

## Subject Index

### **a**

absorption 471  
 acceleration of gravity 414, 417  
 accumulation term energy balance 26  
 accumulation term material balance 11  
 ACSL-OPTIMIZE 82  
 activated sludge continuous reactor 577  
 activation energy 38  
 activity coefficient 167, 505f.  
 – relations 508  
 adaptive control 78  
 adiabatic tank 407  
 adsorption 587  
 advanced control strategies 76  
 aerated tank with oxygen electrode 462  
 agitated extraction columns 459  
 ammonium 471, 547  
 Antoine equation 100, 172  
 aquatic ecosystem 581  
 area for heat transfer 100  
 array facility 535  
 array form 498  
 Arrhenius equation 38  
 Arrhenius relation 104  
 auto-refrigerated reactor 295  
 automatic control 68  
 average holdup time 108, *see also*  
     residence time  
 axial concentration profiles 469  
 axial dispersion 468, 480f.  
 – coefficient 481  
 – flow model 479  
 – model 194, 208, 210, 468  
 axial mixing liquid–liquid extraction  
     columns 205

### **b**

backmixing 149, 454f.  
 backmixing flow rates 137  
 balance region 6, 10  
 – for distributed parameter systems 8

– for lumped parameters 8  
 balances for the end sections 454  
 balancing procedures 6  
 batch continuous stirred tanks 93  
 batch distillation 494  
 – column 158, 490, 504  
 batch extraction 130  
 batch extractor 444  
 batch fermentation 126  
 batch fermenter 126  
 batch liquid–liquid extraction 442  
 batch operation 94, 541  
 batch reactor 102, 399  
 – analogy 189  
 – examples 232  
 batch two-phase extraction system  
 442  
 benzene 501  
 binary batch distillation 158  
 – column 490  
 bio-trickling filter 555  
 biofilm 551  
 – diffusion-reaction process 551  
 biofilter 555  
 biofiltration 555  
 biological flocs and films 533  
 biological reaction examples 538  
 biological reactors, tank-type 124f.  
 biomass 126  
 – retention 547  
 bioremediation 591  
 – time 591  
 BOD profile 572  
 boiling period 508  
 bottom plate 491  
 boundary conditions 192, 195, 197,  
     204, 207, 218, 519, 522, 526–527  
 boundary value problems 527  
 bubble point calculations 504

**c**

cadmium 565  
 cake washing 480  
 calorimetry-differential scanning 258  
 capacity 64  
 cascade control 76  
 cascade of equilibrium stages 449  
 cascade of three reactors 276  
 cascades with side streams 137  
 catalyst effectiveness 527, 531  
 cell concentration 124  
 chemical engineering modelling 1  
 chemical equilibrium 39  
 chemical kinetics 35  
 chemical reaction time constant 65  
 chemical reactor safety 177  
 chemical reactor waste minimisation 120ff.  
 chemostats 126  
 chromatographic processes 207  
 cocurrent flow 516f.  
 Cohen-Coon controller settings controller tuning 75  
 Cohen-Coon settings 422  
 coils or jackets 96f.  
 column hydrodynamics 152  
 column plate 158ff.  
 common time constants 64  
 complex batch reaction sequence 232, 355, 538  
 complex column simulations 167  
 complex reaction 237  
 complex sequential-parallel reaction 276  
 component balance equation 95  
 component balances 5, 18  
 concentration driving forces 48, 131  
 concentration profiles 44  
 – for countercurrent 45  
 concentration response 54  
 condenser 491, 505  
 conditional control 599  
 CONFLO, *see also* continuous flow tank 406  
 constant molal overflow 160  
 contaminant removal in soil 591  
 continuous binary distillation 162  
 – column 496  
 continuous column 123  
 continuous distillation column 163, 497, 501  
 continuous equilibrium multistage extraction 449

continuous equilibrium stage extraction 133  
 continuous-flow 123  
 – equilibrium stage 448  
 – reactor 96  
 – stirred tank 52, 420  
 – tank 406  
 continuous heating tank 27  
 continuous multicomponent distillation column 501  
 continuous operation 94  
 continuous phase 460  
 continuous stirred-tank reactor 7, 32, 106, 400  
 – cascade 93  
 continuous tank reactor 34, 265  
 continuous tubular 123  
 control of extraction cascades 141  
 control of temperature 99, 420  
 control of time 76  
 controller 424  
 – action 69  
 – adjustment 434  
 – equation 117, 428  
 – tuning 73  
 – tuning problem 427  
 convective flow terms 11  
 conversion 39  
 cooling jacket 97, 283, 431  
 countercurrent 214  
 – contactor 44f.  
 – cooling 287  
 – extraction cascade with backmixing 137  
 countercurrent flow 515  
 – heat exchanger 214  
 countercurrent multistage equilibrium extraction 450  
 countercurrent multistage extraction 449  
 countercurrent packed column 471  
 countercurrent stagewise extraction cascade 453  
 curve fit 83, 263  
 cyclic fed batch 129  
 cylindrical coordinates 178

**d**

deactivating catalyst 268  
 dead zones 123  
 defining equations 16  
 degree of segregation 394  
 density 127  
 – influences 409  
 desorption of solute 480 f.

- distillation process examples 490  
difference differential equation 480  
difference equation 173  
difference formulae for partial differential equations 219  
differential column 130  
differential contacting 45, 173  
differential control constant 421  
differential extraction column with axial dispersion 468  
differential flow 173  
differential mass transfer 43, 199  
differential scanning calorimetry 119  
diffusion 13, 521  
diffusion and heat conduction 175  
diffusion and reaction 179, 529, 533  
– in a spherical bead 533  
– split boundary solution 525  
diffusion coefficient 528  
diffusion film 462  
diffusion fluxes 177, 534, 551  
diffusion from the interior of the solid 521  
diffusion model 551  
diffusion process examples 521  
diffusion rate 593  
diffusion time 524  
diffusion-dispersion time constant 65  
dilution rate 128  
dimensionless concentration 481  
dimensionless equations 31, 270  
dimensionless form 480, 536  
dimensionsless groups 63  
dimensionless kinetics 235  
dimensionless model 315  
– equations 31, 527  
dimensionless solute concentration 481  
dimensionless terms 407  
dimensionless variables 464, 527 f.  
discharge nozzle 412  
discharge of molten steel 412  
discrete control systems 78  
dispersed phase 460  
– holdup 153  
dispersion model 193, 196, 198  
dispersion number 197  
dissolved oxygen 569  
– concentration 462  
– profile 572  
distillation period 509  
distributed parameter 8  
distribution 391  
– of residence times 123  
diurnal variation 560  
double Monod kinetics 592  
driving force 97  
drying 521  
– of a solid 521  
dynamic component balances 127  
dynamic difference equation model for chromatography 209  
dynamic diffusion and enzymatic reaction 529  
dynamic method 462  
dynamic models 2, 4  
dynamic simulation 1, 2  
dynamic tubular reactor 190, 332  
dynamics of a shell-and-tube heat exchanger 511  
dynamics of the cooling jacket 97  
dynamics of the metal jacket wall 100
- e**
- e-curve 274  
Eddy dispersion coefficient 469  
effective area for heat transfer 97  
effectiveness factor 528, 536  
effectiveness of the catalyst 525  
eigenvalues 114  
electrode membrane 463  
electrode response characteristic 462  
endothermic reaction 103  
energy balance 169, 420, 472  
– equation 95, 183, 413  
energy balancing 22  
enriching section 163  
enthalpy 23  
entrainment fractions 147  
environmental examples 560  
environmental impact 581  
enzyme 525  
equalisation basin 560  
equation stiffness 90  
equilibrium 129, 445, 494  
– line 48  
– oxygen concentration 463  
– relationship 48, 131, 472, 480  
equilibrium stage 44  
– behaviour 136  
– extraction 134  
– extractor 447  
estimation of rate and equilibrium constants 83  
examples of chemical engineering processes 225  
exothermic reactor 356

exothermic reaction 110, 283, 437  
 – sequence 253  
 exothermic semi-batch reactor 430  
 exponential and limiting growth  
   phases 42, 126  
 exponential response 52  
 extraction cascade 136  
 – with backmixing and control 456  
 – with slow chemical reaction 139  
 extraction column 150  
 extraction from a solid 20  
 extraction vessel 130  
 extractor 468

**f**

Fanning friction factor 417  
 feed composition 503  
 feed control 430  
 feed phase 130  
 feed plate 164  
 feed-batch fermenter 128  
 feed-forward control 77  
 feedback control 68, 430  
 – system 420  
 fermentation 124  
 Fick's law 47, 175, 177, 552  
 field capacity 589  
 filling and emptying tanks 426  
 film heat transfer coefficient 100, 513  
 filter bed 481  
 filter washing 479  
 finite difference 531  
 – approximations 91  
 – elements 468, 522  
 – segments 178  
 finite differencing 176, 336, 511, 529f.,  
   534  
 – of heat exchanger 216  
 – of tubular reactor 174, 191  
 finite elements 204  
 first-order decay 42  
 first-order lag 52, 428  
 – equation 463  
 first-order response 51  
 first-order time lag 420  
 flow phenomena time constant 64  
 flow term energy balance 26  
 flow terms material balance 12  
 fluidised bed 547  
 Fourier's law 175, 518  
 fractional conversion 39, 182  
 fractional holdup 459f.  
 fractional phase holdup 470

fractional yield 40  
 free-radical polymerisation 310  
 frequency of the oscillations 422  
 friction factor 414  
 frictional force 417

**g**

gain coefficient 136  
 gas absorption 154  
 – heat effects 199  
 – steady-state design 200  
 – steady-state simulation 201  
 gas separation by membrane permeation  
   475  
 gas–liquid contacting systems 153  
 gas–liquid interface 46  
 gas–liquid mass transfer 34, 385  
 gas–liquid mixing in a stirred tank 385  
 gas–liquid transfer 462  
 gas-permeation 475  
 – module 475  
 gas-phase reaction with molar change  
   344  
 gas-phase tubular reactors 186  
 general aspects of modelling 3  
 general heat balance 25  
 groundwater pollution 584  
 growth rate 42, 126

**h**

heat balance 428, 516  
 heat capacity 24  
 heat conduction 518f.  
 heat emissivity 519  
 heat exchange 214  
 heat exchanger 96, 511  
 – boundary conditions 218  
 – differential model 216  
 – dynamics 215  
 – steady-state 214  
 heat gain curve 112  
 heat loss 112  
 – by radiation 518  
 heat of reaction 25, 39  
 heat transfer 96, 511  
 – applications 213  
 – area 430  
 – coefficient 509, 514, 516  
 – from metal wall 511  
 – rate 100, 513  
 – steady-state tubular flow 213  
 – energy balance 26  
 – time constant 67

- heating period 508f.  
 heating in a filling tank 28  
 heavy metals accumulation 565  
 heavy phase 143  
 Heerden steady-state stability criterion 297  
 Henry coefficient 465  
 Henry's law 463  
 heterogeneous catalytic reactions 37  
 higher order responses 58  
 holdup 492  
 – distribution 460  
 hot spot effect 327  
 human irrigation 587  
 hydrostatic equation 144  
 hydrostatic pressure force 417
- i**  
 ideal gas law 463  
 immiscible liquid phases 130  
 implicit algebraic loop 155  
 information flow diagram 22, 131, 169, 171, 185, 18f., 228  
 inhibitory substrate 543  
 initial conditions 126  
 inoculum 126  
 input rate 125  
 insecticide distribution 581  
 integral control 428, 458  
 – constant 421  
 integrated extraction 280  
 integration method 90, 600  
 integration parameters 90  
 integration routine 89  
 integration step length 91  
 intensity of segregation 396  
 interacting solute equilibria 133  
 interacting tank reservoirs 416  
 interfacial area 131  
 interfacial concentrations 48  
 internal energy 22f.  
 interphase mass transfer 46  
 interphase transport 14  
 interstage flow rates 137  
 introductory MADONNA example 227  
 irrigation 585  
 ISIM 82  
 isothermal reactor with axial dispersion 335  
 isothermal reactor with complex reaction 265  
 isothermal tank 407  
 isothermal temperature conditions 406
- isothermal tubular reactor 320  
 iterative calculations 504  
 iterative loop for the bubble point calculation 172  
 iterative procedure for parameter estimation 86
- j**  
 jacket cooling 83, 297, 437  
 jacket heating 99  
 jacketed batch reactor 253
- k**  
 KLa 462
- l**  
 lag in the system 424  
 lag phase 126  
 lake ecology 565  
 Langmuir isotherm 587  
 Laplace transformation 464  
 latent heat of vapourisation 428  
 leaching 591  
 lead 565  
 least squares 81  
 level control 424  
 limit cycles 115  
 limiting substrate 126  
 linearisation 113  
 liquid film 463  
 liquid impurities 479  
 liquid stream blending 409  
 liquid-liquid extraction 129, 280  
 – column dynamics 202  
 liquid-phase tubular reactors 185f.  
 liquid-vapour equilibrium 505  
 lumped parameter 7, 8, 100
- m**  
 MADONNA 82, 90, 597  
 manipulation of the cooling-water flow rate 430, 432  
 mass transfer coefficient 47, 131  
 mass transfer process examples 442  
 mass transfer theory 43  
 mass transfer time constant 65  
 mass transfer to a continuous tank reactor 34  
 material balance 4, 10, 95  
 – equations 124  
 material balancing procedures 6  
 mathematical modelling 2  
 MATLAB 82

- maximum likelihood 81  
mean square fluctuations 396  
measured oxygen concentration response curve 462  
measurement and process response 51  
measurement dynamics 56, 463  
measurement lag 57  
measurement time constant 56  
membrane permeabilities 475  
metal balance 565  
metal jacket wall 100  
metal rod 518  
methanol 507  
Michaelis–Menten 528, 530  
– equation 526  
microbial growth kinetics 41  
migration 584  
mixer 142  
– dynamics 143  
mixer-settler 129  
– cascade 147  
– extraction cascades 142  
– stage 148  
mixing history 123  
mixing in chemical reactors 394  
mixing model 374, 378, 381, 390  
mixture of hydrocarbons 494  
modelling a non-isothermal, chemical reactor 22  
modelling approach 3  
modelling fundamentals 1  
modelling of chromatographic processes 207f.  
modelling of cooling effects 99  
modelling procedure 3  
modes of reactor 93  
molar feeding rate 105  
molar quantities 106  
mole ratios 202  
molecular diffusion coefficient 47  
momentum balance 31, 416  
momentum transport 175  
Monod equation 43  
Monod-type equation 43, 535  
Monod-type rate expressions 127  
multicomponent differential distillation 494  
multicomponent extraction 444  
multicomponent mixture 158  
multicomponent separations 165  
multicomponent steam distillation 168  
– semi-batch 508  
multicomponent system 140, 508  
multiple feeds 137  
multiple steady states 91  
multiple tanks in series 58  
multisolute batch extraction 132  
multisolute equilibria 133  
multistage countercurrent extraction cascade 136  
multistage extractor with backmixing 453  
multistage multicomponent extraction cascade 130  
mutual inhibition 555
- n**
- N profile 572  
n-decane 508  
n-octane 508  
naturally occurring oscillations 91  
negative feedback 116  
Nelder–Mead search algorithm 79  
Newton's gradient method 79  
nitrate 547  
nitrification 547, 574  
nitrite 547  
nitrogen 475f.  
non-equilibrium differential contacting 130  
non-equilibrium staged extraction column 150  
non-ideal distillation 504  
non-ideal flow 123  
non-ideal liquid behaviour 504  
non-ideal stirred-tank reactor 374  
non-linear parameter estimation 79  
non-linear systems, parameter estimation 82  
nozzle mass flow 413  
Nth-order reaction 270  
numerical aspects of dynamic behaviour 79  
numerical integration 88
- o**
- objective function 352, 368  
on/off control 70  
optimal cooling 79  
optimal feeding policy 350  
optimisation 79, 600  
order of reaction 37  
organism balance 125  
oscillating tank reactor 290  
oscillations 421, 429  
outlet 128

- output rate 125  
 overall heat transfer coefficient 97  
 overall mass transfer coefficient 131, 446  
 overhead distillation 156  
 oxidation reaction in an aerated tank 250  
 oxygen 475 f., 533  
 – deficit 573  
 – diffusion 594  
 – enrichment 475  
 – limitation 533  
 – sag curve 569  
 – transfer coefficient 462  
 – uptake rate 535  
 oxygen electrode 462  
 – dynamic 463
- p**  
 parallel reaction in a semi-continuous reactor 29  
 parameter estimation 81–82, 600  
 parametric plot 600  
 partial differential equation 480  
 partial molar enthalpy 24  
 Peclet number 193, 480  
 penetration distance 533  
 perfect mixing 102, 123  
 – stirred tank 93  
 permeabilities, membrane 477  
 permeability coefficient 478  
 permeation rate 475, 478  
 perturbation variables 113  
 phase equilibria 45, 171  
 phase flow rate 144  
 phase volume 133, 144  
 phase-plane diagram 92, 546  
 PID control 246, *see also*  
     proportional-integral-derivative  
 plant start up/shut down 107  
 plants ecology 585  
 plate efficiency 166  
 plate hydraulics 162  
 plug-flow 123, 455  
 – reactor 189  
 – tubular reactor 181  
 pollutant transport 584  
 pond ecology 581  
 porosity 481  
 – distributions 480  
 porous biocatalyst 529  
 porous solid supports 525  
 principles of mathematical modelling 2  
 probability density 82  
 – function 81
- process control examples 420  
 process development in the fine chemical industry 119  
 process dynamics and response 51  
 product inhibition 526, 530  
 production rate 15, 125  
 – material balance 15  
 profit function 79  
 programming tips 598  
 proportional control 428, 458  
 – constant 421  
 – equation 425  
 proportional controller 116  
 proportional gain 116, 428  
 proportional plus integral control 456  
 proportional temperature controller 72  
 proportional-integral feedback controller 421  
 proportional-integral-derivative (PID) control 70, 246  
 pulse function 337  
 pulse input 339, 599  
 pure time delay 61
- q**  
 quasi-steady state 129, 155
- r**  
 radiation from metal rod 518  
 raffinate 141  
 rain 587  
 rate 64  
 – expressions 126  
 – of accumulation 11, 125  
 Rayleigh equation prediction 495  
 reaction calorimetry 118  
 reaction enthalpy 25  
 reaction, exothermic 247  
 reaction, fractional conversion 39  
 reaction heat term energy balance 27  
 reaction kinetics 103  
 reaction rate 35, 37, 398  
 – constant 38  
 reaction selectivity 40  
 reaction yield 40  
 reactor 124  
 – cascade 109, 287  
 – configurations 93  
 – control 107, 115  
 – energy balance 254, 301  
 – stability 110  
 – temperature 255  
 reboiler 490, 492, 498, 504

- recovery of valuable filtrates 479  
 rectangular slab 525  
 recycle-loop reactor 268  
 reflux 505  
 – drum 490ff., 499  
 – ratio 158, 491f., 499, 502f., 505f.  
 relative volatility 157, 165, 491–492,  
     495, 498, 502  
 relaxation time 63  
 release of chemicals 581  
 residence time 128, 469  
 – distribution 381  
 response controller 71  
 response measuring element 55  
 response of a stirred tank reactor 55  
 response of the measuring instrument  
     57  
 reversible reaction 299, 305  
 Reynolds number 414  
 river ecology 572  
 root growth 586  
 RTD experiments 123  
 runaway scenario 118
- s**
- sampled data 78  
 second-order kinetics 431  
 second-order measuring element 60  
 second-order response lag 463  
 sediments 565  
 segregation 394, 398  
 – batch reactor 397  
 – continuous reactor 397  
 – semi-continuous reactor 398  
 selectivity 39, 276  
 semi-batch 353  
 – continuous stirred tanks 93  
 – operation 94  
 – reactor 104, 106, 355, 401  
 – system 508  
 semi-continuous reactor 347, 350, 430  
 – adiabatic 29  
 semi-dimensionless form 531  
 sensitivity analysis 85  
 sequential reactions 276  
 setpoint 68ff.  
 settler 142, 577  
 – dynamics 144  
 shell-and-tube heat exchanger 216, 511  
 short-cut flow 123  
 signal and process dynamics 53, 55, 57,  
     59, 61, 92  
 simple overhead distillation 156
- simplified energy balance 27  
 simulation 129  
 – software 226f.  
 – tools 226  
 single batch extraction 130  
 single solute batch extraction 442  
 slip velocity 153  
 sludge recycle 577  
 software links 226  
 soil ecology 584, 591  
 solid drying 522  
 solute 130  
 – transfer rate 131  
 solvent or organic phase 130  
 specific growth phase 42  
 specific growth rate 128  
 specific interfacial area 47  
 spherical balancing aggregate 592  
 spherical bead 534  
 spherical coordinates 178  
 spherical shell 534  
 split-boundary problems 88  
 split-boundary type 174, 527  
 spouted bed reactor 390  
 staged extraction columns 149  
 stagewise absorption 153  
 stagewise contactor 44  
 stagewise discontinuous extraction 451  
 stagewise distillation 156  
 stagewise mass transfer 43, 129  
 stagewise model with backmixing 137  
 stagewise processes 93  
 startup 500  
 steady-state 127, 418  
 – absorption column design 471  
 – balance 4, 503  
 – conditions 126  
 – criterion 115  
 – diffusion 179  
 – energy balance 326, 518  
 – gas absorption 199  
 – operation 95  
 – simulation 174  
 – split boundary problem 530  
 – tubular flow 213  
 – tubular reactor dispersion model  
     196, 315  
 – two-pass heat exchanger 515  
 steam distillation 508  
 steam tables 100  
 steam-heated stirred tank 427  
 steam-heating in jackets 99  
 step-change disturbance 51f.

steps in model building 4

sterile feed 126

still pot 490f., 494

stirred-tank reactors 93, 95, 97, 99, 101, 103, 105, 107, 109, 111, 113, 115, 117,

119, 121, 123, 125, 127

stoichiometric coefficient 25, 36

stoichiometry 103

Streeter and Phelps curves 569

stripping section 163

substrate balance 125

substrate concentration 124

substrate uptake kinetics 43

superficial phase velocity 151, 470

superficial velocities 460

system stability 91

#### **t**

tank 124

– drainage 17

– flow examples 406

– mixing 409

– reactor 317

tanks-in-series 58, 123, 276, 424

– approximation of a tubular reactor 333

Taylor's expansion theorem 113

temperature conditions 406

temperature control 69

– for semi-batch reactor 430

temperature difference 97

temperature distribution 101

temperature measurement 420, 427, 430

– device 420

temperature profile 508, 518

theoretical plate behaviour 491, 498, 505

theoretical plates 490, 504

thermal capacity 100

thermal stability of a CSTR 283, 437

thermally safe process 365

Thiele modulus 528

thin slab 521

time constant 35, 63, 65, 67

– application 67

– for heater 421

– for transfer 466

– measurement 421, 466

time delay 61f., 145

– function 62

time delayed values 144

time integral criteria 76

toluene 501

total energy 23

total mass balance 125

total material balance 5, 16, 95

total reflux 507

tracer experiments 274

tracer information in reactor design 123

tracer response 333, 384

transfer function 62

– in series 435

– simulation 435

transfer rate relationships 131

transient holdup profiles in an agitated extractor 459

transport of heavy metals 565

transport streams 10

trial and error method controller tuning

74

tube 511

tubular reactor 7, 185 ff., 317, 324, 329, 333

– batch reactor analogy 189

– boundary conditions 195

– chemical 180

– component balance dispersion model 181, 193

– energy balancing 184

tubular reactor model for the steady-state 315

tubular reactor with axial dispersion 193, 340

tuning the controller 458

turbulent fluctuations 395

two tank level control 424

two-film theory 46, 131

two-pass heat exchanger 515

two-solute batch extraction 445

– with interacting equilibria 444

#### **u**

ultimate gain method 422

– controller tuning 75

unmixed reactants to a tubular reactor 395

unsteady-state diffusion 175

unsteady-state heat conduction 178

#### **v**

vadose soil 584

van Laar equation 505f.

van't Hoff equation 39, 300, 306

vapour pressure 100

variable heat capacities 299

variable volume reactor 431

volumetric feed rate 105

volumetric flow rate 124

**w**

- washing of filter cake 479
- washout 128
- waste air treatment 555
- waste holding tank 19
- wastewater 551
  - discharge 573
- water 507
  - field capacity 585
  - heater 420
  - jacket 430
  - table 584
- water-methanol system 504
- well-mixed 124
  - region 147
- Whitman two-film theory 46
- work term 23

**x**

- xylene 501

**y**

- yield 39, 117
  - coefficient 125

**z**

- zero-order kinetics 536
- zero-order reaction 531
- Ziegler-Nichols method controller
  - tuning 74
- Ziegler-Nichols-criteria 429
- zinc 565