Travelling Salesman Problem (TSP) based integration of Planning, Scheduling and optimal Control for Continuous Processes

Vassilis M. Charitopoulos, Vivek Dua, Lazaros G. Papageorgiou*

Department of Chemical Engineering, Centre for Process Systems Engineering, University College London, Torrington Place, London WC1E 7JE, United Kingdom

*<u>**Corresponding Author:**</u> l.papageorgiou@ucl.ac.uk

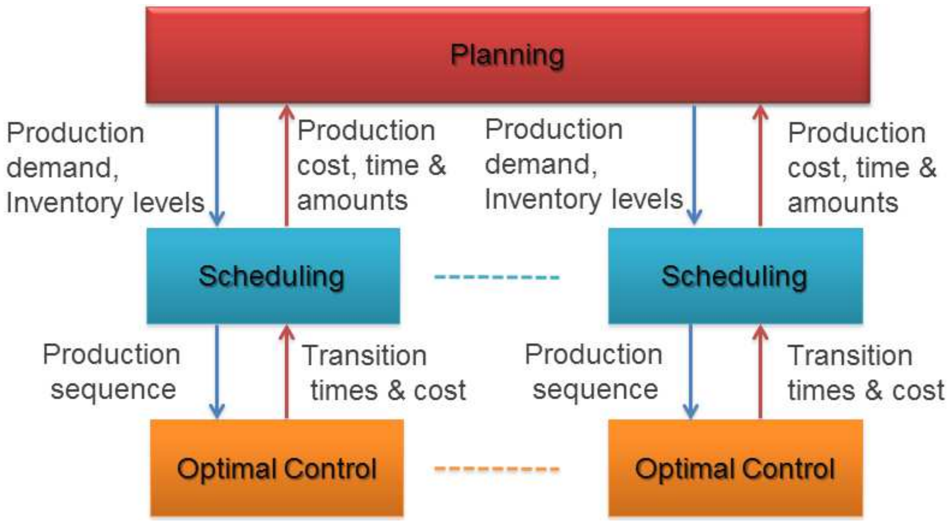


Figure S1: Flow of information across the different levels of decision making within the iPSC

	A	B	C	D	E
A	0	10.435	12.039	15.301	23.679
B	6.4555	0	95.967	91.475	88.432
C	11.71	59.712	0	347.88	248.97
D	22.894	64.231	259.89	0	596.45
E	51.068	89.355	242.84	693.92	0

(a) Slope coefficients (α)

	A	B	C	D	E
A	0	614.43	1360.3	2251.3	4772.1
B	-66.402	0	95.967	1598.1	4078.4
C	-66.891	-141.63	0	797.02	3216.5
D	-66.825	-148.35	-220.62	0	2143.8
E	-66.772	-149.17	-248.86	-343.25	0

(b) Intercept constant (β)

Table S1: Slope and intercept coefficients of the linear metamodels correlating transition cost and transition time, i.e. $\mathrm{CT_{i,j}} = \alpha \mathrm{TT_{i,j}} + \beta$, for the SISO CSTR case study

Table S2: Results of SISO CSTR case study for the case that OCFE is employed with 45 finite elements and 3 collocation points

Model	Monolithic TSP	Decomposed iPSC	
Type	MINLP	MILP (TSP)	Offline: NLP
Constraints	18,607	287	454
Cont. Var.	23,856	256	591
Binary Var.	105	105	-
Solver	SBB/CONOPT3	CPLEX 12.6.1	CONOPT3
Profit ($)	9135867.53	9190849.8263	-
CPU (s)	2220.775	0.078	10.65
Optimal	P1: A→B→D→E→C	P1: A→B→C→D→E	-
Schedule	P2: D→B→A→C→E	P2: E→C→B	-

Table S3: Comparison between the decomposed TSP and T-S formulation for varying planning horizons for the SISO CSTR case study

Planning horizon	4 weeks		6 weeks		12 weeks	
Decomposed Model	**TSP**	**T-S**	**TSP**	**T-S**	**TSP**	**T-S**
Type	MILP	MILP	MILP	MILP	MILP	MILP
Constraints	586	2,209	879	3,287	1,767	6,593
Cont. Var.	516	1,801	776	2,851	1,556	5,701
Binary Var.	235	600	365	900	755	1,800
Solver	CPLEX 12.6.1					
Profit ($)	11018842.48	11018842.48	22168061.83	22168061.83	30425464.1	30425464.1
CPU (s)	0.39	26.162	0.437	382.341	4.4	3440.21
Gap (%)	0	0	0	0	0	0
Sales	1.295400E+7	1.295400E+7	2.672676E+7	2.672676E+7	3.556624E+7	3.556624E+7
Operational cost ($)	27189	27189	169032	169032	75242.66	75242.66
Inventory cost ($)	3597.09	3597.09	289050	289050	14000	14000
Transition cost ($)	97103.638	77237.18	149222.6	149222.6	276475.49	276475.49
Production cost ($)	1806260.509	1806260.509	3746590.50	3746590.50	4847574.78	4847574.78
Backlog cost ($)	1007.273	1007.273	318222.454	318222.454	132154.2	132154.2

Table S4: Economic data for the MIMO CSTR case study

	Price ($/mol)	**Inventory cost ($/mol)**	**Operating cost ($/mol)**
A	17	1.7	0.1
B	25	2	0.2
C	32	1.8	0.35
D	21	3	0.25
E	45	4.5	0.17
F	60	1.5	0.38
G	37	2.3	0.4
H	75	6	0.8

Table S5: Kinetic data for the MIMO CSTR case study

	C_b^{ss} ($\frac{mol}{L}$)	T_l^{ss}(K)	F_l^{ss} ($\frac{m^3}{h}$)	F_c^{ss} ($\frac{m^3}{h}$)	Production rate (mol/h)
A	1	290	1872	792.3	5616
B	1.3	310	1296	270.1	3499.2
C	1.6	325	936	83.4	2246.4
D	2	340	624	15.8	1248
E	2.5	350	374.4	42.2	561.6
F	2.6	355	336	24.6	470.4
G	2.8	310	267.43	279.1	320.914
H	3.3	370	132.36	23.37	92.655

	A	B	C	D	E	F	G	H
A	0	32.823	30.748	29.998	30.291	30.095	32.923	30.081
B	20.831	0	11.094	10.344	10.637	10.440	13.269	10.427
C	13.802	6.782	0	3.315	65.350	3.412	6.240	3.398
D	11.261	3.599	1.694	0	1.067	0.871	3.699	0.857
E	12.255	5.235	2.688	1.768	0	1.865	4.693	1.851
F	11.588	4.568	2.022	1.102	1.395	0	6.351	1.185
G	21.169	13.507	11.433	10.683	10.976	10.779	0	10.766
H	11.543	4.523	1.976	1.056	1.349	1.153	6.181	0

(a) Slope coefficients (α)

	A	B	C	D	E	F	G	H
A	0	$1.12 \cdot 10^{-6}$	$1.5 \cdot 10^{-7}$	0	0	0	0	0
B	$1.07 \cdot 10^{-6}$	0	$1.5 \cdot 10^{-7}$	0	0	0	0	0
C	$1.5 \cdot 10^{-7}$	$1.8 \cdot 10^{-7}$	0	0	$1.13 \cdot 10^{-7}$	0	0	0
D	0	0	0	0	0	0	0	0
E	$1.4 \cdot 10^{-7}$	0	0	0	0	0	0	0
F	0	0	0	0	0	0	0	0
G	0	0	0	0	0	0	0	0
H	0	0	0	0	0	0	$5.11 \cdot 10^{-3}$	0

(b) Intercept constant (β)

Table S6: Slope and intercept coefficients of the linear metamodels correlating transition cost and transition time, i.e. $CT_{i,j} = \alpha TT_{i,j} + \beta$, for the MIMO CSTR case study

Table S7: Demand data for the decomposed iPSC of the MIMO CSTR case study

	P_1	P_2	P_3	P_4	P_5	P_6	P_7	P_8	P_9	P_{10}	P_{11}	P_{12}
A	160000	11000	120000	0	12500	83000	73000	9200	13000	12000	10000	94000
B	80000	5000	7000	43000	21300	4300	12200	12100	132000	32000	22000	12200
C	6000	400	330	420	3000	2900	3400	21000	3200	400	4500	2340
D	30000	5000	23400	12300	11000	13400	4500	3500	2000	3400	2100	1250
E	37000	3000	14000	11500	12800	3400	7200	7260	3720	2890	7210	4030
F	40000	5000	29000	82000	38290	49030	50000	99000	21200	100000	12030	0
G	18500	4000	9400	8300	1200	12000	14000	42000	1300	3200	11000	23000
H	300	300	250	100	280	400	120	115	120	130	140	150

Table S8: Comparison between the decomposed TSP and T-S formulation for varying planning horizons for the MIMO CSTR case study

Planning horizon	4 weeks		6 weeks		12 weeks	
Decomposed Model	**TSP**	**T-S**	**TSP**	**T-S**	**TSP**	**T-S**
Type	MILP	MILP	MILP	MILP	MILP	MILP
Constraints	1,309	8,369	1,971	3,287	3,957	6,593
Cont. Var.	1,209	6,721	1,817	2,851	3,641	5,701
Binary Var.	544	2,304	848	3,456	1,760	6,912
Solver	CPLEX 12.6.1					
Profit ($)	16755710.28	16755710.28	24372569.048	24370455.65	42795858.49	30425464.1
CPU (s)	1.7	2305.43	5.959	382.341	167.405	3440.21
Gap (%)	0	0	0	0	0	0

Table S9: Demand and cost data for the MMA case study

	Planning Period		Operation cost ($/m^3)	Price ($/m^3)
Demand (m^3)	P_1	P_2		
A	30	20	263	288.5
B	16.7	8.3	188	232.8
C	15	10	163	217.8
D	60	10	226	293.0
E	22.2	60.3	220	330.5

	A	B	C	D	E
A	0	0.0452	0.0313	0.0240	0.0163
B	0.0467	0	0.0333	0.0236	0.0140
C	0.0460	0.0261	0	0.0250	0.0141
D	0.0456	0.02562	0.0227	0	0.0148
E	0.0458	0.02563	0.0225	0.1998	0

(a) Slope coefficients (α)

	A	B	C	D	E
A	0	0	0	10^{-7}	0
B	0	0	0	10^{-7}	10^{-7}
C	0	0	0	0	0
D	$1.13{\cdot}10^{-7}$	10^{-7}	0	0	0
E	0	$2 \cdot 10^{-7}$	$5 \cdot 10^{-7}$	10^{-7}	0

(b) Intercept constant (β)

Table S10: Slope and intercept coefficients of the linear metamodels correlating transition cost and transition time, i.e. $\mathrm{CT_{i,j}} = \alpha \mathrm{TT_{i,j}} + \beta$, for the MMA case study

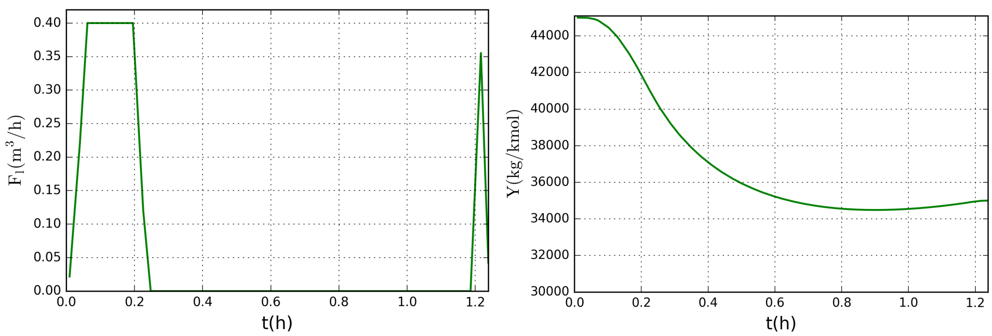
Table S11: Problem statistics for the offline computation of the minimum transition time ($\tau_{\mathrm{i,j}}^{\mathrm{min}}$) for the MMA case study

Solver	CONOPT3	BARON
Type	NLP	NLP
Solution status	Locally optimal	Optimal
Constraints	687	204
Cont. Var.	752	266
CPU (s)*	6.677	36,500

*Cumulative computational time for all the transitions

Table S12: Results of the decomposed iPSC for the MMA case study

	Planning Period I	**Planning Period II**
Production sequence	E → D → C → B → A	A → E → D → C → B
Transition times (h)	1.238, 1.173, 1.278, 2.652	6.505, 1.238, 1.173, 1.278
Production times (h)	22.2, 50, 22.73, 18.55 , 37.5	25, 60.3, 8.33, 9.09, 9.22
Inventory	A:0, B: 0, C: 10, D:0, E:0	A:0, B:0, C:0, D:0, E:0
Sales ($)	73466.25	
Production cost ($)	2071.64	
Inventory cost ($)	0	
Transition cost ($)	60.035	
Backlog cost ($)	0	



(a) $F_l = f(t)$ (b) $y = f(t)$

Figure S2: Transition profiles from E to D

Table S13: Results of the monolithic iPSC for the MMA case study

	Planning Period I	**Planning Period II**
Production sequence	D → B → A → C	E → B
Transition times (h)	1.48, 2.65, 4.45	4.45, 3.47
Production times (h)	58.3, 15.9, 62.5, 22.7	82.5, 11.8
Inventory	A: 20, B: 0, C: 10, D: 10, E: 0	A: 0, B: 0, C: 0, D: 0, E: 0
Backlog	A: 0, B: 2.315, C: 0, D: 0, E: 22.200	A: 0, B: 0, C: 0, D: 0, E: 0

Table S14: Comparison between the decomposed TSP and T-S formulation for the multiple customers case

Planning horizon	8 weeks	
Decomposed Model	**TSP**	**T-S**
Type	MILP	MILP
Constraints	1,736	4,749
Cont. Var.	1,535	4,521
Binary Var.	495	1200
Solver	CPLEX 12.6.1	
Profit ($)	63112.27	63112.27
CPU (s)	30.841	3625.32
Gap (%)	0	0