Electronic Supplementary Material

An efficient multi-objective optimization framework based on data-driven identification and adaptive directed correction for complex distillation processes

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Section S1. Details of Model Elements

As illustrated in **Fig. S1**, a representative model with two inputs and one output is adopted for demonstration purposes. The entrainer feed location and the fresh feed location are treated as the two input variables and are indicated in red and green, respectively. The side-stream location is defined as the sole output variable and is highlighted in blue. Six typical infeasible configurations are shown in **Fig. S1**. In each case, infeasibility originates from improper positional relationships between the specified locations and the total number of trays in the column.

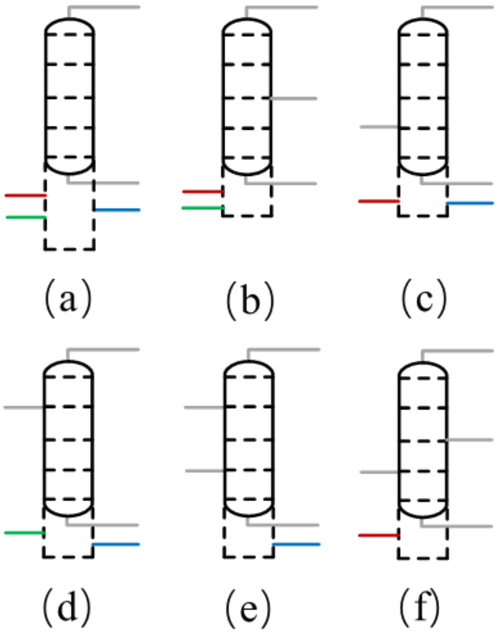

Fig. S1. Illustrative examples of infeasible solutions.

Section S2. Calculation Details for TOPSIS

TOPSIS (Technique for Order of Preference by Similarity to Ideal Solution) is a multi-criteria decision-making technique. It is based on the principle that the selected alternative should has the shortest geometric distance from the positive ideal solution (PIS) and the longest geometric distance from the negative ideal solution (NIS). The calculation details are as follows.

Step 1: Construct the decision matrix $X = \left[x_{i,j}\right]$.

$$X = \begin{bmatrix} x_{1,1}, x_{1,2}, \dots, x_{1,n} \\ x_{2,1}, x_{2,2}, \dots, x_{2,n} \\ \dots \\ x_{m,1}, x_{m,2}, \dots, x_{m,n} \end{bmatrix} \tag{S1}$$

Step 2: Normalize the decision matrix $X' = [x'_{i,j}]$.

$$x'_{i,j} = x_{i,j} / \textstyle\sum_{j=1}^{m} x_{i,j}{}^2 \tag{S2}$$

Step 3: Calculate the weight.

$$W_{i,j} = w_j x'_{i,j} \tag{S3}$$

where w_j is the weight of the j-th criterion. The weighted normalized decision matrix $W = [W_{i,j}]$ reflects the importance of each criterion.

Step 4: Determine the positive ideal solution PIS and the negative ideal solution NIS for each criterion.

$$PIS_j = Max(W_{i,j}) \tag{S4}$$

$$NIS_j = Min(W_{i,j}) \tag{S5}$$

Step 5: Calculate the Euclidean distance DP_i and DN_i for each option i with PIS and NIS respectively.

$$DP_i = \sqrt{\textstyle\sum_{j=1}^{n} \left(x'_{i,j} - PIS_j\right)^2} \tag{S6}$$

$$DN_i = \sqrt{\textstyle\sum_{j=1}^{n} \left(x'_{i,j} - NIS_j\right)^2} \tag{S7}$$

Step 6: Calculate the relative closeness P_i.

$$P_i = DN_i/(DP_i + DN_i) \tag{S8}$$

Step 7: Rank the options based on their proximity to the ideal solution and select the option with the highest P_i as the best alternative solution.

Section S3. Details Related to the SS-DCED Optimization

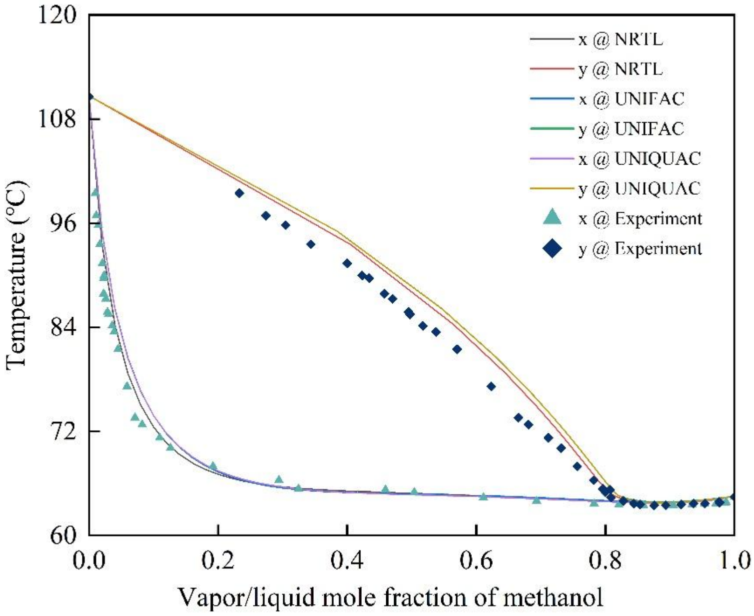

Fig. S2. Comparison of NRTL/UNIQAUC/UNIFAC models and experiment for the Methanol-Toluene.

Table S1. Upper and lower bounds of decision variables in the SS-DCED optimization.

Decision variable	Lower bound	Upper bound
NT_{EDC}	30	80
NE_{EDC}	10	50
NF_{EDC}	20	60
NS_{EDC}	10	60
F_{EDC} (kmol/h)	1.0	20.0
RR_{EDC}	1.5	3.0
NF_{SRC}	20	50
NT_{SRC}	10	40

Table S2. Parameters and formulas used for TAC calculations.

Parameter	Value / Formula	Unit
Condenser:		
Heat transfer coefficient (U_c)	0.852	kW/(°C·m^2)
Temperature difference (ΔT)	$((T_c - 42) - (T_c - 32))/\ln((T_c - 42)/(T_c - 32))$	°C
Heat transfer area (A_c)	$Q_c/(U_C \times \Delta T)$	m^2
Investment costs	$(M\&S/280) \times 1609.13 \times A_c^{0.65}$	$
Reboiler:		
Heat transfer coefficient (U_R)	0.568	kW/(°C·m^2)
Temperature difference (ΔT)	Steam temperature – Base temperature	°C
Heat transfer area (A_R)	$Q_R/(U_R \times \Delta T)$	m^2
Investment cost	$(M\&S/280) \times 1775.26 \times A_R^{0.65}$	$
Column vessel:		
Tray height (h_{tray})	$0.6096 \times (NT - 2)$	m
Column height (h_{col})	$1.2 \times h_{tray}$	m
Column diameter (ID_{col})	Calculated by Aspen Tray Sizing	m
Column internal cost (CIC_{inst})	$(M\&S/280) \times 97.243 \times ID_{col}^{1.55} \times h_{tray}$	$
Column shell cost (CSC_{inst})	$(M\&S/280) \times 3919.32 \times ID_{col}^{1.066} \times h_{col}^{0.802}$	$
Capital cost	$CIC_{inst} + CSC_{inst}$	$
Energy cost:		
HP steam (254°C)	9.88×10^{-6}	$/kJ
MP steam (184°C)	8.22×10^{-6}	$/kJ
LP steam (160°C)	7.78×10^{-6}	$/kJ
Colling water	0.354×10^{-6}	$/kJ
M&S *	1638.2	–
Payback period	3	a
TAC	$TAC = (TCC/Payback\ period) + TOC$	$/a

* Note: *M&S* is the Marshall & Swift Cost Index, which is widely used to update capital costs and account for inflation effects in chemical process economic evaluations.

Table S3. Formulas and parameters for the calculation of carbon dioxide emissions (GGE_{CO_2}).

Parameter	Value / Formula		Unit
	Case 1	Case 2	
Net heating value (*NHV*)	51600	39771	kJ/kg
Carbon content of the fuel (*C*)	75.4	85.5	%
Latent heat (λ_{proc})	2086.00	2083.47	kJ/kg
Enthalpy of the low-pressure steam (h_{proc})	2756.66	2683.64	kJ/kg
Heat duty (Q_{proc})			kJ/h
Molar mass ratio of CO_2 and C (α)	3.67		-
Flame temperature (T_F)	1800		°C
Stack temperature (T_s)	160		°C
Ambient temperature (T_0)	25		°C
Amount of furl burnt (Q_{fuel})	$\left(Q_{proc}/\lambda_{proc}\right) \times \left(h_{proc} - 419\right) \times ((T_F - T_0)/(T_F - T_s))$		kJ
Carbon dioxide emissions (GGE_{CO_2})	$(Q_{fuel}/NHV) \times (C/100) \times \alpha$		t/h

Table S4. Comparison of TAC-optimal, GGE_{CO_2}-optimal, and balanced solutions achieved by MO-DIDC for the SS-DCED process.

		TAC-optimal solution	GGE_{CO_2}-optimal solution	Balanced solution
Decision variable	NT_{EDC}	46	48	46
	NE_{EDC}	18	18	18
	NF_{EDC}	44	43	44
	NS_{EDC}	20	19	19
	F_{EDC} (kmol/h)	5.9135	6.0571	5.7543
	RR_{EDC}	0.105	0.112	0.105
	NF_{SRC}	37	48	40
	NT_{SRC}	20	36	28
Objective function	TAC (10^6 \$/a)	0.6709	0.6847	0.6719
	GGE_{CO_2} (t/h)	0.7466	0.7416	0.7448

Section S4. Details Related to the FCED Optimization

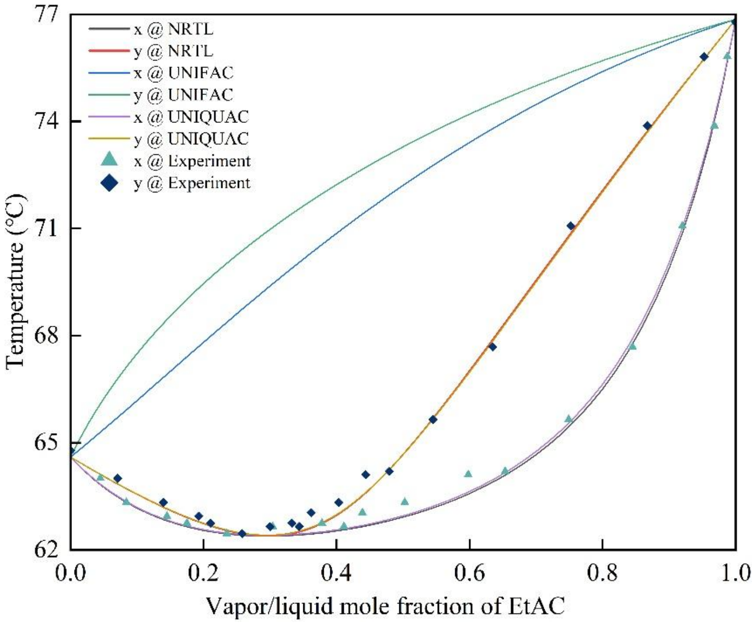

Fig. S3. Comparison of NRTL, UNIQAUC, and UNIFAC models and experiment for the EtAC-MeOH.

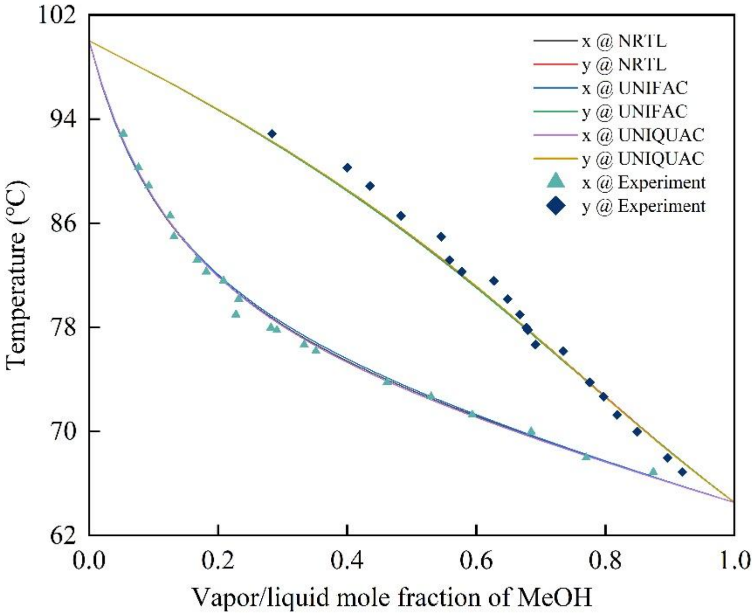

Fig. S4. Comparison of NRTL, UNIQAUC, and UNIFAC models and experiment for the MeOH-Water.

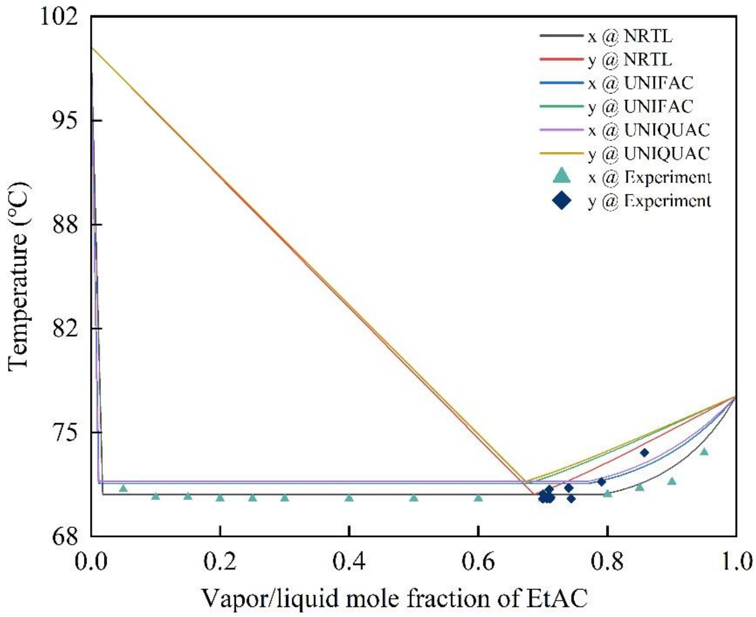

Fig. S5. Comparison of NRTL, UNIQAUC, and UNIFAC models and experiment for the EtAC-Water.

Table S5. Upper and lower bounds of FCED optimization variables.

Decision variable	Lower bound	Upper bound
NT_{PC}	3	15
NF_{PC}	2	13
NT_{EDC}	20	60
NF_{EDC}	10	55
NE_{EDC}	2	20
F_{EDC} (kmol/h)	10	50
RR_{EDC}	0.1	5
NT_{PDC}	15	40
NF_{PDC}	2	20
RR_{PDC}	0.1	5
NT_{SRC}	10	30
NF_{SRC}	2	25
RR_{SRC}	0.1	5

The Process route index (*PRI*) can be estimated via Eq. (S9) as follows:

$$PRI = \frac{AMHV \times AFD \times AP \times AC}{10^8} \tag{S9}$$

where *AMHV* is the average mass heating value in kJ/kg, *AFD* is the average fluid density in kg/m³, *AP* is the average pressure in atm, and *AC* is the average combustibility in %(vol). Associated formulas and parameters for calculating the PRI are presented in **Table S6**.

Table S6. Formulas and parameters for the calculation of process route index (PRI)[1].

Parameter	Value / Formula	Unit
Average mass heating value (*AMHV*)	Obtained from Aspen Plus databanks	kJ/kg
Average fluid density (*AFD*)		kg/m^3
Average pressure (*AP*)		atm
Mole fraction of component i (y_i)		-
Stream temperature (*T*)		°C
Heat of combustion (ΔH_c)		kcal/kmol
Upper flammability limit of a mixture (UFL_{mixture})	$1/\sum_{i=1}^{n}(y_i/UFL_i)$	-
Upper flammability limit of component i (UFL_i)	$UFL \times (1 + 0.75 \times (T - 25)/\Delta H_c)$	-
Lower flammability limit of a mixture (LFL_{mixture})	$1/\sum_{i=1}^{n}(y_i/LFL_i)$	-
Lower flammability limit of component i (LFL_i)	$LFL \times (1 - 0.75 \times (T - 25)/\Delta H_c)$	-
Average combustibility (*AC*)	$UFL_{\text{mixture}} - LFL_{\text{mixture}}$	-

Note: The upper and lower flammability limits at 25 °C are provided in **Table S7**.

Table S7. LFL and UFL of EtAC, MeOH, and DMSO.

Component	UFL	LFL
EtAC	11.5%	2.0%
MeOH	44.0%	5.5%
DMSO	42.0%	0.6%

Table S8. Comparison of TAC-optimal, GGE_{CO_2}-optimal, PIR-optimal, and balanced solutions achieved by MO-DIDC for the FCED process.

		TAC-optimal solution	GGE_{CO_2}-optimal solution	PIR-optimal solution	Balanced solution
Decision variable	NT_{PC}	5	5	4	5
	NF_{PC}	3	3	2	3
	NT_{EDC}	47	48	40	39
	NF_{EDC}	38	38	33	31
	NE_{EDC}	5	4	4	4
	F_{EDC} (kmol/h)	20.3683	20.4248	21.4383	21.9160
	RR_{EDC}	0.731	0.708	0.893	0.754
	NT_{PDC}	28	31	19	23
	NF_{PDC}	14	14	11	13
	RR_{PDC}	2.834	2.742	4.182	3.323
	NT_{SRC}	15	15	15	15
	NF_{SRC}	6	6	6	6
	RR_{SRC}	0.106	0.107	0.112	0.115
Objective function	TAC (10^6 \$/a)	0.5572	0.5576	0.5779	0.5638
	GGE_{CO_2} (t/h)	0.5346	0.5324	0.5669	0.5477
	PRI	4.5603	4.5690	4.5183	4.5292

References

1. Yang A, Ernawati L, Wang M, Kong ZY, Sunarso J, Sun S, Shen W. Multi-objective optimization of the intensified extractive distillation with side-reboiler for the recovery of ethyl acetate and methanol from wastewater. *Separation and Purification Technology*. 2023;310:123131. doi:10.1016/j.seppur.2023.123131