrained mixture or non-mixture experiments that contain a center point and points on at least two layers of the experimental region. CCADs contain all or a subset of the vertices of the constrained region, as well as a set of “star” points (which for mixture experiments are along mixture component effect directions). LDs contain points on the boundary and at least one other layer of the constrained region. Examples of a CCAD and a LD for a 3-component constrained mixture experiment are shown in Figure 7. Both designs have points on

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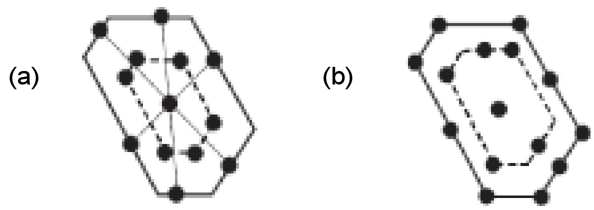

Figure 7. Two New Classes of Designs for a Constrained Three-Component Mixture Experiment: (a) Central-Composite Analogue Design with Inner Layer 0.50 of the Outer, (b) Layered Design with Inner Layer 0.667 of the Outer Layer.

an outer layer (the boundary of the constrained region), an inner layer (a shrunken version of the boundary), and a center point.

Bayesian D-Optimal Mixture Experiment Designs: Simplex & Constrained Regions

DuMouchel and Jones (1994) included a mixture experiment example of Bayesian D-optimal design. Andere-Rendon, Montgomery, and Rollier (1997) extended the Bayesian D-optimal design work to 3- and 4-component simplex and constrained mixture regions.

Andere-Rendon et al. considered a three-component, constrained mixture experiment example where the goal was to generate a 12-point Bayesian D-optimal design assuming a quadratic primary model with cubic potential terms. The prior distribution of the potential terms was chosen as $N(0, \tau^2\sigma^2)$. Parts of Figure 5 from their paper are reproduced in Figure 8. The figure shows a

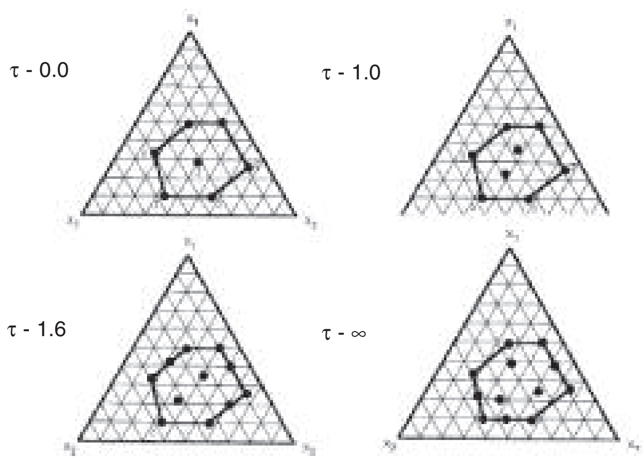

Figure 8. Bayesian D-Optimal Designs for Different Values of the Bias Error

progression of 12-point designs for different values of τ, which corresponds to the relative magnitude of the bias compared to the experimental error variance (σ^2). The authors recommended in general choosing a design with τ = 1.0 to 1.6.

Mixture and Mixture-Process Variable (MPV) Designs using EIMSE Criterion

Chantarat et al. (2006) generated mixture and mixture-process variable (MPV) designs using the EIMSE criterion discussed previously. They presented a 17-point minimum-EIMSE design in their Table 2(b) for the unconstrained MPV region given by

$$0 \le x_i \le 1 \ (i = 1, 2, 3) \qquad -1 \le z_k \le 1 \ (k = 1, 2)$$

where the x_i are the proportions of three mixture components and the z_k are coded values of two process variables. To visualize the design, I plotted the points as projections into the mixture simplex [Figure 9(a)] and the process-variable space [Figure 9(b)]. This design is much different looking than traditional minimum-variance focused MPV designs. For example, a traditional 17-point MPV design might have a fraction of a 7-point simplex centroid design at each vertex of the PV space.

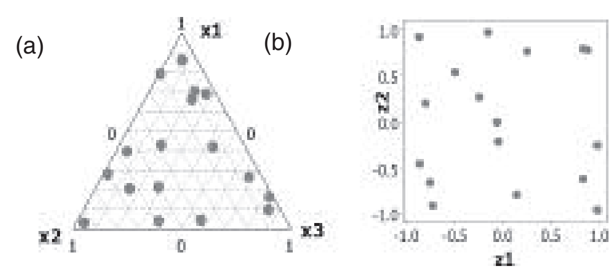

Figure 9. The 17-Point Minimum EIMSE Design Projected into the (a) Mixture Simplex and (b) Process Variable Space

Summary

In response surface methodology, models are used to approximate true, unknown response surfaces. Model predictions are subject to variance errors and bias errors.

In a seminal paper, Box and Draper (1959) considered bias as well as variance properties in developing response surface designs. In the ensuing 50 years (1959-2009) more than 100 research papers have been published on model-robust and model-misspecification designs. Two representative conclusions from the literature are:

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- "…even if the variance error V is several times as large as the bias error B, the best design is much closer to the all-bias design than to the all-variance design." (Draper and Guttman 1992)
- "Studies have revealed that unless the contribution from variance is many times greater than that from bias then the optimal designs are very close to the designs obtained by ignoring variance altogether." (Butler 2006)

Both of these quotes presume that an assumed model will have bias and variance errors, and that best/optimal designs should account for both.

Still, after 50 years of research and many such conclusions, bias (along with variance) is not routinely considered in developing, evaluating, and comparing experimental designs. There are several reasons for this, including:

- Experimenters often believe they have specified an adequate model
- Many papers are difficult to read and contain few examples
- The literature presents many different strategies:
  - Design points restricted to being within the experimental region (R) or allowed to fall outside R in a larger region of operability (O)
  - Minimum-bias vs. MBE with secondary criteria
  - Bayesian
  - Rotation
  - Space-filling/uniform
  - Others
- Designs are developed
  - with different assumptions
  - within a class of designs (e.g., FF, CCD, BBD) considered by the authors

Hence, it is difficult to understand the many approaches and options from the literature and to know what to do in practice.

Recommendations

It is my belief that we (statisticians and practitioners) need to routinely use methods that consider variance and bias properties to develop, evaluate, and compare experimental designs. I have several recommendations for how the statistics community can achieve this:

- Complete a review paper to describe and compare existing research, provide guidance for practitioners and identify gaps/needs (I am working on this with some co-authors).
- Perform new research to fill gaps
- Implement the methods in commercial experimental design software. (This is currently not the case with a few exceptions.)
- Publish some practical examples to aid practitioners
- Routinely include this topic in short courses and statistics department classes on experimental design

Progress in these areas would provide for much wider use of the methods by practitioners.

Acknowledgments

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Closing Comment

The bibliography of articles in the area of methods for experimental designs that account for bias properties of designs is much larger than the number of papers referred to in my Youden Address and referenced in the following section. If you would like a copy of the full bibliography or have feedback about my Youden Address, please feel free to contact me at greg.piepel@pnl.gov.

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