

## Subject Index

### a

abstraction 226 f  
acceptance criterion 117 ff  
accuracy  
– data validation 801 ff, 808 f  
– distributed dynamic models 38 ff  
– simultaneous integration 207  
– stencil methods 43, 47  
acetic acid/methyl acetate process 544  
acetone–chloroform mixtures 785 ff  
acetone–cyclohexane system 127  
acetone–water system 129  
achieve relation 255  
acidification 711  
acoustic databases 734  
action-instrumental artisan model 249  
active pharmaceutical ingredients (API) 405,  
  434, 649 f  
active tablet components 435  
activity coefficients 125 ff, 781  
activity-based costs (ABC) 464  
adaptive grids method 40  
adaptive mesh refinement (AMR) 35 ff, 68 ff,  
  74 ff  
adaptive stencil methods 42, 45 ff  
adaptive supply chains capabilities 702  
adsorption  
– batch chromatography 552  
– distributed dynamic models 75  
– gas separation 3, 11, 138–147  
– model-based control 567  
– separation systems 137 ff  
advanced numerical methods 68  
advanced planning and scheduling systems  
  (APS) 476, 622, 700  
advanced process combinatorics 473  
Advanced Process Control (APC) 820  
advection 99  
advisory system 612, 615 f  
aeroderivative duty gas turbines 336  
affine functions 583 f  
agent-based supply chain management 632,  
  697 ff, 702 ff

agglomeration 75, 87, 90 ff  
aggregate time period (ATP) 455  
aggregation  
– decomposition techniques 447, 454 ff  
– distillation 278, 287  
– granulation process 191  
agitated reactors 307  
agrochemicals 649  
air conditioning 328 ff  
air preheating 355  
Alberta Taciuk Processor (ATP) 684  
alcohols 649  
algebraic systems 2, 15–34, 175, 201  
algorithm implementation 530  
alkane groups 127 ff  
allocation  
– product scheduling 488 ff  
– resource planning 448, 457, 460  
– supply-chain management 624, 637, 708  
allolactose, lac operon 231  
Altshuller method (TRIZ) 428  
aluminum process, carbothermic 399  
amino acid chains 228  
ammonia synthesis 534 ff, 812 ff  
analyses methods 428  
Anderson molecular modeling 117  
Andrecovich–Westerberg model 273  
anisotropic united atoms force fields 123  
Apache standards 752  
application programming interface (API) stan-  
  dards 752  
applications 174, 485, 771–854  
– chemical product-process design 659  
– distributed dynamic models 75 ff  
– embedded integration framework 210  
– flexible recipe model 612  
– frameworks 209–214  
– life cycle modeling 681 ff  
– molecular modeling 125 ff  
– multiscale processes 203  
– product scheduling 506 ff  
– simultaneous integration 207  
l-arabinose (ARA) regulatory networks 242

- arc length 72
- ARMAX package 679
- aromatics groups 130
- Arrhenius temperature dependence 79 ff, 85
- Arrhenius-type kinetic constants 792
- artisan model of instrumental action 249
- ARX model 567
- Aspen Custom Modeler (ACM) 545
- Aspen packages 473, 638
- AspenPlus
  - educational modules 775
  - equipment design 390
  - life cycle modeling 680, 691
  - multiscale process modeling 214
- asphalt production 457
- assumption retrieval 181, 678
- asymmetric traveling salesman problem 490
- asymptotic solutions 162
- asynchronous agent-based team 507
- atmospheric distillation unit (CDU) 323
- attainable region method 306
- AUA4 force fields group 131 f
- auction method, iterative 636
- augmented Lagrangean relaxation 466 ff, 470
- auto-associated software agents 697
- autocorrelation coefficients 116
- automatic differentiation 39 f
- automation OPC standards 755
- autonomic chemical plants 223
- autonomous agents 702
- auxiliary functions 24, 31, 159
- average values
  - data reconciliation 521 f
  - molecular modeling 112 ff
  - supply-chain inventory 634 f
- Avogadro number 126
- azeotropes
  - distillation 278 ff
  - educational modules 782 ff
  - methyl acetate process 544
- b**
- backdiffusion effects 142
- backward allocation 709
- backward differentiation formula (BDF) 36 ff, 57 ff
- balance composite curves 345 f
- balance equations 172–182
  - chemical product-process design 659
  - educational modules 778
  - equipment design 388
  - multiscale process modeling 198
  - process monitoring 520
- balance volumes 172 ff, 180 ff
  - multiscale process modeling 198
  - partial models 201
- Bardenpho process 314
- batch chromatography 552 ff, 562–568
- batch correction procedure 611
- batch crystallization 159
- batch processes 498, 591–620
- batch production 448, 458 ff
- batch reactor model equations 406
- batch scheduling 673
- batch splitting 487
- Bayesian networks 238, 594
- beads model 122
- benzene 388, 785
- benzyl alcohol production 606
- beta-factor 566
- beta-galactoside permease 231, 256 f
- bibliographical thermophysical databases 735
- bid selection problem 466
- bifurcations 237
- bi-Langmuir function 556 ff
- bill of materials (BOM) 698
- binary interaction parameters 127
- binder
  - granulation 196
  - tablet formulation 435
- biochemical processes (BioPro) 75 ff, 408
- biochemical product-process design 656
- biogas outlet temperatures 355
- biological regulatory framework 250
- biological systems/biomolecules 224 ff
- Biot number 80
- biotransformation processes 224 ff
- black-box model
  - flexible recipes 606
  - life cycles 676
  - multiscale processes 199
- blending
  - data validation 827+
  - product development 432
  - product scheduling 484
  - resource planning 448, 456
- block grid structures 69
- blow-down steps 140, 148
- boilers 337, 370 ff
- boiling point 649, 734
- Boltzmann factor 114, 127
- bond molecular models 122
- Boolean matrix 29 f
- Boolean networks 238
- Boolean variables 277, 290 f
- bottom-up approaches 194, 197 f
- boundary conditions 172 ff
  - distillation 281
  - distributed dynamic models 36, 54, 66 ff, 77
  - gas separation 147
  - mesh refinement 70
  - molecular modeling 108 ff

- multiscale processes 198
- partial models 201
- separation systems 139 f
- thermophysical databases 734
- bounds 30
- bovine somatotropin (BST) 409
- Box-Jenkins model 679
- brainstorming product development 427
- branch and bound technique
  - distillation 282
  - hybrid processes 594
  - product scheduling 495 ff
  - resource planning 467 ff
  - supply-chain management 637
- branch-and-cut enumeration 488
- Brdyš model 557 ff
- breakage
  - crystallization processes 162
  - distributed dynamic models 75, 87, 90 ff
- brewery utility management 689
- bromopropyl compound amination 405
- Brownian motion 108
- Broyden condition 28 f, 559
- bubble columns 307
- bubble curve, hexane/cyclohexane system 128
- Buckingham potential 123
- budgeting horizons 714
- buffer times 499
- building blocks
  - chemical product-processes 660
  - distillation 277
- building transformations 177
- bulk chemicals 648
- bullwhip effect 699
- Burger's equation 73
- business strategies 421
- butanoic acid chlorination 308
- butyronitrile 131
- Buzzi-Ferraris property 19, 25, 29
- bypassing strategies 305
- bypproducts 297, 327
  
- C**
- Caballero-Grossmann model 277
- Calderbank-Moo-Young correlation 85
- calibration 182 ff
  - calibration
    - data validation 801
    - equipment design 391
    - life cycle modeling 676
    - multiscale process modeling 194
  - caloric databases 734
  - campaign production 448, 458 ff, 493 f
  - Cannizarro reaction 606
  - canonical models 179
  - canonical NVT 113
- capacities
  - chemical product-processes 657
  - cost-effective manufacturing 831 ff
  - planning 541
  - product scheduling 489, 504
  - resource planning 450
- CAPEC database 780
- CAPE-OPEN
  - standards 750 ff
  - life cycle modeling 680 f, 691
  - multiscale process modeling 214
  - resource planning 476
- carbon catabolite repression 233 f, 256 ff
- carbon dioxide balance 96 ff
- carbon ratio 806 ff
- carbothermic reactors 399 f
- carboxyl groups 130
- carnosic acid manufacture 652
- Carnot efficiency 342
- cascade model 331
- case studies
  - equipment design 393 ff
  - life cycle modeling 681 ff
  - cost-effective manufacturing 834 ff, 844 ff
- case-based reasoning systems (CBR) 423, 434 ff
- cash flow 695, 712
- catabolite repression 233 ff, 256 ff
- catalysts
  - ammonia formation 814
  - design 434, 655
  - educational modules 791
  - flexible recipe model 601
  - intensification 300
  - life cycle modeling 673
  - utility systems 328
- catalytic slurry bed 84
- cause effect analysis 199
- cell compartments 237 ff
- cell division 75
- cell number variation 97
- cell population
  - biochemical process design 409
  - distributed dynamic models 75, 92 ff
- cell state control 224, 244
- central agents 705 f, 727
- central dogma of biology 228 f
- centrifuges 411 f
- chain rule, distributed dynamic models 40, 63
- Chang method 61 ff, 65 ff
- chaos properties, regulatory networks 237
- character string pattern 531
- charge conservation 384
- ChemCad modules 775
- Chemical Abstracts Service (CAS) 419
- chemical engineering, thermophysical databases 733–748

- chemical engineering plant cost index (CEPCI) 335 f
- chemical equilibria 36, 649, 814
- chemical industrial plants 327 ff
- chemical phenomena 301 f, 422
- chemical potential 384
- chemical product-process design, integrated 75 ff, 647–668
- chemical vapor deposition (CVD) 195, 203
- chemistry
  - computer-theoretical 108 ff
  - intensification 302
  - quantum models 121 ff
- chemistry WebBook, thermophysical databases 736 ff
- CHEMKIN software 214
- chi-square test 528, 809 f, 817 f
- chlorination, butanoic acid 308
- chloroform 649
- chloroform–acetone mixture separation 785 ff
- chocolate couverture, house of quality 426
- Cholesky algorithm 22
- CHP schemes 349
- chromatographic separation 6, 552
- chromatography 35, 75 ff
- chromosomes 532
- classification
  - integration methods 204
  - life cycles 679
  - linking frameworks 205 f
  - multiscale process modeling 199
  - partial models 198 ff
- cleaning 328
- client agents 705, 722
- clinical trial outcomes 462
- closed-loop control 542
- coagulation 150 ff, 155 ff
- coal outlet temperatures 355
- coalescence 196
- concurrent beds 307
- COGents standards 766
- COLaN standards 751 ff
- cold streams 329 ff, 334 ff, 370
- collision frequency 153
- collocation method
  - crystallization processes 155
  - distributed dynamic models 52
  - intensification 315
- columns
  - batch chromatography 552
  - distillation 270–295
  - intensification 307
  - methyl acetate process 544
- COM standards 754, 758
- COMBO system 598
- combustion 328, 351 ff, 686
- commissioning 669 ff
- common grid approach 490
- communicative actions 250
- compensated disturbances 612, 616
- complementary slackness 582
- complex column sequences 285–296
- complex multiphase reactor 393 ff
- complex separation systems 137–170
- complexity
  - batch chromatography 552
  - chemical product-process design 656
  - product scheduling 489
  - regulatory networks 229 ff, 236 ff
- component integration 7
- component-based hierarchical explorative process simulator (CHEOPS) 214
- components 171 ff
- composite curves 331
- compositions 171
- compositions
  - multiscale process modeling 197
  - utility systems 345 f, 371 ff, 375
- compound balances 811 ff, 827
- compound selection 660
- compressed gases 328
- compression
  - ammonia synthesis 536
  - refrigeration cycles 359
- computer theoretical chemistry 108 ff
- computer-aided educational modules 9
- computer-aided equipment/process design 383–418
- computer-aided flow sheet design (CAFD) 662
- computer-aided integration, utility systems 327–382
- computer-aided intensification methods 297–326
- computer-aided mixture-blend design (CAM<sup>b</sup>D) 649 ff, 653 ff
- computer-aided modeling/simulation 11–264
- computer-aided molecular design (CAMD) 422, 649 ff, 653 ff
- computer-aided process modeling (CAPM) 1 ff, 181
- computer-aided process operation 443–642
- computer-aided process/product design 1 ff, 265–442
- computer-aided production engineering (CAPE) 1, 5, 643–770
  - *see also:* CAPE, CAPE-OPEN
- computer-integrated manufacturing (CIM) 1 ff, 98–106
- computational fluid dynamics (CFD) 11, 35, 383
- equipment design 383
- life cycle modeling 673
- parallel integration framework 212
- simultaneous integration 207

concentration dynamics, regulatory networks 233  
 concentration profiles  
   - ammonia formation 815  
   - model-based control 568  
 conceptual design  
   - life cycles (Clip) 669, 676 ff, 691  
   - multiscale process modeling 203  
   - shale oil processing 682  
 condensers  
   - complex multiphase reactor 394  
   - data validation 812  
   - distillation 283, 291  
 condition number 24  
 conditioning 519  
 conductive media simulation 401  
 configuration  
   - interaction methods 121 ff  
   - nonazeotropic mixtures 286  
 conjoint analysis 424  
 connection relation 255  
 conservation balances 176 ff  
 conservation element/solution element (CE/SE)  
   method 39, 57, 61 ff  
 conservation laws  
   - distributed dynamic models 43, 62  
   - equipment design 384, 388 ff  
 consistency 183  
 constitutive equations 173–182  
   - multiscale process modeling 191 ff, 202 ff  
 constraint logic programming (CLP)  
   - product scheduling 500 ff  
   - resource planning 469  
   - supply-chain management 627  
 constraint propagation methods 30  
   - chemical product-process design 659  
   - cost-effective manufacturing 831 f  
   - data validation 802  
   - educational modules 778  
   - flexible recipe model 613  
   - hybrid processes 594, 601 ff  
   - model-based control 558 ff  
   - process monitoring 520 ff, 529 ff  
   - product scheduling 483, 489 f, 496 f  
   - real-time optimization 581 ff  
   - resource planning 456  
   - supply chain management 714  
   - utility systems 350, 365 f  
 construction projects 465 ff  
 consumer requirements 5, 424  
 contaminant profiles 322 ff, 375 ff  
 continuation methods 31 f  
 continuity, boundaries 54  
 continuous multiscale process modeling 199  
 continuous time discretization 490, 497  
 continuous time representation 594

control  
   - hybrid processes 599  
   - model-based 541–576  
   - multiscale process modeling 194  
   - resource planning 453  
   - transcriptional regulation 235 f  
 controllability  
   - complex multiphase reactor 397  
   - dynamical properties 185  
   - life cycles 676  
   - product development 431  
 convection  
   - cell population dynamics 93  
   - complex multiphase reactor 401  
   - distributed dynamic models 35, 43, 59, 75  
 convergence 17 f, 25  
   - material flows 448  
   - real-time optimization 589  
   - separation systems 142  
 conversion systems 329 ff  
 convex hull disjunction formulation 277, 284 f  
 cooling requirements 330, 370  
 coordinate transformation 177  
 CORBA-IIOP standards 750, 754 f  
 Corporate Web site management 764  
 correction model  
   - distributed dynamic models 60  
   - flexible recipes 610  
 correlations  
   - molecular modeling 114 ff  
   - multiscale process modeling 204  
   - utility systems 335  
 cosmetics 438  
 costs  
   - chemical product-process design 648 f  
   - correlations 335  
   - data validation 810  
   - effective manufacturing 829–854  
   - flexible recipe model 603 ff  
   - model-based control 548, 566  
   - nonlinear functions 361  
   - process monitoring 537  
   - real-time optimization 580  
   - resource planning 450  
   - supply-chain management 623  
   - utility systems 334 ff  
 Coulombic interactions 109, 121 f, 124 f  
 counter currents  
   - carbothermic aluminum process 400  
   - utility systems 330  
   - intensification 307  
   - separation systems 142  
 coupling  
   - multiscale process modeling 189  
   - regulatory networks 244  
 Courant–Friedrichs–Lowy (CFL) number 59

- covariance matrix 521
- CPLEX solver 469
- CPU conditions 28
- CPU time
  - distributed dynamic models 51
  - water systems 324
- cradle-to-the-grave process 667
- Crank–Nicolson central difference scheme 61
- creative templates 430
- critical region 579 ff, 588 ff
- crude desalting 323
- crude oil distillation
  - data validation 819
  - inventory management 457
  - real-time optimization 580
- crystal fragmentation 150 ff
- crystal growth
  - distributed dynamic models 75, 87 ff
  - separation systems 150 ff
- crystal size distribution (CSD) 87, 152
- crystallization 13, 159
  - chemical product-process design 653
  - distributed dynamic models 35
  - separation systems 149 ff
- customers demands
  - cost-effective manufacturing 829
  - product development 430
  - supply-chain management 621, 630 f
- customers service level (CSL) 622, 631, 635
- cutoff distance 124
- cycle periods, batch chromatography 552
- cyclic adenosine monophosphate (cAMP) 234
- cyclic material flows 448
- cyclic steady state (CSS)
  - model-based control 565, 570
  - separation systems 139
- d**
- Daesim dynamics 680
- Damkohler number 80, 85, 387
- Danckwert's boundary condition 36 ff, 66, 77, 86
- DARX standards 766
- data analysis
  - chemical product-process design 660
  - life cycle modeling 681
  - multiscale process modeling 194
  - product development 423, 438 ff
- data handbooks 735 ff
- data quality 182
- data reconciliation 6, 517–540, 802 ff, 810 ff
- data validation 801–828
- data validation
  - computer-aided integration 329
  - process monitoring 519 ff, 524 f
  - utility systems 330
- databases
  - educational modules 779
  - thermophysical properties 733–748
- Datacon package 527
- debottle-necking 303,674
- decay rates, regulatory networks 240
- decentralized decision making 704
- DECHEMA databases 735 ff, 744 ff, 753
- decommissioning 669 ff
- decomposition techniques
  - fluid bed reactor 414
  - life cycle modeling 675
  - product scheduling 495 ff
  - resource planning 447, 454 ff, 469 ff
  - structural 184
- decoupling frameworks 205 f
- default values 181
- definition phase, product development 421 ff
- deformation rate, granulation 196
- degradation 502, 816
- delay differential equations (DDEs) 231 f
- delta function 164
- demand data 451
  - cost-effective manufacturing 829–854
  - expected 833
  - manager agent system 723
  - product scheduling 484
  - supply-chain management 621, 626
  - water usage 376
- demonstration, multiagent system 726
- dense overlapping regions (DOR) 243
- densities, thermophysical databases 734
- density functional theory (DFT) 121 ff, 130 f
- desalter 323
- design
  - chemical product-processes 648, 657
  - complex multiphase reactor 399 f
  - documentation standards 764
  - equipment 390
  - life cycle modeling 669
  - product development 421, 424 ff, 431
  - supply-chain management 624
  - utility systems 367 f
- design institute for physical property data (DIPPR) 735, 739 ff
- desorption 139147
- deterministic methods
  - life cycle modeling 674, 679
  - multiscale process modeling 199
  - product scheduling 505
  - resource planning 469
  - supply chain management 698 f
- DETERM thermophysical databases 736, 762
- diabatic distillation column 394
- DICOPT MINLP solver 276
- Diesel engines 336, 343

- diethyl ether 649
  - difference schemes 60
  - differential equations
    - partial models 201
    - regulatory networks 239 ff
  - differential index 177, 184 f
  - differential-algebraic equation (DAE) 2, 13–34, 171 ff
    - educational modules 778
    - life cycle modeling 680
    - model-based control 545 ff
  - diffusion
    - computational fluid dynamics 80, 99
    - distributed dynamic models 35 f, 75
    - gas separation 145
    - intensification 311
  - diffusion coefficients
    - distributed dynamic models 59
    - molecular modeling 114
    - thermophysical databases 734
  - dilution loss 93
  - DIMA block standards 765
  - dimension analysis 183
  - dipolar interactions 121
  - Dirac delta function 164
  - Dirichlet's boundary condition 36
  - discontinuities 30
  - discretization
    - crystallization processes 156 ff
    - distributed dynamic models 35 ff
    - fixed-bed reactors 83
    - hybrid processes 591 ff
    - multiscale process modeling 199
    - partial differential equations 55
    - time grids 488, 490 ff, 494 ff
  - discrimination process models 171–188
  - disintegrant 435
  - disjunctions 277
  - dispersion
    - crystallization processes 155, 161
    - distributed dynamic models 36
    - shale oil processing 684
  - displacements 119
  - dissipation 59
  - distance, linear systems 18
  - distillation 4, 17, 27, 32
    - chloroform–acetone mixture 787 ff
    - columns 17 f, 27, 32
    - data validation 811, 818 f
    - equipment design 388 ff, 393 ff
    - intensification 297, 310
    - model-based control 543 ff
    - molecular modeling 109
    - process synthesis 269–296
    - separation systems 138 ff
    - solvents 787
  - distributed dynamic models 35–106
  - distributed parameter multiscale process modeling 199
  - distribution centres 623 f, 696 ff, 717
  - disturbances
    - feed compositions 397
    - flexible recipe corrections 610 ff, 616
    - methyl acetate process 550
    - model-based control 543 f
  - divergent material flows 448
  - divided differences method 45
  - dividing wall column 286
  - DNA replication 224, 228 ff
  - Documentum package 679, 692
  - domain relationship 206
  - Dorf–Drury method 71
  - Dortmunder database (DDB) 736 ff, 745
  - drum design 196
  - Dufort–Frankel method 59, 67
  - duty gas turbines 336
  - dyes 437
  - dynamic data reconciliation 517, 524 ff
  - dynamic models
    - environment 696
    - life cycles 678
    - plants 541 ff
  - dynamic population balance 75, 87, 92
  - dynamic simulation
    - equipment design 390
    - process operation scheduling 501
  - dynamical properties 185
- e**
- Eastman process 297 f
  - echelons supply chain 699 ff, 708 f
  - Eclipse standards 500, 752
  - eco-label (ecological card) 710
  - e-commerce 697, 750
  - economic lot scheduling 491
  - economic models
    - life cycle modeling 672
    - supply chain management 700
  - eco-toxicological impact 711
  - edge effects 110
  - educational modules 9, 775–800
  - effect modeling and optimization (EMO) 349 ff
  - efficiency
    - data validation 809
    - utility systems 335, 362
  - effluents 328
  - eigenvalues 38
  - ELDAR, thermophysical databases 738, 743 ff
  - electrode heating 403
  - electrodeposition 203
  - electrolyte solution data bases 742 ff
  - electrostatic interactions 123, 131

- elementary functions, regulatory networks 251 f
- embedded integration framework 210
- embedding relations 252
- emergency response 673
- emissions
  - utility systems 328
  - water use 374
- empirical model building 181, 199, 674
- encapsulation 653
- energetic-interaction-related phenomena 109
- energy balances 173, 180 ff
- energy balances
  - chemical product-process design 654
  - distributed dynamic models 36
  - educational modules 793
  - equipment design 384
  - process monitoring 535
- energy consumption
  - data validation 810
  - distillation 270
  - formic acid plant 825
  - utility systems 328–382
- energy dissipation 150 f
- energy eStandards 753, 757 ff
- energy recovery 330
- energy recycling 80
- engineering
  - life cycle modeling 669 ff
  - shale oil processing 684
- enterprise content management (ECM) 692
- enterprise resource planning (ERP) 463 ff, 472 ff
- enthalpy
  - balance equations 18
  - thermophysical databases 734
  - utility systems 340 ff
- entrainer selection 281
- entropy
  - complex multiphase reactor 395
  - equipment design 384 ff
  - thermophysical databases 734
- enumeration
  - distillation 271
  - product scheduling 488 f
  - resource planning 459, 467 ff
- environmental impact
  - chemical product-process design 649
  - life cycles 668, 672, 680
  - manager agent module 707, 725
  - shale oil processing 684
  - supply chain management 696, 710, 727
- environment–health–safety (EHS) 785
- enzyme activity 568
- equation construction procedure 172
- equation partitioning 795
- equation weights 18 f
- equation-oriented packages 392
- equidistribution principle 71
- equilibrium
  - adsorption 144
  - chemical product-process design 649
  - data validation 814
  - ethanol–water mixture 782
  - thermodynamics 384 ff
- equipartition of entropy production (EDF) 389, 395 f
- equipment
  - costs 335 ff
  - design 383–418
  - failure 505, 517
  - process intensification 299 ff
- errors
  - adaptive mesh refinement 68
  - covariance matrix 521
  - data validation 801 ff, 805 ff
  - distributed dynamic models 37, 51
  - model-based control 560, 564 f
  - molecular modeling 115
  - multiscale process modeling 216
  - process monitoring 518 ff
  - UNIQUAC model 131
- Escherichia coli*
  - biochemical process design 409
  - regulatory networks 224–235, 242 ff
- essentially nonoscillatory (ENO) schemes 42–47, 57 ff, 71 ff
- esterification, methyl acetate process 544
- ethanol oxidation 94
- ethanol–water system 129, 782
- ethylbenzene separation 811
- ethylene dichloride (EDC) fraction 398
- ethylene glycol production 312
- Euclidean norm 19, 25
- eukaryotes 237
- Euler central difference method 60 ff
- Euler discretization 156 f
- Euler equation 100
- EURECHA Web site 798
- European Symposium on Computer-Aided Process Engineering (ESCAPE) 763
- eutrophication 711
- event operation network (EON) 595 ff
- event tree 673, 679
- evolutionary algorithms 487, 597
- Ewald summation 124
- exact solution approaches 469
- exchange rates 623
- exergy analysis 341 ff
- exergy losses 362 ff, 395
- exhaust gas flow 98
- exothermic behavior 146

- experimental design
  - model-based control 569
  - product development 422, 432 ff
- experts systems 778
- explicit time discretization 58, 60 f
- extended Kalman filter 525
- extensible markup language (XML) 750, 757
- extension conditions 181
- extensive quantities 174, 387
- extracellular glucose 229
- extracts, separation systems 140 f
  
- f**
- Factory Planner software 473
- FACT thermophysical databases 736
- factorization 24
- failure
  - methyl acetate process 550
  - process monitoring 517
  - product scheduling 505
- fault diagnostics 251, 673, 678 f
- feasibility studies 520, 531
- feed compositions 270, 397, 680
- feed flow rates 275, 282
- feedback control 541–576
- feedforward loop 243
- feeding strategies 305
- FEMLAB multiphysics module 401
- Fenske–Gilliland–Underwood short cut
  - model 283 f
- fentanyl analysis 779 ff
- fermentation 318, 408
- field molecular orbital concept 122
- fill rate maximization 624
- fillers 435
- filtering 519
- financial analysis models 673, 696
- financial module 711, 725
- finishing 651
- finite difference methods (FDM)
  - batch chromatography 563
  - distributed dynamic models 41, 54, 86
- finite element methods (FEM)
  - complex multiphase reactor 401
  - crystallization processes 154
  - distributed dynamic models 41, 51 ff
  - life cycles 680
  - stress modeling 686
- finite intermediate storage (FIS)
  - hybrid processes 593
  - product scheduling 485
- finite volume method (FVM) 41, 55 ff
- first principals model 234
- Fischer–Tropsch synthesis 83
- fitness function 533
- fixed-bed gas separation 143 f
- fixed-bed reactors 35, 75, 79 ff
- fixed-grid method 40
- fixed-point homotopy 31
- fixed-stencil approximation 42 ff
- flexible cost-effective manufacturing 829–854
- flexible environment modeling 594 ff
- flexible recipe model 597–613
- Floudas optimization 274, 305 f
- flow rates
  - batch chromatography 552
  - complex multiphase reactor 396
  - distributed dynamic models 49
  - real-time optimization 580
  - refrigeration cycles 359
  - regulatory networks 256
  - resource planning 448
  - utility systems 340 ff
- flow sheets
  - chemical product-process design 651, 661
  - distillation 284
  - educational modules 778
  - life cycle modeling 672
  - shale oil processing 683
- fluctuations, molecular 108, 113 ff
- flue-gas flow 352
- FLUENT software 214
- fluid bed reactor 413 ff
- fluid concentration propagation 78
- flux terms, gas separation 145
- food additives plant 834 ff
- force equipartition 389
- force fields 110 ff, 114 ff, 123 ff
- forecast management 696, 703 ff
- forecasting module (FOREST) 714
- forecasting techniques 830
- formalization, regulatory networks 251
- formic acid plant 825
- formulation
  - process monitoring 520
  - product development 432
- forward allocation 709
- Fourier transform 114
- fractionation 686
- fragmentation 150 ff, 160 ff
- frameworks
  - integrated chemical product-process design 658
  - multiscale process modeling 205 ff, 215 f
  - regulatory networks 249
- free software standards 752
- freedom degrees 157, 183 f
- frequency response approximation 548
- freshwater consumption 320
- fruit cooperative 714
- fuel additives 436
- fuel cells 338

- fuel consumption 334 ff, 352 f
- fuel oil production 457
- fuel outlet temperatures 355
- fully discretized methods 35 ff, 58
- fully thermally coupled column sequences 288
- functional analysis 251 f
- functional B-splines 163
- functional equivalence 172
- functional genomics 224, 236 f
- functionalities 599
- function – property – composition relations 420 ff
- Furzeland method 71
- fuzzy modeling
  - cost-effective manufacturing 833
  - resource planning 452
  - supply-chain management 637
- g**
- gain matrix 558, 562
- galactoside permease 231
- Galerkin residuals 155 ff, 163
- gamma distribution 165
- gamma-phi equilibrium model 782
- Gantt charts 447, 608
- gas concentration factor 85
- gas constant 95
- gas engines 336
- gas permeation 314
- gas phase, Fischer–Tropsch synthesis 84
- gas processes, eStandards 757 f
- gas separation 3, 11, 138–148
- gas turbines 336, 351, 373
- gas–liquid–liquid reactors 311
- gas–oil systems 457
- gasoline blending 456
- gasoline data 580
- Gauss divergence 62
- Gauss integration 166
- Gauss law 115
- Gaussian waves 50
- Gear-like algorithms 116
- Gebhard–Seinfeld collocation 155
- gene interactions 224
- gene population 532
- gene transcription 228, 233 ff
- general flexible recipe algorithm 602 f
- general purpose solutions 483
- general rate model (GRM) 553
- generalized disjunctive programming (GDP) 277
- generalized Maxwell–Stefan (GMS) equation
  - 145
- generic activity-based product development 421 ff
- generic algorithms
  - investment cost function 361
  - life cycle modeling 680
- process monitoring 528, 532
- product development 423 ff, 438
- product scheduling 487, 503
- resource planning 468 ff
- generic manipulation 223 ff
- genericity tests 131
- genetic code, *lac* operon 229
- genome sequencing 224
- genome wide molecular interactions 246
- geographical information system (GIS) 626
- Gibbs ensemble Monte Carlo 119 ff, 125 f
- Gibbs model 386
- Gibbs–Duhem relation 125 f
- Gilliland–Fenske–Underwood method 276, 283 ff
- Gill–Murray criterion 25
- global supply chain management (GSCM) 696 ff
- global warming 710
- glucose
  - fermentation/oxidation 94
  - regulatory networks 229 f, 258
- glycols 649
- Goffman framework 249
- gPROMS package
  - educational modules 775
  - equipment design 392
  - gas separation 148
  - life cycle modeling 680, 691
  - model-based control 545 f
  - multiscale process modeling 214
- gradient methods 20 ff, 26, 39, 557 ff
- gradual model enrichment 197
- grafcat logic models 673
- grand composite curves 331–346, 375
- granulation 3, 189–197, 408
- graphic user interface (GUI) 719 ff, 724 ff
- graphical representations
  - intensification 305, 310 f
  - resource planning 469
  - utility systems 333 ff, 339 ff
  - water usage 377
  - water-pinch concept 320 ff
- Green's theorem 56, 62
- green-kubo formulas 116
- grey-box model
  - life cycles 676
  - multiscale process modeling 199
- grid methods
  - crystallization processes 156
  - distributed dynamic models 40, 52, 69
  - hybrid point timing 594
- grinding processes 13, 151 ff, 160 ff
- gross errors 809 f, 817
  - data validation 803, 809
  - process monitoring 518 ff, 528

Grossmann model 277  
 Grossmann–Pinto method 490 ff  
 group contribution methods 662  
 growth, crystallization 150 ff, 155 ff

**h**

Habermas approach 249 f  
 HAD process standards 765  
 Hamiltonian operator 121 f  
 Hangos–Cameron model 172 ff, 390  
 hardware, process intensification 299 ff  
 Hartree–Fock method 128  
 heat balances  
   – educational modules 792  
   – gas separation 146  
   – utility systems 330 f, 335 f  
 heat cascades 331  
 heat exchange  
   – ammonia synthesis 536  
   – distillation 270  
   – educational modules 791  
   – granulation process 191  
   – intensification 297, 300 f  
 heat exchange network (HEN) 276, 328 f, 349 ff  
 heat integrated column sequences 279 ff  
 heat pumps 337, 360, 372  
 heat recovery boilers 337  
 heating requirements 370  
 heating system failure 550  
 heat-power combination 329  
 heavy duty gas turbines 336  
 height equivalent to theoretical plate (HETP)  
   value 545  
 Hendry–Hughes technique 274  
 Henry coefficients 569, 734  
 Henry's law 95  
 heptanone 649  
 Hermite polynomials 155 f, 165  
 Hessian matrix 23 f  
 heuristic methods  
   – distribution planning 624  
   – product scheduling 484, 487 ff  
   – supply chain management 698 f  
 hexanone 649  
 hidden components 174  
 hierarchical approaches  
   – hybrid processes 594  
   – product scheduling 481  
   – resource planning 459  
 high-temperature reaction zone 400  
 high-throughput experimentation (HTE) 433  
 Hildebrandt solubility 649, 779  
 Hill coefficient 240  
 Hill–Ng procedure 163 f  
 Hoffmann's number 59 ff  
 homogeneous azeotropic separation 281 f

homotopy 31  
 Honeywell's database 681  
 horizon methods  
   – data reconciliation 526  
   – flexible recipe model 605  
   – model-based control 542  
   – real-time optimization 586  
   – resource planning 454, 457  
   – supply-chain management 628, 633 f, 714  
 horizon-averaged finished product (SKU) inventory 634  
 hot streams 329 ff, 334 ff, 352 ff, 370  
 house of quality 425  
 Huang–Russell approach 71  
 Hückel calculations 121  
 human factors  
   – life cycles 674  
   – supply chains 702  
 hybrid methods 7, 16, 27 ff  
 hybrid methods  
   – embedded integration framework 211  
   – life cycle modeling 671  
   – multiscale processes 199  
   – product development 438  
   – product scheduling 483, 498 ff, 506 f  
   – real-time optimization 584  
   – resource planning 469  
   – *see also: Powell method*  
 hybrid multizonal/CFD modeling 160  
 hybrid processes 591–620  
 hybrid separation 137, 297, 301, 314–321  
 hydrocarbon-based fuels 682, 686  
 hydrocarbons 323  
 hydrogen bonding interactions 123  
 hydrogen catalytic oxidation 79  
 hydrogen energy balances 84  
 hydrogen plant process 806 f  
 hydrogen production 414  
 hydrogen recovery 316  
 hydrogen sulfide 323  
 hydrogenation 686  
 hydrotreating system (HDS) 323  
 hydroxyl groups 130  
 hyperplanes 386  
 hypertext markup language (HTML) standards 750  
 hypertext transfer protocol (HTTP) standards 750  
 HYSIS package 680

**i**

i2 packages 473, 638  
   – factory Planner 473  
 IBIS system 679  
 ICAS package 680  
 ICV-SEV electrolyte solution data 745

- ideal adsorption solution theory (IAST) 144 f
- ideal gas law 143, 545
- ideality product development 429
- identification problem 248, 676
- ill-conditioned approximations 16, 24, 73
- ILOG solver 469
- implementation
  - cost-effective manufacturing 851
  - supply chain management 710
- implicit constraints 594
- implicit enumeration approaches 467
- implicit time discretization 60
- improvement algorithms 471
- incidence matrix 795
- inclusion body (IB) 408, 410 ff
- incorporation techniques 280
- incremental assumption-driven models 29, 181
- independence constraint quality 582
- individual resource grid 490
- inducer exclusion 233 ff, 258 ff
- industrial applications
  - process intensification 302
  - product scheduling 506 ff
  - supply chain management 710 ff
- industrial source complex version 3 (ISC3) 684
- inequality constraints 174
- information flows, multiscale processes 204 ff
- Information Society Technologies (IST) standards 764
- information technology standards 758
- INFOTHERM thermophysical databases 736 ff
- infrastructure
  - life cycle modeling 667
  - supply chains 697
- initial conditions 171 ff
- cell population dynamics 96
- distributed dynamic models 36 f, 49 f
- educational modules 796
- partial models 201
- regulatory networks 255
- initialization
  - flexible recipe model 602 f
  - mixed-integer linear program 587 ff
- injection period 552
- inlet temperatures 332
- integer cut 360
- integral/partial differential/algebraic equations (IPDAE) 161 f, 592
- integrality gap 494
- integrated chemical product-process design 647–668
- integrated composite curves 345 f
- integrated computer-aided system (ICAS) 777–800
- integrated supply chains management 695–732
- integrated system optimization and parameter estimation (ISOPe) 557 ff
- integrated system production planning (SIPP) 456
- integration methods
  - crystallization processes 158
  - flexible recipe model 605
  - multiscale process modeling 196, 202
  - ODE 38
  - production/resource planning 453
  - supply chain management 695–732
  - utility systems 327–382
- integropartial differential equations (IPDEs) 87
- intelligent manufacturing, data validation 801–828
- intensive variables 384 ff
- interactions, molecular 108, 121 ff, 127
- interactive multiscale frameworks 205 f
- interface
  - environmental module 725
  - financial module 725
  - negotiation agent 727
- intermediates 448 ff, 485
- interoperability, supply chains 697
- interpolation
  - crystallization processes 165
  - distributed dynamic models 43, 53, 70
- interpretation frameworks, regulatory networks 248 ff
- introduction strategy 461
- inventory-replenishing dynamics 622, 630 f, 710
- investment costs
  - generic function 361
  - resource planning 450
  - utility systems 334
- investment decision calendar 628
- ISA S88 framework 598
- Ising method 132
- ISO10303 691
- ISO14000/15288 668
- isobaric/thermal distillation 274
- isobar-isothermal *NPT* 113
- isopryl acetate 649
- iso-risk contours 687
- iterative methods 20 ff, 64
- iterative methods
  - model-based control 557 ff
  - multiscale process modeling 197
  - supply-chain management 636
- IUPs software 214
- Jacobian matrices 2, 15, 19–31
  - data reconciliation 523 ff, 529 ff, 802
  - distributed dynamic models 38 ff, 64 f, 96

**j**

- Jacob–Monod model 229 ff
- Java platform standards 751
- Jboss standards 752
- jobshops 485 ff
- Jonsdottir–Rasmussen–Fredenslund method 128

**k**

- Kalman filter 525
- Keesman quadratic model 606
- kernel functions 197
- kerosene data 580
- ketones 649
- ketones/alkanes system 127
- key assumptions 678
- key performance indicators (KPI) 802–827
- kinetic cell population rates 94
- kinetic constants 792
- knowledge-based methods 422, 434 ff, 503
- Kotler concept 419 ff
- Kronecker factor 530
- Kumar–Ramkrishna discretization 156 ff, 164 ff
- $k-\varepsilon$  turbulence model 401

**l**

- lac operon (lactose) 225–235, 256 ff
- ladder logic models 673
- Lagrange decomposition 455 ff, 466 ff, 470 ff
- Lagrange multipliers
  - cost-effective manufacturing 848
  - crystallization processes 155 f
  - data reconciliation 521 ff, 529 ff
  - distributed dynamic models 53
  - model-based control 558 ff
  - real-time optimization 582 f
- Laguerre polynomials 155 f, 165
- Langmuir isotherm 144 ff, 553 ff
- large-scale algebraic systems 2, 15–34
- large-scale process modeling 190
- large-scale simultaneous integration 207
- Lax–Wendroff scheme 59, 67
- ICA evaluation 708
- leaching models 684
- leaks detection 816 ff
- lean burn configurations 336
- Leapfrog scheme 58 f, 67
- least-impact heuristic schedules 503
- Legendre polynomials 52
- Lengeler model 244, 256
- length scale models 190 f, 203
- length scale models
  - chemical product-processes 655
  - life cycle modeling 674

- Lennard–Jones functions 123, 130 f
- Levenberg–Marquardt method 24 ff
- life cycle modeling 8, 667–694
  - chemical product-process design 647
  - product development 420
  - supply chain management 707 f
- lignite 355
- Lim–Jorgenson method 65
- linear data reconciliation 810
- linear discrete time system 577 ff
- linear driving force approximation (LDF) 146
- linear independence constraint quality 582
- linear multiscale process modeling 199
- linear programming 489, 531
- linearization, piecewise 361, 842
- links
  - hybrid processes 594 f
  - process monitoring 528 ff
  - see also: constraints
- Linux standards 752
- liquefied petroleum production 457
- liquid phase, Fischer–Tropsch synthesis 84
- liquid streams 270, 328 ff
- liquid–liquid mass exchanger 311
- liquid–vapor equilibria 812
- list splitting technique 274
- location–allocation problem 450, 624
- logical checking 183
- lognormal distribution 165
- long-term planning 207, 502 ff, 449 ff
- Lorentz–Berthelot rule 124
- LQ factorization 25
- LU factorization 530
- lubricants 435
- Ludzak–Ettinger process 314
- lumped parameter multiscale processes 199

**m**

- MacCormack method 60, 67
- macroscale multiscale process modeling 204 ff
- maintenance costs 334 f
- make-to-order/stock 484
- management agent system 703, 706 ff, 718
- manufacturing process
  - life cycles 667–694
  - supply chains 696
- manufacturing resource planning (MRP-II) 463 ff
- Manugistics packages 474, 638
- mapping regulatory networks 236 ff
- market potentials 672
- Markov chain 679
- Marshall Swift index tables 335
- mass balances
  - chemical product-process design 654
  - crystallization processes 154, 159 ff

- data validation 810, 827
- distillation 274
- equipment design 384
- gas separation 143 f
- utility systems 335
- mass exchange network (MEN) 276, 311, 321
- mass recycling 80
- mass transfer
  - granulation 191, 196
  - intensification 304, 311
  - model-based control 569
- master recipes
  - flexible 615
  - hybrid processes 598
  - real-time optimization 589
- material balances
  - distributed dynamic models 36
  - product scheduling 483, 489 f
  - resource planning 450
- material data
  - hybrid processes 597
  - product scheduling 484, 493
  - resource planning 448
- material requirement planning (MRP) 463 ff, 497
- mathematical educational modules 775
- mathematical models
  - batch chromatography 552
  - cost-effective manufacturing 832
  - equipment design 384
  - life cycle modeling 672 ff
- mathematical programming
  - product scheduling 484–500
  - resource planning 456
  - utility systems 349 f
- MATLAB
  - educational modules 775, 781 ff
  - flexible recipe model 614
  - life cycle modeling 674
- maximum product yield 405
- Maxwell–Stefan surface diffusivities 145
- mean variance 407
- means-end analysis 227 ff, 251 ff, 255 ff
- measurement system 5, 518 f, 528, 556
- measurements optimization 801, 808
- mechanical simulation 673
- mechanical vapor recompression (MVR) 360 f, 366
- mechanistic models 198 ff
- mediation regulatory relation 255
- melting point 649, 734, 779
- membrane
  - compartments 143
  - distillation 297, 314 ff
  - separation systems 3, 137, 142 ff
  - surface effects 144
- merit function 17 ff
- MESH column model 276 ff
- mesh refinement 68 ff
- messenger RNA (mRNA) 228 ff, 236 f, 240 ff
- metabolic cell reactions 94
- metaheuristic approaches 469 ff, 484, 487 ff
- methods of characteristics (MOC) 88 ff, 96
- methods of lines (MOL) 37, 40 ff, 67 f
- methods of moments 154 f, 157 ff
- methyl acetate process 297 f, 544–551
- methylisobutyl ketone 649
- Metropolis sampling 117
- microbial culture processes 35, 75 ff
- microbial systems 247 ff
- microcanonical NVE 114
- microcapsule encapsulation 653
- microelectronic industries 413
- microorganisms 3, 223–264
- microreaction technology 300
- microscale multiscale process modeling 206
- middle-out strategies 195
- middleware standards 760
- minimum energy requirement (MER) 328–382
- minimum exergy losses 395
- minimum temperature difference 331
- mining operation 672
- Minsky model 672
- mixed-integer linear programming (MILP)
  - educational modules 778
  - hybrid processes 594
  - life cycle modeling 673
  - real-time optimization 586
  - refrigeration cycles 360, 364 ff
  - resource planning 449 ff, 469 ff
  - supply-chain management 624, 636 ff
- mixed-integer nonlinear programming (MINLP)
  - resource planning 448 ff, 469 ff
  - distillation 274 f, 290 ff
  - educational modules 778
  - electrode heating 403
  - intensification 305 ff, 310 ff, 315 f, 320 ff
  - life cycle modeling 673
  - product scheduling 483, 489, 497 f, 500 ff
  - separation systems 141
  - supply chain management 698 f
  - utility systems 333 ff
- mixed-integer programming (MIP) 271
- mixed-integer quadratic program (MIQP) 586
- mixed-logical dynamics (MLD) optimization 584
- mixer superstructures 321
- MIXPROPS thermophysical databases 736
- mixture design 648 ff
- model integration
  - batch chromatography 554 ff

- chemical product-process design 657 ff
- equipment design 390 f
- life cycle modeling 678
- multiscale process modeling 189, 193, 197
- model tuning/discrimination 171–188
- Model.La package 680
- model-based control 541–576
- model-based predictive control (MPC) 577 ff, 631
- model-based statistical methods 517 ff
- ModelEnterprise package 499
- Modelica package 680, 691
- modeling 171–188
  - computer-aided 11–264
  - equipment design 390 f
  - lac operon 232 ff
  - life cycle modeling 675
  - molecular 2, 13, , 107–136
  - multiscale process modeling 195 ff
  - partial models 202
  - supply chains 712
- modeling functions of microbial systems (MFM) 254 ff
- ModKit package 680
- modules
  - educational 775–800
  - environmental 707
  - financial 711, 725
  - supply chain management 703 f, 707
- modulons, regulatory networks 241, 244 ff
- mole balances 792
- molecular dynamics 115, 204
- molecular electrostatic potential (MEP) analysis 131
- molecular interactions 246
- molecular mechanics 110, 122 f
- molecular modeling 2, 13, , 107–136
- molecular properties 734
- molecule structure design 648 ff, 661
- molten aluminum 399
- moments methods 154 ff, 163 ff
- momentum transfer 191
- monetary units (ME) 349
- monitoring 517–540
- monitoring/forecasting techniques 830
- monodimensional approach 25
- monolithic reactors 297
- Monte Carlo methods
  - crystallization processes 154, 163
  - life cycle modeling 679
  - molecular modeling 108
  - product scheduling 505
- morphological analysis 428
- MOT/ICAS modules 790 ff
- mother-cell division death term 93
- moving finite difference (MFD) 71
- moving finite element (MFE) 71
- moving grid methods 35 ff, 68–75
- Mozilla standards 752
- MS Excel 674
- Mulliken population analysis 131
- multiagent systems (MAS) standards 702 f, 712, 718 f, 765
- multicomponent distillation 272
- multicomponent molecular systems 124
- multicriteria piecewise linearization 842
- multidimensional optimization 23
- multidisciplinary tools, process–product design 777
- multidomain framework 211
- multiechelon supply-chain 700
- multienterprise supply-chain management 635
- multifunctional heat exchangers 300
- multilevel flow modeling (MFM) 251 ff, 257 f
- multimedia collection standards 764
- multiobjective generic algorithms (MOGA) 471
- multiparametric quadratic programming (mp-QP) 582, 586 ff
- multiperiod problems
  - location-allocation 624
  - product scheduling 504
  - resource planning 459
  - utility systems 367 f
- multiphase reactor equipment 393 ff
- multiphase systems 130
- multiple crew strategies 468
- multiple sensors 532
- multiple-input multiple-output (MIMO) block architecture 242, 820
- multiprocess plants 329 f
- multiproduct batch plant 831
- multiproduct plants
  - cost-effective manufacturing 829
  - product scheduling 485 ff
  - supply-chain management 621
- multipurpose batch processes 609
- multipurpose equipment 448
- multipurpose plants 485 ff, 493 ff
- multipurpose supply-chain management 621
- multiresource generalized assignment problem (MRGP) 471
- multiscale capacity planning 462
- multiscale modeling 3, 189–222
- multiscale modeling
  - chemical product-process design 655 f
  - life cycle modeling 675
  - life cycles 675
  - molecular modeling 107 f, 111 ff
- multisite planning
  - integer optimization 627
  - product scheduling 481 ff
  - supply-chain management 621, 628 ff, 696

- multiskill strategies 468
- multistage production 448
- multistage stochastic programming 505
- multizonal computational fluid dynamics 100f
- MySQL standards 752
  
- n**
- Nash-type objective functions 637
- natural frameworks, regulatory networks 249
- natural gas 355, 812
- Navier – Stokes equation 100, 389
- negated regulatory conditions 255
- negotiation module 703–716, 726 ff
- Nelder–Mead algorithm 831, 843 ff
- net present values (NPV) 450, 461
- network regulatory motifs 241 ff, 246 f
- network representations 392
- network superstructures *see: superstructures*
- Neumann's boundary condition 36
- neural networks
  - life cycle modeling 674, 680
  - model-based control 567
  - product development 423, 436 ff
- new product development (NPD) 421 ff, 427 ff, 460
- new-born cell birth term 93
- Newton homotopy 32
- Newton methods 20–30
  - distributed dynamic models 39, 64
  - separation systems 142
- Newtonian fluids 209
- Newton–Raphson method 523
- NIST chemistry WebBook 736 ff
- nitrile groups 131 f, 824
- no intermediate storage (NIS) 485, 593
- noise 542, 560, 673
- nominal optimization 405
- nonazeotropic mixture distillation 286
- nonconvex optimization model 637
- nonisothermal systems 308
- noniterative CE/SE method 65
- nonlinear cost functions, utility systems 361
- nonlinear equation systems (NLS) 15–34
- nonlinear isotherms 562 f
- nonlinear model predictive control (NMPC) 6, 542 ff, 567 ff
- nonlinear multiscale process modeling 199
- nonlinear Nash-type objective functions 637
- nonlinear ODE-based models 246
- nonlinear optimization strategies 365 f
- nonlinear programming (NLP)
  - data reconciliation 523 ff
  - distillation 287
  - intensification 305, 315 f
  - resource planning 456
- nonlinear-based control 545
  
- o**
- OASIS standards 751 f, 759
- object management group (OMG) standards 751
- objective functions
  - cost-effective manufacturing 831–849
  - exergy model 362
  - model-based control 557 ff
  - real-time optimization 583 f
  - supply-chain management 637
- observable variables 185, 524 f, 531 ff, 676
- octanol–water partition coefficient, fentanyl 779
- offline initialization 610
- offline optimization 541, 585
- oil processing
  - data validation 826
  - eStandards 756 f
  - life cycle modeling 682 ff
- oilfields 456 f
- oleic acid methyl ester removal 649
- one-way coupling 207
- online monitoring 823
- online parameter adaptation 542, 556, 568 ff
- online production accounting 827
- online scheduling 482
- ontology web language (OWL) 767
- ontological representation (OntoCAPE) 691, 765
- OPC process /control system standards 750 ff
- open standards 750 ff
- operation conditions
  - chemical product-processes 654
  - data validation 802, 822
  - flexible recipe model 601 ff, 613
  - hybrid processes 594
  - life cycle modeling 669 ff
  - multiscale processes 195

- process monitoring 517, 531f
- supply-chain management 630
- operation costs
  - resource planning 450
  - supply-chain management 623
  - utility systems 334
- operation modeling
  - shale oil processing 687
  - supply chain management 714
- operational planning, gas fields 458
- operons 244f
- optical databases 734
- optimization
  - biochemical processes 409ff
  - complex multiphase reactor 405
  - costs 361, 842f
  - crystallizers 159
  - data reconciliation 526, 529ff
  - distillation 271
  - intensification 305, 320f
  - life cycles 675
  - membrane-based gas separation 143f
  - model-based control 541ff
  - product scheduling 483, 490f
  - real-time 577–590
  - supply-chain management 621–642
  - utility systems 333f, 345ff, 369f
- ordinary differential equations (ODE) 15–34
  - computational fluid dynamics 101
  - crystallization processes 155f, 158, 165f
  - data reconciliation 526
  - distributed dynamic models 36ff
  - educational modules 778
  - life cycle modeling 680
  - process models 171, 184
  - regulatory networks 238f
- organic Rankine cycles 344
- orthogonal collocation 51, 315
- orthogonal systems 18
- oscillatory cell population behavior 75
- oscillatory yeast rates 94
- outlet temperatures 355
- overall modeling
  - biochemical processes 410
  - masses 173
  - multiscale processes 195
- P**
- paper manufacturing 508
- parallel multiscale process modeling 204–216
- parameters 182
  - continuation method 32
  - molecular modeling 110
  - multiscale process modeling 217
  - partial models 201
  - real-time control 578–585
  - recommended 735
  - shale oil processing 682
- Pareto curves 319, 716f
- partial consistency 183
- partial differential algebraic equations (PDAsEs)
  - 2, 13–106
- partial differential equations (PDEs) 173ff
  - complex multiphase reactor 402
  - computational fluid dynamics 35–106
  - distributed dynamic models 35
  - large-scale algebraic systems 2, 13–34
  - regulatory networks 238
- partial models 196ff, 200ff
- partial pressure 142
- particle size distribution (PSD)
  - crystallization processes 153ff, 161ff, 164f
  - distributed dynamic models 87
- particle surface effects 144
- partitioning 15
  - educational modules 795
  - molecular modeling 114, 117ff
- partnerships, supply chains 716
- pdXmL standards 753, 757
- peak demand period 452
- Peclet number 80, 85
- penalty composite curves 373
- penalty function 532, 802
- penalty parameters 548
- pentane/hexane system 127
- performance criterion 602, 606
- performance indicators 518, 802–827
- permeate compartment 147
- permeation modeling 684
- permutation schedule 487
- perturbations
  - flexible recipe model 614
  - model-based control 560ff
- pesticides 653
- Petyluk columns 282, 286
- Petri-nets 631, 679
- petroleum fractions 192, 818
- petroleum supply chains 457
- Petrov–Galerkin method 155
- pharmaceuticals
  - chemical product-process design 648
  - product development 432–437
  - supply chain 460, 632
- phase boundary 311
- phase diagrams 778ff
- phase equilibrium 8, 734
  - educational modules 779
  - methyl acetate process 545
  - molecular modeling 109, 119ff
- phase stability 386
- phosphoenopyruvate (PEP) 234

- phosphoric acid fuel cells 338
- phosphotransferase (PTS) 234
- photochemical oxidant formation 711
- photovoltaic industries 413, 466
- physical agents 703 ff
- physical models
  - distillation 271 ff
  - life cycles 672 ff
- physical phenomena 17
  - distributed dynamic models 75
  - equipment design 383
  - hybrid processes 592
  - intensification 301
  - product development 422
- physical properties 171
- molecular modeling 107–136
- process monitoring 530
- PHYSPROPS, thermophysical databases 736
- phytochemical manufacturing 650
- piecewise affine systems (PWA) 584
- piecewise linearization 361, 842
- pilot plants 303, 508
- pinch point analysis
  - complex multiphase reactor 396
  - intensification 320 ff, 328 ff
  - utility systems 331, 361
  - water use 374
- Pinto–Grossmann method 490 ff
- planning techniques
  - cost-effective manufacturing 830–852
  - experimental product development 432
  - resources 452
  - supply-chain management 624
- plant design 303
- plant management 10
  - product scheduling 504
  - resource planning 452
  - supply-chain management 621
- plant measurements 801
- plant simulation 592
- plant structure 815
- plug flow grinding process 161
- poly(ether urethane urea) membrane 317
- polymer composites 438
- polymerase enzymes 228
- polysulfone membranes 315
- population balance equation (PBE)
  - computational fluid dynamics 100
  - crystallization processes 151 f, 160 f
  - distributed dynamic models 75, 87 ff, 92 ff
  - fluid bed reactor 414
- population generation 532
- porcine somatropin (pST) 409
- POSC standards 753, 757
- powder feed rate, granulation 196
- Powell method 16, 27 f, 39
- Powell's dogleg algorithm 523
- power market, resource planning 465 ff
- Poynting correction factor 782
- precedence constraints 714
- precipitation 152
- precision
  - data validation 807
  - process monitoring 531
- prediction
  - distributed dynamic models 60
  - flexible recipes model 610
  - real-time control 577, 586
- preferential sampling 118
- prefractionator 286
- preparative chromatography 35,
- pressure 171
  - distillation 283
  - equipment design 384
  - flexible recipe model 601
  - gas separation 148
  - molecular modeling 113
- pressure drop
  - gas separation 147
  - methyl acetate process 545
- pressure-swing adsorption (PSA) separation 13, 137 ff, 789
- pricing optimization 636, 639
- principal component analysis (PCA) 520, 527, 821
- prize collecting salesman problem 490
- proactive capabilities 702
- probability demand function 833 ff, 852
- probability density, molecular modeling 113 f
- probability of stock-outs (PSO) 631 ff, 635
- ProCAMD modules 785 f
- process and materials network (PMN) 594
- process control OPC standards 755
- process design 383–418
  - chemical products 648
  - decision chain 527
  - integrated 647–668
- process flow diagrams (PFD)
  - chemical product-process design 651
  - data validation 804, 812
- process history database (PHD) 681
- process intensification 4, 297–326
- process life cycle modeling 667–694
- process models
  - computational fluid dynamics 98–106
  - flexible recipe model 613
  - hybrid processes 592, 597
  - resource planning 448 ff
  - scheduling 482 ff, 501
  - separation systems 137
  - utility systems 329
- process monitoring 5, 517–540

- process simulation
    - educational modules 775
    - hybrid processes 592
    - *see also:* simulation
  - process solvent systems 317 ff
  - process synthesis
    - intensification 302 ff
    - separation 269–296
  - process system enterprise (PSE) 474
  - process-molecule synthesis supermodel 318 f
  - producer–product relation 255
  - product demand *see:* demands
  - product development 4, 419–442
  - product engineering 189 f
  - product portfolio 462
  - product scheduling 481–516
  - product selectivity 823
  - product specifications
    - chemical process design 647 ff
    - flexible recipe model 602 ff
    - multiscale process modeling 190
    - needs 657
  - product testing 431
  - product yield 405
  - production accounting 827
  - production life cycle 669 ff
  - production planning
    - cost-effective manufacturing 830–852
    - flexible recipe model 603
    - resource planning 472
  - production profiles 450
  - production recipes 483
  - production scheduling 5
  - production time 832
  - production–distribution–inventory systems 696
  - productivity, biochemical processes 412
  - product-oriented methods 431, 650 ff, 661
  - product-process design, integrated 647–668
  - profile-based approach 308
  - profit profiles
    - cost-effective manufacturing 831–852
    - expected 716, 838
    - real-time optimization 580
    - supply-chain management 624
  - PRO-II simulator 680, 775, 789 f
  - prokaryotic organisms 224, 228 ff, 237 ff, 244 f
  - ProPred module 780
  - property relations 173 f
  - property relations
    - educational modules 779 f
    - multiscale process modeling 198
  - propionitrile 131
  - PROSYN-MINILP synthesizer 276
  - protein networks 223–264
  - protein–DNA interactions 224, 247
  - protein–protein interactions 224, 237, 247
  - proteins 409
  - proton exchange membranes 338
  - pseudocomponent concept 818
  - purge separation 141
  - purification
    - batch chromatography 552 ff, 568
    - biochemical process design 409 ff
    - carbothermic aluminum process 400
    - chemical product-process design 651
    - fluid bed reactor 413 f
  - PVT behavior, thermophysical databases 734
  - pyrolysis 682
- q**
- quadratic programming problems 582
  - qualitative differential equations (QDEs) 238
  - quality
    - chemical product-process design 647 ff
    - equipment design 384
    - hybrid processes 597, 601 ff
    - thermophysical databases 733
  - quality function deployment (QFD) 424 ff
  - quantitative performance measurements 623
  - quantum models 110, 121 ff, 673
  - quasi-Newton family 2, 13, 23, 27 ff
  - quaternary separation 272
  - queuing models 673
  - quick-to-market 671
- r**
- radiation risk 688
  - raffinates 139 ff
  - rain water percolation 684
  - Randolph–Larson model 151 f
  - random noise 527
  - random number generation 115 ff
  - Rankine cycles 344
  - raw materials 327, 597
  - Rayleigh number 387
  - reactant conversion 607, 649
  - reaction rates 173
    - educational modules 792
    - model-based control 569
  - reaction system models 673
  - reaction transfer models 304
  - reactive distillation process 543 ff
  - reactive scheduling 482, 503 ff
  - reactive separations 301, 309 ff
  - reactive simulated moving bed (SBM) 565
  - reactor/mass exchanger (RMX) 311, 315
  - reactors
    - educational modules 791
    - intensification 311
  - reactor–separator–recycle process network synthesis 310

- real models 562
  - real physical distributed systems control 702
  - real-time adjustments 697
  - real-time control 518
  - real-time environment 697
  - real-time expert system 674
  - real-time optimization (RTO) 577–590
  - real-time scheduling 503
  - reboilers 270 ff, 283–291, 394
  - receding horizon 586
  - recipe-based representations 501, 591–615
  - recommended parameters 735
  - reconciliation tools 330
  - reconfiguration, supply chains 697
  - recovery
    - batch chromatography 562
    - carbothermic aluminum process 401
    - chemical product-processes 651
  - rectifier 282, 311
  - recycling 79, 305, 668
  - redundancy analysis
    - data validation 803 ff, 815 ff
    - process monitoring 517, 519 ff
    - real-time optimization 582
  - refineries
    - blending 579
    - data validation 826
    - resource planning 448 ff, 456 ff
  - refinery and petrochemical modeling system (RPMS) 456
  - reflux ratio 548
  - refrigeration
    - computer-aided integration 369
    - product development 437
    - utility systems 359, 370
  - regression analysis
    - complex multiphase reactor 407
    - distillation 285
    - life cycle modeling 679
    - molecular modeling 126
  - regulatory control 525, 568
  - regulatory microorganism networks 223–264
  - regulons 244 f
  - rehabilitation phase 672
  - relative concentration dynamics 233
  - remediation 669 ff
  - repartitioning 452
  - report generation 533
  - repository of modeling environment (ROME) 690
  - represilators 239 ff
  - repressor gene, *lac* operon 231 f, 258 ff
  - requirement-parameter translation 424 ff
  - rescheduling strategy 610 f
  - research modeling 682
  - residuals 19
  - crystallization processes 163
  - distributed dynamic models 55
  - real-time optimization 580
  - residues curves 787
  - resource planning 447–480
    - constraint frameworks 467, 483 f, 489 f
    - cost-effective manufacturing 830
    - decomposition methods 498
    - hybrid processes 592
    - life cycle modeling 673
    - product development 429
    - supply chain management 696
  - resource-task network (RTN) 454, 496 f, 592
  - responsiveness 398, 696
  - restricted matches 364, 373
  - retentate compartment 147
  - retiming strategy 611
  - retrofit 674
  - reuse models 690
  - reverse engineering 117 ff, 226 ff
  - Reynolds number 387
  - ribosome-binding site 241
  - risk-based management (RBM)
    - life cycle modeling 671
    - shale oil processing 687
    - supply-chain 626
  - RNA polymerase enzymes 228 ff
  - rolling horizon algorithm 454, 457
  - rubber mixtures 436
  - rule-based methods
    - chemical product-process design 661
    - product development 423, 438 ff
    - product scheduling 488
  - Runge–Kutta method 37 ff, 96
  - run-time deviations 610
- S**
- Saccharomyces cerevisiae* 93, 224, 237 f
  - safety
    - chemical product-process design 649
    - data validation 807
    - thermophysical databases 734
  - safety–health–environment (SHE) concept 667
  - sales maximization 624, 831
  - salts–water systems 323
  - sampling 111, 115 ff
  - SAP packages 474, 638
  - satisfaction level 716
  - saturation composition 781
  - scale identification 193, 697
  - scale invariance homotopy 32
  - scaling laws 387
  - scenario-based approaches 451
  - scheduling techniques 481–516
    - flexible recipe model 603 f, 609 f, 614

- life cycle modeling 673
- resource planning 452
- Schrödinger equation 110 ff, 121 ff
- Schubert formula 29
- search techniques
  - intensification 310
  - product scheduling 484
- segmentation methods 154 ff, 162 ff, 431
- self consistent field molecular orbital concept 122
- self-diffusion 116
- self-organization 697, 703
- semantic networks 439
- Semantic Web standards 9, 750 ff, 763–769
- semibatch reactive distillation process 543 ff
- semibatch reactor 791
- semiconductor fabrication 203, 508
- semidiscretized methods 35,
- semiempirical methods 121
- sensitivity analysis
  - cost-effective manufacturing 847 ff
  - process monitoring 517, 524 ff, 535
  - real-time optimization 580
  - supply-chain management 627
- sensor network optimization 518, 528, 531 f, 801
- sensors 110
- separation 137–170
- separation
  - chemical product-process design 660
  - chromatographic 552
  - costs 566
  - product scheduling 484
  - synthesis 269–296
- separator–centrifuge settling area 411
- sequential approach 448, 715
- sequential quadratic programming (SQP) 523 ff, 531 ff, 802, 810 f
- serial integration framework 208
- serial multiscale process modeling 204 f
- series reactions 791 ff
- service-oriented architecture (SOA) standards 761
- set-point perturbation finite difference method (FDPN) 563
- set-point tracking
  - flexible recipe model 602
  - methyl acetate process 549
  - model-based control 559, 564
- set-up times 448
- seven-step procedure 172, 182 f, 193
- shadow compartment concept 311
- shale oil processing 682 ff
- shared intermediate storage (SIS) 485
- sharp split assumptions 272 ff
- shock transition 45
- shortcut models 271, 274, 283 f
- short-term scheduling 493
- short-term scheduling
  - flexible recipe model 602
  - uncertainties 451, 502
- shut-down resource planning 450
- side rectifier 282, 286
- side stripper column 282
- signal converters 518
- signaling molecules 223 ff
- signal-oriented modeling 244 ff
- signed directed graph (SDG) 185
- silane feed 414
- silicon 413 f
- simple distillation columns sequences 272–286
- simple object access protocol (SOAP), Web services 750, 758 ff, 763 ff
- simplex method 843
- simplified solutions 177
  - distillation 271 ff
  - model-based control 545 f
  - multiscale process modeling 207 ff
- simulated annealing
  - intensification 310, 315
  - product scheduling 487 ff, 506 f
  - resource planning 469 ff
- simulated moving bed (SMB) process 565
- simulation
  - computer-aided 11–264, 329
  - hybrid processes 592
  - life cycle modeling 673, 680
  - model-based control 568
  - supply-chain management 631, 701 ff
- simultaneous approaches 195, 207, 661
- single-input multiple-output (SIMO) block architecture 242
- single-level mathematical formulation 459
- single-multiphase reactors 307
- single-phase flow model 402
- single-site scheduling 483, 492
- single-stage refrigeration cycle 359
- singular Jacobi matrix 24
- site recipes 598
- size factor 595
- size reduction 287
- size–shape relation 387
- slack real-time optimization 582
- slack resource iterative auction approach 636
- slurry bubble column reactor (SBCR) 35, 75, 83 ff
- smart agents 697
- smelting zone 400
- SMILES strings 780
- smoothness 195
- SO<sub>2</sub> levels 684

- social frameworks 249
- socioeconomic impact analysis 687
- sociotechnical risk assessment 667, 673
- soft sensors 808
- software packages 9
  - data reconciliation 527
  - multiscale process modeling 214 ff
  - process intensification 299 ff
  - product scheduling 483, 499 ff
  - resource planning 472 ff
  - standards 765
  - supply-chain management 637 f
- solar cell production 414
- solid conversion 401
- solid oxide fuel cells 338
- solid phase 84
- solubilities 649
- SoluCalc toolbox 781
- solution methods
  - crystallization processes 154 ff, 162 ff
  - distributed dynamic models 70
  - multiscale process modeling 193, 203 ff, 215
- solvents
  - design 649 ff, 653 ff
  - utility systems 328
- solver modules 778, 782, 786
- source terms
  - computational fluid dynamics 99
  - multiscale process modeling 197
- space segmentation 431
- sparse systems 28
- spatial discretization 37, 41, 48
- spatial finite volume method 58
- spatial step size 38
- specifications
  - chemical products 647 ff, 651 ff
  - equipment design 383
  - *see also: product specifications*
- spinning disk reactor (SDR) 297 ff
- splitter superstructures 272 ff, 321
- spring model 122
- SQP package 406
- stability
  - distributed dynamic models 50
  - dynamical properties 185
- standard deviation
  - data validation 802, 806
  - molecular modeling 108, 112
  - process monitoring 531 f, 535
- standard for exchange of product model data (STEP) 691
- standards 749–770
  - partial model ingredients 201
- Stanton number 85
- STAR-CD software 214
- state operator network (SON) 276, 289
- state transitions 216
- state-of-the-art control 585
- state-sequence network (SSN) 499
- state-space representation 581
- state-task network (STN)
  - hybrid processes 592
  - product scheduling 493 ff
  - resource planning 464
- statistical error
  - molecular modeling 115
  - *see also: error*
- statistical laws 803
- statistical thermodynamics 108 f, 112 ff
- steady-state distillation 17
- steady-state properties 194
- steady-state systems 521 f, 678
- steam networks 356–372
- steep moving fronts 64, 75
- steepest descent method 20 ff
  - *see also: gradient method*
- steering relation 255
- stencil methods 42
- stiffness problem 15, 41, 60, 73
- stochastic methods
  - crystallization processes 159, 163 f
  - intensification 307, 310 f
  - life cycle modeling 674, 679
  - multiscale process modeling 199
  - supply chain management 699 f
- stochastic programming
  - product scheduling 487, 505
  - resource planning 451
- stochastic uncertainty model 406
- stock imperatives 483
- stock-outs 631 f
- stoichiometric equations 18
- stop criteria 30
- storage
  - product scheduling 485
  - resource planning 448
  - shale oil processing 683
- strategic planning
  - intensification 305
  - life cycle modeling 669
  - multiscale process modeling 216
- stratospheric none depletion 710
- stream flows
  - chemical product-processes 654
  - utility systems 329 ff
- stretching 122
- stripping 287, 311
- structural analysis
  - computational properties 183
  - distillation 276
- structural decomposition 184
- structural plant-model 542

- structures 171 ff
- structures
  - catalyst intensification 300
  - dynamical properties 185
  - process design 383
  - regulatory networks 226 f
- styrene separation 811
- substitution method 20
- sulfuric acid 791
- Sum-Sandler method 128
- superposition principle 199
- supersaturation profile 159
- superscheduling problem 454
- superstructure methods
  - complex columns 287
  - distillation 273–296
  - intensification 305, 312, 321 f
  - steam network 358
- supplier's reliability 830
- supply-chain management (SCM) 8, 621–642
- supply-chain management (SCM)
  - capacities 473
  - integration 695–732
  - life cycle modeling 673
  - product scheduling 481 ff
- support technologies 680
- supporting hyperplanes 386
- surface potentials 131
- surface segmentation 431
- surface tension 734
- surfactants 653
- sustainability 667 f
- synchronization 518
- synetics 427
- syntactical verification methods 183
- synthetic regulatory networks 226 ff, 239 ff
- system for chemical engineering model assembly (SCHEMA) 680, 690
- systems biology markup language (SBML) 245
  
- t**
- tablet formulation 435
- Tabu search 311, 469 ff
- tactical resource planning 462 ff
- target modeling
  - chemical product-process design 657 ff
  - shale oil processing 684
- tasks
  - hybrid processes 592
  - product scheduling 484, 493 ff
- tax regimes 623
- Taylor series 21, 27
  - distributed dynamic models 59, 65
  - molecular modeling 116
- TCP/IP standards 750
- tearing 15
- temperature profiles 171
- temperature profiles
  - carbothermic aluminum process 400
  - complex multiphase reactor 396
  - equipment design 384
  - flexible recipe model 601, 607
  - intensification 308
  - molecular modeling 108
  - process monitoring 519
  - utility systems 332, 340–366
- temperature-swing adsorption (TSA)
  - separation 139
- temporal stepsize 38
- termination criterion 561
- ternary column sequencing 273, 280 f
- testing
  - product development 431
  - resource planning 461
  - supply chain management 710
  - *see also:* applications
- thermal coupling 270, 285, 290 f
- THERMAL databases 736
- thermal radiation 688
- thermal/PV batteries 467
- THERMODATA databases 736
- thermodynamics
  - data validation 810 f
  - distillation 284
  - distributed dynamic models 35
  - equipment design 384 ff
  - heat pumps 337
  - methyl acetate process 545
  - molecular modeling 111 ff
  - multiscale processes 189
  - process monitoring 530
  - utility systems 330 ff, 350
- thermoeconomic models 333
- thermophysical databases 733–748
- thermophysical properties 8
- Thiele modulus 209
- thiol groups 130
- Thompson-King model 275
- three-point backward (TPB) method 44
- time discretization
  - product scheduling 490 ff
  - distributed dynamic models 58
  - resource planning 450, 458
- time horizon
  - data reconciliation 526
  - model-based control 543 ff
  - multiscale process modeling 190 ff
  - product scheduling 484
  - supply-chain management 628
- time integrators 38
- time-based decomposition approaches 470
- time-colored Petri-nets 631

- time-scale models 215
  - chemical product-process design 655
  - life cycle modeling 674
- time-to-market 461
- timing standards 752
- tolerance values 563
- toolboxes *see: educational / modules / software packages*
- top-down approaches 194
- torsion 122
- total annualized cost (TAC)
  - distillation 272 ff, 282 ff
  - water systems 323
- total site integration 363
- toxic release models 673
- trading structure 629, 716
- transcriptional regulation 228, 232 ff
- transcriptional repressors 239 f
- transfer coefficients 114, 173, 198
- transfer prices 623
- transfer times 505
- transformations
  - algebraic 176 f
  - integration framework 208
- transient operations 35
- transition probability 117
- translation models
  - educational modules 795
  - regulatory networks 228
- transport mechanisms 175, 282
- transport properties 116
  - equipment design 387
  - thermophysical databases 734
- transportation 623
- trapezoidal rules 96
- tray cascades 270
- tray-by-tray model, distillation 287
- TRC thermophysical databases 735 ff
- triangle distribution 833
- triplet assumption variable relation keyword 175
- TRIZ method 423, 428 ff, 439
- trouble-shooting 303
- true boiling point (TBP) 818
- trusted solutions 216
- tuning process models 171–188
- turbulence model 401
- two-phase flow models 401 ff
  
- U**
- UDDI standards 758
- uncertainty
  - clinical trial outcomes 462
  - complex multiphase reactor 404 ff
  - cost-effective manufacturing 829–854
  - data validation 806
  
- process monitoring 535
- resource planning 448, 451 ff
- supply chain management 396, 399 ff, 622, 626, 639,
- uncertainty product scheduling 483, 502 ff
- UNIFAC activity coefficients 781 ff
- unified modeling language (UML), standards 710 f, 720, 751, 754 ff
- uniform sampling 118
- UNIQUAC model 125 ff
- unique assignment case 493
- unit operation (UO) specifications, standards 755
- unit-based approach (UBS) 308
- united atoms force fields 123 f
- unit-to-task allocation 460, 488, 493
- unlimited intermediate storage (UIS) 485, 593
- upwind schemes 43 f, 80
- USTI method 429
- utility systems
  - computer-aided integration 327–382
  - life cycle modeling 689
  
- V**
- vacuum distillation unit (VDU) 323
- vacuum-swing adsorption (VSA) separation 139
- validation 181
  - equipment design 391
  - life cycle modeling 676
  - multiscale process modeling 216
  - process monitoring 517 ff
  - UNIQUAC model 125 ff
  - Vali package 527
- van der Waals repulsion 109, 124 f, 130 f
- vapor behavior
  - distillation 270
  - methyl acetate process 545
  - molecular modeling 110
  - UNIQUAC model 130
- vapor recovery reactor (VRR) 400
- vapor–liquid equilibria
  - crystallization processes 158
  - Dortmund database 745
  - molecular modeling 108–108
- vapor–liquid–liquid systems 311
- variables
  - process monitoring 521, 524
  - partial models 201
- variance, molecular modeling 114
- variational multiscale process modeling 205
- vector spaces 384
- Verdict package 499
- verification
  - life cycle modeling 676
  - multiscale process modeling 194, 216

- PDS-ICAS 790
- process models 171–188
- Verlet algorithm 116
- vessel design 673, 686
- vibration phenomena 122
- Villadsen–Michelsen collocation 52
- vinyl chloride monomer (VCM) purification
  - 394
- viscosity 80, 99, 114
- volatilities 270 f
- von Wright actions 253
  
- W**
- W3C standards 751 ff, 763 ff
- waiting times 604, 611
- warehouse agent 689, 705, 717
- waste products
  - scheduling 508
  - intensification 297
  - utility systems 328
- water management 684
- water pinch analysis 320 ff
- water systems 319 f, 328 ff, 374 ff
- water/ethanol system 129
- w-commerce 697
- Web portals standards 764
- Web services 9
- Web services-SOAP standards 750, 758 ff, 763 ff
- Web thermophysical databases 735 ff
- Web-oriented interfaces 697
- weight matrix 18 f, 521, 529 f
- weighted residuals 163
- weighted stencil methods (WENO)
  
- distributed dynamic models 42, 46 ff, 71 ff, 81, 91
- fixed-bed reactors 81
- well-conditioned differential equations 16
- wet-etching 508
- White–Ydstie model 414
- Wilkinson algorithm 455 f
- Wilson activity coefficient 126 ff
- Wilson equations 545 ff
- workflow
  - chemical product-process design 660
  - life cycle modeling 675 ff
- working fluids 372
- World-Wide Web standards 750 ff
  
- X**
- XML (extensible markup language) 680, 750, 757
- XPRESS-MP solver 469
  
- Y**
- Yeomans–Grossmann model 278
- yield stress 196
- yields 809, 822
- Yildirim–Mackey model 230 ff
- Young's modulus 196
  
- Z**
- zeolite membranes 137 f, 146 ff
- zero integration error 207, 216
- zero-wait (ZW) mode 458 ff, 485, 491 f
- zero-wait intermediate storage 593