ADAPTATIONS OF MULTI-OBJECTIVE EVOLUTIONARY ALGORITHMS AND THEIR APPLICATIONS TO CHEMICAL PROCESSES

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by

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Dedicated

To

Mamma

Certificate

This is to certify that the thesis entitled “**ADAPTATIONS OF MULTI-OBJECTIVE EVOLUTIONARY ALGORITHMS AND THEIR APPLICATIONS TO CHEMICAL PROCESSES**” being submitted by **Mr. Vibhu Trivedi** to the **Indian Institute of Technology Delhi** for the award of the degree of **Doctor of Philosophy** is a bonafide record of research work carried out by him under my supervision and guidance. The thesis work, in my opinion, has reached the requisite standard fulfilling the requirements for the degree of Doctor of Philosophy.

The results contained in this thesis have not been submitted, in part or full, to any other University or Institute for the award of any degree or diploma.

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Abstract

Chemical engineering systems involve a concatenating of various units such as reactors, crackers, distillation columns, froth floatation cells, absorbers, crystallizers, etc. To maximize the profit, these units should be operated, planned and scheduled optimally. This often leads to the formulation of multi–objective optimization (MOO) problems. Such MOO problems involve solving complicated model equations which require inordinately large computational time for each function calculation (i.e. solving the model once). For these cases, the algorithms which converge to the acceptable Pareto optimal solutions in a small number of function calculations (= population size × maximum number of generations) or in a small number of generations (for fixed population size) are always recommended.

In the present study, five evolutionary algorithms with the aim of producing better results in limited number of generations are developed by introducing improved operators in the framework of existing algorithms or hybridizing different algorithms and their performance is tested rigorously using more than thirty standard test problems with two and three objectives from ZDT, MOP, DTLZ and WFG test suits. These algorithms are then used to solve various complex MOO problems of chemical engineering systems. In the first algorithm, a new operator, simulated binary jumping gene (SBJG), is introduced to enhance the convergence speed of real-coded elitist non – dominated sorting genetic algorithm (RNSGA-II). The developed algorithm is then used to solve the MOO problems of a dynamic steam reformer (a problem with two-objectives) and a phthalic anhydride reactor (a two-objective and a three objective problem). The second algorithm, simplified multi-objective particle swarm optimization (SMPSO), provides a fine balance between exploration and exploitation using two simple operators that are developed on the basis of a detailed qualitative analysis of similar operators used in PSO and NSGA-II. SMPSO is then used to solve a newly formulated MOO problem of resid fluid catalytic cracking unit (a problem with two objectives). The third algorithm is a multi-objective variant of bat algorithm (BA) which is used to solve the two-objective problem of the phthalic anhydride reactor. The fourth algorithm, NSDE1-FH, is a hybridization of a multi-objective variant of differential evolution (DE) with a recently developed concept of following heroes. It is applied to a novel MOO problem of a dual lithium ion insertion cell (a problem with two-objectives). In the fifth algorithm, an improved DE strategy is used to enhance the convergence speed of multi-objective DE which is then used for optimized on-line control (OOC) of Poly Methyl Methacrylate (PMMA) reactor where MOO problem must be solved in a time period of few minutes. The industrial problems solved in this study belong to different categories, e.g. first three problems represent process optimization, the MOO problem of dual lithium ion insertion cell represents design optimization and the last problem represents control optimization. The results obtained for these problems show that the proposed algorithms perform well in limited number of generations without compromising with the computational time. Also, for each industrial problem, the optimal operating points obtained using developed algorithms are better than the reported industrial values and these can be applied to real systems for an optimal operation.

सारांश

रासायनिक अभियांत्रिकीय निकायों में विभिन्न इकाइयां जैसे कि रिएक्टर, क्रैकर्स, डिस्टीलेशन कॉलम, फ्रॉथ फ्लोटेशन सेल, अब्सॉर्बर, क्रिस्टलाइज़र आदि श्रृंखलाबद्ध रूप में उपस्थित रहतीं हैं। अधिकतम लाभ प्राप्त करने के लिए, इन इकाइयों का संचालन, नियोजन और समय प्रबंधन बेहतर ढंग से करने की आवश्यकता होती है। इससे प्रायः मल्टी-ऑब्जेक्टिव ऑप्टिमाइजेशन प्रॉब्लम्स का निर्माण होता है। ऐसी मल्टी-ऑब्जेक्टिव ऑप्टिमाइजेशन प्रॉब्लम्स में जटिल मॉडल एक्वेशन्स को कई बार हल करना होता है जिन्हें प्रत्येक फंक्शन कैलकुलेशन के लिए मात्र एक बार हल करने में ही अत्यधिक कम्प्यूटेशनल समय की आवश्यकता होती है। ऐसी स्थिति में, कम फंक्शन कैलक्युलेशन्स (= पॉपुलेशन साइज़ x जेनरेशन्स की अधिकतम संख्या) अथवा कम जेनरेशन्स (निश्चित पॉपुलेशन साइज़ के लिए) में परेटो ऑप्टिमल सोल्यूशन्स प्रदान करने वाले एल्गोरिदम्स की सदैव आवश्यकता होती है।

वर्तमान शोध प्रबंध में, सीमित जेनरेशन्स में बेहतर परिणाम प्राप्त करने के उद्देश्य से, प्रचलित एल्गोरिदम्स में उन्नत ऑपरेटर्स का प्रयोग करके अथवा विभिन्न एल्गोरिदम्स के संकरण द्वारा, पाँच एवोलूशनरी एल्गोरिदम्स विकसित किये गए हैं। इन एल्गोरिदम्स की कार्यक्षमता के सघन परीक्षण के लिए, ज़ेडडीटी, एमओपी, डीटीएलजेड और डब्ल्यूएफजी टेस्ट सुइट्स की, दो और तीन ऑब्जेक्टिव वाली, तीस से अधिक मानक टेस्ट प्रॉब्लम्स को हल किया गया है। तत्पश्चात इन एल्गोरिदम्स का उपयोग रासायनिक अभियांत्रिकीय निकायों से सम्बंधित विभिन्न जटिल मल्टी-ऑब्जेक्टिव प्रॉब्लम्स को हल करने में किया गया है। पहले एल्गोरिदम में, रियल-कोडेड एलीटिस्ट नॉन-डॉमिनेटेड सॉर्टिंग जेनेटिक एल्गोरिदम (आरएनएसजीए-II) की कन्वर्जेन्स गति बढ़ाने के लिए, एक नया ऑपरेटर, सिम्युलेटेड बाइनरी जंपिंग जीन (एसबीजेजी) विकसित किया गया है। तत्पश्चात, विकसित किये गए एल्गोरिदम का उपयोग एक डायनामिक स्टीम रिफॉर्मर (दो ऑब्जेक्टिव युक्त प्रॉब्लम) और एक थैलिक एनहाइड्राइड रिएक्टर (एक दो ऑब्जेक्टिव युक्त प्रॉब्लम और एक तीन ऑब्जेक्टिव युक्त प्रॉब्लम) की मल्टी-ऑब्जेक्टिव प्रॉब्लम्स को हल करने के लिए किया गया है। दूसरा एल्गोरिदम सिम्प्लीफाइड मल्टी-ऑब्जेक्टिव पार्टिकल स्वार्म ऑप्टिमाइजेशन (एसएमपीएसओ) है जो कि पीएसओ और एनएसजीए-II में प्रयुक्त समरूप ऑपरेटर्स के विस्तृत गुणात्मक विश्लेषण के आधार पर विकसित किए गए दो सरल ऑपरेटरों का उपयोग करके अन्वेषण और शोषण के बीच एक अच्छा संतुलन प्रदान करता है। तत्पश्चात, एसएमपीएसओ का उपयोग रेसिड फ्लुइड कैटेलिटिक क्रैकिंग इकाई (दो ऑब्जेक्टिव युक्त प्रॉब्लम) की एक नवरचित मल्टी-ऑब्जेक्टिव प्रॉब्लम को हल करने में किया गया है। तीसरा एल्गोरिदम, बैट एल्गोरिदम (बीए) का मल्टी-ऑब्जेक्टिव संस्करण है, जिसका उपयोग थैलिक एनहाइड्राइड रिएक्टर की दो-ऑब्जेक्टिव युक्त प्रॉब्लम

को हल करने में किया गया है। चौथा एल्गोरिदम, एनएसडीई1-एफएच, डिफरेंशियल एवोलूशन (डीई) के एक मल्टी-ऑब्जेक्टिव संस्करण और फॉलोविंग हीरोज़ की नवविकसित अवधारणा के संकरण द्वारा विकसित किया गया है। इसे डुअल लीथियम आयन इंसर्शन सेल (दो ऑब्जेक्टिव युक्त प्रॉब्लम) की एक नवीन मल्टी-ऑब्जेक्टिव प्रॉब्लम को हल करने के लिए प्रयोग किया गया है। पांचवें एल्गोरिदम में, मल्टी-ऑब्जेक्टिव डीई की कन्वर्जेन्स गति बढ़ाने के लिए एक उन्नत डीई स्ट्रैटेजी का उपयोग किया गया है और फिर इस एल्गोरिदम को पॉली मिथाइल मेथाक्राइलेट (पीएमएमए) रिएक्टर के ऑप्टीमाइज़्ड ऑनलाइन कंट्रोल (ओओसी) के लिए प्रयोग किया गया है जिसमें मल्टी-ऑब्जेक्टिव ऑप्टिमाइजेशन प्रॉब्लम को मात्र कुछ मिनट की समयावधि में ही हल करना आवश्यक होता है। इस अध्ययन में हल की गई औद्योगिक प्रॉब्लम्स विभिन्न श्रेणियों से संबंधित हैं, उदाहरणार्थ, पहली तीन प्रॉब्लम्स प्रोसेस ऑप्टिमाइजेशन का प्रतिनिधित्व करती हैं, डुअल लीथियम आयन इंसर्शन सेल की प्रॉब्लम डिजाइन ऑप्टिमाइजेशन को दर्शाती है और अंतिम प्रॉब्लम कंट्रोल ऑप्टिमाइजेशन का प्रतिनिधित्व करती है। इन समस्याओं के लिए प्राप्त परिणाम बताते हैं कि प्रस्तावित एल्गोरिदम कम्प्यूटेशनल समय के साथ समझौता किए बिना सीमित जेनरेशन्स में अच्छा प्रदर्शन करते हैं। साथ ही, प्रत्येक औद्योगिक प्रॉब्लम के लिए, विकसित किये गए एल्गोरिदम्स द्वारा प्राप्त ऑप्टिमल ऑपरेटिंग पॉइंट्स उप्लब्ध औद्योगिक आंकड़ों से बेहतर हैं और इनका प्रयोग वास्तविक निकायों के उपयुक्त संचालन के लिए किया जा सकता है।

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Nomenclature

a	specific interfacial area, m^2/m^3 in Eq. (6.6)
a_s	surface area of catalyst, $m^2\ kg^{-1}$
A	fractional length of the half-catalyst slab in which the concentration varies in Table 3.2
A_c	inside cross-sectional area of the reformer tube, m^2
A_f	surface area of the flame produced by a single burner, m^2
A_i	loudness of i^{th} bat
$A_{\min}$	minimum loudness
$A_{\max}$	maximum loudness
A_p	cross-sectional area of the catalyst slab, m^2
A_{ref}	surface area of the refractor, m^2
A_{ris}	cross-sectional area of the riser, m^2
A^t	average loudness of all the bats at t^{th} iteration
$A_{t,i}$	total internal surface area of reformer tubes, m^2
ASE	adaptive social evolution
A_i, B_i	Constants
BA	bat algorithm
c_s	ion concentration in the solid phase, mol/dm^3
C	ion concentration in the electrolyte, mol/dm^3
$C_{cat,ck}$	coke on the catalyst (in the matrix) at any location, (kg coke) (kg porous catalyst)$^{-1}$
$\overline{C}_{cat,ck}$	coke on the catalyst (in the zeolite crystallite) at any location, (kg coke) (kg porous catalyst)$^{-1}$

$C_{cat,i}$	concentration of the i^{th} lump at any radial position in the matrix at location, h, of the riser reactor, kmol m^{-3}
$\overline{C}_{cat,i}$	concentration of the i^{th} lump in the zeolite crystallite at any location, kmol m^{-3}
c_i	concentration of species i in the catalyst slab, kmol m^{-3}
C_i	concentration of species i in the gas phase, kmol m^{-3}
c_{in}	concentration of OX in feed [g OX (m^3 air at NTP)$^{-1}$]
C_p	specific heat, J kg^{-1} K^{-1}
$C_{p,c}$	heat capacity of the catalyst, kJ kg^{-1} K^{-1}
$C_{p,fl}$	heat capacity of the vapour feed, kJ kg^{-1} K^{-1}
$C_{p,g}$	specific heat of the process gas, kJ $kmol^{-1}K^{-1}$
$C_{ris,i}$	concentration of the i^{th} lump in the gas phase at any location in the riser, kmol m^{-3}
$C_{p,s}$	specific heat of the solid (catalyst), kJ $kmol^{-1}K^{-1}$ in Table 3.2
$C_{p,s}$	heat capacity of steam, kJ kg^{-1} K^{-1} in Table 4.2
$C_{p,t}$	specific heat of the bed, kJ $kmol^{-1}K^{-1}$
C_t	molar concentration of the gas mixture (= P/RT), kmol m^{-3}
D	diameter of single tube of the reactor, m in Table 3.3
D	diffusion coefficient of electrolyte in the solid matrix, cm^2/s in Eq. (6.6)
D/C	ratio of carbon dioxide to methane in feed, (kmol/h of CO_2) / [kmol/h of methane fed ($F_{CH_4,in}$)]
d_i, d_o	inner and outer diameters, respectively, of the reformer tube, m
D_i^e	effective diffusivity of species i in the catalyst at axial location Z and time t, m^2 h^{-1}

D_p	equivalent diameter of the catalyst pellet (Raschig ring), m in Table 3.2
D_p	diameter of the catalyst particle, m in Table 3.3
D_s	diffusion coefficient of Li in the solid matrix, cm^2/s
DE	differential evolution
e	Exponential
E	quantity defined in Eq. (T.11) of Table 3.2
E_d, E_p, E_{td}	activation energies for the reactions, kJ mol^{-1}
E_i	activation energy of the *i*th reaction; $i = 1, 2, \ldots, 8$, $Jmol^{-1}$
f	the fraction of population directed to DE operations in NSDE1-FH
f_A	activity coefficient of salt
f_i	frequency of i^{th} bat
$f_{\min}$	minimum frequency
$f_{\max}$	maximum frequency
F	total feed rate, kmol h^{-1} in Table 3.2
F	Faraday's constant, 96,487 C/eq in Eq. (6.9)
F	initiator efficiency in Table 7.1
F_{cat}	flow rate of the catalyst in the riser, kg s^{-1}
F_{CH_4}	flow rate of methane, kg h^{-1}
F_{ck}	average concentration of coke in the catalyst in the riser at any location, kg coke (kg catalyst)$^{-1}$
F_{CO}	flow rate of methane, kg h^{-1}
F_{feed}	mass flow rate of the feed in the riser, kg s^{-1}
F_{H_2}	flow rate of H_2, kg h^{-1}
fi	objective function, $i = 1, 2$
F_i	molar flow rate of the i^{th} lump in the riser at any location, kmol s^{-1}

F_s	molar flow rate of dispersion steam at the inlet of the riser, kmol s^{-1}
FH	following heroes
G	mass velocity of the process gas in the reformer, kg m^{-2} h^{-1} in Table 3.2
G	mass flux of the gas phase, kgm^{-2} s^{-1} in Table 3.3
GA	genetic algorithm
GM	guided move
h	gas phase film heat transfer coefficient, Wm^{-2} K^{-1} in Table 3.3
h	axial location in the riser, m in Table 4.2
H/C	ratio of hydrogen to methane in feed, (kmol/h of hydrogen recycled) / [kmol/h of methane fed ($F_{CH_4,in}$)]
H_{ris}	height of the riser, m
ΔH_i	heat of reaction of the *i*th reaction; $i = 1, 2, \ldots, 8$, J mol^{-1} in Table 3.3
ΔH_i	enthalpy of the i^{th} reaction, kJ $kmol^{-1}$ in Table 4.2
ΔH_j^{ads}	heat of adsorption of the *j*th component; *j* = OX, OT, P, PA,MA, O_2, J mol^{-1}
i_n	interfacial reaction rate, mA/cm^2
I	superficial current density, mA/cm^2 in Eq. (6.10)
I	moles of initiator at any time *t*, mol in Table 7.1
IRN	integer random number
j_n	pore-wall flux across the interface
JG	jumping genes
K_I, K_{II}, K_{III}	equilibrium constants of reactions I-III, respectively
k_d, k_i, k_p, k_t, k_{tc}, k_{td}, k_{tm}	rate constants at any time t, s^{-1} or $m^3mol^{-1}s^{-1}$
$k_{d,0}$, $k_{p,0}$, $k_{td,0}$	intrinsic (in absence of gel and glass effects) rate constants, m^3 mol^{-1} s^{-1}
k_g	thermal conductivity of the process gas, kJ h^{-1} m^{-1} K^{-1}
k_i	Rate constant of the *i* th (*i* = I-III) reaction, kmol $kPa^{0.5}$ kg cat^{-1} h^{-1} or

	kmol kPa^{-1} kg cat^{-1} h^{-1} in Table 3.2
k_i	rate constant of the *i*th reaction; $i = 1, 2, \ldots, 8$, mol m^{-3} s^{-1} $(MPa)^{-2}$ in Table 3.3
K_i	equilibrium adsorption constant for species *i* (*i* = CH4, H2, CO, H_2O), kPa^{-1}
k_{io}	frequency factor of the *i*th reaction; $i = 1, 2, \ldots,$ 8, mol m^{-3} s^{-1} $(MPa)^{-2}$
$k_{j,M}$	rate constant for the i^{th} reaction in the matrix, m^3 kg-$matrix^{-1}$ s^{-1}
$k_{j,Z}$	rate constant for the i^{th} reaction in the zeolite crystallite, m^3 kg-$zeolite^{-1}$ s^{-1}
K_j	equilibrium adsorption constant of the *j*th component; *j* = OX, OT, P, PA,MA, O_2 , $(MPa)^{-2}$
K_{jo}	pre-exponential factor in the equation of *Kj*; *j* = OX, OT, P, PA,MA, O_2 $(MPa)^{-2}$
k_w	thermal conductivity of the tube-wall material, kJ h^{-1} m^{-1} K^{-1}
l	axial location in the catalyst slab, m
l_c	thickness of the wall of the Raschig ring, m
l_p	length of the Raschig ring, m
L	total length of the reactor, m in Table 3.2
L	length of the reactor tube , m in Table 3.3
L_{cat}	total length of all catalyst zones, m
L_i	length of catalyst zone *i*; $i = 1, 2, \ldots, 9$, m
L_1 and L_2	lower and upper limits used for generating $\eta = IRN[L_1, L_2]$
$\bar{m}$	coolant flow rate, kg (kg process $gas)^{-1}$
$\dot{m}_c$	coolant flow rate, kg s^{-1}

M	number of internal collocation points in Table 3.2
M	moles of monomer in liquid phase, mol in Table 7.1
M_F	average molecular weight of the gas mixture at any axial location, kg mol^{-1}
$M_{W,ck}$	molecular weight of coke, kg kmol^{-1}
$M_{W,g}$	average molecular weight of the gas in the riser at any location, kg kmol^{-1}
$M_{W,i}$	molecular weight of the i^{th} lump, kg kmol^{-1}
$M_{W,s}$	molecular weight of steam, kg kmol^{-1}
(MW_m)	molecular weights of pure monomer and solvent, kg mol^{-1}
N_b	number of burners in the reformer furnace
N_c	number of lumps in the lumped reaction scheme
N_C	number of carbon atoms
N_{DB}	number of double bonds
N_g	bats having rank 1
N_gen	number of generations
N_H	number of hydrogen atoms
N_i	flux of species i at any axial locationl inside the catalyst slab, kmol m^{-2} h^{-1}
N_maxgen	user-specified maximum number of generations
N_p	total number of solutions in the population
N_r	total number of reactions
N_V	total number of variables
N/C	ratio of carbon dioxide to methane in feed, (kmol/h of nitrogen) / [kmol/h of methane fed ($F_{CH_4,in}$)]

r_i

NSBAT-II	elitist non-dominated sorting BA
NSDE	non-dominated sorting DE
NSDE1	NSDE with DE/rand/1 strategy
NSDE2	NSDE with DE/best/1/bin strategy
NSDE1-FH	NSDE1 with FH operation
NSGA-II	elitist non-dominated sorting GA
NSPSO	non-dominated sorting PSO
p_i	partial pressure of the i^{th} lump in the gas in the riser at any location, kPa
P	operating pressure at axial location Z and time t, kPa
P_{GM}	probability of guided move
P_t	total pressure, Pa
$P_{T,ris}$	total pressure in the riser, kPa
PSO	particle swarm optimization
q_{cond}	conductive heat flux based on the average surface area of the tube, kJ m^{-2} h^{-1}
q_{conv}	convective heat flux based on the inner surface area of the tube, kJ m^{-2} h^{-1}
q_{rad}	radiative heat flux based on the outer surface area of the tube, kJ m^{-2} h^{-1}
r	radial position, m in Table 3.2
r	pulse emission rate in Chapter 5
r_i	rate of the i th reaction (i = I-III) corresponding to conditions at the catalyst surface at axial location Z and time t, kmol h^{-1} kg cat^{-1} in Table 3.2
r_i	rate of the ith reaction; $i = 1, 2, \ldots, 8$, mol m^{-3} s^{-1} in Table 3.3
r_i	pulse emission rate at i^{th} bat in Chapter 5
$r_{i,t}$	pulse emission rate at t^{th} iteration

R	sum of feed molar ratios in Table 3.2
R	universal gas constant, kPa m^3 $kmol^{-1}$ K^{-1} in table 4.2
R	universal gas constant, 8.3143 J/mol.K in Eq. (6.9)
R	primary radical in Table 7.1
R	universal gas constant, atm-m^3 mol^{-1} K^{-1} in Table 7.1
R_g	universal gas constant, J mol^{-1} K^{-1}
R_{gas}	volume of recycle gas (at actual conditions) mixed with volume of incoming feed at NTP
R_i	rate of production of the i th component at the catalyst surface at any axial location Z and time t, kmol h^{-1} kg cat^{-1}
$R_{i,n}$	rate of production of the i th component at the n th collocation point inside the catalyst slab at axial location Z and time t, kmol h^{-1} kg cat^{-1}
R_{li}, R_{lm}	rate of continuous addition of (liquid) initiator, monomer, or solvent to reactor, mol s^{-1}
R_s	radius of solid particles, m
R_{vm}	rate of evaporation of monomer or solvent, mol s^{-1}
RJG1	real-coded jumping gene adaptation proposed by Sankararao and Gupta.
RJG2	real-coded jumping gene adaptation proposed by Ripon et al.
RM	random move
RNSGA-II	real-coded NSGA-II
RNSGA-II-SBJG	RNSGA-II with SBJG operator
$\Re^*_{ck}$	net rate of formation of coke in the porous catalyst macro-particle, kmol $(kg)^{-1}$ s^{-1}
$\Re^*_{ck,cat}$	rate of formation of coke in the matrix at any location, kmol $(kg)^{-1}$ s^{-1}
$\overline{\Re}^*_{ck,cat}$	rate of formation of coke in the zeolite at any location, kmol $(kg)^{-1}$ s^{-1}
$\Re^*_i$	overall rate of reaction of the i^{th} lump, kmol (kg porous catalyst)$^{-1}$ s^{-1}

$\Re_j$	rate of consumption of the i^{th} lump by the j^{th} reaction in the matrix, kmol ξ (kg porous catalyst)$^{-1}$ s^{-1}
$\overline{\Re}_j$	rate of the j^{th} reaction in the zeolite crystallite, kmol (kg porous catalyst)$^{-1}$ s^{-1}
$\overline{\Re}_j^*$	overall rate of the j^{th} reaction, kmol (kg porous catalyst)$^{-1}$ s^{-1}
S_i	spacing after the *i*th zone of catalyst, m
S/C	ratio of carbon dioxide to methane in feed, (kmol/h of steam recycled) / [kmol/h of methane fed ($F_{CH_4,in}$)]
SBJG	simulated binary jumping gene
t	time, h in Table 3.2
t	time, s in Table 7.1
t	number of iterations in Chapter 5
$t_{\max}$	user-specified maximum number of iterations
T	process gas temperature at axial location *Z* and time *t*, K in Table 3.2
T	bulk gas temperature at any axial location, K in Table 3.3
T	temperature, K in Table 7.1
$T_{b,i}$	normal boiling point (at 1 atm), K
T_C	coolant temperature, K
T_f	adiabatic flame temperature at any axial location in the reactor, K
T_g	temperature of the furnace gas, K
T_{ref}	reference temperature, K
T_{ris}	temperature in the riser at any location, K
T_s	temperature of the catalyst at any axial location, K
T_w	tube-wall temperature, K

U	film heat-transfer coefficient on the inside of the tube (to gas + catalyst), kJ h^{-1} m^{-2} K^{-1} in Table 3.2
U	overall heat transfer coefficient between the jacket fluid and the bulk gas, J m^{-2} s^{-1} K^{-1} in table 3.3
U_i	i^{th} trial vector
v	dimensionless distance within the catalyst slab (= l/lc) (v = 0 at catalyst surface)
v_+	number of cations into which a mole of electrolyte dissociates
v_{cat}	velocity of catalyst in the riser at any location, m s^{-1}
v_g	velocity of gas in the riser at any location, m s^{-1}
$\boldsymbol{v}_i$	current velocity of i^{th} bat
v_l	superficial velocity of gas in the reformer, m h^{-1}
$v_{i,j}^0$	initial i^{th} bat velocity
$v_{i,j}^t$	j^{th} component of i^{th} bat velocity at t^{th} iteration
V	pore volume in the matrix, cm^3 g^{-1}
$V_{b,i}$	liquid molar volume of i, cm^3/gmol
$V_{c,i}$	critical volume of i, cm^3/gmol
V_i	i^{th} perturbed vector
V_l	volume of liquid at time t, m^3
w_i	inertia weight for i^{th} bat
$\boldsymbol{x}_i$	current position of i^{th} bat
$x_{i,j}^0$	j^{th} component of i^{th} position at 0^{th} iteration
$x_{i,j}^t$	j^{th} component of i^{th} position at t^{th} iteration
x_j^{Low}	lower limit of decision variable

x_j^{High}	upper limit of decision variable
x_g^{best}	total number of solution having rank 1
x_n	n^{th} variable of solution X_i
X	real value of a variable
X_i	mass-based yield of *i*, kg of species *i* produced per kg of OX consumed in Table 3.3
X_i	i^{th} solution point in Chapter 6
y_i	mole fraction of species *i* in the gas phase at axial location *Z* and time *t*
$\bar{y}_{i,n}$	mole fraction of component *i* at the *n* th collocation point inside the catalyst slab at axial location *Z* and time *t*
$Y_{Bottoms}$	yield (wt %) of bottoms in the riser at any location
Y_i	yield (wt %) of the i^{th} lump in the riser at any location
Y_j	mole fraction of the *j*th component; *j* = OX, OT, P, PA, MA, O_2, COx, H_2O
Z	axial location, m
z	charge number

Greek Symbols

β	distribution function for guided move operator
ε	random number between -1 and 1
ε_b	void fraction in the catalyst bed (outside the porous catalyst pellet) in Table 3.2
ε_b	void fraction in the bed in table 3.3
ε_c	volume fraction of pores inside a catalyst pellet
ε_{ris}	void fraction in the riser at any location
$\in$	Porosity
ξ_f	emissivity of the flames

ξ_g	emissivity of the furnace gas
ξ_M	pore radius in the matrix, Å
ζ_m, ζ_{m1}	initial monomer concentration
η	index for calculating β
η_I , η_{II} , η_{III}	effectiveness factors for reactions *I-III*, respectively, at axial location Z and time t
η_i	effectiveness factor for component i at axial location Z and time t in Table 3.2
η_i	effectiveness factor of the ith reaction; i=1, 2, . . ., 8 in Table 3.3
θ	random number (*RN*)
κ	conductivity of electrolyte, S/cm
λ_k	k^{th} ($k = 0, 1, 2,\ldots$) moment of live (P_{n}) polymer radicals
μ	viscosity of the gas mixture at axial location Z and time t, kg m^{-1} h^{-1}
μ_k	k^{th} ($k = 0, 1, 2,\ldots$) moment of dead (P_{n}) polymer chains
ρ	density, kg m^{-3}
ρ_{cat}	density of the porous catalyst macro-particle, kg m^{-3}
ρ_m, ρ_p	density of pure (liquid) monomer, polymer or solvent at temperature $\boldsymbol{T}$ (at time t), kg m^{-3}
ρ_V	density of the vapour in the riser at any location, kg m^{-3}
σ	conductivity of solid matrix, S/cm
φ	random number between -1 and 1
ϕ_m, ϕ_p	volume fractions of monomer, polymer or solvent in liquid at time t
ϕ_M	deactivation function in the matrix
ϕ_Z	deactivation function in the zeolite crystallite
Φ_1	potential in the solid phase, V

Φ_2	potential in the liquid phase, V

Subscript/Superscript

add	Addition
b	bulk gas phase
cat	Catalyst
$correl$	as obtained from the correlation
C	Coolant
CO_x	combustion products
F	bulk gas phase
H_2O	Steam
in	Inlet
mix	Maximum
MA	maleic anhydride
O_2	Oxygen
OT	*o*-tolualdehyde
OX	*o*-xylene
P	Phthalide
PA	phthalic anhydride
s	surface of the impervious catalyst
0	inlet of the riser in table 4.2
0	initial value or value without gel and glass effects in Table 7.1
+, -	positive electrode, negative electrode