SUPPORTING INFORMATION

Novel Formulation for Optimal Schedule with Demand Side Management in Multi-product Air Separation Processes

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Hull Reformulation

The Big-M reformulation generates a smaller mixed-integer problem, while the Hull Reformulation, provides in general a tighter formulation. There is a trade-off between the size of the model and the tightness of its LP relaxation. Therefore, we apply the Hull reformulation only to the constraint related to the power consumption (S1). As the power consumption is directly involved in the objective function, its HR will have the greatest impact on the LP relaxation. We disaggregate the following variables: power consumption, $P_{c,t}$, inlet air flow rate, $QA_{c,t}$, and compressed air production, $QCA_{c,t}$, described by equations (S2), (S3) and (S4), respectively. Then we apply the hull reformulation, Eqs. (S5) to (S8).

$$\bigvee_{s \in S_c} \begin{bmatrix} y_{c,s,t} \\ P_{c,t} = \alpha 3_{c,s} \cdot QA_{c,t} + \beta 3_{c,s} \cdot QCA_{c,t} + \gamma_{c,s} \end{bmatrix} \forall c \in C, s \in S_c, t \in T \quad \text{(S1)}$$

$$P_{c,t} = \sum_{s \in S_c} \overline{P}_{c,s,t} \forall\ c \in C, t \in T \quad \text{(S2)}$$

$$QA_{c,t} = \sum_{s \in S_c} \overline{QA}_{c,s,t} \forall\ c \in C, t \in T \quad \text{(S3)}$$

$$CA_{c,t} = \sum_{s \in S_c} \overline{QCA}_{c,s,t} \forall\ c \in C, t \in T \quad \text{(S4)}$$

$$Q\overline{P}_{c,s,t} \leq \alpha 3_{c,s} \overline{QA}_{c,s,t} + \beta 3_{c,s} \overline{QCA}_{c,s,t} + \gamma_{c,s} y_{c,s,t}\ \forall\ c \in C, s \in S_c\ t \in T \quad \text{(S5)}$$

$$P_{c,s}^{min} y_{c,s,t} \leq \overline{P}_{c,s,t} \leq P_{c,s}^{max} y_{c,s,t}\ \forall\ c \in C, s \in S_c\ t \in T \quad \text{(S6)}$$

$$QA_{c,s}^{min} y_{c,s,t} \leq \overline{QA}_{c,s,t} \leq QA_{c,s}^{max} y_{c,s,t}\ \forall\ c \in C, s \in S_c\ t \in T \quad \text{(S7)}$$

$$QCA_{c,s}^{min} y_{c,s,t} \leq \overline{QCA}_{c,s,t} \leq QCA_{c,s}^{max} y_{c,s,t}\ \forall\ c \in C, s \in S_c\ t \in T \quad \text{(S8)}$$

We apply the Hull Reformulation to the power constraint of the different formulations (PB, PSTN and APSTN) for the instance with five states with minimum operating time and different time horizons and time resolutions. Table 3 is extended to incorporate the results.

As expected, the application of the Hull Reformulation increases the number of constraints of the model, leading to improvements in the LP relaxation gap for all the instances. The reductions range between 27% and 42%. It is interesting to note, that the HR reformulation has the greatest impact on the PSTN representation. Without the HR, it was not possible to obtain the optimal solution within an hour of computational time. For the case of the PB representation, the computational times for instances #3 to #5 are reduced, whereas for instance #6 it is increased. Therefore, the effects of the HR on the PB model seems to be instance dependent. Finally, the computational times of the APSTN are increased in all instances, even when the LP relaxation gap is reduced.

Table S1. Comparison between Big-M and Hull Reformulation.

Formulation	Instance	Model size			Cost	LP relaxation gap	# of Nodes	CPUs
		# bin. vars.	# cont. vars.	# constraints				
PB	#3	10,748	24,194	56,452	32,089,462	7.69%	539	44.67
	#4	5,372	12,098	28,228	31,089,044	7.77%	513	11.38
	#5	2,684	6,050	14,116	31,089,230	7.73%	528	4.50
	#6	5,372	12,098	28,228	62,281,349	9.29%	486	11.27
PB-HR	#3	10,748	36,290	69,892	32,089,462	4.43%	3	30.22
	#4	5,372	18,146	34,948	31,089,044	4.54%	0	7.06
	#5	2,684	9,074	17,476	31,089,230	4.50%	0	2.28
	#6	5,372	18,146	34,948	62,281,349	6.20%	1,144	15.55
PSTN	#5	2,686	7,724	27,066	31,089,230	*opt gap: 2.882%*	118,241	3600
PSTN-HR	#4	5,374	31,580	73,656	31,089,012	14.58%	4,559	656.08
	#5	2,686	15,788	37,818	31,089,230	8.30%	1,230	120.11
	#6	5,374	31,580	69,738	62,280,726	*opt gap: 0.001%*	22,775	3600
APSTN	#3	7,385	27,548	83,296	32,089,462	9.17%	515	39.42
	#4	3,689	13,772	41,632	31,089,044	9.19%	0	6.74
	#5	1,841	6,884	20,800	31,089,230	9.17%	0	3.19
	#6	3,689	13,772	41,632	62,281,349	10.76%	0	7.47
APSTN-HR	#3	7,385	39,644	95,392	32,089,462	6.24%	264	117.70
	#4	3,689	19,820	47,680	31,089,044	6.31%	1	20.56
	#5	1,841	9,908	23,824	31,089,230	6.30%	0	5.53
	#6	3,689	19,820	47,680	62,281,349	7.85%	795	25.39