

## Index

### a

- acid detergent fiber (ADF), chemical analysis of 109
- active ingredients 19, 41–43
- additives 4, 12, 49, 92, 106, 126, 149
- amino acid concentration
  - effect on biomass production 79
  - in fresh and first supernatant 79
- analysis of variance (ANOVA) 51, 53, 59–60, 77, 84–85, 134–135, 138
- Analytic Hierarchy Process (AHP) 147, 155
  - applications 156
  - random index used in 158
  - sustainable gasoline blend selection 156
- animal-derived medium components 73
- antimicrobial active ingredients 19, 42
- antimicrobial activity
  - experimental design for 47
  - artificial neural networks 51–54
    - historical data augmentation 49
    - linear least squares regression analysis 49–51
    - prior knowledge 48
- artificial neural networks (ANNs) 14, 28–30, 51–54, 65–66, 70–71, 73, 127
  - corrosion tests 64
- aspartic acid, importance of 87
- aspect ratio 8, 105, 107–108, 110–112, 114–118, 122, 164
- attribute-based models 127

### b

- batch 609 quality variables 99
- Bayesian D-optimality approach 55–61
- Bayesian design of fractional factorial experiments 27
- bill of material (BOM) 198

- bio-ethanol 150
- Bode plots, for bare copper, PEI and PEI/G coated copper 175–176
- Boston Consulting Group (BCG) Business Portfolio Matrix 197–201, 204, 205
- Bowyer–Bader model 13, 126
- Box–Behnken (BB) design, for corrosion tests 63, 64
- Box–Cox transformation methodology 49
- Business Growth Rate 197

### c

- capacity tests 42
- carrier tests 42
- Cash Cows business category 198, 200, 201, 204
- central composite design (CCD) 25, 26, 63
- chemical process industries 3
- chemical product design (CPD) 2
  - defined 4–6
  - definition 125, 127
  - property functions and models 126
  - reverse property prediction 5
- chemical products
  - classification 3
  - engineering 2, 125
- chemical toner manufacturing process 91, 92
  - model cross validation technique 93–97
  - process and data description 92–93
- chemical vapor deposition (CVD) approach 15
- chemically defined medium
  - design and optimization technique 78
  - materials and methods
    - analytical methods 74–76
    - experimental design analysis 76–77

- chemically defined medium (*contd.*)  
 microorganism and medium 74  
 optimization by mixture design method  
 82–87  
 screening mixture experiments 80–82  
 starvation trials 79  
 composite mechanical properties 10, 107  
 computer-aided chemical product design  
 5–6  
 Computer-Aided Mixture/Blend Design  
 (CAM<sup>b</sup>D) 4, 5, 126  
 Computer-Aided Molecular Design (CAMD)  
 4, 5, 126  
 computer-aided techniques 4, 126  
 consistency index (CI) 156–158  
 constant phase elements (CPE) 174  
 constrained mixture design 34  
 copper, corrosion mechanism 163  
 corrosion protection 163  
 epoxy/glass composites coatings 16–17  
 fluorographene particles into polyvinyl  
 butyral composite coatings for 16  
 of epoxy and graphene oxide (GO)  
 composites coatings 16  
 using polymer composites 15–17  
 corrosion test  
 artificial neural networks 64–66  
 preliminary experimental design 62–63  
 response surface methodology 63–64  
 cost versus tensile modulus 186, 189  
 cost-benefit analysis 147, 159  
 cost-benefit (KPI) analysis, of blends 147,  
 159–161  
 coupling agents, on polymer blends and  
 composites 9  
 critical length theory 107  
 cross-validation evaluation method 94
- d**  
 Dangerous Substances Directive (Directive  
 67/548/EEC) 44  
 3<sup>k</sup> design 25  
 disinfectant products 42–43, 62, 70–71, 127  
 disinfectants  
 characteristics 42  
 antimicrobial tests 42–43  
 corrosion tests 43–44  
 stability tests 43  
 formulation  
 antimicrobial activity 47–54  
 constraints in 41  
 optimization problem 67  
 optimized verification 69–70  
 optimized vs. available products 70  
 properties 67  
 in healthcare settings 41  
 toxicity of 44–47  
 use of 41  
 disinfecting product design 41  
 distance-based multivariate response matrix  
 78, 80, 82, 87  
 distance-based redundancy analysis  
 (db-RDA) 77  
 DISTLM *forward* 77, 82  
 DISTLM *forward* software 80  
 Dogs business category 198  
 D-optimality 26–27, 55–61
- e**  
 E5, M5 and I5 impacts  
 on environment 152–154  
 on safety risk 154–155  
 electrochemical corrosion parameters  
 for bare copper and PEI/G coated copper  
 173  
 for copper, PEI and PEI/G coated copper  
 176  
 electrophoretic deposition (EPD) 15–16  
 energy impact index 152  
 environmentally friendly product design 2  
 experimental design of mixtures 31
- f**  
 face-centered composite design 26  
 factorial design 23, 76  
 2<sup>k</sup> factorial 23, 24  
 benefit of 23  
 effect of a factor in 23  
 fermentation medium, design of 73  
 fiber-matrix bonding theory 107  
 fiber orientation coefficient 13, 126  
 fiber quality 10  
 finite element method 181  
 Fisher's Least Significant Difference method  
 111, 117–118  
 Fisher's statistical test 83–84  
 formulated products 3  
 2<sup>k</sup> factorial design 23–25  
 fractional factorial design (FFD) 23–25, 27,  
 31, 34, 48–51, 55–56, 58–59, 61–64  
 for brass corrosion test 62  
 2<sup>k-p</sup> fractional factorial design 24

fractional two-level factorial designs 49  
 fractured surface morphology, of composite  
 10  
 freshness index 1

**g**

gasoline blends  
 and ethanol, impacts of 149–150  
 octane number of  
 effects of ethanol, methanol, isooctane  
 on 150  
 impact on 148–149  
 price comparisons 153  
 and methanol blends with HYSYS 2006  
 153  
 utilization of 148  
 genetic algorithms 73  
 glass fibers 8, 14, 105, 126  
 global atmospheric impacts 153  
 graphene 164  
 based coating 16  
 composites 14–15  
 greenhouse ventilation system 2  
 growth dependence, on amino acid  
 combinations 80

**h**

hidden layer feed-forward neural network  
 29  
 homopolypropylene 12, 106, 108, 131–134,  
 136–137, 139–140, 144  
 hybrid-wise unfolding approach 36  
 hydrogen peroxide stability  
 experimental design  
 historical data analysis 54–55  
 historical data augmentation using  
 Bayesian D-optimality approach  
 55–61

**i**

impedance spectroscopy, of bare and coated  
 metal substrate 174  
 in vitro tests 42, 47  
 in vivo test methods 42, 44  
 inert ingredients 42  
 innovation 1, 198  
 innovation and technology strategy 196  
 input and output neurons, for network  
 architecture 30  
 in situ polymerization method 14

interface adhesion property, of corrosion  
 resistance coating 170, 177  
 intermediate chemicals 195  
 inverted model technique 185

**k**

Kelly–Tyson modified rule of mixture 13,  
 126  
 Key Performance Indicators (KPI) 147,  
 158–161  
 K-fold cross validation method 94

**l**

latent variable modeling 38–39, 95–102  
 lignin content test 109  
 linear least squares regression analysis  
 49–51  
 linear programming, for petrochemical  
 industry planning 195  
 local toxicological impacts 152

**m**

machine learning models 28  
 main effect 23–24, 49, 183  
 maleic anhydride grafted polypropylene  
 (MA-g-PP) 9, 106, 108  
 manufacturing strategy 196–199  
 mass heat value  
 of blends (E5, M5 and I5) 151  
 of pure chemical 151  
 material impact index 152  
 mathematical programming models 195  
 mechanistic model 13, 91, 126  
 melt intercalation method 15  
 method of least squares 27  
 method of steepest ascent 26  
 mileage loss, of blends 151  
 Mixed Integer Linear Programming (MILP)  
 model 195, 205  
 mixture design method 82–87  
 chemically defined medium optimization  
 87  
 Mixture Design of Experiments 31–35  
 mixture design problems, variations of 34  
 mixture model-based MICA approach 38  
 mixture variables 129–130, 142  
 mixture/blend design 4, 126  
 model-based principal component analysis  
 (MB-PCA) 37–38  
 model cross validation technique 93–97  
 molecular design 4, 126

- multiscale modeling approach 181
- multiway independent component analysis (MICA) 37–38
- multi-way partial least square method (MPLS) 38–39, 101
- multi-way principal component analysis (MPCA) 35, 101
  - batch process variables 35
  - features of 35
- multiple linear regression model 27–28
- multiple regression model 27
  
- n**
- N&M method 36
- natural fiber plastic composites 7–10, 13
  - statistical models of 14, 126–127
- natural fiber polymer composites, modeling 12–14, 126
- natural fibers 105–106
- neural network-based analysis 14, 127
- neural networks 28, 53
- neutral detergent fiber (NDF), chemical analysis of 109
- New Sustainable Indices, principal metrics of 160
- non-mixture variables 129
- nonlinear iterative partial least squares (NIPALS) algorithm 38–39, 93, 99
  - for PLS 98
- Nyquist plots, for bare copper, PEI and PEI/G coated copper 174, 175
  
- o**
- object-oriented finite element modeling (OOF) 182
- octane number (ON) 147–152, 158, 160
- OFAT testing 55
- “one-factor-at-a-time” approach 23
- operational boundaries, of latent variables 98, 99, 101
- optical density (OD) measurements 75, 79
- organic-inorganic polymer nanocomposites 181
  
- p**
- Partial Least Squares (PLS) 38, 97–98
- patents 17–19
- PEI/G composite coatings
  - corrosion resistance properties of 174
  - electrochemical measurements 166–167
  - in situ polymerization approach 165
  - interface adhesion 165
  - morphology characterization 165
  - synthesis of 165, 166
- peroxide based disinfectant product
  - product design framework for 127
- petrochemical industry
  - modeling, multiobjective analysis in 195
  - sustainable development 196
- pharmaceutical drugs 3, 17–18
- pitting corrosion 163
- polyimide/graphene composites coatings 16
- polymer/fiber composites
  - fiber quality 106
- polymer-layered silicate nanocomposites 35, 183–187, 192–193
  - factorial and mixture design models 182
- polypropylene-organically modified montmorillonite PP-OMMT nanocomposites
  - cost minimization 185
  - mathematical models 183
  - modified organic component effect 192
  - modified organic weight fraction 191
  - nonlinear regression models 192
  - optimization mechanism 183–185
  - systematic modeling and optimizing product design 184
  - tensile modulus and gas permeation behaviors of 183
  - tensile modulus and oxygen permeation for 183
  - variances of permeation values 188
  - variances of tensile modulus values 187, 188
  - variance vs. cost function vs. tensile modulus 190
- polypropylene properties 106
- polypropylene, selection factors of 10
- polypropylene types 106
- potential environmental impacts (PEIs)
  - corrosion resistance property 164
  - E5, M5 and I5 impacts on environment 152–154
- PP/ICP blend properties measurements 131
- prediction error sums of residual 96
- processing property models 12, 126
- process-mixture design 34, 128
- process simulation techniques 5, 91
- process system engineering (PSE) 91

process variables 34–38, 49, 92–93, 95–96, 100–102, 129–130

product design 2, 125

- defined 4
- design process for 5
- four steps design process 4
- objectives for 147
- studies 147

product design frameworks 127

- for peroxide based disinfectant product 127
- for under eye cream product 127

product design problems

- mixture/blend design 126
- molecular design 126

product engineering 197

product formulation 4, 26, 34, 48, 62, 127

product optimization 23, 67, 130

product selection

- in investment strategies 195
- case study 201–205
- manufacturing strategy 196–199
- model development 199–201
- in petrochemical industry 205

pseudo-simplex design 34, 138

pure gasoline and chemicals prices, comparison of 152

## q

quadratic polynomial model 33

quality assurance protocol, for natural fibers 10

quantitative carrier test method 42

Question Mark stage 198

## r

random index (RI) 158

recombinant *Streptomyces lividans* NCIMB 11416/IL3 p002 74

regression analysis 27–28, 31, 49–51, 64, 70, 130, 183

Relative Competitive Position 197

representative volume element (RVE) 181, 182

resolution IV fractional factorial design 49, 55, 56, 58, 59

response surface composite property models 130

response surface designs 31

response surface methodology (RSM) 31, 63

and designs 25–26

- for WS-PP/ICP blend composite 131

response surface, of linear polynomial model 33

rHuIL-3 production

- contour plot of 86
- response surface model for 85
- by *S. lividans* 66 83

rHuIL-3 production vs. biomass 83–87

## S

safety risk index 152, 155, 158, 159

- for methanol, ethanol and isooctane blends 155

scanning electron microscopy (SEM) image

- for bare copper and PEI coated copper substrate
- before and after conducting Tafel polarization and EIS tests 167–168

for graphene dispersion in PEI/G composite coatings 169

of PEI/G<sub>2</sub> coated copper 170

of post-adhesion test copper substrates coated with PEI 171

of post-adhesion test copper substrates coated with PEI/G<sub>0.5</sub> composites 171

of post-adhesion test copper substrates coated with PEI/G<sub>1</sub> composites 172

of post-adhesion test copper substrates coated with PEI/G<sub>2</sub> composites 172

Scheffe's canonical polynomial models 130

semi-empirical models 14, 127

sensitivity to change (STC) 199

simplex lattice design 32, 76, 78

solution method 14

specialty chemicals, defined 3

specific modulus, defined 120, 121

squared prediction error (SPE) 37

S-shaped logistic sigmoid transfer function 29

*Staphylococcus aureus*

- historical data for antimicrobial tests 48

star business category 197, 198

statistical software 2, 80, 84, 130

statistically designed experiments 48, 73

*Streptomyces lividans*

- minimum nutrient requirement 79

*Streptomyces lividans* 66 73–87

- growth associated rHuIL-3 production 83

- structural property models 12, 126
  - subscription-based patent databases 19
  - surface morphology, of bare and PEI/G coated copper surfaces 167
  - suspension tests 42
  - sustainability 147–161, 195, 196, 198, 201, 205
  - synergy 19
- t**
- Tafel plots, for bare copper, PEI, PEI/G coated copper electrodes 172, 173
  - TEM images 167
    - for graphene dispersion in PEI/G composite coatings 169
  - thermoplastic resins 7
  - thiostrepton containing complex medium 74
  - toxicity of disinfectants
    - eye irritant, *Xi* (R36) 46
    - harmful (*Xn*) 45
    - respiratory irritant, *Xi* (R37) 47
    - severe eye damage (*Xi*) 45–46
    - skin irritant, *Xi* (R38) 46–47
  - Trainlm 52
- v**
- validation data set for antimicrobial tests 54
- w**
- Waste Reduction (WAR) algorithm 152, 159, 160
  - wheat straw polypropylene composites (WSPPC) 107, 108, 125
    - in automotive application 125
    - fiber fractionation 110
    - fiber fractions
      - cellulose, hemicellulose and lignin content 114
      - chemical analysis 113
      - degradation temperatures 114
      - TGA analysis 113
    - fiber preparation 108
    - fiber size measurement 108, 110
    - fiber size reduction 110
    - fiber size reduction during compounding process 114–117
    - fiber thermal and chemical analyses 109, 113
    - flexural and impact properties 109
    - flexural modulus of 117–118
    - impact strength measurement 118–120
    - melt-blending method 109
    - product design framework for 128
      - customer needs 129
      - illustration for 128
      - mixture and/or process-mixture experiments 129–130
      - model simulation and optimization 130
      - multiple-product specifications 128
      - relevant data organizing and analysis 129
      - response surface composite property models 130
      - result confirmation 130
      - variable screening of 129
    - product design methodology 125
    - sample preparation 109
    - specific modulus 120
    - systematic representation 129
    - variables in formulation and manufacturing of 11
  - Wold's approach 35, 36
  - WS-PP/ICP blend composite system
    - ANOVA-test results summary 135
    - in automotive industry 130
    - component price per mass unit 143
    - components 131
    - constrained pseudo-simplex design 138
    - flexural and impact properties
      - comparison matrix 140
    - flexural modulus 134–136
    - izod impact strength 136–137
    - materials and methods 133–134
    - mixture experiment, design of 131
    - optimization case study 141
    - optimum proportions 144
    - parameter estimates 142
    - product specifications 138
    - property models 137
    - superiority 138