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Research Tutorials in Chemistry (RTC)

## Chemical Aims Today (Cat)

## One. (Statistical Evolving) Experimental design (Seed) in Omni_metrics (O!M)

**K. Somasekhara Rao[1], K. Ramakrishna[2] and R. Sambasiva Rao[3]**

1. Dept. Of Chemistry, Acharya Nagarjuna Univ., Dr. M.R.Appa Rao Campus, Nuzvid,521 201, **INDIA**
2. Department of Chemistry, Gitam Institute of Science, Gitam University, Visakhapatnam, 530 017, **INDIA**
3. School of Chemistry, Andhra University, Visakhapatnam 530 003, **INDIA**

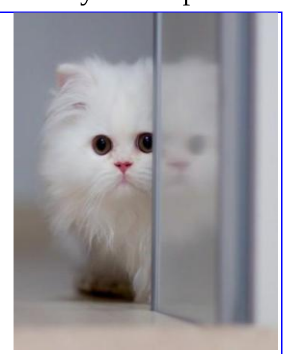
Email: sraokaza1947@gmail.com, karipeddirk@gmail.com, rsr.chem@gmail.com

In chemistry, the application disciplines, instrumental sensors in operation and thought experimental/ computational/ experimental methods in vogue span a wide spectrum with high fidelity in scope and precision. Chemical aims today (Cat, Chart 1) are after hundreds of years of evolution and further evolve to adapt to the challenges of twenty second century.

During twentieth century, the designing of experiment, varying magnitudes of relevant chemical/physico-chemical factors/catalysts etc. was believed to be in the minds/ genes of trained chemists. Statistical experimental design (ED) developed in first half of last century was used in agricultural trials for maximum yield of rice and other cereals. In 1970s, design of experiments using factorial/central composite entered into quantitative and kinetic methods of chemical analysis. With evolutionary changes of Chemometrics, ED has become an integral part chemical activity. The breadthwise application endorsed the positive benefits compared to equal/unequal interval trials and set the flag for its indispensability in critical tasks. Now, Omnimetrics dealing with diverse disciplines with chemical component in the interdisciplinary task from high end contributions employ most of state- of-knowledge tools to ensure not only value-added-end-

**Chart 1: Cat in nature**

Cat belongs to felidae family and species range from domestic cat to wild leopard/lion. The magnificent integrity/ diversity is along nature's evolution.



**CAT (computerized axial tomography) in Medical diagnosis:** is a state-of-knowledge instrument in medical

Diagnosis, an outcome of decades' experts' effort; it sees soft-tissues, which are not perceived by X-rays except mapping bones.

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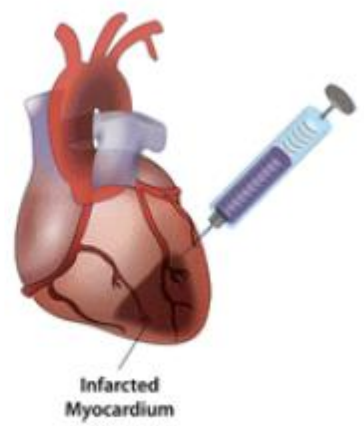
**Applications-Instruments-Methods**

products but also high quality with desired range of characteristics for foolproof functional utility. Chemical aims today (Cat) with chemical aims in the past (Cap) shall adapt to chemical aims of future evolution (Café).

Statistical *experimental evolving* design (Seed: Statistical *evolving experimental* design) occupies a niche and a high contributing tool in synthesis, manufacturing, quantitative analysis, computations and free parameter setting in instruments. The increasing number of published papers in high impact journals year by year endorses still its shelf life. The hands-on-experience will yield synergistic information/quality in future high-tech ventures in chemical sciences. A select set of current literature reports from ACS (American chemical society) dealing with proved benefit of Seed methods in diverse disciplines involving chemical species follow. The chosen display format is to browse through the crisp information fast and not dilating into hierarchical details. The target readers are researchers to appreciate the high potency of the tool in the arsenal of research methodology. The experts in one field may be inspired to think of its use in their field to extract increased amount of information with relatively less number of experiments.

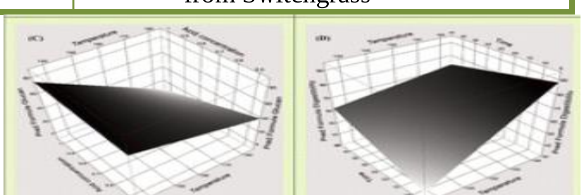
**Factorial design (FD, FactDes)**

| Task: | **Response** | **Variables in ED** |
|---|---|---|
| Rat MI (Myocardial infarction) model   Opt( multiple protein therapy) | ☼ Ejection fraction 4 weeks after MI after injecting protein combination<br>☼ Factorial design | ✈ Tissue inhibitor of metalloproteinases 3 (TIMP-3)<br>✈ Interleukin-10 (IL-10)<br>✈ Basic fibroblast growth factor (FGF-2)<br>✈ Stromal cell-derived factor 1 alpha (SDF-1α) |

Factorial Design of Experiments to Optimize Multiple Protein Delivery for Cardiac Repair

ACS Biomater. Sci. Eng., 2016, 2 (5), pp 879–886 DOI: 10.1021/acsbiomaterials.6b00146

Hassan K. Awada, Louis A. Johnson, T. Kevin Hitchens, Lesley M. Foley, and Yadong Wang∇

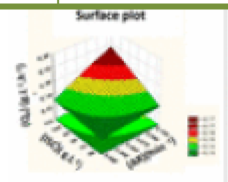
| **Expdes (ED)** | **Discipline** | **Variables in ED** | **Resp** |
|---|---|---|---|
| Full factorial design | ▪ Biochemical Sugar Production from Switchgrass  | ✈ Temperature 140 to 180 °C;<br>✈ Time 10 to 40 min;<br>✈ Sulfuric acid 0.5% or 1% (v/v) | ® Prehydrolyzate xylose<br>® Glucose concentrations etc. |

Three way factor interaction has significant influence on prehydrolyzate glucose concentrations

Effects of Dilute Acid Pretreatment Parameters on Sugar Production during Biochemical Conversion of Switchgrass Using a Full Factorial Design

*ACS Sustainable Chem. Eng.*, **2016**, *4* (8), pp 4124–4130; **DOI:** 10.1021/acssuschemeng.6b00441

Angele Djioleu and Danielle Julie Carrier

| Expdes (ED) | Task | Variables in ED | Resp |
|---|---|---|---|
| $2^2$-full factorial design | ▪ Hemicellulosic Ethanol Production in Fluidized Bed Reactor | ✈ Aeration rate (0.027, 0.069, and 0.111 min–1)<br>✈ carrier concentration (55.55, 83.33, and 111.11 g. L–1)). | ® On the ethanol yield ($Y_{P/S}$) and productivity ($Q_P$) |
|   | | | |

Hemicellulosic Ethanol Production in Fluidized Bed Reactor from Sugar Cane Bagasse Hydrolysate: Interplay among Carrier Concentration and Aeration Rate

ACS Sustainable Chem. Eng., 2017, 5 (9), pp 8250–8259; DOI: 10.1021/acssuschemeng.7b01916

Felipe A. F. Antunes, Anuj K. Chandel, Julio Cesar dos Santos, Thais S. S. Milessi, Guilherme F. D. Peres, and Silvio Silvério da Silva

| Expdes (ED) | Variables in ED | Resp |
|---|---|---|
| Full factorial ($2^4$) | ✈ pH<br>✈ Nps loading<br>✈ Initial drug concentration<br>✈ Contact time | ® Efficiency of adsorption of two photosensitive fluoroquinolones Ciprofloxacin (CIP) and Moxifloxacin (MOX) on the surface of synthesized magnetite/pectin nanoparticles |

Adsorptive Removal of Fluoroquinolones from Water by Pectin-Functionalized Magnetic Nanoparticles: Process Optimization Using a Spectrofluorimetric Assay

ACS Sustainable Chem. Eng., 2017, 5 (1), pp 133–145; DOI: 10.1021/acssuschemeng.6b01003

Olivia A. Attallah, Medhat A. Al-Ghobashy, Marianne Nebsen, and Maissa Y. Salem

| Task: | Resp | Variables in ED (X) |
|---|---|---|
| Novel biomaterials are suitable for extrusion-based 3D printing applications. Poly(propylene fumarate) (PPF) as a model material<br><br>ED: Full factorial design | Viscosity<br>Fiber diameter<br>And pore size<br>Layer-by-layer on 3D scaffolds<br><br>Viscosity = linfn([PPF]..) | ✈ [PPF]<br>✈ Printing pressure,<br>✈ Printing speed<br>✈ Programmed fiber spacing |

Extrusion-Based 3D Printing of Poly(propylene fumarate) in a Full-Factorial Design
ACS Biomater. Sci. Eng., 2016, 2 (10), pp 1771–1780
DOI: 10.1021/acsbiomaterials.6b00026
Jordan E. Trachtenberg, Jesse K. Placone, Brandon T. Smith, Charlotte M. Piard, Marco Santoro, David W. Scott, John P. Fisher, and Antonios G. Mikos

| Expdes (ED) | Discipline | Reduce to |
|---|---|---|
| ☼ Generalized fractional factorial design | ▪ Multivariate calibration using microwave resonance spectroscopy for (a) determination of water in tablets, (b) stability study in drug product development (c) representative sample selection in clinical studies | ✈ Complementary and balanced sub designs analogous to a fold-over in two-level reduced factorial designs . |

| Expdes (ED) | Discipline | Variables in ED | Resp |
|---|---|---|---|
| Factorial | ▪ Renewable energy | ✈ Compression ratio<br>✈ Injection pressure<br>✈ Injection timing | ® Variable compression ratio |

Fueled with Diesel–Aegle Marmelos Oil–Diethyl Ether Blends Using Response Surface Methodology
*Energy Fuels*, **2017**, *31* (10), pp 11362–11376; **DOI:** 10.1021/acs.energyfuels.7b01515
M. Krishnamoorthi and R. Malayalamurthi

| Expdes (ED) | Discipline | Variables in ED | Resp |
|---|---|---|---|
| Factorial design | ▪ Adsorption | ✈ Aptes concentration<br>✈ reaction temperature<br>✈ and reaction duration | ® Silica adsorbent BET surface area |
| **Software:** Minitab-15 | | | |

Benzene, Toluene, m-Xylene Adsorption on Silica-Based Adsorbents
Energy Fuels, 2017, 31 (2), pp 1882–1888; DOI: 10.1021/acs.energyfuels.6b03192
T. Ncube, K. Suresh Kumar Reddy, Ahmed Al Shoaibi, and C. Srinivasakannan

## Fractional Factorial design (Fr.FD, Fract.FactDes)

| Expdes (ED) | Discipline | Variables in ED | Resp |
|---|---|---|---|
| ☼ fractional factorial design | ▪ MALDI-TOF-MS | ✈ Matrix preparations<br>✈ Matrix additives<br>✈ Additive concentrations<br>✈ Deposition | ® Detection of Phospholipids and Acylglycerols |

| | |
|---|---|
| | methods |
| 720 key experiments by FrFd instead of 8064 possible trials; Pareto optimality used | |

Fractional Factorial Design of MALDI-TOF-MS Sample Preparations for the Optimized Detection of Phospholipids and Acylglycerols

Anal. Chem., 2016, 88 (12), pp 6301–6308; DOI: 10.1021/acs.analchem.6b00512

Najla almasoud, Elon Correa, Drupad K. Trivedi, and Royston Goodacre

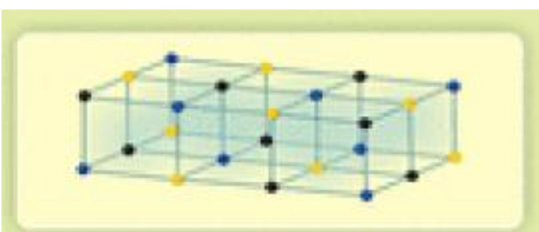
| Expdes (ED) | Task | Variables in ED | Resp |
|---|---|---|---|
| $2^{5-1}$ factorial design | ▪ Bioethanol Production | ✈ Temperature (80–120 °C)<br>✈ Solid loading (2.5–7.5%)<br>✈ Glycerol (85–95%)<br>✈ Acid concentrations (0.5–3%)<br>✈ Reaction time (10–60 min), | ® Glycerol acid-pretreatment of sugar cane bagasse |

Organosolv Pretreatment of Sugar Cane Bagasse for Bioethanol Production

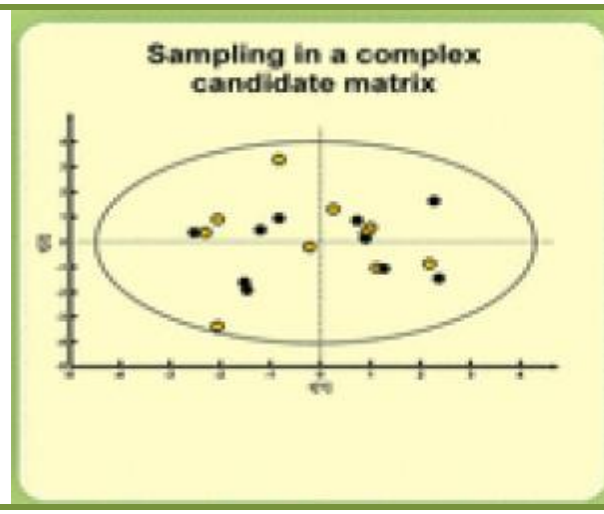
Ind. Eng. Chem. Res., 2017, 56 (14), pp 3833–3838
DOI: 10.1021/acs.iecr.7b00079

Ruly Terán Hilares, Mateus Pereira Swerts, Muhammad Ajaz Ahmed, Lucas Ramos, Silvio Silvério da Silva, and Júlio César Santos

**Generalized Fr FD**



| Qualitative factors | Factor levels |
|---|---|
| Strength | [10mg, 40mg] |
| Container | [3;30;500;1000] ml |
| Batch | [Batch1; batch 2;batch 3] |




Generalized Subset Designs in Analytical Chemistry

Anal. Chem., 2017, 89 (12), pp 6491–6497; DOI: 10.1021/acs.analchem.7b00506

Izabella Surowiec, Ludvig Vikström, Gustaf Hector, Erik Johansson, Conny Vikström, and Johan Trygg

## Central Composite design (CCD, Central Comp. Desig.)

| Expdes (ED) | Discipline | Process Variables in ED | Resp |
|---|---|---|---|
| Central composite design | Biodiesel | Reaction time<br>Methanol/oil ratio<br>Catalyst loading | Biodiesel yield |

Transesterification of Rubber Seed Oil to Biodiesel over a Calcined Waste Rubber Seed Shell Catalyst: Modeling and Optimization of Process Variables

Energy Fuels, 2017, 31 (6), pp 6109–6119; DOI: 10.1021/acs.energyfuels.7b00331

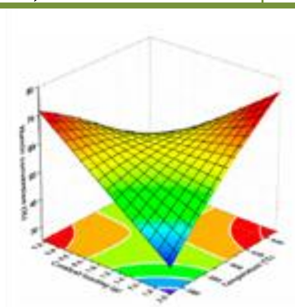
Samuel Erhigare Onoji, Sunny E. Iyuke, Anselm I. Igbafe, and Michael O. Daramola

| Expdes (ED) | Discipline | Variables in ED | Resp |
|---|---|---|---|
| Central composite | Synthesis | Acetone to monoacetin mole ratio<br>Reaction temperature<br>pressure<br>Flow rate<br>Catalyst | Yield of the second stage of the reaction |

Optimization of Solketalacetin Synthesis as a Green Fuel Additive from Ketalization of Monoacetin with Acetone

Ind. Eng. Chem. Res., 2016, 55 (25), pp 6904–6910; DOI: 10.1021/acs.iecr.6b00929

Yadollah M. Gorji and Hassan S. Ghaziaskar

| Expdes (ED) | Discipline | Variables in ED | Resp |
|---|---|---|---|
| Central composite (19 experiments) | Catalysis | T<br>Humin intake<br>Catalyst intake<br>Batch time | Humin conversion<br>Alkylphenolics yield |
|  | | | |

Catalytic Liquefaction of Humin Substances from Sugar Biorefineries with Pt/C in 2-Propanol

ACS Sustainable Chem. Eng., 2017, 5 (1), pp 469–480; DOI: 10.1021/acssuschemeng.6b01834

Y. Wang, S. Agarwal, and H. J. Heeres

| Expdes (ED) | Variables in ED | Resp |
|---|---|---|
| Central composite | Hydrotreating conditions<br>Temperature, pressure | Fines deposition on nimo/γal2o3 catalyst |

| | |
|---|---|
| | Particle loading |

The Impact of Process Parameters on the Deposition of Fines Present in Bitumen-Derived Gas Oil on Hydrotreating Catalyst

Energy Fuels, 2017, 31 (6), pp 5969–5981; DOI: 10.1021/acs.energyfuels.7b00554

Rachita Rana, Sandeep Badoga, Ajay K. Dalai, and John Adjaye

| Expdes (ED) | Discipline | Resp | Variables in ED | Optimum values |
|---|---|---|---|---|
| Central composite | Extraction | Extraction yield (7.9936 ± 0.0364 mg/g) | Solvent/solid ratio | 17.5:1 |
| | | | Ultrasonic power | 180 W, |
| | | | Temperature | 45 °C, |
| | | | Particle size | 80 mesh |
| | | | Extraction time | 70 min |

Well-Designed Hydrophobic Deep Eutectic Solvents As Green and Efficient Media for the Extraction of Artemisinin from Artemisia annua Leaves

ACS Sustainable Chem. Eng., 2017, 5 (4), pp 3270–3278; DOI: 10.1021/acssuschemeng.6b03092

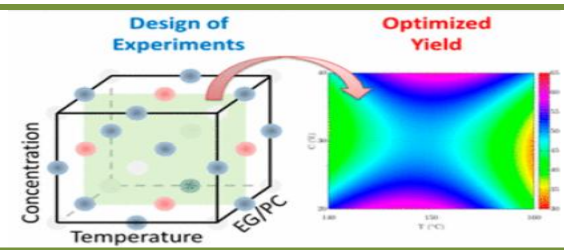
Jun Cao, Meng Yang, Fuliang Cao, Jiahong Wang, and Erzheng Su

| Expdes (ED) | Task: | Variables in ED [opt values] |
|---|---|---|
| Composite fractional factorial | Synthesis of gold nanorods | Experimental factors<br>- Amount of sodium borohydride<br>- Rate of stirring when producing seed nanoparticles<br>- Age of and amount of seeds added<br>- Reaction temperature<br>- Amounts of silver nitrate<br>- Amount ascorbic acid added<br>- Age of reduced growth solution before seed nanoparticles are added to initiate rod formation |

| | |
|---|---|
| Understanding the Seed-Mediated Growth of Gold Nanorods through a Fractional Factorial Design of Experiments | Langmuir, 2017, 33 (8), pp 1891–1907<br>DOI: 10.1021/acs.langmuir.6b03606 |
| Nathan D. Burrows, Samantha Harvey, Fred A. Idesis, and Catherine J. Murphy | |

## Box–Behnken

| Expdes (ED) | Discipline | Variables in ED | Resp |
|---|---|---|---|
| Box–Behnken | Synthesis | Temperature | ® PC(OH)2 |

| | | |
|---|---|---|
|  | ✈ ethylene glycol (EG)/PC molar ratio<br>✈ polymer solution conc. | molar mass and on reaction yield |



Telechelic Poly(bisphenol A carbonate) Synthesis by Glycolysis: A Response Surface Methodology Approach
Eng. Chem. Res., 2017, 56 (14), pp 3983–3992; DOI: 10.1021/acs.iecr.6b04614
Thiago do Carmo Rufino, Márcia Cristina Breitkreitz, and Maria Isabel Felisberti

| Expdes (ED) | Discipline | Variables in ED | Resp |
|---|---|---|---|
| ✈ Box-Behnken<br>✈ Central composite | ▪ Catalysis | ✈ Methanol/oil ratio<br>✈ Catalyst amount<br>✈ Reaction time on, | ® Acid value<br>® Biodiesel yield |
| ✓ Scanning electron microscopy (SEM)<br>✓ X-ray diffraction (XRD)<br>✓ Fourier transform infrared (FTIR)<br>✓ Elemental analysis | | | |

Two-Step Conversion of Neem (Azadirachta indica) Seed Oil into Fatty Methyl Esters Using a Heterogeneous Biomass-Based Catalyst: An Example of Cocoa Pod Husk
Energy Fuels, 2017, 31 (6), pp 6182–6193; DOI: 10.1021/acs.energyfuels.7b00604
Eriola Betiku, Anietie Okon Etim, Omoniyi Pereao, and Tunde Victor Ojumu

| Expdes (ED) | Discipline | Variables in ED | Resp |
|---|---|---|---|
| Box–Behnken | ▪ Synthesis-- methyl acrylate<br>▪ Fluidized Bed Reactor | Process parameters<br>✈ Reaction temperature<br>✈ Molar ratio of Ma and FA<br>✈ Liquid hourly space velocity (LHSV) | Yield |

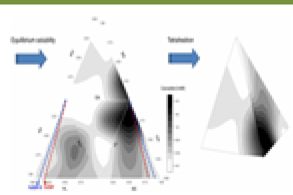
One-Step Synthesis of Methyl Acrylate Using Methyl Acetate with Formaldehyde in a Fluidized Bed Reactor
Ind. Eng. Chem. Res., 2017, 56 (33), pp 9322–9330; DOI: 10.1021/acs.iecr.7b02522
Shifeng Jiang, Chunshan Li, Hongnan Chen, Dan Yang, and Suojiang Zhang

## Taguchi

| Expdes (ED) Discipline | Variables in ED | Resp |
|---|---|---|
| Taguchi factorial design | ✈ ABP concentration<br>✈ Acetone concentration<br>✈ Volume ratio of acetone to ABP<br>✈ Drug concentration | ® Nanocarrier characteristics<br>® Particle size, polydispersity index, zeta potential, and percentage drug loading |

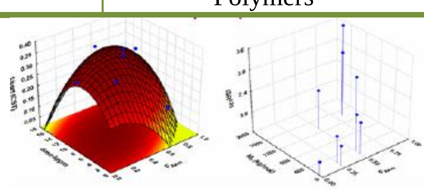
Factorial Design Based Multivariate Modeling and Optimization of Tunable Bioresponsive Arginine Grafted Poly(cystaminebis(acrylamide)-diaminohexane) Polymeric Matrix Based Nanocarriers
Mol. Pharmaceutics, 2017, 14 (1), pp 252–263; DOI: 10.1021/acs.molpharmaceut.6b00861
Rongbing Yang, Kihoon Nam, Sung Wan Kim, James Turkson, Ye Zou, Yi Y. Zuo, Rahul V. Haware∇, and Mahavir B. Chougule

## Mixture design

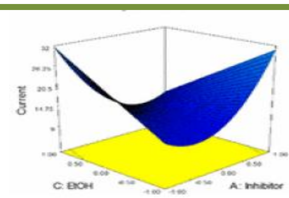
| Expdes (ED) | Task | Variables in ED | Resp |
|---|---|---|---|
| Four-component mixture design<br>Factorial design | ▪ Solubility of drugs<br>○ acidic (zafirlukast)<br>○ basic (aprepitant, carvedilol)<br>○ neutral (fenofibrate, felodipine, griseofulvin, and spironolactone) | ✈ digested lipids | ® Solubility variation |
|  | | | |

Influence of Physiological Gastrointestinal Surfactant Ratio on the Equilibrium Solubility of BCS Class II Drugs Investigated Using a Four Component Mixture Design
Mol. Pharmaceutics, Article ASAP; DOI: 10.1021/acs.molpharmaceut.7b00354
Zhou Zhou, Claire Dunn, Ibrahim Khadra, Clive G. Wilson, and Gavin W. Halbert

## Response Surface Methodology (RSM)

| Expdes (ED) | Discipline | Variables in ED | Resp |
|---|---|---|---|
| RSM | ▪ Polymers | ✈ Chemical composition<br>✈ Average molecular weight of poly(acrylamide-co-diallyldimethylammonium chloride) in | ® Dewatering mfts |
|  | | | |

Dewatering Oil Sands Mature Fine Tailings (mfts) with Poly(acrylamide-co-diallyldimethylammonium chloride): Effect of Average Molecular Weight and Copolymer Composition
Ind. Eng. Chem. Res., 2017, 56 (5), pp 1256–1266; DOI: 10.1021/acs.iecr.6b04348
Vahid Vajihinejad, Rina Guillermo, and João B.P. Soares

| **Expdes (ED)** | **Resp** | | **Variables in ED** | **Optimum values** |
|---|---|---|---|---|
| RSM | Corrosion inhibition efficiency of 2-(2-hydroxyphenyl)-benzothiazole |  | ▪ Inhibitor concentration | 433.7 µm |
| | | | ▪ Hydrochloric acid | 3.38 M for |
| | | | ▪ Ethanol | 0.36 M for |

Experimental and Theoretical Investigation of Inhibition Efficiency of 2-(2-Hydroxyphenyl)-benzothiazole Using Impedance Spectroscopy, Experimental Design, and Quantum Chemical Calculations
Ind. Eng. Chem. Res., 2017, 56 (32), pp 9035–9044; DOI: 10.1021/acs.iecr.7b02030
Marzie Afzalkhah, Saeed Masoum, Mohsen Behpour, Hossein Naeimi, and Adel Reisi-Vanani

Typical books on experimental design (Seed)

Experimental Design and Analysis — http://www.stat.cmu.edu/~hseltman/309/Book/Book.pdf data files : http://www.stat.cmu.edu/~ hseltman/309/Book/data/ **2015**
Howard J. Seltman,

Statistical Design and Analysis of Experiments, Chapters 7 to 10 — Society for Industrial and Applied Mathematics Philadelphia, **1998**
Peter W. M. John

A First Course in Design and Analysis of Experiments, Chapters 18, 19. — ISBN 0-7167-3510-5, **2010**
Gary W. Oehlert

Design and Analysis of Experiments, Chapter s, 15 and 16. — Springer,New York, **1999**
Angela Dean, Daniel Voss,

Computer applications in chemistry
Chapter 11: Experimental designs — Himalaya publishing House, 2005, Mumbai, India,
R Sambasiva Rao, G Nageswara Rao

The role of Simplex method in chemical research — J.Chem.Sci. 14(1993)23-44
Review: state-of-knowledge algorithms –applications kinetic method of analysis-chromatography-instrumental parameters
R. Sambasiva Rao

**Object Oriented Vocabulary of**
**Design of Experiments (DOE)**
**Statistical Evolving experimental design (stat.evol.expdes, SEED)**

Sampling points : statistical
XY_Model : [Mathematical ; statistical; Fuzzy]
Objfn: [Mathematical ; statistical; Fuzzy]

| | | |
|---|---|---|
| | Goal: | Opt(Fn{residual in response}) |
| Expdes.Methods | | [sample space;<br>Response surface modelling;<br>Prediction → Experiment ; refinement [ coarse; fine];] |
| Expdes.Applications | | Optimum<br>[Operating conditions [exptal variables];<br>Instrumental parameters;] |
| Optimum | | [maximum ;<br>Minimum;] |
| $$$_Design | | |
| Multiple variables: | | [single variable;<br>Multiple variable;]<br>[one variable at a time (OVAT);<br>Multiple variables at a time (MVAT);]<br>[Sequential ;<br>Parallel;]<br>[one method;<br>Hybrid [binary; ternary;] |
| Uniform | | |
| Factorial | : | [mixed; fractional; confounded ]<br>[full ;<br>Fractional;<br>Central composite] |
| Fractional factorial | : | |
| Central composite | : | [simple; with star points] |
| Orthogonal | : | [Plackett-Burma<br>Box Behnken |
| | : | |
| $$$ optimal designs | : | [A ;<br>D;<br>E;] |
| Hybrid | | [factorial + simplex]<br>[factorial + random]<br>[factorial + random + simplex] |

| | |
|---|---|
| Mixture | |
| Simplex | [Basic;<br>Modified simplex;<br>Super modified simplex; |
| Taguchi design | |
| Surrogate-Enhanced Evolutionary Annealing-Simplex (SEEAS) | [evolutionary search + simulated annealing + downhill simplex) |
| Model ; | [multiple-linear;<br>Multiple-linear with cross producdts;<br>Multiple-polynomial [ square; cubic; quatric];<br>Full quadratic;<br>Full polynomial];<br>Neural networks |
| Stochastic response surface method (Stochast.RSM) | [non-Gaussian dependent random variables used under incomplete probability information] |
| Model.objective | Prediction of extremum in m-D space of experimental variables<br>Objective: (optimum) Parametrization but not curve fitting |