

Index

a

absorption-selectivity-desorption index (ASDI) 93
 adsorption isotherms 146, 147, 150, 155, 156, 164, 166, 167
 advanced data analysis and pattern recognition toolkit 24
 AI-assisted process design 14–17
 AI-assisted property modeling 1–10
 AI-assisted solvent tailoring 10–14
 AI-driven property modeling 1
 air-cooled heat exchanger system 192
 ALAMO framework 302
 ammonia synthesis 224
 aqueous biphasic systems (ABS) 2, 9, 13
 aqueous two-phase systems (ATPS) 1, 2, 6, 7, 10, 13, 14
 Arrhenius equation 225
 artificial intelligence (AI) 1, 106, 107, 211, 268, 290
 artificial neural networks (ANN) 3–8, 10, 12–14, 27, 34–36, 42, 43, 48, 49, 57, 89, 95, 150, 151, 159, 164, 165, 248–250, 269, 290, 293, 296–300, 302, 303
 Aspen Plus 12, 91, 92, 94, 110, 111, 135
 attentive neural process (ANP) 228
 automatic differentiation 175, 177, 178

b

backpropagation 111–114, 296
 baseline models 227–230

Bayesian framework 211–233
 Bayesian networks (BNs) 214
 Bayesian regularization 249
 Bernoulli distribution 216, 232
 bi-level reduced-order models (ROM) 244
 multi-sample CFD simulations 247–248
 optimal experiment design 245–247
 boundary conditions 159, 173, 175–178, 183, 192, 196
 bounded domain 176
 1-butyl-3-methylimidazolium chloride ($[C_4mIm][Cl]$) 15

c

Cambridge Structural Database
 non-disordered MOF (CSDSS-MOFs) 266
 carbon dioxide capture 93
 catalytic shift conversion (CSC) 223, 224, 226, 227, 229–233
 unit 224
 cheminformatics 23, 81, 149, 164
 cis-3-hexenyl propionate 48–51
 classification and regression tree (CART) algorithm 294
 closed-type cooling tower models 239
 computational fluid dynamics (CFD) 173, 185, 187, 189, 239–241, 244, 245, 247–248, 251, 258, 261, 298–300
 simulations 245

- Computation-Ready, Experimental MOF Database (CoREMOF) 160, 161, 239, 266, 276
- computer-aided aroma design (CAAD) framework
- case studies
- mixture aroma design for aroma substitutes 48–51
 - mixture aroma design for odor tuning 51–53
 - pure aroma design for shampoo additives 44–45
 - pure aroma design for the ingredient in insect repellent spray 45–48
 - mixture aromatic chemicals 39–43
 - pure aromatic chemicals 36
- computer-aided IL design (CAILD)
- approach 12, 79–82, 85, 93–95, 98, 99
- computer-aided IL screening 81, 90–92
- computer-aided material 265, 270
- conductor-like screening model (COSMO)
- derived fingerprints and descriptors 83
 - theory 83
- conductor-like screening model for real solvents (COSMO-RS) 83–85, 87, 90, 91, 96, 97
- conductor-like screening model-segment activity coefficient (COSMO-SAC) model 11, 31, 33, 43, 84, 90
- continuous stirred-tank reactor (CSTR) 297, 298
- convection-diffusion equation 243
- conventional method 212
- convolutional neural networks (CNNs) 15, 27, 98, 211
- cooling tower systems
- bi-level reduced-order models 244–251
 - model reduction 248–251
 - multi-sample CFD simulations 247–248
 - optimal experiment design 245–247
 - full-scale physical model 241–244
- optimization model 253–254
- small-size cooling tower 254
- thermodynamic performance indicators 251–253
- 3-D CFD model 247
- d**
- data-driven inferential sensor models
- baseline models 227–228
 - CSC Process 225, 226
 - evaluation metrics 224
 - industrial process 214
 - knowledge representation 216–220
 - GCN & Sam 217–219
 - knowledge description 216
 - knowledge section via self-attention mechanism 216–217
 - sampling from posterior 219–220
- L1 & L2 regularization terms 229–230
- loss function derivation 215
- model expressions 221–223
- model performance comparisons 228–229
- prior knowledge analysis 225–227
- process description 224–225
- sensitivity analysis 230
- transport process scale 213
- unit operation scale 214
- data-driven models 93, 147–149, 151, 167, 240, 261
- decision-making methods 176, 180–181
- decision trees (DT) 3, 4, 6, 115, 243, 290, 294, 298
- deep belief networks (DBN) 106, 111–113, 119–125
- deep factorization machine (DeepFM) 12
- deep learning (DL) method 3, 17–18, 81, 86, 89, 97–98, 105–139, 175, 176, 205, 211–212, 214, 220, 221, 223, 230, 232, 233, 302
- deep neural networks 18, 109, 111–112, 122, 302
- deodorizer distillate 90, 91
- descriptor optimization 148

Cu-BTC 154
material-property relationship of MOF 148–151
optimal MOF 154–157
P/VSA-based PE/PA separation 155
workflow 147, 148
design of experiments (DoE) 241, 245, 261
design optimization 13, 175, 177, 180–181, 187, 204
Dirichlet boundary conditions 176, 177
Dirichlet distribution 220
distillation 15, 16, 79, 85, 90, 94, 147, 265, 287, 299
DL-based Transformer-CNN framework 89
double-salt ILs (DSILs) 80, 95–97
“dual-core drive” model 125
“dual-core-driven” deep learning HDM model 117
“dual-core driven” deep learning model 107
“dual-core driven” HDM model 119–121
dual-site Langmuir (DSL) isotherm models 148

e

electronic structure informatics approach 12
electronic van der Waals surface descriptors 24
empirical methods 189, 204
energy conservation equations 242
equilibrium separation 145, 147, 153
Ergun equation 153, 226
4-ethoxybenzaldehyde 26
1-ethyl-3-methylimidazolium bis (trifluoromethylsulfonyl) amide [EMIM][Tf₂N] 12
1-ethyl-3-methylimidazolium tricyanomethanide [EMIM][TCM] 11
Euclidean distances 181, 293, 295
Eulerian–Lagrangian approach 242

Eulerian wall film model 243
Evidence Lower Bound (ELBO) 232
Exclusive Feature Bundling (EFB) 6
exergy analysis 251
exergy efficiency ratio (EER) 253, 255–257, 260, 261
exothermic reaction 224
extensions to IL Mixtures 95–97
extraction distillation (ED) 85, 91, 94

f

feature detectors 113
feature important analysis 118–125
feedforward neural networks (FNNs) 111, 211
finned heat sink model
PINN structure 185
system description and objectives 181–185
Flory–Huggins model 10
Fourier network (FN) 196, 199
fragment (group)-based representation 26
full-order model (FOM) 174, 239–241
full-scale physical model 241–244
fully-connected network (FCN) 196, 199
fully connected residual networks 114–115

g

gas separation processes
descriptor optimization 147–157
MOF 148–149
gas separation/purification 265
Gaussian distribution 216, 291
Gaussian measures 291
Gaussian process-based kriging method 303
Gaussian process regression (GPR) 291
generalized Polynomial Chaos (gPC) 194
“Generate-and-Test” method 24
genetic algorithm (GA) 93, 107, 109, 116, 180, 298

- geometry optimization 31, 204
glycolic acid (GA)
 analysis of experimental data 117
 database generation 109–111
 data dependence analysis 117
 deep learning
 deep belief networks 112–113
 deep neural networks 111
 fully connected residual networks 114–115
 random forest (RF) 115–116
 selected features and desired targets 109
experimental data 133
feature important analysis 123–125
genetic algorithm (GA) 116
hydrolysis 106
LCSA based on the optimized parameters
life cycle inventory analysis 128, 130
life cycle sustainable interpretation and assessment 129, 131
original life cycle framework 128, 129
life cycle multi-dimensional evaluation 116
model comparison 118–123
optimized FC-ResNet-GA model 125–126
Pareto optimization set 132
process multi-objective optimization and experimental verification 126–127
Pt-Mn₂O₃ nanocatalysts 106
reaction mechanism 134–139
gradient boosting (GB) 3, 4, 6, 106
Gradient Boosting Decision Tree (GBDT) algorithm 5, 6
Gradient-based One-Side Sampling 6
gradient-based optimization algorithms 174
gradient-based particle swarm optimization (GBPSO) 12
gradient descent 111, 178, 214, 220, 296
gradient descent optimization method 111
grand canonical Monte Carlo (GCMC) simulations 149, 163–165, 168, 269, 270, 274, 282
graph attention networks (GAT) 227, 232
graph neural network (GNN) models 212, 214, 217, 219, 221, 228, 232
group-based machine learning method 25–29
group contribution (GC) method 81
- h***
Halton sequence sampling method 193
Hamiltonian operator 182
heat capacity 2, 7, 15, 16, 82, 83, 94, 226, 244, 252
heat exchange and integration 300
heat exchanger system
 PINN models 200–201
Henry's coefficient 266, 276, 277
Henry's constants 159
Hermite interpolation 289
Hermite polynomials 291
high-dimensional model representation (HDMR) 290, 293–294
high-throughput screening
 AI-aided 266, 267
 hydrogen purification, MOF 273–282
 practical factors 277–282
 prescreening 273
 rapid screening 274
 rigorous validation 274–276
 structure-property-relationship analysis 276–277
machine learning model
 diversity analysis and dataset splitting 268
 molecular characterizationb 266–267
 performance evaluation metrics 268–269
 structural/chemical analysis-based prescreening 267–268

methodology 266–272
 process level simulation 270
 reverse molecular design 270–272
 histogram-based GBDT algorithm 6
 hybrid simulated annealing-genetic
 algorithm (MSAGA) algorithm
 93, 95
 hydrogen purification, MOF
 practical factors 277–282
 prescreening 273
 rapid screening 274
 rigorous validation 274–276
 structure-property-relationship
 analysis 276–277
 hydrophilic ILs 13, 15
 hyperparameters 35, 150, 180, 197, 198,
 223, 230, 232, 233, 296
 CSC dataset 232–233
 hypothetical MOF (h-MOF) 147, 155,
 161–164, 168, 266

i

IL-H₂O mixture systems 7
 ILTransR 84
 IL trihexyl(tetradecyl)phosphonium
 perfluorooctanesulfonate
 ([P66614][PFOS]) 12
 imidazolium-based ILs 6, 83
 45 imidazolium-based ILs 83
 incomplete knowledge 212, 216
 inferential sensors 211–214, 223
 inlet air 187, 188, 191, 192, 202–204,
 247, 251, 256, 259, 261
 inlet gas composition 270, 280, 283
 International Chemical Identifiers
 (InChI) 83
 ionic liquids (ILs) 1
 computer-aided IL design 93–95
 computer-aided IL screening
 90–92
 extensions to IL Mixtures 95–97
 machine learning for COSMO-based
 models 84–86
 machine learning for UNIFAC
 extensions 86–89

molecule representation of 80–84
 COSMO-derived descriptors or
 fingerprints 83
 groups or fragment-based
 representation 81–83
 machine-learned representations
 83–84

j

Jessen's inequality 215

k

kernel-based methods 292
 k-nearest neighbor (KNN) 3, 6
 algorithm 3
 Kriging 174, 248, 290–293, 298–303

l

Lagrangian multiplier method 215
 Laplace's equation 183
 large Eddy simulation 213
 largest cavity diameter (LCD) 149, 152,
 266, 271, 273, 274, 276–278
 Le Chatelier's principle 224
 least-square minimization (LSM) 291
 Lennard-Jones (LJ) potentials 165
 life cycle assessments (LCAs) 92
 life cycle inventory analysis 128–130,
 132
 life cycle multi-dimensional evaluation
 116, 129
 life cycle sustainability assessment
 (LCSA) 116, 128, 132
 life cycle sustainable interpretation and
 assessment 129–131
 lightweight gradient boosting machine
 (LightGBM) 3, 5–8
 Linux Ubuntu operating system 186
 liquid-liquid equilibrium (LLE) 85–87,
 90, 91, 94, 97
 log-normal distribution 220, 227

m

machine learning algorithm (MLA) 2, 3,
 6, 7, 11, 13, 15–18, 53, 89, 211

- machine learning-based atom contribution (MLAC)-CAMD framework 11
- machine learning-based odor prediction models group-based machine learning method 25–29 σ -profiles-based machine learning method 29–31
- machine learning (ML) models 1 for COSMO-based models 84–86 diversity analysis and dataset splitting 268 molecular characterization 266–267 performance evaluation metrics 268–269 structural/chemical analysis-based prescreening 267–268 for UNIFAC extensions 86–89
- mean absolute error (MAE) 89, 150, 224, 231, 270
- mean absolute percentage error (MAPE) 187, 224, 231
- meshing module 247
- meta-models 288
- metal-organic framework (MOF) 145, 147
- computational design building blocks identification 161–162 *in silico* hypothetical synthesis 162–164 screening PSA process optimization 165 screening *via* GCMC simulations 165 SMOF-1 165–167 validity and feasibility constraints 164–165
- integrated design process 154–157
- material-property relationship 471 CoRE 159–161
- multi-component dual-site Langmuir isotherm model 150–151
- PE/PA separation 157–159
- representation 148–149
- single-component adsorption isotherm 149–150
- mechanisms 145
- PSA operating conditions descriptor design space 151–152 integrated design formulation 153–154 P/VSA process model 152–153 structural features of 266
- mixed-integer linear/non-linear programming (MILP/MINLP) problem 12, 14, 25, 38, 39, 93, 303
- mixed-integer linear programming (MILP) 300
- mixture aroma design for aroma substitutes 48–51
- mixture aroma design for odor tuning 51–53
- mixture aromatic chemicals 25–36, 39–43, 53
- ML-based hybrid process design method 15
- ML-based IL solvent design method 12
- model parameters 57, 87, 109, 116, 118, 125, 150, 151, 158, 245, 292
- modified Fourier network (MFN) 196, 199
- Monte Carlo integral approximation 184
- Monte Carlo method 178, 246
- Monte Carlo sampling 198, 245
- multi-component dual-site Langmuir isotherm model 150–151
- multi-layer perceptron (MLP) 3, 4, 6, 228
- multi-objective optimization 107, 125–128, 132, 176, 180, 188, 189, 204, 287, 299, 300
- multiple linear regression (MLR) 3, 6, 24, 106
- n**
- natural language processing (NLP) 6, 148, 153, 154, 159, 168, 216, 301
- Navier-Stokes equations 182, 185, 213, 242

n-butylpyridinium trifluoromethanesulfonate ($[C_4Py][TfO]$)
13, 15

Neumann boundary conditions 176
neural networks, as surrogate models
174

nitrogen-oxygen ratio (NOR) 266
non-linear programming (NLP) 6, 148,
153, 154, 159, 168, 301
problem 148

normalized mean absolute percentage
error (NMAPE) 187, 199
PINN models 199

Northwestern Hypothetical MOF
Database (hMOFs) 266

Nusselt numbers 200, 202–204
NVIDIA modulus 185

o

odor characters, radar chart 25–26
open metal site (OMS) 148, 156
operation temperature 280–283
OptCAMD 39, 40, 45, 47, 48
optimal experiment design 241, 245
optimization algorithm 174, 205, 246,
296
optimization model 38, 39, 43, 184, 194,
195, 253–254, 256, 261
optimization problems 5, 38, 39, 95, 116,
146, 147, 154, 159, 181, 195, 215,
287, 288, 290, 302
optimization solver BARON 93
optimized FC-ResNet-GA model
125–126
ordinary differential equations (ODEs)
213, 288
organic Rankine cycle (ORC) 300
organic solvent N-methyl-2-pyrrolidone
91
oxygen-metal ratio (OMR) 266

p

Pareto-optimal solutions 176, 180, 187,
189
Pareto optimization set 132

Pareto solutions 126, 181, 190, 195
partial differential equations (PDEs)
154, 174–179, 185, 204, 213, 240,
247, 288

partial least squares 248
physics-based ROM 240, 245, 249, 251,
254–258, 261

physics-informed neural network (PINN)
175, 212, 213

based inverse design method
design optimization and
decision-making methods
180–181

inverse design 176–177
standard 177–180
vs. CFD 187

hyperparameters setting 198
NMAPEs 199
standard 177

point density adjustment (PDA) 198,
200, 201

poly(ethylene glycol)-dextran
ATPS 7

poly(glycolic acid) (PGA) 105

polymer–polymer aqueous two-phase
systems 10

polynomial chaos 194, 240, 290, 291

polynomial chaos expansion (PCE) 240,
290, 291, 297, 298

polynomials regression (PR) 95,
290–291, 293, 298–301

pore limiting diameter (PLD) 152, 266,
267, 273, 276–278

Prandtl numbers 243

pressure swing adsorption (PSA) 145,
146

descriptor design space 151–152

integrated design formulation
153–154

P/VSA process model 152–153

principal component (PC) matrix 12, 16,
250, 254

principal component analysis (PCA)
240, 245, 250, 254, 261

process variations 155



product attributes 36–38, 41–42, 48
 σ -profiles-based machine learning method 29–35
protic IL (PIL) 6
pure aroma design for shampoo additives 44–45
pure aroma design for the ingredient in insect repellent spray 45–48
pure aromatic chemicals 25–29, 36–39, 53
P/VSA process model 152–153

q
quantitative structure-property relationships (QSPR) model 6, 42, 80, 97, 269–270, 283

r
radial basis function (RBF) 5, 151, 174, 240, 290, 292–293
random forest (RF) 3, 4, 24, 106, 115–116, 149, 269, 294
rapid screening 269–270, 274
reaction engineering 212, 225, 291, 297–299
recommender systems 84, 88, 212
rectified linear unit (ReLU) 111, 196, 296
recurrent neural networks (RNNs) 211
reduced-order model (ROM) 194, 239–261
residual network (ResNet) 109, 114–115
restricted Boltzmann machines (RBM) 112, 113
Reynolds-averaged Navier-Stokes equations 213
Reynolds number 226, 242
root mean square error (RMSE) 118–122, 124–126, 224, 231, 270

s
Screening Charge Density (SCD or σ) distribution 83
self-attention mechanism (SAM) 211, 214, 216–219, 223
separation engineering 299–300

sequential-conceptual methods 301
shape optimization 173
single-component adsorption isotherms 149, 150, 167
singular values 249, 254, 255
Softmax operator 217, 221, 223
solvent screening 10, 11, 90, 91
solvent tailoring 1–19
stacked-autoencoders (SAEs) 211
state-space model 244, 250
Stefan–Boltzmann constant 244
stochastic optimization models 194, 253, 261
stochastic reduced-order model (SROM) 194, 245–247, 250, 253–255, 257
structure-odor relationship (SOR) 23–25, 27, 29, 31, 34, 39, 42, 43, 48, 53
structure–property–relationship 2, 6, 42, 80, 146, 269–270, 273, 276–277
supervised-learning paradigm 174
supervised variational autoencoder (SVAE) 228
support vector machine (SVM) 1, 3–7, 24, 89, 106, 151, 165, 290, 295, 298, 299
surrogate model 174, 240
basic workflow 289
benefits 288
chemical processes 297–303
heat exchange and integration 300
process design and synthesis 301
reaction engineering 297–299
separation engineering 299–300
construction 289
optimization problems 287
segregated-network PINN architecture 196
techniques 289–297
artificial neural network 296–297
decision tree 294–295
high-dimensional model representation 293–294
Kriging 291–292
polynomial chaos expansion 291



- polynomial regression 290–291
 radial basis functions 292–293
 support vector machine 295
 two types 194
 types of 241
 syntax-directed variational autoencoder (SDVAE) 12
 synthesizer 227–228
 synthesizer-based models 227–228
- t**
- task-specific ILs 80, 90, 97
 techno-economic analysis 265
 TensorFlow 185, 198, 200
 thermal conductive adhesive 181
 thermophysical property 182
 Thiele modulus 226
 three-layer ANN 4, 5, 296
 “Tommy Girl” fragrance 23
 topology optimization 173, 174
 TOPSIS method 180, 189, 195, 200
 total degree of molecular unsaturation (TDU) 266, 280
 traditional mesh-based numerical method 174
 transfer learning 86, 176, 191, 194, 196–200, 205
 air velocities and temperatures 200
 transformer models 217
 transport process scale 212, 213
 trial-and-error 145, 173, 189, 204, 265
 trihexyl(tetradecyl)phosphonium bis(trifluoromethanesulfonyl) amide ($[P_{\{6,6,6,14\}}][TFSA]$) 12
- tubular air cooler model
 PINN structure 195–196
 system description and objectives 191–195
 transfer learning 196–199
 Tyrosine (CAS No. 60-18-4) 31
- u**
- UNIFAC-IL model 82, 86, 87, 89, 93, 94
 unit operation scale 212–214
 unsupervised layer-by-layer learning 113
 unsupervised layer-by-layer training 112
- v**
- vacuum swing adsorption 146, 147
 vapor-liquid equilibrium (VLE) 85, 87, 89
 variational autoencoder (VAE) 11, 12, 215, 228
 variational inference over graph (VIOG) module 213, 214, 221, 223, 227–230, 232
 viscosity 1, 2, 6, 7, 11, 15, 16, 36, 38, 82, 92, 93, 95, 152, 182, 242
 volumetric/accessible/gravimetric surface area (VSA/ASA/GSA) 266
- w**
- weighted electronegativity per atom (WEPA) 266
 Wiener chaos expansion 291
- x**
- XGBoost 3, 5–8, 107





