Electronic Supplementary Material

Design and optimization of reactive distillation: a review

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Table S1 List of the reactive phase diagram

Reference	Application case
Barbosa & Doherty [1]	A+B⇌C, MTBE production, A+B⇌C+D, ethyl acetate production
An isobaric system with simultaneous chemical reaction and phase equilibrium, and the standard Gibbs free energy change of reaction is used to calculate the chemical reaction equilibrium constant. 3-D temperature-composition diagram for both ternary and quaternary systems. In the quaternary system, the T-axis represents the non-reactive binary mixture of one reactant and one product.	
Barbosa & Doherty [2]	A+B⇌C+D
The transformed composition variables [3] are applied in reactive phase diagrams. The bubble-point surface in the temperature-transformed composition variable diagram is simpler than the corresponding surface in the temperature-mole fraction diagram.	
Ung & Doherty [4]	A+B⇌C 2C⇌B+D, MTBE production with inert, alkylation of xylenes with di-tert-butylbenzene
The new set of transformed composition variables reduces the problem's dimensionality, which simplifies the analysis. In the MTBE system, the usage of TCVs reveals the existence of the pseudo-reactive azeotrope, and in multi-reaction systems, this approach finds the existence of hidden dissociation reactions.	
Pérez Cisneros et al. [5]	Formaldehyde-water system, MTBE production with inert, ethyl acetate production
The elemental composition variables are used to calculate the isothermal reactive phase diagram, which determines the conditions of element azeotropes.	

Table S2 List of the reactive residue curve map

Reference	Application case
Barbosa & Doherty [3]	A+B⇌C, MTBE production, A+B⇌C+D, ethyl acetate production
The standard Gibbs free energy change of reaction is used to calculate the reaction equilibrium constant. Using TCVs, both 3-D RCMs using the liquid mole fractions and plane RCMs using TCVs represent RCMs for quaternary systems.	
Rev [6]	A+B⇌C, tert-pentyl formate production, A+B⇌C+D
Both reaction rate and the evaporation rate are used to calculate RCMs of the non-equilibrium reversible reaction.	
Ung & Doherty [7]	A+B⇌C 2C⇌B+D, MTBE production with inert, alkylation of xylenes with di-tert-butylbenzene
The TCVs are used to calculate RCMs for multiple equilibrium reaction systems, which determine the presence of reactive azeotropes.	
Ung & Doherty [8]	MTBE production with inert, alkylation of xylenes with di-tert-butylbenzene
RCMs using TCVs provide the feasibility of separating multi-reaction mixtures by RD, the unstable node (lightest) and the stable node (heaviest) in RCMs are candidate distillate and bottoms products.	
Thiel et al. [9,10]	MTBE, TAME, and ETBE production
The Damköhler number and alterable operating pressure are used to calculate RCMs for the heterogeneously catalyzed system. Values of these two parameters influence both the existence and position of saddles, stable nodes, and separatrices in the RCM.	
Song et al. [11]	Methyl acetate production with methanol dehydration as side reaction
The experimental residue curves agree well with RCMs from the model prediction, and effects of catalyst loading are considered, which are represented by different Damköhler numbers.	
Wasylkiewicz & Ung [12]	N-butyl acetate production
Reactive phase diagrams and reactive RCMs with liquid split are calculated using transformed coordinates.	
Jiménez et al. [13]	Toluene production using chlorobenzene as entrainer, transesterification between methyl acetate and butanol using o-xylene as entrainer, MTBE production using n-pentane as entrainer, formaldehyde-water mixtures with methanol
The influence of entrainer in the extractive RD process is evaluated by reactive RCMs using TCVs.	
Qi et al. [14]	A hypothetical ternary system with liquid-liquid split, cyclohexene hydration
The Damköhler number is applied to describe the chemical kinetics effects on reactive RCMs for the liquid-liquid split system.	
Duarte & Loureiro [15]	TAME production
The effects of adsorption are studied by reactive RCMs using the Damköhler number.	
Sánchez-Daza et al. [16]	MTBE, methyl acetate, and ethyl lactate production
The element concept is applied in calculating reactive RCMs, which reduces the number of composition variables and simplifies the graphical representation.	
Carrera-Rodríguez et al. [17]	A hypothetical senary system with three reactions, MTBE, ETBE, and TAME production

Based on the usage of reaction-invariant composition variables and the assumption that phase equilibrium constants are independent of the temperature, the calculation of reactive RCMs is simplified.

Table S3 List of the fixed point method

Reference	Application case
Barbosa & Doherty [18,19]	A+B⇌C+D, methyl acetate production
The boundary value method is applied, and the equilibrium reaction on each plate is assumed. On the composition profiles diagram, there are two pinch zones at minimum reflux condition, which determines the minimum reflux of single or double feed RDC.	
Buzad & Doherty [20,21]	2A⇌B+C
The Damköhler number is applied in the fixed-point method to determine the minimum reflux and minimum total liquid holdup in kinetically controlled RDC.	
Espinosa et al. [22-24]	A hypothetical ternary reaction with inert, MTBE production with inert butane
The fixed-point method is applied in the RDC design with inert, and different RDC configurations with or without non-reactive sections are analyzed.	
Mahajan & Kolah [25], Mahajani, [26,27]	2A⇌B+C, A+B⇌C+D
Two dimensionless numbers are applied for the Design of packed-bed RDC: HTU (height of the transfer unit) representing the influence of distillation efficiency, and the Damköhler number representing for reaction kinetics efforts.	
Okasinski & Doherty [28]	2-Pentene metathesis, ethylene oxide hydration, and methanol dehydration
Reaction kinetics effects (using the Damköhler number), non-ideal vapor-liquid equilibrium (Wilson, NRTL and UNIFAC model), heat effects, and distribution of catalyst loading and liquid holdup are taken into account for the design of kinetically controlled staged RDC.	
Chen et al. [29]	Methyl acetate production, 2-pentene metathesis, MTBE production, ethylene glycol production is
Side reactions, reaction heat, non-constant latent heat, and liquid holdups distribution are taken into account, and the Damköhler number is selected to characterize kinetic effects.	
Chadda et al. [30]	A hypothetical equimolar ternary decomposition reaction, 2-pentene metathesis
The attainable product composition regions at intermediate reaction rates are obtained, and the location and movement of the product regions changed by different reaction rates are studied.	
Avami et al. [31], Avami [32]	Methyl formate production, xylenes alkylation, methyl acetate production with inert, butyl levulinate production, ethyl acetate production
A modified feed angle method developed from pinch point analysis is proposed to determine the assess feasibility product and the minimum energy demand of single and double feed RDCs.	
Li et al. [33]	Amyl acetate production, MTBE production with inert, TAME production
The fixed-point method is combined with the element concept, and the Z-axis is introduced for temperature, which considers the effect of temperature on both separation and reaction.	

Table S4 List of the statics analysis

Reference	Application case
Giessler et al. [34,35]	MTBE production with or without inert, acetic anhydride hydrolysis, cumene production, ethylene glycol production, alcohol acetate production, methyl acetate hydrolysis
Based on the distillation diagram and distillation lines, the application of static analysis is extended to the feasibility study of the RD process.	
Giessler et al. [36,37]	MTBE production, methyl acetate production, methyl acetate hydrolysis.
The static analysis generates the RDC process structure with a different number of columns for different feed compositions.	
Shuvalov et al. [38]	Ethyl acetate production, allyl acetate hydrolysis
Degrees of freedom analysis is applied in the statics analysis. A criterion involving the concentration quotient and reaction equilibrium constant is proposed to estimate the realizability and realization conditions for the RD process.	
Pisarenko et al. [39]	A hypothetical quaternary multi-reaction system ($2A \rightleftharpoons B$, $B \rightleftharpoons C+D$)
Based on the construction of the modified reactive distillation trajectory, the statics analysis is applied in the conceptual design of the RD process involving multiple chemical reactions.	
Sun et al. [40]	$A+B \rightleftharpoons C$
The Z-axis is introduced for temperature in stereo distillation diagram for statics analysis, hence the effects of temperature, which is changed by a variable pressure, are considered, while the previous graphical method is be acquired at a fixed pressure.	

Table S5 List of the reactive cascade

Reference	Application case
Chadda et al. [41]	Isopropyl acetate production
The co-current flash cascades, consist of the rectifying cascade and the stripping cascade, predict the feasible products of single-feed RDC.	
Chadda et al. [42]	Butyl acetate, isopropyl acetate, and methyl acetate production
The co-current cascades consist of both rectifying and stripping cascades represent the single-feed fully RDC. The co-current cascades, consist of both reactive and non-reactive cascades, represent the single-feed hybrid RDC. The counter-current cascades with non-reactive rectifying and stripping cascades represent the double-feed hybrid RDC.	
Nisoli et al. [43]	A+B⇌C, isopropyl acetate production
The Stefan–Maxwell model is applied to evaluate the effect of mass-transfer resistance, the Damköhler number and the Peclet number is introduced to quantify the effect of finite mass-transfer rates.	
Gadewar et al. [44]	Isopropyl acetate production and methyl acetate production
A cross-flow cascade model is developed to determine feasible product compositions of double-feed RDCs.	

Table S6 List of the attainable region

Reference	Application case
Nisoli et al. [45]	Methanol dehydration and MTBE production
A hybrid reactor-separator model based on two-phase CSTR and PFR with vapor removal is proposed to obtain the attainable region for the reactive separation process. The proposed model is described by the Damköhler number, and the vapor fraction depends on the heating policy.	
Gadewar et al. [46]	A hypothetical ternary reaction(A→B→C), trans-alkylation of toluene, and isopropyl acetate production
The attainable region of reactive-separation systems is obtained from a counter-current cascade of two-phase CSTRs model, a surrogate for the rectifying or stripping sections of an RDC.	
Gadewar et al. [47]	Isopropyl acetate production
The attainable region is obtained from counter-current cascades of vapor-liquid CSTRs, and the feasible process alternative with recycling loop is generated from attainable regions methodology.	
Agarwal et al. [48,49]	Isobutylene dimerization, aldol condensation of acetone, two multi-reaction systems with undesired reactions, hypothetical ternary multi-reaction systems with azeotrope
A reactive condenser model is proposed to represent the reactive rectification section, and a reactive reboiler model is proposed to represent the reactive stripping section, which expands the feasible region method.	
Amte et al. [50,51]	Van de Vusse reaction (A→B→C, 2A→D)
Four building blocks, continuous reactive reboiler, continuous reactive condenser, and their cascade versions, cascade continuous reactive reboilers and cascade continuous reactive condensers, are introduced to determine the desired RD network and conventional reactor network.	

Table S7 List of mixed integer nonlinear programming problems in reactive distillation design

Reference	Production or reaction, and catalyst	Algorithm	Optimization variable
Ciric & Gu [52]	Ethylene glycol, sodium hydroxide	GBD	NS, FS, RR, LH per tray, temperature and composition profiles
The double feed column and distributed feed column are compared.			
Frey & Stichlmair [53]	Methyl acetate, sulfuric acid	OA/ER/AP	QC, QR, TF, NS, NRS, LRS, FS
The energy demand is decreased by vaporizing and splitting methanol feed.			
Stichlmair & Frey [54]	MTBE, resin; Methyl acetate, sulfuric acid	OA/ER/AP	TF, RR, FS, NNRS, NRS, LRS
The multiple feeding generates a drastic reduction of TAC for both systems.			
Poth et al. [55]	Methyl acetate, resin	OA/ER/AP	TF, RR, FS, NNRS, NRS, LRS
The dimerization of the acetic acid is considered, and an adsorption-based reaction kinetic model is applied.			
Jackson & Grossmann [56]	2-Pentene metathesis, molybdenum complex Ethylene glycol, sodium hydroxide	OA	NS, FS, LH per tray, RR, BUR, QC, QR
A disjunctive programming approach is applied, therefore only the selected trays are modeled with the MESH and reaction kinetics equations.			
Sand et al. [57]	MTBE, resin	BB, GRG	NS, LRS, FS, RR
The MINLP problem is decomposed into an IP-master-problem (optimization of integer variables, NT) and NLP-sub-problems (optimization of continuous variables with a fixed number of trays, solved by GRG). Three algorithms solve the IP problem: branch and bound algorithm, an interval reduction algorithm and complete enumeration of the subspace of binary variables.			
Gangadwala et al. [58]	Isomerization of 2,3-dimethylbutene-2 to 2,3-dimethylbutene-1, resin	BB	NS, FS, LRS, NRS, NNRS, catalyst amount, RR
The polyhedral relaxation is applied to obtain global bounds on the objective function value, and MINLP is relaxed into MILP.			
Gangadwala & Kienle [59]	Butyl acetate, resin	BB	QR, NRS, FS, amount and distribution of catalyst
Both RDC and non-reactive DC coupled with side reactors are optimized.			
Gangadwala et al. [60]	2-Pentene metathesis, molybdenum complex 2,3-Dimethylbutene-1, resin	BB	NS, FS, NRS
Nonlinear model reduction using polyhedral relaxations of wave functions is applied to reduce the complexity of MINLP.			
Filipe et al. [61]	2-Pentene metathesis with different relative volatilities	ε-constraint method	NS, FS, LRS, NRS, RR, BR, DF reactive holdup distribution
The reactive holdup and the cost indicator are selected as two objective functions. The Pareto surface is built to depict the trade-off between NS, reactive holdup, and cost indicator.			
Amte et al. [62]	Isobutene dimerization, resin	BB	FS, reflux stage, RR, DB, amount and location of catalyst
A multiple reaction system. The objective function is the maximization of the desired product (di-isobutene) selectivity.			

Bildea et al. [63]	Di-n-pentyl ether, resin	SQP	NS, FS, NRS, LRS, OP, DR, catalyst amount
The conventional reaction–separation–recycle process is also optimized and compared with the catalytic distillation process.			
Karacan & Karacan [64]	FAME, resin	[65-69], Fletcher–Reeves, Quasi-Newton	RR, QR, OP, FF
The objective function is maximizing the FAME mole fraction in the bottom stream. The highest concentration is obtained from the Fletcher–Reeves method.			
Ismail et al. [70,71]	Ethyl acetate, sulfuric acid; methyl acetate, sulfuric acid; MTBE, resin	GRG	QR, QC, feed rate
The RDC is representated by Generalized Modular Representation Framework, the Gibbs free energy-based driving force constraints are introduced. The modular results agree well with the equilibrium model.			
Cardoso et al. [72]	Ethylene glycol, sodium hydroxide	SA, adaptive random search	NS, FS, RR, LH per tray, QC, QR
The number of theoretical stages is not an important decision variable in this system, therefore the MINLP problem can be simplified into an NLP problem by fixing integer variables. Both algorithms perform well.			
Gómez et al. [73]	ETBE, resin	SA, SQP	NS, FS, LRS, RR, QR, geometrical parameters of column and trays
The NEQ model simulates the RDC, which considers tray efficiencies and geometrical parameters of the column's hardware. The NLP subproblem is solved by SQP, and the MINLP master problem is solved by SA.			
Babu & Khan [74]	Ethylene glycol, sodium hydroxide	DE	NS, FS, LH per tray, RR, QC, QR
The simulation is improved by the relaxation method and the homotopy method, and the proposed homotopy-continuation method with differential evolution strategy performs better than the previous work.			
Babu et al. [75]	An ideal quaternary reaction with the most favorable ranking of relative volatilities	GA	NS, NRS, NNRS, catalyst loading per tray, OP, FS
Feeding reactants into reactive section results in energy saving, and a two-point temperature inferential control structure is presented.			
Cheng et al. [76]	Methyl acetate, resin, butyl acetate, resin	SA	NRS, NNRS, FS
The SA method has a smaller probability of getting trapped in a local minimum than the sequential optimization approach. The result obtained from SA is similar to the result from evaluating all solution space, but takes less computation time.			
Urselmann et al. [77], Urselmann & Engell [78]	MTBE, resin	MA	NS, FS, RR, OP, catalyst amount
The proposed algorithm finds all global optimal solutions of four different RDC configurations, while deterministic methods, such as BB, could not provide global optimum which depends strongly on the initial value.			
Niesbach et al. [79]	N-butyl acrylate, resin	EA	OP, DF, RR, NRS, NNRS, FR
The non-equilibrium stage model simulates the RDC, and pilot-scale experimental studies validate the optimal solution.			
Domingues et al. [80]	ETBE, resin	GA, PSO	NS, FS, LRS, NRS, OP, bottom flowrate, column diameter
Consider the effect of catalyst deactivation, and PSO solves the optimization problem faster than GA.			

Bîldea et al. [81]	Dimethyl ether, γ-alumina for gas-phase reaction, ion exchange resin for liquid-phase reaction	GA	NS, FS, NRS, RR, OP, catalyst amount
The RDC process is more economical than the classic reactor-separator-recycle process and the combined gas-phase reactor-RD process.			
Xiao et al. [82]	MTBE, resin	NSGA-II	NS, RR, FS, NRS, LH, FF
A multi-objective optimization problem, including the maximization of isobutene conversion and the minimization of TAC.			
Lu et al. [83]	Methyl acetate, resin; Methyl laurate, niobium oxide	BA	NS, FS, RR, the number and locations of side reactor
The side-reactor column process facilitates the integration between high-temperature reaction and low-temperature distillation, which expands the application areas of RD.			

Table S8 List of mixed integer nonlinear programming problems of reactive distillation with heat integration

Reference	RDC type	Production or reaction, and catalyst	Algorithm	Optimization variable
Behroozsarand & Shafiei [84]	RDTC	Transesterification reaction of methyl acetate and n-butanol, resin	NSGA-II	FR, RR, TF, FS, OP, location and flowrate of side stream
Three objective functions are selected: reboiler duty, RDC productivity, and non-reactive distillation column productivity.				
Miranda-Galindo et al. [85]	RDTC	FAME, sulfuric acid	GA	RR, FS, NS, LRS, NRS, BUR, DR, location and flowrate of interconnection flow
A multi-objective optimization problem, total heat duty, NS in each column, and the size of the reactive section of RDC are optimized, three RDTC sequences and two RD-separation sequences are optimized and compared.				
Kiss et al. [86]	RDWC	FAME, sulfated zirconia	SA	TF, NRS, NS, DR, BUR, location and flowrate of side stream, liquid and vapor split
The computational time of SA is lower than that of Harmony Search and GA, especially in the optimal design of complex distillation sequences.				
Vázquez-Ojeda et al. [87]	RDTC	FAME, resin	DE	RR, DR, NS, FS, NRS
Four reactive distillation sequences, including RDTC with side rectifier or side stripper, and RDC with a non-reactive column, are studied and compared.				
Ignata & Kiss [88]	RDWC	FAME, sulfated zirconia	SQP	TF, NS, NRS, FS, FR, BUR, RR location and flowrate of side stream, wall size and location, liquid and vapor split
The objective function is to minimize the total reboiler duty and NT, which approximates to TAC.				
Qian et al. [89]	RDWC	Selective hydrogenation of methyl acetylene and propadiene in C3 stream, palladium	PSO	FS, NS, MRS, RR, BR of depropanization column and propylene distillation column, liquid split ratio
A detailed capital cost is applied, considering fixed costs, including maintenance expense and wages, the fixed capital depreciation rate and the minimum return on investment.				
Santaella et al. [90]	RDWC	Ethyl acetate, sulfuric acid	SQP	NS, FS, number of stages above and below dividing wall, RR, BR, liquid and vapor split ratio, QR, DF, decanter temperature
Several RD schemes are optimized and evaluated. after the preliminary economic evaluation, those schemes are characterized by sustainability indicators, include conversion, productivity, mass productivity, mass intensity, Sheldon's Factor, energy intensity, and water-free Sheldon's factor.				
Santaella et al. [91]	RDWC	Triethyl citrate, resin	DE, tabu list	FR, RR, NS, FS, NRS, QR for both sides of RDWC, catalyst loading,
A multi-objective optimization problem, TAC is selected as profitability objective function, and the condition number integral in the frequency range is chosen as the				

controllability objective function.				
Yang et al. [92]	RDWC with heat pump	Diethyl carbonate, sodium ethoxide	GA	flow rate of working fluid, output pressure of the turbine and the pump, and the output temperature of the waste heat
The organic Rankine cycle (ORC) is applied to the proposed heat pump-assisted RDWC, the net revenue and the ORC thermal efficiency are selected as the objective function to optimize. The ORC system is optimized alone while RDWC's parameters are fixed.				
Chen et al. [93]	RDC with middle vapor recompression	Methyl acetate hydrolysis, resin	GA	MS, FS, RR, liquid and vapor split ratio, compress ratio
Five different schemes are optimized and compared, and the relation between the TAC and products quality is analyzed				

Table S9 List of orthogonal collocation on finite elements in reactive distillation design

Reference Algorithm	Production or reaction, and catalyst	Optimization variable
Seferlis & Grievink [94]	Ethyl acetate, sulfuric acid	NRS, NNRS, FS, LH per tray, DR, BUR, RR
Both reactive column and recovery column are approximated by OCFE model, and optimization results obtained from OCFE and tray-by-tray model are in good agreement.		
Dalaouti & Seferlis [95]	Reactive absorption of nitrogen oxides, ethyl acetate production, sulfuric acid	NRS, NNRS, FS, LH, QC, QR
A modeling approach that combines OCFE technique and NEQ model is applied for both optimal steady design and dynamic simulation, which governs the behavior of the packed column.		
Damartzis & Seferlis [96]	Butyl acetate, resin	NS, FS, RR, BUR, QC, QR, FR, LH
The NEQ/OCFE model is applied for simulating the non-ideal system with potential liquid-phase split, which is validated by experimental results.		

Table S10 List of response surface methodologies in reactive distillation design

Reference	Production or reaction, and catalyst	Objective function	Optimization variable
Noshadi et al. [97]	FAME from transesterification, heteropolyacid	Maximizing FAME yield	FF, QR, TF, FR
The pilot plant scale experiment validates the optimal solution.			
Giwa & Giwa [98]	Isopropyl myristate	Maximizing the bottom mole fraction of isopropyl myristate	RR, FR, QR
The reaction equilibrium constant on each reactive stage is calculated by Gibbs free energy			
Mallaiah & Reddy [99]	Methyl acetate, resin	Maximizing the methyl acetate concentration in the distillate	Reboiler temperature, RR, FR, FF, FS
The experimental results are in good agreement with that predicted by the regression model.			
Feyzi & Beheshti [100]	Acetic acid production, rhodium complex	Minimizing exergy loss	FS, TF, BUR, RR, FR
The exergy analysis method is applied to evaluate the performance of the RD process, and a remarkable reduction in energy consumption is obtained			
Deng et al. [101]	Ethyl acetate, zeolite	Maximizing the yield and purity of ethyl acetate	QR, FR, RR, catalyst amount, weight hourly space velocity
The Box–Behnken design is applied to analyze the effects of five design variables, and a laboratory-scale RDC is used to examine the optimal result.			
Kaur & Sangal [102]	ETBE, resin	QB, QC, mole fraction of bottom, distillate and withdrawal, CO_2 emission	NS, RR, withdrawal stage, liquid and vapor flowrate to the post-fractionator part, location of liquid and vapor split
The RDWC is applied for ETBE synthesis, and the Box–Behnken design is used to solve this multi-objective optimization problem.			

Table S11 List of optimization-based reactive distillation dynamic design

Reference	Application case	Algorithm	Objective function
Cervantes & Biegle [65]	Ethyl acetate production in batch RDC Ethylene glycol production in continuous RDC	OCFE, SQP	Maximizing the amount of distillate product of batch RD, minimizing the heat required to start up the column of continuous RD
The differential-algebraic equation optimization is converted into an NLP by applying OCFE, solved by SQP. The objective functions are maximizing the amount of distillate product for batch ethyl acetate RD process by manipulating RR as a function of time, and minimizing the heat required to start up the column for continuous ethylene glycol RD process by controlling the fraction of the bottoms.			
Kawathekar & Riggs [66]	Ethyl acetate production	OCFE	Maximizing the impurity in the overhead product
The OCFE technique transforms the control problem into an NLP problem, and the nonlinear model predictive control is applied, which provides significantly better control performance than the PI controller.			
Venkateswarlu & Reddy [67]	Ethyl acetate production	SQP, GA, SA	Minimizing an objective function based on a desired output trajectory over a prediction horizon
The proposed stochastic optimization (GA and SA) based NMPCs perform better than the conventional PI controller, the linear model predictive controller, and the NMPC based on SQP.			
Behroozsarand & Shafiei [68]	TAME production	NSGA-II	Minimizing overshoots and integral of absolute errors of controllers.
This work presents the tuning of 7 PI and PID controllers by solving the multi-objective optimization problem.			
Lopez-Saucedo et al. [69]	Light alcohols batch distillation Ethyl acetate batch RD	OCFE, SQP	Maximizing the profit of non-reactive column, maximizing the reactant conversion of RDC.
Two different dynamic optimization approaches are proposed: equation-oriented approach based on OCFE using the interior-point algorithm as the NLP solver, and control vector parameterization using SQP as the NLP solver.			
Raghavan et al. [103]	A+B⇌C+D	recurrent neural network	Response and estimator performance
The RD process is controlled by controlling the composition estimated from available temperature measurements. The Recurrent Neural Network-based estimator than the standard Extended Kalman filter-based and the Feed forward Neural Network-based.			
Sharma & Singh [104]	TAME production	neural network	Minimization of cost
The neural network predictive control provides smoother and better control performance than PID control and MPC.			
Ge et al. [105]	Formic acid production	GA, convolutional neural network	Minimization of TAC for steady design, reduction of response for dynamic design
GA solves the steady optimization. The fault detection and diagnosis model based on convolutional neural network effectively drives RD to steady-state under disturbance.			

Table S12 List of mixed-integer dynamic optimization problems in reactive distillation design

Reference	Production or reaction, and catalyst	Algorithm	Controller	Objective function
Georgiadis et al. [106]	Ethyl acetate, sulfuric acid	GBD	PI	Minimizing TAC
The MIDO problem is decomposed into a multi-period design and control sub-problem, and the simultaneous approach results in both economic and operability benefits over the sequential approach.				
Panjwani et al. [107]	Ethyl acetate, sulfuric acid	GBD	PI	Minimizing TAC
The MIDO problem is differentiated into an NLP-primal-problem and a MILP-master-problem. The high-fidelity dynamic model predicts the process behavior under time-varying disturbances.				
Paramasivan & Kienle [108]	A+B⇌C+D	GBD	PI	Minimizing the combination of the expectation and the variance of the performance index
The MIDO problem is decomposed into a series of NLP subproblems by fixing binary variables, and MILP master problems, which determine a new binary configuration for the next NLP subproblem.				
Contreras-Zarazúa et al. [109]	Diphenyl carbonate, orthotitanate	DE with tabu list		Minimizing TAC Minimizing condition number
The Condition Number is chosen as the index to evaluate the control properties related to the minimum singular value and the maximum singular value. Three RDTC configurations are presented.				
Bernal et al. [110]	ETBE, resin	GRG	NMPC	Minimizing a linear combination of tracking performance and economic costs.
This design and control optimization problem is fully discretized by the orthogonal collocation method.				
Tian et al. [111]	MTBE, resin	shooting algorithm	MPC	Minimizing TAC
A high-fidelity dynamic model that considers both time-invariant design and time-variant operating variables is developed to describe dynamic process behavior accurately.				

Abbreviation

A+B⇌C, a hypothetical ternary synthesis reaction

2A⇌B+C, a hypothetical equimolar ternary decomposition reaction

A+B⇌C+D, a hypothetical quaternary reaction

A+B⇌C 2C⇌B+D, a hypothetical quaternary double-reaction system based on formaldehyde-water mixtures

CSTR, continuous stirred tank reactor

DC, distillation column

ETBE, ethyl tert-butyl ether

FAME, fatty acid methyl ester

IP, integer programming

MIDO, mixed-integer dynamic optimization

MILP, mixed integer linear programming

MINLP, mixed integer nonlinear programming

MTBE, methyl tert-butyl ether

MPC, model predictive control

NEQ, non-equilibrium stage

NLP, nonlinear programming

NMPC, nonlinear model predictive controller

OCFE, orthogonal collocation on finite elements

PFR, plug flow reactor

PI, proportional integral

PID, proportional integral derivative

RCM, residue curve map

RD, reactive distillation

RDC, reactive distillation column

RDTC, reactive distillation with thermal coupling

RDWC, reactive dividing wall column

RSM, response surface methodology

TAC, total annualized cost

TAME, t-amyl-methyl-ether

TCV, transformed composition variable

Abbreviation for algorithms

BA, bat algorithm

BB, branch and bound algorithm

DE, differential evolution algorithm

EA, evolutionary algorithm

GBD, generalized Benders decomposition algorithm

GRG, generalized reduced gradient algorithm

MA, memetic algorithm

NSGA-II, non-dominated sorting genetic algorithm II

OA, outer-approximation algorithm

OA/ER/AP, outer-approximation/equality-relaxation/augmented-penalty algorithm

PSO, particle swarm optimization algorithm

SA, simulated annealing algorithm
SQP, sequential quadratic programming algorithm

Abbreviation for variables
BR, bottom rate
BUR, boil-up ratio
DB, distillate rate to bottoms rate ratio
DF, distillate rate to feed rate ratio
DR, distillate rate
FF, feed flowrate
FR, feed ratio
FS, feed stage
LH, liquid holdup
LRS, the location of reactive stages, or the position of the reactive section
NNRS, the number of non-reactive stages
NRS, the number of reactive stages
NS, total number of stages
QC, condenser duty
QR, reboiler duty
OP, operating pressure
RR, reflux ratio
TF, temperatures of feed stream

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