Index

а

acid catalysts ethylbenzene production 193–194 FCC 191–192 Lewis acid 191 acrylic acid production 196 activated carbons (AC) 180, 181, 183 active metals 185–186 alumina 179–182, 184, 185, 190, 191, 195, 200, 203, 204, 215, 241, 278 ammonia absorption 269–272 aqueous glass 184

b

bacterial growth 308-310 batch tank stirred reactor example of 130-136 temperature control heat transmission 130 biocatalysts immobilization 310-313 biological reactions 289 biomass-substrate yield 305 bioreactors batch reactors 315 CSTB 315-319 CSTR 315 fed-batch 315 fed-batch culture 321-323 tubular bioreactor 316 tubular fermenters with flocs 319-320 biotechnology 289, 315

С

calcination oven 185 catalysts characteristics of 207 definition 207 external diffusion 219 fluid-fluid reactions 245-261 internal diffusion 221-236 monolithic catalytic reactors 237 - 245rate equation heterogeneous systems 208 mechanism of 215-216 porosity and void volumes 214 second-order decomposition reaction 209 theory of adsorption 217-219 resistance combination 236-237 catalyst support 178, 180, 198 cell growth 304-310 cell recirculation 319-320 chemical engineering boundary conditions 94 Chemical Reaction Engineering 87, 262 chlorine removal 282-283 cobalt 186 CO₂ elimination 245, 267–268 continuous stirred tank bioreactor (CSTB) 316-317 continuous stirred tank reactor (CSTR) 63, 111, 112, 315 bioreactor 323-325 complex system 28-30

Chemical Reactor Design: Mathematical Modeling and Applications, First Edition. Juan A. Conesa. © 2020 Wiley-VCH Verlag GmbH & Co. KGaA. Published 2020 by Wiley-VCH Verlag GmbH & Co. KGaA.

continuous stirred tank reactor (CSTR) (contd.) dead volume and short circuit 23 - 25exchange of matter 22-23 exothermal reaction 118-125 experimental solid flow reactor 53 - 54non-ideal 32 PFR in series 13–14 RTD 4, 12-13 RTD Laplace transform 62 second-order reaction in a series 30 - 32tanks-in-series model 16 unsteady state 111-113 conventional scaling process 128 convolution calculation of 38-41 definition 35 RTD reactor 38 of signals experimental solid flow reactor 53 - 55properties 37-38 pulse input tracer 51-52 three reactors connected in series 50, 51 two functions 36 cordierite structure 184 Cumene 189, 191, 220 cyclic operation 158, 159

d

Danckwerts boundary conditions 20, 27, 102 deconvolution calculation of 42–43 of signals 50 deep stirred reactor 77 De-NOx via SCR 238–241 diesel cracking 230–231 diesel oxidation catalyst (DOC) 157, 201, 204 diesel particulate filter (DPF) 204–205 dispersion model 15–18, 27, 81–84

е

entrained-flow reactors 175, 176 environmental catalysis cleaning systems 202 DOC 204 DPF system 204-205 exhaust gases 200 SCR 203-204 three-way catalyst 202-203 enzymatic catalysis characteristics of 291 inhibitors 295-296 metabolism of ethanol 294-295 Michaelis constant 293 Michaelis-Menten equation 293 substrates 296-304 enzyme-substrate complex 291, 292, 296 ethylbenzene production 193–194 ethylene oxide 194–195, 241, 242, 244 exothermal first-order reaction 118 explicit method 93-94 external diffusion 215, 219-221, 232, 233, 237, 239, 241, 242, 259, 260, 280 extruder 185

f

fed-batch bioreactor 320-325 fermentation 168, 289, 290 first order approximation 88, 90, 95, 105, 122, 260 fixed-bed reactor 164, 165, 175, 176, 231 - 232fluid catalytic cracking (FCC) 176, 191-192 fluid-fluid reactions gas/liquid reactions 256-261 in industry 245 transfer models 245-247 two-film theory Hatta modulus 250-251 instantaneous reaction 247-250 rate reaction 251-256 fluidized-bed reactor 176 forced unsteady state operation (FUSO) objective 158-159

oscillating pressure 169–170 periodic flow-reversal 166 periodic operation/cyclic operation 158 periodic variation of concentration 163-164 design strategy 162-163 flow rate 164 flow variation of reagents 159, 160 input signals and process rate 160, 161 modes of operation 160 - 162temperatures 165 variables 160 types of 159 VVO reactor 168

g

γ-alumina 181 gas-liquid reaction 247, 256–261, 275 gas-solid reactors 175

h

Hatta modulus 250–251, 255 Henry's law 246, 248, 252, 284 hydrothermal process 184

i

industrial catalysis acid catalysts 190-194 commercial catalysts active metals 185-186 catalytic support manufacturing 185 zeolites synthesis 184-185 environmental pollutants 200 oxidation products 194 oxidation/reduction reactions 188 reactions catalyzed, solids 175 - 177solid catalysts 178-183 internal diffusion 313 first-order kinetics flat particles 222-225 porous pellet 225 Thiele and Weisz modulus 229-236 irreversible inhibition 295

j

jacketed piston flow reactor 146–147

k

kinetic law 301-304

I

lanthanum oxide (LaO₂) 202 Laplace transform (L.T.) basic functions 61 example of 82–83 properties of 58, 59 pulse function 60–61 ramp function 59–60 RTD in CSTR 62–65 PFR 65–66 sinusoidal function 60 technique 66 Lewis acid 185, 190, 191 liquid-liquid reaction 266

т

mass transfer effect 310-314 matrix convolution 39, 45, 54 membrane reactor 254-256 metal active particles 184 methanation 197-200 Michaelis complex 291 Michaelis constant 293 Michaelis-Menten equation 292 - 293, 313 microbial growth 318-319 microbial kinetics cell growth 305-310 product formation 305-310 stoichiometry of growth 304–305 modified Bessel function 227 modulation lean-rich "poor-rich" 204 mole balance, PFR 113 molybdenum 186, 196, 216 Monod equation 306-308, 317 Monod kinetics 307, 309, 310, 318-320 monolithic catalytic reactors De-NOx via SCR 238-241

monolithic catalytic reactors (contd.) fluidized bed reactor 241, 242, 244 pore diffusional resistance 237-238 structure 238 multiphase reactors design models, flow ammonia absorption 269–272 cases and situations 269-284 catalytic system 278 chlorine removal 282-283 fluid-fluid reaction over catalyst 276 - 277fluid-fluid reaction, tower 283 - 284isomerization in fluidized bed reactor 279-280 nomenclature 263 pure absorption 263–265 reactor of known volume 275 - 276second order isomerization 278 - 279sucrose acid treatment 281 sulfur oxides removal 273-275 systems with reaction 265–268 trickle-bed type reactor 272–273 flow types 261-262

n

Nerst's law 248 nickel 185, 186, 196, 199 non-ideal CSTR 32, 74–76 non-ideal flow CSTR and PFR complex system 28–30 second-order reaction 30–32 tubular reactor 25–28 types of 26 RTD 3–11

0

oscillating pressure 157, 159, 169–170 oxidation catalysis acrylic acid production 196 ethylene oxide 194–195 reduction catalysis 197

р

parametrically sensitive areas 139 partial differential equations (PDE) classification of 87-88 finite differences explicit method 93-94 first order approximation 88 gas phase 91 initial and boundary condition 94-96 second-order approximation 89-91 stability 96-98 numerical methods catalytic flat wall reaction 107 flow and dispersion 104-106 RTD of complex system 98-104 particulate matter (PM) 201, 204 Peclet-Bodenstein module 19 periodic operation 158–160, 162, 163, 167, 170 platinum (Pt) 191, 197, 202-204 plug flow reactor (PFR) CSTR in series 13–14 dynamic regime no dispersion 113–15 real reactors 25-32 with dispersion 115–118 RTD 4, 11-12, 14 system of two reactors 80-81 tubular reactor 136-155 pre-drying oven 185 protonic acids 190 pulse function 60-61 pulse input tracer 51-52 pulse modes 160, 161 pure types of inhibition 295

q

quasi-steady mode 161

r

ramp function 59–60 reactor of known volume 275–276 recipient dispersion module 19 reduction catalysis methanation 199–200

steam reforming of alcohols 197 syngas production 197 residence time distribution (RTD) characteristics of cumulative distribution curve, F(t) 8 mean residence time 9–10 second and third moments 10–11 convolution 38-41 CSTR with dead volume and short circuit 23–25 dispersion model 18 experimental measurement of in heterogeneous systems 7-8 pulse input 4 step input 6–7 ideal reactors batch and PFR reactors 11–12 CSTR 12-13 PFR/CSTR in series 13–14 Laplace transform CSTR 62-65 PFR 65-66 tanks-in-series model 15–18 two CSTR with exchange of matter 22 - 23reversible inhibition 295 rhodium (Rh) 197, 202, 204

S

safe approach 141 scaling of chemical reactor batch tank stirred reactor example of 130 temperature control heat transmission 130 definition of 127 maximum factor, equipments 127 production rate and the time intervals 127 rules 129 second-order approximation 88–91, 95 selective catalytic reduction (SCR) 176, 201, 203–204, 238–241 semi-batch reactor 130-136, 320 Sherwood module 220

sifting machine 185 silica 179-181, 190, 191, 195, 215, 230 sinusoidal function 60 slurry reactors 176 solid catalysts activated carbons 183 catalyst support 180 characteristics of 180 requirements 178 silica and alumina 181 spherical pellet 179, 180 zeolites 181–183 space velocity 186, 187 spherical catalyst 231, 233 square pulse of tracer 77–78 steam reforming alcohols 197-198 of hydrocarbons 199 sucrose acid treatment 281 sulfur oxides removal 273-275

t

tanks-in-series model 15-18, 30, 31, 69 tank-type reactor 13 theory of adsorption 217-219 thermal control 130 Thiele modulus 228–236 time-dependent functions 57 transfer function CSTRs and PFRs parallel systems 69–71 recycle system 71–81 series systems 67-69 definition 57 dispersion model 81-84 Laplace transform 58–61 non-ideal chemical reactors 57 pulse input signal 58 transfer models 245-247 trickle-bed reactor 177, 272-273 tubular bioreactor (TB) 316, 320 tubular reactor 25 isothermal operation 138 optimum length, conversion and performance for 138, 139 PFR 136

332 Index

tubular reactor (contd.) piston flow 137 stability process areas of runaway 139 batch tank stirred reactor 145 energy balance 141 initial concentration changes 152-155 jacketed piston flow reactor 146-147 Matlab 148-152 parametrically sensitive areas 139 temperature profiles 141, 142 van Welsenare and Froment method 145 two-film theory Hatta modulus 250–251

instantaneous reaction 247–250 rate reaction 251–252

и

unsteady state, CSTR 111–113

V

variable volume (VVO) 157, 159, 168–169

W

washcoat 184, 237 Weisz modulus 229–236 wet mixer 185 Würtz synthesis 194

Ζ

zeolites 179–184, 190, 191, 216