

Index

Note: Page numbers in *italics* and **bold** refers to figures and tables respectively.

a

- absolute error 32
- acid pretreatment 224
- activation energy 82
- AD. *see* anaerobic digestion (AD)
- AdaBoost 6
- adaptive-network-based fuzzy inference systems (ANFISs) 30
- adiabatic calorimetry 102
- ADM1. *see* Anaerobic Digestion Model No. 1 (ADM1)
- agent-based hybrid modeling 153
- agricultural residues 21
- AI. *see* artificial intelligence (AI)
- AIDMS. *see* artificial intelligence-based decision-making system (AIDMS)
- algae 4
- algorithm performance
 - assessment 191–193
- alkaline pretreatment 225
- anaerobic digestion (AD) 25, 34, 59–63, 184, 198, 60
- Anaerobic Digestion Model No.1 (ADM1) 140–141, 184
- ANFISs. *see* adaptive-network-based fuzzy inference systems (ANFISs)
- ANNs. *see* artificial neural networks (ANNs)
- antioxidants 241–242, 242
- artificial bee colony (ABC) method 147
- artificial intelligence (AI) 6, 27, 222
 - AI-assisted data acquisition 10–11
 - AI-assisted process modeling 12, 13
 - AI-assisted system
 - optimization 12–14, 13
 - AI-driven high-throughput experimentation 267
 - AI-MOO frameworks 205
 - biomass property prediction 263–264
 - biomass supply chain modeling 263
 - hybrid modeling approaches 264
 - integrated biomass valorization 8–14
 - integration in biomass conversion processes 37–63
 - integration in biomass valorization 263–265
 - keyword clusters **9–10**
 - keyword co-occurrence, analysis of 9
 - multidimensional framework of AI integration 29–37
 - multi-objective optimization 264–265
- artificial intelligence-assisted biomass
 - fractionation and dissolution 223
- biomass processing 229–232, 230
- conventional solvent system 223–226, 224
- green solvent system 226–229, 226, 227, 229

- artificial intelligence-assisted cellulose products 232, 233
 - cellulose-derived chemicals 235–236
 - cellulose-derived materials 236–239, 239
 - conventional bulk products 233–235
 - artificial intelligence-assisted
 - hemicellulose products 243, 244
 - pharmaceutical delivery carriers 244–245, 245
 - sugars 244
 - artificial intelligence-assisted lignin
 - products 240, 240
 - antioxidants 241–242, 242
 - dispersants and ethers 243
 - lubricating additives 240–241, 241
 - artificial intelligence-based
 - decision-making system (AIDMS) 224–225
 - artificial neural network-genetic
 - algorithms (ANN-GA) framework 231
 - artificial neural networks (ANNs) 3, 30, 145, 175, 225
 - Aspen Plus (software package) 121, 188–189
 - simulation 12
 - Aspen Plus V14, 123
 - AspenTech 140
 - automated workflows and continual learning 205
- b**
- backpropagation (BP) networks 7
 - batch ethanol fermentation 34
 - Bayesian optimization (BO) 7, 92
 - BDC. *see* bio-derived catalyst (BDC)
 - big data fusion 64
 - bio-based functional materials 5
 - bio-based high-energy fuels 5–6
 - bio-based platform chemicals 5
 - biochar 26, 246–247
 - biochemical approaches 56
 - biomass anaerobic digestion 59–63, 60
 - biomass fermentation 57–59, 57
 - biochemical conversion 24
 - bio-derived catalyst (BDC) 45
 - biodiesel 34
 - bioethanol 58
 - biomass 1, 21, 28, 79–80, 221
 - biomass coupling processes 262
 - exergy prediction 104–107, **105**
 - fermentation 57–59, 57
 - hydrolysis 53–56, 54
 - hydrothermal conversion 46–50
 - processing 229–232, 230
 - property database 262
 - property prediction 263–264
 - pyrolysis 41–45, 41, 197
 - resources 21, 22
 - transesterification 50–53, 50
 - biomass activation energy, prediction of 107–114, 109, 110, 113
 - biomass biorefining, system integration in 267–268
 - biomass conversion 121, 122, 133, 262
 - AI integration in 37
 - biochemical approaches 56–63
 - challenges and opportunities 265
 - chemical approaches 50–56
 - complexity and conflicts in 166–167, 261–262
 - digital twin for online MOO 189–190
 - fermentation process
 - modeling 139–142, 140
 - gaps to be filled in 262
 - hydrothermal treatment process
 - modeling 134–135, 135
 - kinetic and heat-mass models 178–185, 183, 185
 - multiscale modeling 187–188
 - renewable-hydrogen system coupling
 - models 185–187
 - simulation platforms and data
 - interfaces 188–189
 - and system modeling 178–190
 - thermochemical approaches 37–50
 - torrefaction process modeling 135–139, 137, 139
- biomass-derived carbon 1

biomass gasification 37–41, 38, 178
 drying stage 178–179
 oxidation stage 179
 pyrolysis stage 179
 reduction stage 179
 biomass heat capacity, prediction
 of 101–103, **102–103**
 biomass HHV estimation 82
 empirical correlations in HHV
 estimation 82–86
 ML in HHV prediction 86–100
 biomass process modelling, ML and
 mechanistic integration for 266
 biomass–renewable electricity–hydrogen
 system 168
 biomass-specific data, databases, and
 descriptors 265–266
 biomass standard entropy, prediction
 of 100–101, **101**
 biomass supply chains (BSCs) 2, 263
 biomass thermodynamic parameters
 basic 81
 derived and correlated parameters 82
 prediction of 80
 thermochemical conversion process
 parameters 81–82
 biomass-to-hydrogen (BTH)
 pathway 148
 biomass-to-X (BTX) electrification
 roadmap 1
 biomass valorization
 AI/ML integration in 263–265
 technologies 3–4
 bio-oil 42, 245–246, 246
 biorefinery 25–26
 biorefining poly-generation 6
 biphasic solvents 225
 BO. *see* Bayesian optimization (BO)
 BSCs. *see* biomass supply chains (BSCs)

C

calorific values 82–83
 carbon neutrality 107
 cascade-forward neural network
 (CFNN) 147

case-level parallelization 194
 CatBoost 44
 cellulose (CELL) 22, 127
 cellulose-derived chemicals 235–236
 cellulose-derived materials 236–239, 239
 CFD. *see* computational fluid
 dynamics (CFD)
 CFNN. *see* cascade-forward neural
 network (CFNN)
 “characterization-to-data” paradigm 11
 ChatGPT 153
 chemical analysis, HHV estimation based
 on 83, **84**
 chemical approaches 50–56
 chemical conversion 24
 chemical exergy 104–107, **105**
 chemical looping reforming
 approach 127
 circulating fluidized-bed (CFB)
 gasification process 181
Clostridium 60
 CNNs. *see* convolutional neural networks
 (CNNs)
 Coats–Redfern method 108, 124
 co-conversion strategies and MOO
 frameworks 267
 coefficient of determination (R^2) 32
 COMBUST unit 131
 combustion 24
 computational fluid dynamics
 (CFD) 121
 modeling 132–133, **133**, 134
 consensus yeast (CY) model 59
 conventional bulk products 233–235
 conventional solvent system
 223–226, 224
 convolutional neural networks (CNNs) 7
 co-pyrolysis 126–127
 Corncob 55
 coupling validation 195

d

DAEMs. *see* distributed activation energy
 models (DAEMs)
 data assimilation 189

- data-driven models 2, 121, 146
 - data generation and simulation support 266
 - data interfaces 188–189
 - data-model uncertainty management 204–205
 - dataset construction 31
 - “data-to-data” approach 11
 - decision dimension 35–37
 - decision support 176–177
 - decision support system (DSS) 47
 - decision trees (DTs) 30, 189–190
 - deep eutectic solvents (DESs) 228
 - deep learning (DL) 6, 30–31
 - deep neural networks (DNNs) 43
 - DeepSeek 153
 - DEM. *see* discrete element method (DEM)
 - density 81
 - DESs. *see* deep eutectic solvents (DESs)
 - differential scanning calorimetry (DSC) 102
 - digital twin
 - deployment 64
 - for online MOO 189–190
 - for operation and maintenance 206
 - Digital Twin for Biomass Gasification Power Plant (DT-BGPP) 153
 - dilute acid hydrolysis 55
 - 2,5-dimethylfuran (DMF) 25
 - direct hybrid modeling 143
 - hybrid residual modeling 144–146, 145
 - parallel direct hybrid modeling 143–144, 143
 - series direct hybrid model 146–148, 147
 - direct numerical simulation (DNS) 133
 - discarded wood 39
 - discrete element method (DEM) 151
 - disentangled representation-aided PINN (DR-PINN) 150
 - dispersants 243
 - distributed activation energy models (DAEMs) 126, 136, 183
 - DL. *see* deep learning (DL)
 - DMOO. *see* dynamic MOO (DMOO)
 - DNNs. *see* deep neural networks (DNNs)
 - DNS. *see* direct numerical simulation (DNS)
 - DR-PINN. *see* disentangled representation-aided PINN (DR-PINN)
 - DSC. *see* differential scanning calorimetry (DSC)
 - DSS. *see* decision support system (DSS)
 - DT-BGPP. *see* Digital Twin for Biomass Gasification Power Plant (DT-BGPP)
 - DTs. *see* decision trees (DTs)
 - Dulong formula 83
 - dynamic MOO (DMOO) 203
- e**
- ECs. *see* empirical correlations (ECs)
 - elemental features 87
 - ELM. *see* extreme learning machine (ELM)
 - empirical correlations (ECs) 83
 - chemical analysis 83, **84**
 - in HHV estimation 82–86
 - proximate analysis 84, **85**
 - ultimate analysis 84–86, **86**, 87
 - energy, exergy, economics, environment, and safety (4E+1S) 40
 - energy potential of biomass 82
 - energy return on investment (EROI) 45
 - engineering-scale validation with pilot data 195
 - EnKF. *see* ensemble Kalman filters (EnKF)
 - ensemble Kalman filters (EnKF) 189
 - enthalpy 81
 - entropy 81
 - enzymatic hydrolysis 33–34
 - equilibrium-based model 130
 - EROI. *see* energy return on investment (EROI)
 - ethanol 234
 - ethers 243
 - exergy 104

extreme gradient boosting (XGBoost)
 algorithm 6, 30, 44, 176
 extreme learning machine (ELM) 62

f

FAME. *see* fatty acid methyl ester (FAME)
 fast pyrolysis 41, 81, 197, 3
 fatty acid methyl ester (FAME) 33
 FC. *see* fixed carbon (FC)
 feedforward backpropagation artificial
 neural network (BP-ANN)
 model 62
 feed-forward neural network 39
 fermentation 25, 34
 process modeling 139–142, 140
 first-generation biorefineries 26
 Fischer–Tropsch synthesis 24
 fixed carbon (FC) 84
 flash pyrolysis 24, 182
 Flynn–Wall–Ozawa (FWO)
 approach 112
 food waste leachate (FWL) 61
 forward feedforward neural network
 model 34
 FWL. *see* food waste leachate (FWL)

g

GA. *see* gluconic acid (GA)
 GAN. *see* generative adversarial
 networks (GAN)
 Garson algorithm 58
 GAs. *see* genetic algorithms (GAs)
 gasification 24, 32, 37–41
 equilibrium modeling 130–131,
 130, 131
 kinetics modeling 131–132, 132, 132
 gasification process modeling 130
 CFD modeling 132–133, 133, 134
 gasification equilibrium
 modeling 130–131, 130, 131
 gasification kinetics modeling
 131–132, 132, 132
 gas production 61
 GBDTs. *see* gradient-boostered decision
 trees (GBDTs)

GD metric 191
 gene expression programming (GEP) 49
 General Process Modeling System
 (GPROMS) 187, 189
 generative adversarial networks
 (GAN) 11
 genetic algorithms (GAs) 7, 30
 GEP. *see* gene expression
 programming (GEP)
 Gibbs free energy 81
 minimization technique 130
 global bioenergy system modeling 65
 global warming potential (GWP) 44–45
 gluconic acid (GA) 148
 glucose 25
 gorilla community optimization
 algorithm (GTO) 94
 GPROMS. *see* General Process Modeling
 System (GPROMS)
 gradient-boostered decision trees
 (GBDTs) 6
 gradient boosting regression (GBR)
 algorithm 148
 green multi-objective design 206–207
 green solvent system 226–229, 226, 227
 GTO. *see* gorilla community optimization
 algorithm (GTO)
 GWP. *see* global warming potential (GWP)

h

HCE. *see* hemicellulose (HCE)
 HDO. *see* hydrodeoxygenation (HDO)
 heat-mass models 178–185, 183, 185
 heat of combustion 81
 heating rate (HR) 87
 hemicellulose (HCE) 22, 127, 243
 HHV. *see* higher heating value (HHV)
 hierarchical cluster analysis 85
 high-dimensional optimization
 issues 203–204
 higher heating value (HHV) 2, 81, 263
 high-performance computing for
 MOO 190
 algorithm performance
 assessment 191–193

- high-performance computing
 - for MOO (*Cont.*)
 - engineering-scale validation with pilot data 195
 - high-performance parallel
 - computing 194
 - software environment 190–191
 - surrogate-assisted MOO 193
 - high-performance parallel
 - computing 194
 - high-value conversion
 - technologies 4–6, 4
 - HMF. *see* 5-hydroxymethylfurfural (HMF)
 - HR. *see* heating rate (HR)
 - HRM. *see* hybrid residual
 - modeling (HRM)
 - HRT. *see* hydraulic retention time (HRT)
 - HTG. *see* hydrothermal
 - gasification (HTG)
 - HTL. *see* hydrothermal liquefaction (HTL)
 - HTT. *see* hydrothermal technology (HTT)
 - hybrid modeling 142, 142
 - agent-based hybrid modeling 153
 - approaches 264
 - direct hybrid modeling 143–148
 - integration 64
 - physics-informed neural
 - networks 149–151, 150
 - reduced-order models 148–149
 - TG profile-assisted hybrid
 - modeling 151–153, 152
 - hybrid neural network (HNN)
 - models 181
 - hybrid residual modeling (HRM)
 - 144–146, 145
 - hydraulic retention time (HRT) 198
 - hydrochar 49
 - hydrodeoxygenation (HDO) 148
 - hydrogen-yield prediction 33
 - hydrolysis 24–25
 - hydrothermal carbonization 24
 - hydrothermal conversion 24
 - hydrothermal gasification (HTG) 24
 - hydrothermal liquefaction (HTL) 24, 135, 148
 - hydrothermal technology (HTT) 46
 - of bio-oil 48
 - hydrothermal treatment process
 - modeling 134–135, 135
 - 5-hydroxymethylfurfural (HMF) 5, 25

i

 - IESs. *see* integrated energy
 - systems (IESs)
 - INN. *see* inverse neural network (INN)
 - integrated biomass–renewable–hydrogen
 - energy systems 172
 - integrated continuous catalytic
 - strategy 5
 - integrated energy systems
 - (IESs) 166, 168
 - integrated modeling strategies 122
 - inverse neural network (INN) 34

j

 - JMetal 190

k

 - Kalman filters (KF) 189
 - Keras 7
 - KF. *see* Kalman filters (KF)
 - kinetic modeling/models 141–142, 178–185, 183, 185
 - kinetic simulations 131
 - Kissinger–Akahira–Sunose (KAS)
 - methods 110

l

 - landfill leachate (LFL) 61
 - large-Eddy simulation (LES) 133
 - large language models (LLMs) 268
 - application of 268
 - layered neural networks (LNNs) 7
 - LCCs. *see* lignin–carbohydrate complexes
 - (LCCs)
 - LCOE. *see* levelized cost of energy
 - (LCOE)
 - least-squares boosting (LSBoost)
 - method 148
 - least-squares support vector regression
 - (LSSVR) 103

LES. *see* large-Eddy simulation (LES)
 leveled cost of energy (LCOE)
 172–173, 199–200
 Levenberg–Marquardt algorithm 54
 LFL. *see* landfill leachate (LFL)
 LHV. *see* lower heating value (LHV)
 life cycle 202–203
 light gradient boosting machine
 (LightGBM) 43
 LightGBM. *see* light gradient boosting
 machine (LightGBM)
 lignin 22–23, 127, 243
 lignin-carbohydrate complexes
 (LCCs) 242
 lipid feedstocks 50–51
 LLMs. *see* large language models (LLMs)
 LNNs. *see* layered neural networks
 (LNNs)
 long short-term memory (LSTM)
 networks 7
 low-temperature transesterification
 system 52
 lower heating value (LHV) 81, 263
 LSSVR. *see* least-squares support vector
 regression (LSSVR)
 lubricating additives 240–241, 241

m

machine learning (ML) 2, 6–8, 7, 27,
 121, 242
 advances in research combining
 biomass with 11
 biomass property prediction 263–264
 biomass supply chain modeling 263
 correlation heatmap of studied
 variables 88
 dataset characteristics and feature
 selection 86–89
 in HHV prediction 86–100, **90**
 hybrid modeling approaches 264
 integration in biomass valorization
 8–14, 263–265
 key influence mechanisms 95–100
 and mechanistic integration for
 biomass process modeling 266

models and performance
 comparison 89–95, 93, 95
 multi-objective optimization 264–265
 in process modeling 13
 MAE. *see* mean absolute error (MAE)
 manure 4
 mathematical models (MMs) 171–172,
 179
 MATLAB 121
 MCDA. *see* multi-criteria decision
 analysis (MCDA)
 mean absolute deviation 32
 mean absolute error (MAE) 32
 mean squared error (MSE) 32
 mechanism-driven modeling 122
 biomass conversion
 modeling 133–142
 gasification process
 modeling 130–133
 pyrolysis process modeling 123–130
 strengths and limitations of diverse
 modeling techniques **123**
Methanococcus 60
Methanosarcinales 60
 MFM. *see* multifluid modeling (MFM)
 microbial fermentation technologies 139
 MIMO. *see* multiple input multiple output
 (MIMO)
 MISO. *see* multiple input single output
 (MISO)
 mixed-sugar fermentation process 58–59
 ML. *see* machine learning (ML)
 MMs. *see* mathematical models (MMs)
 model deployment 31
 model evaluation 31
 “model-to-data” strategy 11
 model training 31
 MOEA/D. *see* multi-objective
 evolutionary algorithm based on
 decomposition (MOEA/D)
 MOEAs. *see* multi-objective evolutionary
 algorithms (MOEAs)
 Monte Carlo simulation 177
 MOO. *see* multiobjective
 optimization (MOO)

- MSE. *see* mean squared error (MSE)
 - multi-criteria decision analysis (MCDA) 176
 - multidimensional framework of AI
 - integration 29–37
 - decision dimension 35–37
 - process dimension 32–35
 - technical dimension 29–32, 31
 - multi-energy integration trends 165–166
 - multifluid modeling (MFM) 149
 - multi-objective evolutionary algorithm
 - based on decomposition (MOEA/D) 175
 - multi-objective evolutionary algorithms (MOEAs) 173
 - multiobjective optimization (MOO) 166, 264–265
 - advantages of 167–168
 - application and evaluation
 - cases 196
 - automated workflows and continual learning 205
 - biomass conversion, complexity and conflicts in 166–167
 - biomass conversion and system modeling 178–190
 - co-conversion strategies and 267
 - core concepts 171
 - data-model uncertainty
 - management 204–205
 - digital twin for operation and maintenance 206
 - frameworks 166, 173, 267
 - green multi-objective design, promoting 206–207
 - high-dimensional and real-time optimization issues 203–204
 - high-performance computing
 - for 190–195
 - integrated energy systems 168
 - life cycle and sustainability
 - assessment 202–203
 - mathematical modeling
 - framework 171–172
 - methodology of 171–178
 - multi-energy integration
 - trends 165–166
 - objective conflict analysis 172–173
 - post-processing and decision
 - support 176–177
 - process-level optimization
 - examples 196–198
 - solution strategies, comparison
 - of 173–176
 - structure and technical road
 - map 168–170, 169, **170**
 - system-level demonstration 199–202
 - technology 262
 - trends, challenges, and
 - deployment 203
 - uncertainty in 177–178
 - multi-objective process
 - intensification 64
 - multi-omics 64
 - multiple input multiple output (MIMO) 59
 - multiple input single output (MISO) 59
 - multiscale modeling 187–188
- n**
- natural language processing (NLP) 227
 - neural network (NN)
 - algorithms 7–8, 181
 - NIST 11
 - NLP. *see* natural language processing (NLP)
 - Non-dominated Sorting Genetic Algorithm II (NSGA-II), 40, 175
 - nonstoichiometric methods 180
 - NSGA-II. *see* Non-dominated Sorting Genetic Algorithm II (NSGA-II)
- o**
- objective conflict analysis 172–173
 - online MOO, digital twin for 189–190
 - open multiprocessing (OpenMP) 191
 - OpenMP. *see* open multiprocessing (OpenMP)
 - oxygen bomb calorimeter 83

p

PA. *see* proximate analysis (PA)
 parallel direct hybrid modeling
 (PDHM) 143–144, 143
 Pareto front 176
 partial dependence plots
 (PDPs) 43
 partial dependency analysis (PDP) 96
 particle filters (PF) 189
 particle size (PS) 87
 particle swarm optimization (PSO) 7
 PCC. *see* Pearson correlation
 coefficient (PCC)
 PDHM. *see* parallel direct hybrid
 modeling (PDHM)
 PDP. *see* partial dependency
 analysis (PDP)
 PDPs. *see* partial dependence plots
 (PDPs)
 Pearson correlation coefficient
 (PCC) 88, 89
 PF. *see* particle filters (PF)
 PHA. *see* polyhydroxyalkanoates (PHA)
 pharmaceutical delivery
 carriers 244–245, 245
 Phyllis 11
 physics-informed neural networks
 (PINNs) 8, 8, 143, 149–151, 150
 PINNs. *see* physics-informed neural
 networks (PINNs)
 plant-based biomass 22, 23
 poly-generation 6
 polyhydroxyalkanoates (PHA) 144
 population-level parallelization 194
 post-processing 176–177
 power balance equation 186
 Preference Ranking Organization
 Method for Enrichment Evaluations
 (PROMETHEE) 176
 problem identification 31
 process dimension 32–35
 process features 87
 process-level optimization
 examples 196–198
 process modeling 2

PROMETHEE. *see* Preference
 Ranking Organization Method
 for Enrichment Evaluations
 (PROMETHEE)
 prompt engineering, application of 268
 proximate analysis (PA) 84
 features 87
 HHV estimation based on 84, 85
 PS. *see* particle size (PS)
 PSO. *see* particle swarm
 optimization (PSO)
 PT. *see* pyrolysis temperature (PT)
 pyrolysis 24, 32
 enthalpy 81
 equilibrium modeling 124, 125
 models 121
 pyrolysis kinetics
 modeling 127–130, 128–129
 from TG profile 124–127
 pyrolysis process 80
 environmental benefits 80
 modeling 123
 phases of reaction scheme 129
 pyrolysis equilibrium
 modeling 124, 125
 pyrolysis kinetics from TG
 profile 124–127
 pyrolysis kinetics modeling 127–130,
 128–129
 raw material adaptability 80
 technical characteristics 80
 pyrolysis temperature (PT) 87
 Python 190
 PyTorch 7

r

radial basis function (RBF) neural
 network 7, 53
 random forests (RFs) 6, 30, 121
 RANS. *see* Reynolds-averaged
 Navier–Stokes (RANS)
 Ranzi's method 127, 129
 reaction-order approach 136–137
 real-time optimization issues 203–204
 recurrent neural network (RNN) 144

- reduced-order models (ROMs) 148–149
 - reduction-zone temperature 33
 - reference vector–guided evolutionary algorithm (RVEA) 175
 - regularization parameter 89
 - reinforcement learning 30
 - renewable-hydrogen system coupling
 - models 185–187
 - representative pseudo-compound 102
 - residence time 107
 - residual-focused hybrid simulation
 - method 144
 - response surface methodology (RSM) 46
 - Reynolds-averaged Navier–Stokes (RANS) 133
 - RFs. *see* random forests (RFs)
 - RMSE. *see* root mean squared error (RMSE)
 - RNN. *see* recurrent neural network (RNN)
 - ROMs. *see* reduced-order models (ROMs)
 - root mean squared error (RMSE) 32
 - rough set ML (RSML) 228
 - RSM. *see* response surface methodology (RSM)
 - RSML. *see* rough set ML (RSML)
 - RVEA. *see* reference vector–guided evolutionary algorithm (RVEA)
- S**
- SA. *see* simulated annealing (SA)
 - scenario-level parallelization 194
 - SCWG. *see* supercritical water gasification (SCWG)
 - second-generation biorefineries 26
 - self-learning framework 36
 - semi-supervised learning 30
 - series direct hybrid model 146–148, 147
 - SHapley Additive exPlanations (SHAP)
 - value 96, 96, 98, 99
 - simulated annealing (SA) 7
 - simulation platforms 188–189
 - single input single output (SISO) 59
 - SISO. *see* single input single output (SISO)
 - slow pyrolysis 81, 3
 - software environment 190–191
 - solution strategies, comparison
 - of 173–176
 - solvent dissolution 223
 - specific heat capacity 81
 - specific heat ratio 82
 - stoichiometric methods 180
 - succinic acid 141
 - supercritical water gasification (SCWG) 40
 - supervised learning 30
 - supervised regression learning 6
 - support vector machines (SVMs) 30
 - support vector regression (SVR) 231
 - surrogate-assisted MOO (SA-MOO)
 - methods 193
 - sustainability assessment 202–203
 - SVMs. *see* support vector machines (SVMs)
 - SVR. *see* support vector regression (SVR)
 - syngas 24, 3
 - system integration in biomass
 - biorefining 267–268
 - system-level demonstration 199–202
 - system modeling 178
 - digital twin for Online MOO 189–190
 - kinetic and heat-mass models 178–185, 183, 185
 - multiscale modeling 187–188
 - renewable-hydrogen system coupling
 - models 185–187
 - simulation platforms and data
 - interfaces 188–189
 - system resilience 167
- t**
- technical dimension 29–32, 31
 - TensorFlow 7
 - TG profile-assisted hybrid
 - modeling 151–153, 152
 - TG-DSC. *see* thermogravimetric transient plane source differential scanning calorimetry (TG-DSC)
 - TGA. *see* thermogravimetric analysis (TGA)
 - thermal conductivity 81

thermochemical approaches 37
 biomass gasification 37–41, 38
 biomass hydrothermal
 conversion 46–50
 biomass pyrolysis 41–45, 41
 thermochemical conversion 24
 process parameters 81–82
 thermochemical gasification
 process 178
 thermogravimetric analysis
 (TGA) 82, 124
 thermogravimetric transient plane source
 differential scanning calorimetry
 (TG-DSC) 102
 third-generation biorefineries 26
 TOPSIS algorithm 176–177
 torrefaction 27
 process modeling 135–139, 137, 139
 total volatile solids (TVSs) 61
 traditional conversion
 technologies 3–4, 3
 transesterification 33
 transient plane source (TPS)
 technology 102
 TVSs. *see* total volatile solids (TVSs)

U

UA. *see* ultimate analysis (UA)
 ultimate analysis (UA) 84, 87
 HHV estimation based on 84–86, 86
 uncertainty in MOO 177–178
 unsupervised learning 30

V

variable-importance analysis 49
 VFAs. *see* volatile fatty acids (VFAs)
 VM. *see* volatile matter (VM)
 volatile fatty acids (VFAs) 61
 volatile matter (VM) 84
 VOSviewer software 27

W

wet torrefaction. *see* hydrothermal
 carbonization

X

XAI 64
 XDEM. *see* Xtended DEM (XDEM)
 Xtended DEM (XDEM) 151
 xylose 25

