ISSN: 2278-1862

Journal of Applicable Chemistry

2017, 6 (6): 1234-1239

(International Peer Reviewed Journal)

New Chemistry News

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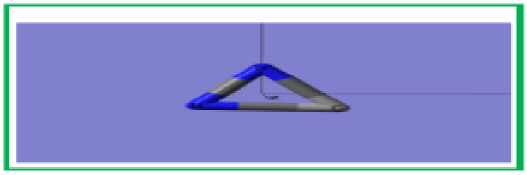
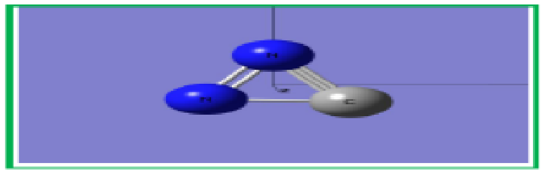


New News of Chem (NNC)



ChemNewsNew (CNN)

Experimental Design (ED) -- Chemometrics

Tutorials & Reviews

Experimental Design in Clinical 'Omics Biomarker Discovery

J. Proteome Res., Article ASAP
DOI: 10.1021/acs.jproteome.7b00418

To avoid unpleasant surprises of statistical analysis. --avoids bias--to improve the chance of answering the clinical questions-- statistical power, to avoid confounding factors

Jenny Forshed

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

A Tasty Approach to Statistical Experimental Design in High School Chemistry: The Best Lemon Cake

J. Chem. Educ., 2017, 94 (4), pp 465–470

Lucia Liguori

Extraction and Antibacterial Properties of Thyme Leaf Extracts: Authentic Practice of Green Chemistry

J. Chem. Educ., 2016, 93 (8), pp 1422–1427
DOI: 10.1021/acs.jchemed.5b00891

Sean C. Purcell, Prithvi Pande, Yingxin Lin, Ernesto J. Rivera, Latisha Paw U, Luisa M. Smallwood, Geri A. Kerstiens, Laura B. Armstrong, maryann T. Robak, Anne M. Baranger, and Michelle C. Douskey

The Alcohol Dehydrogenase Kinetics Laboratory: Enhanced Data Analysis and Student-Designed Mini-Projects

J. Chem. Educ., 2016, 93 (5), pp 963–970
DOI: 10.1021/acs.jchemed.5b00610

Todd P. Silverstein

The Coffee Project Revisited: Teaching Research Skills to Forensic Chemists

J. Chem. Educ., 2017, 94 (4), pp 445–450
DOI: 10.1021/acs.jchemed.6b00600

Hilary J. Hamnett and Ann-Sophie Korb

Nano Science

Understanding the Seed-Mediated Growth of Gold Nanorods through a Fractional Factorial Designof Experiments

Langmuir, 2017, 33 (8), pp 1891–1907
DOI: 10.1021/acs.langmuir.6b03606

Nathan D. Burrows, Samantha Harvey, Fred A. Idesis, and Catherine J. Murphy

Laser Ablation of Silver in Liquid Organic Monomer: Influence of Experimental Parameters on the Synthesized Silver Nanoparticles/Graphite Colloids

J. Phys. Chem. B, 2017, 121 (27), pp 6646–6654
DOI: 10.1021/acs.jpcb.7b05409

Factorial design;

Maxime Delmée, Grégory Mertz, Julien Bardon, Adeline Marguier, Lydie Ploux, Vincent Roucoules, and David Ruch

Submicrometric Magnetic Nanoporous Carbons Derived from Metal–Organic Frameworks Enabling Automated Electromagnet-Assisted Online Solid-Phase Extraction

Anal. Chem., 2016, 88 (14), pp 6990–6995
DOI: 10.1021/acs.analchem.6b02065

☼ Full factorial design; Doehlert Matrix

Rejane M. Frizzarin, Carlos Palomino Cabello, Maria del Mar Bauzà, Lindomar A. Portugal, Fernando Maya, Víctor Cerdà, José M. Estela, and Gemma Turnes Palomino

Nanovesicles

Using Factorial Experimental Design To Prepare Size-Tuned Nanovesicles

Ind. Eng. Chem. Res., 2016, 55 (34), pp 9164–9175
DOI: 10.1021/acs.iecr.6b01552

Soft nanoparticles-- suitable in food, cosmetic, pharmaceutical, or medical diagnosis/therapy

Pablo García-Manrique, María Matos, Gemma Gutiérrez, Oscar R. Estupiñán, María Carmen Blanco-López, and Carmen Pazos

Nanotoxicology

Kriging-Based Design of Experiments for Multi-Source Exposure–Response Studies in Nanotoxicology

ACS Sustainable Chem. Eng., 2017, 5 (4), pp 3223–3232
DOI: 10.1021/acssuschemeng.6b02981

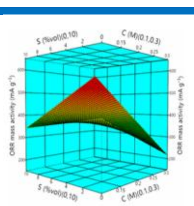
Ying Pei, Feng Yang, Xi Chen, Nianqiang Wu, and Kai Wang

Evaluating the Combined Toxicity of Cu and ZnO Nanoparticles: Utility of the Concept of Additivity and a Nested Experimental Design

Environ. Sci. Technol., 2016, 50 (10), pp 5328–5337 DOI: 10.1021/acs.est.6b00614

Yang Liu, Jan Baas, Willie J. G. M. Peijnenburg, and Martina G. Vijver

Controlling the Interfacial Environment in the Electrosynthesis of mnox Nanostructures for High-Performance Oxygen Reduction/Evolution Electrocatalysis



ACS Appl. Mater. Interfaces, 2017, 9 (32), pp 26771–26785
DOI: 10.1021/acsami.7b05501

☼ Statistical experimental design;

Pooya Hosseini-Benhangi, Chun Haow Kung, Akram Alfantazi, and Elöd L. Gyenge

Extraction of Cellulose Nanocrystals with a High Yield of 88% by Simultaneous Mechanochemical Activation and Phosphotungstic Acid Hydrolysis

ACS Sustainable Chem. Eng., 2016, 4 (4), pp 2165–2172
DOI: 10.1021/acssuschemeng.5b01620

Qilin Lu, Zhenghan Cai, Fengcai Lin, Lirong Tang, Siqun Wang, and Biao Huang

Hospital and Urban Residues

Fully Automated System for 99Tc Monitoring in Hospital and Urban Residues: A Simple Approach to Waste Management

Anal. Chem., 2017, 89 (11), pp 5857–5863
DOI: 10.1021/acs.analchem.7b00184

Marina Villar, Antoni Borràs, Jessica Avivar, Fernando Vega, Víctor Cerdà, and Laura Ferrer

Proteomics

Identification of Analytical Factors Affecting Complex Proteomics Profiles Acquired in a Factorial Design Study with Analysis of Variance: Simultaneous Component Analysis

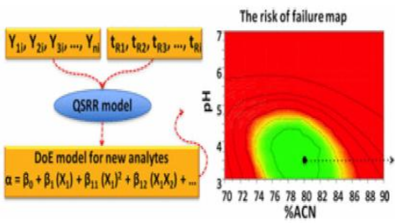
Anal. Chem., 2016, 88 (8), pp 4229–4238
DOI: 10.1021/acs.analchem.5b03483

Two-level fractional factorial design ; preprocessing: Threshold Avoiding Proteomics Pipeline

Vikram Mitra#⊗, Natalia Govorukhina⊗, Gooitzen Zwanenburg, Huub Hoefsloot, Inge Westra, Age Smilde#, Theo Reijmers, Ate G. J. Van der Zee, Frank Suits, Rainer Bischoff#⊗, and Péter Horvatovich

Pharmaceutical Analysis

Rapid Method Development in Hydrophilic Interaction Liquid Chromatography for Pharmaceutical Analysis Using a Combination of Quantitative Structure–Retention Relationships and Design of Experiments



Anal. Chem., 2017, 89 (3), pp 1870–1878
DOI: 10.1021/acs.analchem.6b04282

Maryam Taraji, Paul R. Haddad, Ruth I. J. Amos, Mohammad Talebi, Roman Szucs, John W. Dolan, and Chris A. Pohl

Technology

Probability-Based Design of Experiments for Batch Process Optimization with End-Point Specifications;

Find optimal policies for runs involving stochastic binary outcomes; acetoacetylation of pyrrole with diketene

Ind. Eng. Chem. Res., 2016, 55 (5), pp 1254–1265
DOI: 10.1021/acs.iecr.5b01295

Estefanía Colombo, Martin Luna, and Ernesto Martínez

Optimization of Catalytic Glycerol Etherification with Ethanol in a Continuous Reactor

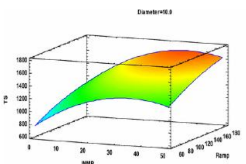
Energy Fuels, 2017, 31 (5), pp 5158–5164
DOI: 10.1021/acs.energyfuels.7b00194

Central composite design;for performance of Amberlyst 15

Caroline O. T. Lemos, Leticia L. Rade, Marcos A. De S. Barrozo, Lindoval D. Fernandes, Lucio Cardozo-Filho, and Carla E. Hori

Experimental and Statistical Optimization of the Tensile Strength of Carbon Fibers from Pitches with Different Composition

Factorial design;



Ind. Eng. Chem. Res., 2017, 56 (12), pp 3243–3250
DOI: 10.1021/acs.iecr.6b04045

Noel Diez, Patricia Álvarez, Clara Blanco, Ricardo Santamaría, Marcos Granda, and Rosa Menéndez

Ultraviolet-Photoassisted Advanced Oxidation of Parabens Catalyzed by Hydrogen Peroxide and Titanium Dioxide. Improving the System

Ind. Eng. Chem. Res., 2016, 55 (18), pp 5152–5160
DOI: 10.1021/acs.iecr.5b04560

☼ Factorial central composite orthogonal and rotatable design

Eduardo M. Cuerda-Correa, Joaquín R. Domínguez-Vargas, María J. Muñoz-Peña, and Teresa González

Biodiesel

Biodiesel Production via Transesterification of Soybean Oil Catalyzed by Superhydrophobic Porous Poly(ionic liquid) Solid Base

Energy Fuels, 2017, 31 (5), pp 5203–5214
DOI: 10.1021/acs.energyfuels.7b00443

☼ Three-level and three-factorial central composite

Bin Jiang, Yumei Wang, Luhong Zhang, Yongli Sun, Huawei Yang, Baoyu Wang, and Na Yang

Steam Deacidification of High Free Fatty Acid in Jatropha Oil for Biodiesel Production

Energy Fuels, 2017, 31 (6), pp 6206–6210
DOI: 10.1021/acs.energyfuels.7b00700

Central composite design; temperature; amount of steam

Godlisten G. Kombe and Abraham K. Temu

Combination of Dispersive Liquid–Liquid Micro-extraction and Emulsion Breaking for the Determination of Cu(II) and Pb(II) in Biodiesel and Oil Samples

Energy Fuels, 2017, 31 (9), pp 9491–9497
DOI: 10.1021/acs.energyfuels.7b01430

Central composite design and a univariate analysis; exptvar: [complexant concentration, ph value, and extractant solvent volume]

Lucas C. Lima, Thiago R. L. C. Paixão, Cassiana S. Nomura, and Ivanise Gaubeur

Chemical Kinetics

Reaction Kinetic Study of Solketal Production from Glycerol Ketalization with Acetone

Ind. Eng. Chem. Res., 2017, 56 (2), pp 479–488
DOI: 10.1021/acs.iecr.6b03581

Ketalization reaction [catalyst: zeolite H-BEA]: glycerol + acetone → solketal ;
Solketal is a green solvent

Vinicius Rossa, Yolanda da S. P. Pessanha, Gisel Ch. Díaz, Leôncio Diógenes Tavares Câmara, Sibele B. C. Pergher, and Donato A. G. Aranda

Experimental Design for Discrimination of Chemical Kinetic Models for Oxy-Methane Combustion

Energy Fuels, 2017, 31 (5), pp 5533–5542 DOI: 10.1021/acs.energyfuels.6b03025

Liming Cai, Stephan Kruse, Daniel Felsmann, Christoph Thies, Kiran K. Yalamanchi, and Heinz Pitsch

Enzymatic Hydrolysis of Steam-Treated Sugarcane Bagasse: Effect of Enzyme Loading and Substrate Total Solids on Its Fractal Kinetic Modeling and Rheological Properties

Energy Fuels, 2017, 31 (6), pp 6211–6220
DOI: 10.1021/acs.energyfuels.7b00818

☼ Central composite design;

Douglas H. Fockink, Mateus B. Urio, Jorge H. Sánchez, and Luiz P. Ramos

Multi-variate Analysis

Multivariate Analysis in Selective Nitroacetophenone Conversion by Hydrogen Sulfide under Phase Transfer Catalysis

Org. Process Res. Dev., 2017, 21 (1), pp 23–30
DOI: 10.1021/acs.oprd.6b00287

Ujjal Mondal and Sujit Sen

Miscellaneous

Development of an Adaptive Experimental Design Method Based on Probability of Achieving a Target Range through Parallel Experiments

Ind. Eng. Chem. Res., 2016, 55 (19), pp 5726–5735
DOI: 10.1021/acs.iecr.6b00852

Adaptive experimental design- parallel experiments--Gaussian process regression

Atsuyuki Nakao, Hiromasa Kaneko, and Kimito Funatsu

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

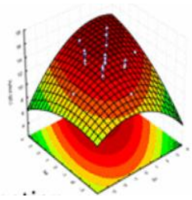
Optimization of Solketalacetin Synthesis as a Green Fuel Additive from Ketalization of Monoacetin with Acetone

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

Central composite design-RSM

Yadollah M. Gorji and Hassan S. Ghaziaskar

Optimization of Salts Supplementation on Xylitol Production by Debaryomyces hansenii Using a Synthetic Medium or Corncob Hemicellulosic Hydrolyzates and Further Scaled Up



Ind. Eng. Chem. Res., 2017, 56 (23), pp 6579–6589
DOI: 10.1021/acs.iecr.7b01120

- Central composite design;

Guadalupe Bustos Vázquez, Noelia Pérez-Rodríguez, José Manuel Salgado, Ricardo Pinheiro de Souza Oliveira, and José Manuel Domínguez

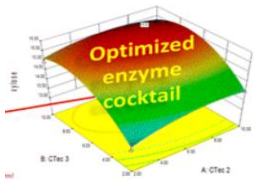
Direct Determination of Contaminants and Major and Minor Nutrients in Solid Fertilizers Using Laser-Induced Breakdown Spectroscopy (LIBS)

J. Agric. Food Chem., 2016, 64 (41), pp 7890–7898
DOI: 10.1021/acs.jafc.6b04028

- Factorial design- using laser-induced breakdown spectroscopy (LIBS) parameters

Daniel F. Andrade and Edenir Rodrigues Pereira-Filho

Enzymatic Hydrolysis of Industrial Derived Xylo-oligomers to Monomeric Sugars for Potential Chemical/Biofuel Production



ACS Sustainable Chem. Eng., 2016, 4 (12), pp 7130–7136
DOI: 10.1021/acssuschemeng.6b02008

Jinguang Hu, Joshua Davies, Yiu Ki Mok, Bryan Gene, Quak Foo Lee, Claudio Arato, and Jack N. Saddler

Adsorbent Screening for Postcombustion CO2 Capture: A Method Relating Equilibrium Isotherm Characteristics to an Optimum Vacuum Swing Adsorption Process Performance

Ind. Eng. Chem. Res., 2016, 55 (8), pp 2447–2460
DOI: 10.1021/acs.iecr.5b04531

Centralcomposite; neural-network-based model; meta-models

Maninder Khurana and Shamsuzzaman Farooq

A Bioinspired Alginate-Gum Arabic Hydrogel with Micro-/Nanoscale Structures for Controlled Drug Release in Chronic Wound Healing

ACS Appl. Mater. Interfaces, 2017, 9 (27), pp 22160–22175
DOI: 10.1021/acsami.7b04428

Orthogonal experimental design

Mi Li, Haichang Li∇, Xiangguang Li#, Hua Zhu, Zihui Xu, Lianqing Liu, Jianjie Ma, and Mingjun Zhang

Statistical Optimization of Heavy Metal (Cu2+ and Co2+) Extraction from Printed Circuit Boards and Mobile Batteries Using Chelation Technology

Ind. Eng. Chem. Res., 2017, 56 (23), pp 6805–6819
DOI: 10.1021/acs.iecr.7b01481

Box–Behnken design + central compositedesign

Nitin Sharma, Garima Chauhan, Arinjay Kumar, and S. K. Sharma

Process Parameters in the Purification of Curcumin by Cooling Crystallization

Org. Process Res. Dev., 2016, 20 (9), pp 1593–1602
DOI: 10.1021/acs.oprd.6b00153

Scooling rate, seeding, seed polymorph, agitation conditions -- statistical experimental design

Marko Ukrainczyk, B. Kieran Hodnett, and Åke C. Rasmuson

An In-Depth Study of the Use of Eosin Y for the Solar Photocatalytic Oxidative Coupling of Benzylic Amines	ACS Sustainable Chem. Eng., Article ASAP DOI: 10.1021/acssuschemeng.7b01754

Joshua D. Tibbetts, David R. Carbery, and Emma A. C. Emanuelsson

Single-Step Assembly of Multifunctional Poly(tannic acid)–Graphene Oxide Coating To Reduce Biofouling of Forward Osmosis Membranes Taguchi's design	ACS Appl. Mater. Interfaces, 2016, 8 (27), pp 17519–17528 DOI: 10.1021/acsami.6b03719

Hanaa M. Hegab, Ahmed elmekawy, Thomas G. Barclay, Andrew Michelmore, Linda Zou#, Christopher P. Saint, and Milena Ginic-Markovic

Hitchhiker's Guide to Voltammetry: Acute and Chronic Electrodes for in Vivo Fast-Scan Cyclic Voltammetry	ACS Chem. Neurosci., 2017, 8 (2), pp 221–234 DOI: 10.1021/acschemneuro.6b00393

Nathan T. Rodeberg, Stefan G. Sandberg, Justin A. Johnson, Paul E. M. Phillips, and R. Mark Wightman

Strecker Aldehyde Formation in Wine: New Insights into the Role of Gallic Acid, Glucose, and Metals in Phenylacetaldehyde Formation Full factorial [ph; Temp];	J. Agric. Food Chem., Article ASAP DOI: 10.1021/acs.jafc.7b00264

Ana Rita Monforte, Sara I. F. S. Martins#⊗, and Antonio C. Silva Ferreira

Elementary Transformation of Glycerol to Trivalerin: Design of an Experimental Approach Central composite; two factors and three levels;	ACS Sustainable Chem. Eng., 2017, 5 (1), pp 802–808 DOI: 10.1021/acssuschemeng.6b02133

Kamalpreet Kaur, Ravinder Kumar Wanchoo, and Amrit Pal Toor

Credit: Acs.org