Supporting Information

Integrated Proactive and Reactive Scheduling for Refinery Front-end Crude Movement with Consideration of Unit Maintenance†

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This supporting information contains model sections regarding general logic, vessel unloading, material balance, and LDPL transfer, as well as variable bounds. These developments are based on our previous works[9, 34].

S1. Constraints for general logic

If a transfer operation is scheduled ($X(u,u',n)=1$), then the total transferred volume ($V^t(u,u',n)$) should be constrained within a reasonable range; otherwise it equals zero In addition, the volume of each type of crudes ($V^c(u,u',c,n)$) is bounded as well. The two constraints are expressed in Eqs. (S1) and (S2).

$$S\, X(u,u',n) \le V^t(u,u',n) \le M\ X(u,u',n), \quad \forall u \in CU; u' \in RU(u); n \in N, n \ge 1 \tag{S1}$$

$$V^c(u,u',c,n) \le M\ X(u,u',n), \quad \forall u \in CU; u' \in RU(u); c \in C; n \in N, n \ge 1 \tag{S2}$$

Furthermore, the total transferred volume is restricted by feeding flowrate range and the transfer duration, which is displayed in Eqs. (S3) and (S4).

$$\begin{aligned} &FR^{lo}(u')(Te(u,u',n) - Ts(u,u',n)) - FR^{lo}(u')\, H\,(1 - X(u,u',n)) \le V^t(u,u',n), \\ &\quad \forall u \in CU; u' \in RU(u); n \in N, n \ge 1 \end{aligned} \tag{S3}$$

$$\begin{aligned} &V^t(u,u',n) \le FR^{up}(u')(Te(u,u',n) - Ts(u,u',n)) - FR^{up}(u')\, H\,(1 - X(u,u',n)), \\ &\quad \forall u \in CU; u' \in RU(u); n \in N, n \ge 1 \end{aligned} \tag{S4}$$

S2. Constraints for vessel unloading timing

For transfer operations associated with unloading a vessel, the starting time should be after that of vessel unloading ($TV^s(u)$), and the ending time should be ahead of that of vessel unloading ($TV^e(u)$). The two constraints are formulated in Eqs. (S5) and (S6).

$$TV^s(u) \le Ts(u,u',n) + H\,(1 - X(u,u',n)), \quad \forall u \in V, u' \in RU(u); n \in N, n \ge 1 \tag{S5}$$

$$TV^e(u) \ge Te(u,u',n) - H\,(1 - X(u,u',n)), \quad \forall u \in V,\, u' \in RU(u);\, n \in N,\, n \ge 1 \tag{S6}$$

As required, the unloading operation of one vessel should be completed prior to that of later vessels. This constraint is implemented by Eq. (S7).

$$TV^e(u) \le TV^s(u'), \quad \forall u, u' \in V,\, u < u' \tag{S7}$$

S3. Constraints for material balance

The material balance is applied to both unit inventory and transferred volume in terms of total volume and the volume of each type of crudes. For each charging unit, its total inventory ($Inv^t(u,n)$) is composed by all possible crudes ($Inv^c(u,c,n)$) at every time event. In addition, the inventory of each type of crudes can be calculated by the total inventory and its volume fraction ($f(u,c,n)$). These logics are formulated by Eqs. (S8) through (S10), where $Inv^0(u)$ and $f^0(u,c)$ represent the initial inventory and crude fraction in unit u.

$$Inv^t(u,n) = \sum_{c \in C} Inv^c(u,c,n), \quad \forall u \in CU;\, n \in N,\, n \ge 1 \tag{S8}$$

$$Inv^c(u,c,n) = Inv^0(u)\, f^0(u,c), \quad \forall u \in CU;\, c \in C;\, n \in N,\, n = 0 \tag{S9}$$

$$Inv^c(u,c,n) = Inv^t(u,n)\, f(u,c,n), \quad \forall u \in ST \bigcup CT;\, c \in C;\, n \in N,\, n \ge 1 \tag{S10}$$

For each vessel, its initial inventory should be totally unloaded within the scheduling time horizon. At each time event, its current inventory of crude c equals that in previous time event minus its transferred quantity. The two constraints are formulated in Eqs. (S11) and (S12).

$$Inv^0(u) = \sum_{u' \in RU(u)} \sum_{n \in N, n \ge 1} V^t(u,u',n), \quad \forall u \in V \tag{S11}$$

$$\begin{aligned} Inv^c(u,c,n) = Inv^c(u,c,n-1) - \sum_{u' \in RU(u)} V^t(u,u',n)\, f^0(u,c), \\ \forall u \in V;\, c \in C;\, n \in N,\, n \ge 1 \end{aligned} \tag{S12}$$

Considering the input and output, the inventory of crude c in tank units at time event n can be calculated following Eqs. (S13) and (S14). Due to the presence of the LDPL, the composition of received slots of CTs may be different from that of charged slots from STs. Thus, the transferred volume of crude c can be corrected by $V1^c(u,u',c,n)$, which will be explained later, following Eq. (S14). The input and output volume should be constrained by unit maximum and minimum capacity, and the inventory at previous time event as displayed in Eqs. (S15) and (S16).

$$\begin{aligned} & Inv^c(u,c,n) = Inv^c(u,c,n-1) + \sum_{u' \in CU(u)} V^c(u',u,c,n) - \sum_{u'' \in RU(u)} V^c(u,u'',c,n), \\ & \quad \forall u \in ST; c \in C; n \in N, n \geq 1 \end{aligned} \tag{S13}$$

$$\begin{aligned} & Inv^c(u,c,n) = Inv^c(u,c,n-1) + \sum_{u' \in CU(u)} V1^c(u',u,c,n) - \sum_{u'' \in RU(u)} V^c(u,u'',c,n), \\ & \quad \forall u \in CT; c \in C; n \in N, n \geq 1 \end{aligned} \tag{S14}$$

$$Inv^t(u,n-1) + \sum_{u' \in CU(u)} V^t(u',u,n) \leq Inv^{\max}(u), \quad \forall u \in ST \bigcup CT; n \in N, n \geq 1 \tag{S15}$$

$$Inv^t(u,n-1) - \sum_{u' \in RU(u)} V^t(u,u',n) \geq Inv^{\min}(u), \quad \forall u \in ST \bigcup CT; n \in N, n \geq 1 \tag{S16}$$

Specially, to ensure the continuous supply for CDUs in the next scheduling problem, each CT need to maintain necessary inventories at the end of scheduling time horizon, as constrained by Eq. (S17).

$$Inv^t(u,n) \geq S\ Inv^{\max}(u), \quad \forall u \in CT; n \in N, n = |N| \tag{S17}$$

Similar to tank inventory $Inv^t(u,n)$, $V^t(u,u',n)$ is also composed by all possible crudes ($V^c(u,u',c,n)$) as shown in Eq. (S18), and the transferred volume of crude c can be calculated following Eq. (S19).

$$V^t(u,u',n) = \sum_{c \in C} V^c(u,u',c,n), \quad \forall u \in ST \bigcup CT, u' \in RU(u); n \in N, n \geq 1 \tag{S18}$$

$$V^{c}(u,u',c,n) = V^{t}(u,u',n)\ f(u,c,n-1), \quad \forall u \in ST \cup CT; u' \in RU(u); c \in C; n \in N, n \geq 1 \tag{S19}$$

The key component (i.e., sulfur content) of crude mixtures inside CTs should be strictly constrained following the blending specifications and its fraction is estimated following linear combination. The constraints are displayed in Eqs. (S20) through (S22).

$$Inv^{k}(u,k,n) = \sum_{c \in C} Inv^{c}(u,c,n)\ f^{k}(c,k), \quad \forall u \in CT; k \in K; n \in N, n \geq 1 \tag{S20}$$

$$Inv^{t}(u,n)\ f^{k,lo}(u,k) \leq Inv^{k}(u,k,n), \quad \forall u \in CT; k \in K; n \in N, n \geq 1 \tag{S21}$$

$$Inv^{k}(u,k,n) \leq Inv^{t}(u,n)\ f^{k,up}(u,k), \quad \forall u \in CT; k \in K; n \in N, n \geq 1 \tag{S22}$$

S4. Constraints for LDPL transfer

In this work, the LDPL is utilized to connect STs and CTs. The following part is designated to model the LDPL transfer. One type of crudes or crude mixtures inside the LDPL denotes one slot. There are one or more slots existing in the LDPL as initial status. During the scheduling time horizon, STs charge new slots into the LDPL and "old" slots are discharged into CTs. Binary variable $W(u,l,n)$ is employed to represent the charging operation of STs, if unit u feeds slot l into the LDPL at time event n, then $W(u,l,n)=1$; otherwise, $W(u,l,n)=0$. If a new slot is scheduled, it should be continuously fed by one unit at one time event, as constrained by Eq. (S23); and only after one slot has been fed, its later slot can be charged, as expressed by Eq. (S24).

$$\sum_{u \in ST} \sum_{n \in N, n \geq 1} W(u,l,n) \leq 1, \quad \forall l \in L^{new} \tag{S23}$$

$$W(u,l+1,n) \leq \sum_{u' \in ST} \sum_{n' \in N, 1 \leq n' \leq n} W(u',l,n'), \quad \forall u \in ST; l \in L^{new}; n \in N, n \geq 1 \tag{S24}$$

In addition, if a transfer operation takes place between one ST and one CT (*X(u,u',n)=1*), it indicates that this ST charges a new slot into the LDPL (*W(u,l,n)=1*), meanwhile, this slot is pushing crudes into that CT (*XL(l,u',n)=1*). This logic can be expressed by Eqs. (S25) and (S26).

$$\sum_{l \in L^{new}} W(u,l,n) = \sum_{u' \in RU(u)} X(u,u',n), \quad \forall u \in ST; n \in N, n \geq 1 \tag{S25}$$

$$XL(l,u',n) \geq X(u,u',n) + W(u,l,n) - 1, \quad \forall u \in ST, u' \in RU(u); l \in L^{new}; n \in N, n \geq 1 \tag{S26}$$

Associated with *W(u,l,n)*, $VL^t(u,l,n)$ represents the total charging volume of new slot *l*. Similar to Eq. (S18), it is composed by the volume of each type of crudes as shown in Eq. (S27).

$$VL^t(u,l,n) = \sum_{c \in C} VL^c(u,l,c,n), \quad \forall u \in ST; l \in L^{new}; n \in N, n \geq 1 \tag{S27}$$

The transferred volume of crude *c* in slot *l* cannot exceed the total transferred volume of crude c and the unit maximum inventory as constrained by Eqs. (S28) through (S30).

$$VL^c(u,l,c,n) \leq \sum_{u' \in RU(u)} V^c(u,u',c,n), \quad \forall u \in ST; l \in L^{new}; c \in C; n \in N, n \geq 1 \tag{S28}$$

$$VL^c(u,l,c,n) \leq Inv^{\max}(u) W(u,l,n), \quad \forall u \in ST; l \in L^{new}; c \in C; n \in N, n \geq 1 \tag{S29}$$

$$\begin{aligned} VL^c(u,l,c,n) \geq & \sum_{u' \in RU(u)} V^c(u,u',c,n) - Inv^{\max}(u)(1 - W(u,l,n)), \\ & \forall u \in ST; l \in L^{new}; c \in C; n \in N, n \geq 1 \end{aligned} \tag{S30}$$

For the sequencing of ST charging operations, the starting time of charging later slots should take place after the ending time of charging previous slots, as formulated in Eq. (S31).

$$\begin{aligned} & Ts(u,u',n) + H(-X(u,u',n)) + H(1 - W(u,l,n)) \geq \\ & Te(u'',u''',n') - H(1 - X(u'',u''',n')) - H(1 - W(u'',l',n')), \\ & \quad \forall u, u'' \in ST, u' \in RU(u), u''' \in RU(u''); l, l' \in L^{new}, l > l'; n, n' \in N, n > n' \geq 1 \end{aligned} \tag{S31}$$

If slot *l* is charged by unit *u* (*W(u,l,n)=1*), then the slot composition should be equal to that of unit u at previous time event as expressed by Eqs. (S32) and (S33). On the other hand, if slot l is not charged, then the slot composition will be enforced as zero. This logic is expressed in Eq. (S34)

$$f^{l}(l,c) \geq f(u,c,n-1) - (1 - W(u,l,n)), \quad \forall u \in ST; l \in L^{new}; c \in C; n \in N, n \geq 1 \tag{S32}$$

$$f^{l}(l,c) \leq f(u,c,n-1) + (1 - W(u,l,n)), \quad \forall u \in ST; l \in L^{new}; c \in C; n \in N, n \geq 1 \tag{S33}$$

$$f^{l}(l,c) \leq \sum_{u \in ST} \sum_{n \in N, n \geq 1} W(u,l,n), \quad \forall l \in L^{new}; c \in C \tag{S34}$$

Note that transfer operations through the LDPL are not instantaneous. A binary variable $Y(l,l',n)$ is introduced to present such a behavior. If slot l is charged at time event n and it pushes slot l' out from the LDPL, then $Y(l,l',n)=1$; otherwise, $Y(l,l',n)=0$. When STs feed first new slots into the LDPL, the first slot initially existing inside the LDPL will be pushed out, as constrained by Eq. (S35).

$$\sum_{u \in ST} W(u,l,n) = Y(l,l',n), \quad \forall l \in L^{new}, l = \left|L^{new}\right| + 1, l' \in L^{ini}, l' = 1; n \in N, n \geq 1 \tag{S35}$$

Corresponding to $Y(l,l',n)$, the discharged volume of slot l' ($VD^{t}(l,l',n)$) should be bounded by Eqs. (S36) and (S37). In addition, the total discharged volume equals the injected volume of slot l as represented by Eq. (S38). The transferred volume of crude c during the injection of slot l ($VD^{c}(l,c,n)$) can be calculated following Eq. (S39).

$$VD^{t}(l,l',n) \leq VD^{t,up}(l,l',n) Y(l,l',n), \quad \forall l \in L^{new}; l' \in L, l' \geq l; n \in N, n \geq l \tag{S36}$$

$$VD^{t}(l,l',n) \geq S\, Y(l,l',n), \quad \forall l \in L^{new}; l' \in L, l' \leq l\ n \in N, n \geq l \tag{S37}$$

$$\sum_{u \in ST} VL^{t}(u,l,n) = \sum_{l' \in L, l' \leq l} VD^{t}(l,l',n), \quad \forall l \in L^{new}; n \in N, n \geq l \tag{S38}$$

$$VD^{c}(l,c,n) = \sum_{l' \in L, l' \leq l} VD^{t}(l,l',n)\, f^{l}(l',c), \quad \forall l \in L^{new}; n \in N, n \geq l \tag{S39}$$

Based on $VD^{c}(l,c,n)$, the volume discharged from slot l into CTs ($VL1^{c}(l,u,c,n)$)can be correctly determined; if slot l is discharged into unit u at time event n ($XL(l,u,n)=1$), then

$VL1^c(l,u,c,n)$ equals $VD^c(l,c,n)$; otherwise, it equals zero. This logic is expressed by Eqs. (S40) though (S42).

$$VL1^c(l,u,c,n) \le VD^c(l,c,n), \quad \forall l \in L^{new}; u \in CT; n \in N, n \ge l \tag{S40}$$

$$VL1^c(l,u,c,n) \le VD^{c,up}(l,c,n)\, XL(l,u,n), \quad \forall l \in L^{new}; u \in CT; n \in N, n \ge l \tag{S41}$$

$$\begin{aligned} &VL1^c(l,u,c,n) \ge VD^c(l,c,n) - VD^{c,up}(l,c,n)(1 - XL(l,u,n)), \\ &\quad \forall l \in L^{new}; u \in CT; n \in N, n \ge l \end{aligned} \tag{S42}$$

The obtained discharged volume is exactly the corrected transferred volume from STs to CTs, corresponding to the transfer operation $X(u,u',n)$ as expressed in Eq. (S43). And the sum of the corrected volume of each type of crudes should equal the total transferred volume as shown in Eq. (S44).

$$\sum_{l \in L^{new}} VL1^c(l,u,c,n) = \sum_{u' \in CU(u)} V1^c(u',u,c,n), \quad \forall l \in L^{new}; u \in CT; n \in N, n \ge l \tag{S43}$$

$$\sum_{c \in C} V1^c(u,u',c,n) = V^t(u,u',n), \quad \forall u \in ST, u' \in RU(u); n \in N, n \ge l \tag{S44}$$

To characterize the material balance inside the LDPL, variable $Invl(l,l',n)$ is used to denote the leftover inventory of slot l' after slot l has been charged into the pipeline at time event n. The leftover inventory of slot l' can be calculated following Eqs. (S45) and (S46).

$$\begin{aligned} &\sum_{u \in ST} VL^t(u,l,n) + Invl(l',l,n-1) = Invl(l,l'',n) + VD^t(l,l'',n), \\ &\quad \forall l,l'' \in L^{new}, l = l'', l' \in L, l' = |L|; n \in N, n \ge 1 \end{aligned} \tag{S45}$$

$$Invl(l,l',n) = Invl(l-1,l',n) - VL^t(u,l,n), \quad \forall l \in L^{new}, l' \in L, l > l'; n \in N, n \ge 1 \tag{S46}$$

Associated with $Invl(l,l',n)$, binary variable $Z(l,l',n)$ is introduced to indicate the status of slot l'. If slot l' has inventory left after the injection of slot l, then $Z(l,l',n)=1$; otherwise, $Z(l,l',n)=0$. This constraint is expressed in Eqs. (S47) and (S48).

$$Invl(l,l',n) \le VOL\, Z(l,l',n), \quad \forall l \in L^{new}; l' \in L, l \ge l'; n \in N, n \ge 1 \tag{S47}$$

$$Invl(l,l',n) \ge S\, Z(l,l',n), \quad \forall l \in L^{new}; l' \in L, l \ge l'; n \in N, n \ge 1 \tag{S48}$$

In addition, if slot l pushes slot $l'+1$ out at time event n, it means that slot l has no inventory left; thus, $Z(l,l',n)=0$. This logic is formulated by Eq. (S49).

$$Z(l,l',n) \le 1 - Y(l,l'+1,n), \quad \forall l \in L^{new}; l' \in L, l \ge l' \ge 2; n \in N, n \ge 1 \tag{S49}$$

Equations (S50) and (S51) are employed to initialize $Invl(l,l',n)$.

$$Invl(l,l',n) = Invl^{0}(l), \quad \forall l,l' \in L, l = |L|; n \in N, n = 0 \tag{S50}$$

$$Invl(l,l',n) = Invl(l'',l',n-1), \quad \forall l,l' \in L^{ini}, l = |L^{ini}|; l'' \in L, l'' = |L|; n \in N, n \ge 1 \tag{S51}$$

S5. Variable bounds

The following constraints (Eqs. (S52) through (S69)) impose variable bounds.

$$0 \le f(u,c,n) \le 1 \tag{S52}$$

$$0 \le f^{k}(c,k) \le 1 \tag{S53}$$

$$0 \le f^{l}(l,c) \le 1 \tag{S54}$$

$$0 \le Inv^{c}(u,c,n) \le Inv^{\max}(u) \tag{S55}$$

$$0 \le Inv^{k}(u,k,n) \le \max_{c}(f^{k}(c,k))\, Inv^{\max}(u) \tag{S56}$$

$$Inv^{\min}(u) \le Inv^{t}(u,n) \le Inv^{\max}(u) \tag{S57}$$

$$0 \le Invl(l,l',n) \le VOL \tag{S58}$$

$$0 \le Ts(u,u',n) \le H \tag{S59}$$

$$0 \le Te(u,u',n) \le H \tag{S60}$$

$$TV^{arr}(v) \le TV^{s}(v) \le H \tag{S61}$$

$$TV^{arr}(v) \le TV^{e}(v) \le H \tag{S62}$$

$$0 \le V^{t}(u,u',n) \le Inv^{\max}(u) - Inv^{\min}(u) \tag{S63}$$

$$0 \le V^{c}(u,u',c,n) \le Inv^{\max}(u) - Inv^{\min}(u) \tag{S64}$$

$$0 \le V1^{c}(u,u',c,n) \le Inv^{\max}(u) - Inv^{\min}(u) \tag{S65}$$

$$0 \le VD^{t}(l,l',n) \le VOL \tag{S66}$$

$$0 \le VL^{t}(u,l,n) \le Inv^{\max}(u) - Inv^{\min}(u) \tag{S67}$$

$$0 \le VL^{c}(u,l,c,n) \le Inv^{\max}(u) - Inv^{\min}(u) \tag{S68}$$

$$0 \le VL1^{c}(l,u,c,n) \le Inv^{\max}(u) - Inv^{\min}(u) \tag{S69}$$