Multi-Objective Optimization of Non-Isothermal Simulated Moving Bed Reactor: Parametric Analyses

Supplementary Materials

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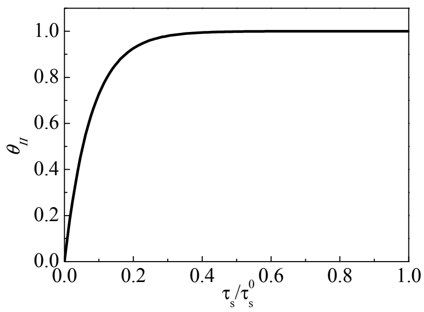

Figure S1 Temperature transition in Zone II during a switch (Case 3)

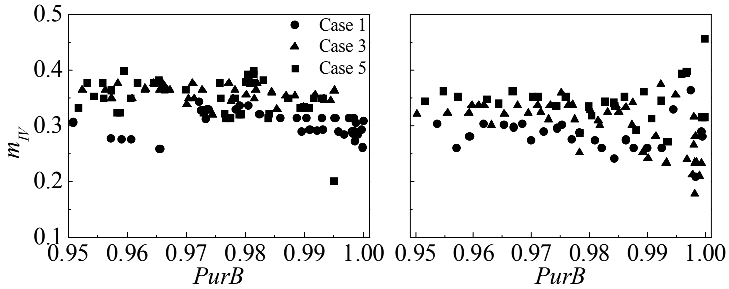

Figure S2 m_{IV} values corresponding to simultaneously maximized *PurB* and *UT*. Cases 1, 3 and 5, α_I equal to 1 and 100.

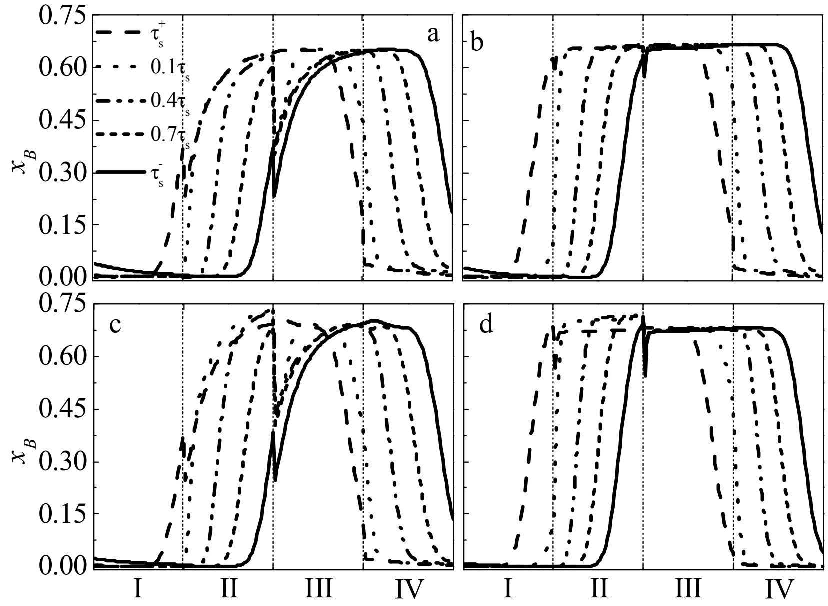

Figure S3 Internal concentration profiles of product *B* corresponding to *PurB*=0.99. a: Case 1, α_1=1; b: Case 1, α_1=100;c: Case 3, α_1=1; d: Case 3, α_1=100.

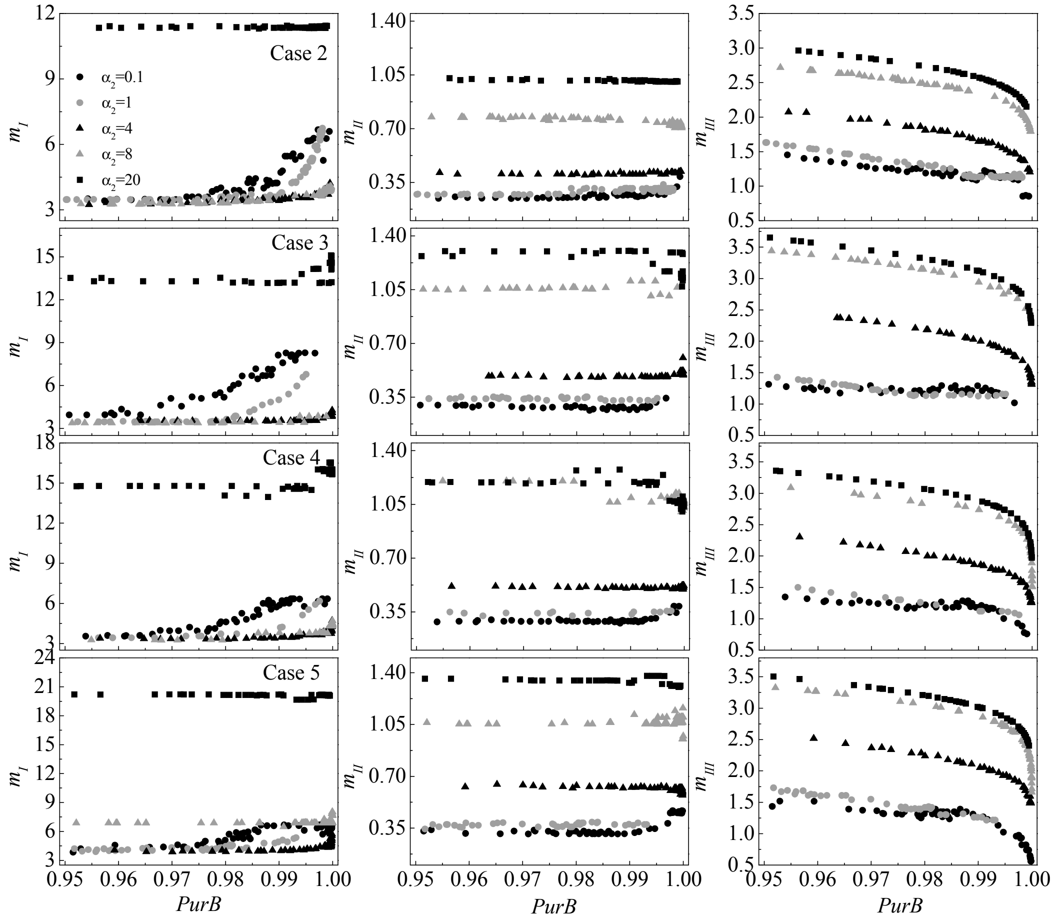

Figure S4 Effects of α_2 on *m* values corresponding to the Pareto solutions for Cases 2, 3, 4, 5.

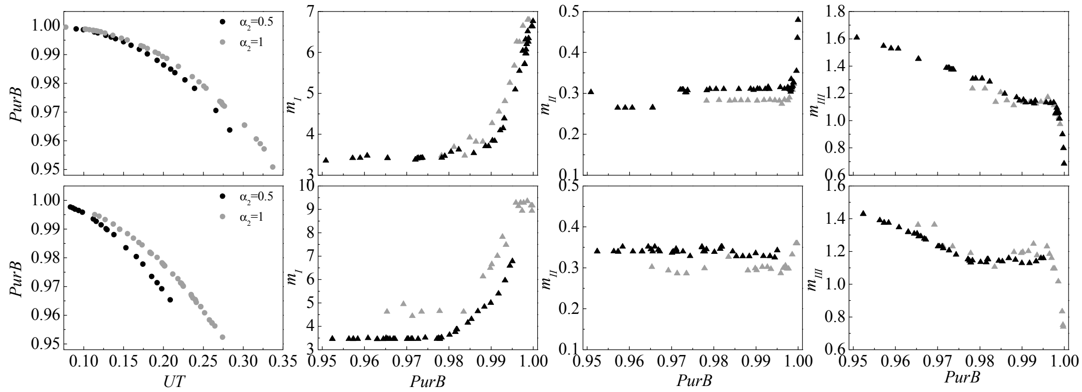

Figure S5 Comparison of α_2 equal to 0.5 and 1. Upper and lower channels are for Cases 1 and 3. From left to right are Pareto curves, m_I, m_{II} and m_{III}.

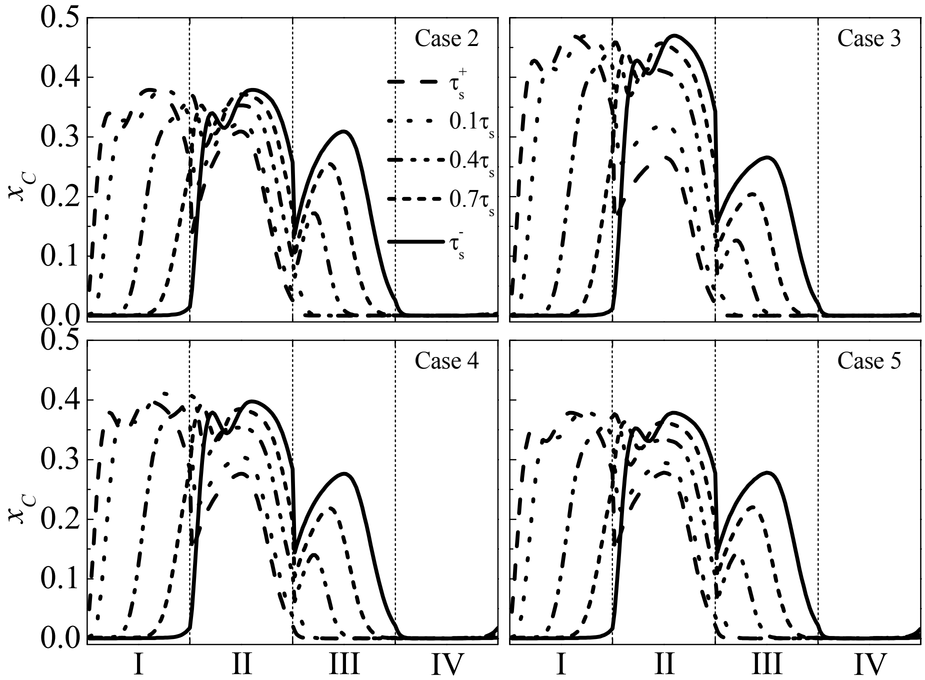

Figure S6 Internal concentration profiles of by product *C* at optimal conditions for *PurB*=0.99, α_2=4, Cases 2, 3, 4, and 5.

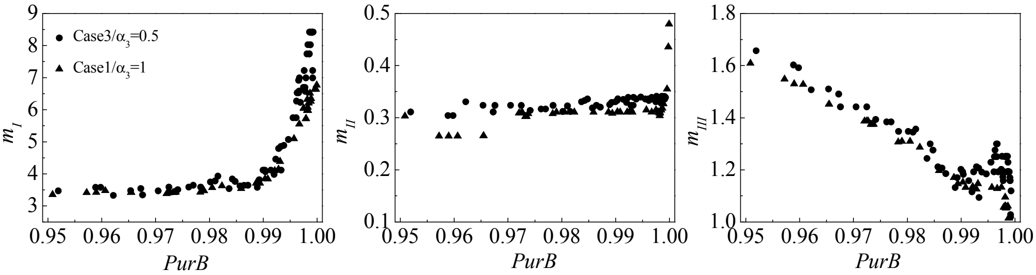

Figure S7 Comparison of *m* values optimized for Case 3/α_3=0.5 and Case 1/α_3=1.

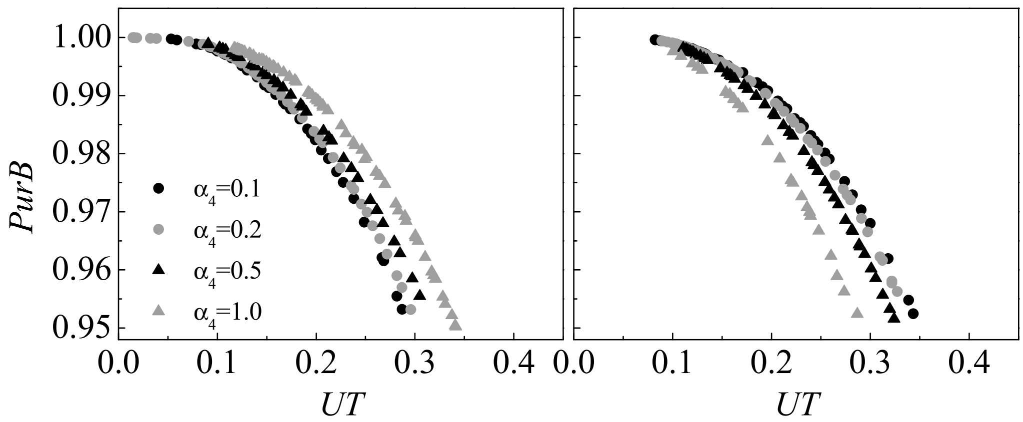

Figure S8 Effects of α_3 on Pareto curves for Cases 2 (left) and 4 (right).

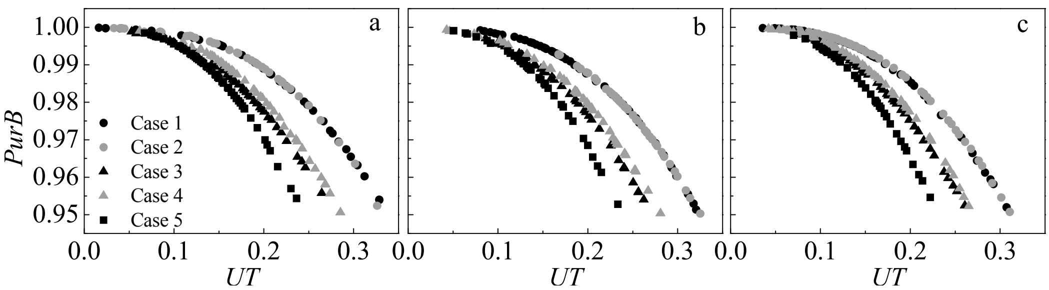

Figure S9 Pareto curves obtained at various feed concentrations. a, b, c for α_4 equal to 2, 5, 10.

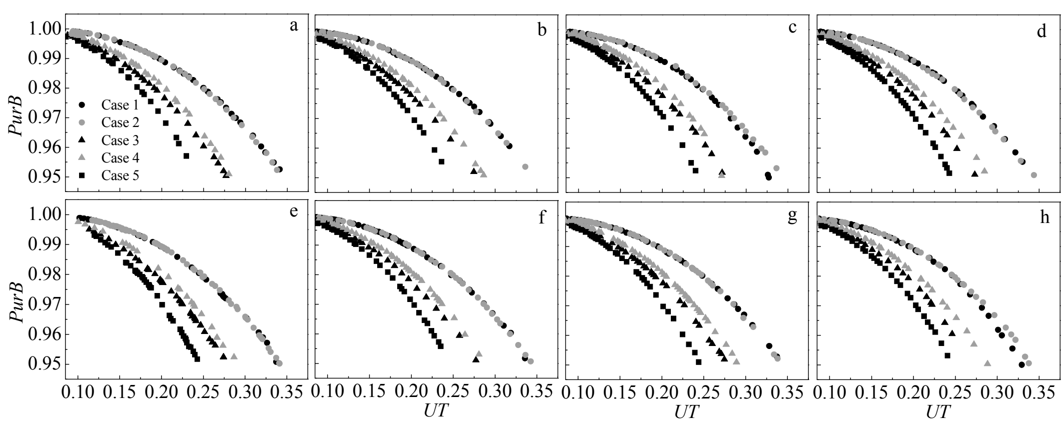

Figure S10 Pareto curves obtained for various reaction enthalpy. a-h are for α_3 equal to -10, -5, -2, -1, 1, 2, 5, 10.

Table S1 Dimensional model parameters

Column		Adsorption equilibrium			Kinetics	
L (m)	0.25		H^0	ΔH_{ads} (kJ·mol^{-1})	k_f^0 / min^{-1}	1.07
d (10^{-3} m)	9.4	A	0.426	-19.64	E_f (kJ·mol^{-1})	44.2
ε	0.4	E	0.375	-9.10	K_{eq} (kJ·mol^{-1})	334.78
N	50	W	2.92	-8.53	ΔH_{rxn} (kJ·mol^{-1})	-5.83
Q^0_{Max} (10^{-8} m^3/s)	5.0	$c_{A,feed}$ (10^3 mol/ m^3)		2.0	$\lambda(10^{-2} s^{-1})$	1.67
T_{max} (K)	308	T_{min} (K)		323	T^{ref} (K)	318

Table S2 Preset upper and lower bounds of variables for the use of NSGA

Para#	Mult$	Bounds of Variables			
		m_I	m_{II}	m_{III}	m_{IV}
Da^{ref}	α_1=1	(2.5,7.5)*	(0.2,0.5)	(0.5,2.0)	(0.1,0.5)
	3	(2.5,6.0)	(0.1,0.5)	(1.0,2.8)	(0.1,0.5)
	4	(2.5,6.0)	(0.1,0.45)	(1.0,2.8)	(0.15,0.5)
	5	(2.8,5.5)	(0.1,0.5)	(1.0,3.0)	(0.15,0.5)
	10	(2.8,5.0)	(0.1,0.45)	(1.3,3.0)	(0.15,0.5)
	100	(2.8,5.0)	(0.1,0.45)	(1.3,3.3)	(0.15,0.5)
H_A^{ref}	α_2=0.1	(2.8,8.75)	(0.15,0.5)	(0.5,1.8)	(0.1,0.5)
	0.5	(2.5,8.75)	(0.15,0.5)	(0.5,2.0)	(0,0.5)
	4	(2.8,7.0)	(0.3,0.75)	(1.0,2.8)	(0.1,0.5)
	8	(2.8,9.5)	(0.5,1.3)	(1.25,3.8)	(0.1,0.5)
	20	(8.0,22.3)	(0.75,1.45)	(1.5,3.8)	(0.1,0.5)

e_f	α_3=0.5	(2.8,9.0)	(0.23,0.45)	(0.5,2.2)	(0.15,0.5)
	0.2	(2.8,9.0)	(0.2,0.5)	(0.5,2.35)	(0.1,0.5)
	0.1	(2.8,9.0)	(0.2,0.5)	(0.5,2.35)	(0.1,0.5)

#:parameter; $: multiplier; *: (lower bound, upper bound).

The bounds for α_1=1 are for original parameters and were also applied to all α_4 and α_5 values.