Computational Experience with Piecewise-Linear Relaxations for Petroleum Refinery Planning

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Supplementary Materials

Appendix A: Mathematical Formulation

A.1. Crude Distillation Unit

Total crude oil feed to CDU is given by:

$$\sum_p Q_{u,p} \leq \sum_{cr} F_{cr}\,, u = \text{CDU} \qquad \text{(A1)}$$

where F_{cr} = flow rate of crude oil type cr and $Q_{u,p}$ = flow rate of CDU fraction (i.e., cut) p.

CDU capacity is described by:

$$L_u \leq cp_u^{\max}, \quad \forall u \in U \tag{A2}$$

where L_u = load of unit u and $cp_u^{\max}$ = maximum capacity of u.

CDU outlet flow rate of cut p is given by:

$$Q_{u,p} = L_u W_p, \quad u = \text{CDU}, \quad \forall p \in P \tag{A3}$$

where W_p = weight transfer ratio of p that is determined based on true boiling point data of cr.

Weight transfer ratio of p sums to unity:

$$\sum_p W_p = 1 \tag{A4}$$

Middle-of-point (or midpoint) weight transfer ratio MW_p of fraction p is given by:

$$MW_p = 100\left(\sum_{p'} W_{p'} + \frac{1}{2} W_p\right), \quad \forall\, p \in P \backslash \{BR\}. \tag{A5}$$

A.2. Fluid Catalytic Cracking Unit

CDU cut of bottom residue is fed to FCC to be converted into more valuable products. FCC outlet flow rate of product fraction f is given by:

$$Q_{\text{FCC},f} = L_{\text{FCC}} Y_f, \quad \forall f \in F \tag{A6}$$

where $Q_{\text{FCC},f}$ = flow rate of f from FCC and Y_f = weight transfer ratio of f from FCC.

All weight transfer ratios of $f \in F$ sums to unity:

$$\sum_f Y_f = 1. \tag{A7}$$

Y_f is determined using the following regression-based relation:

$$Y_f = a_f^0 + a_f^1(\text{conv} - z_f) + a_f^2(\text{conv} - z_f)^2, \quad \forall f \tag{A8}$$

where regression coefficients given by a_f^0, a_f^1, and a_f^2 are known constants.

To achieve a desired FCC conversion level, part of its outlet flow of total gas oil (TGO) is recycled (as Q_p^R) and mixed with total inlet feed (Q_u^T):

$$Q_{\mathrm{FCC}}^T = Q_{\mathrm{CDU,BR}} + Q_{\mathrm{TGO}}^R \quad \text{(A9)}$$

where Q_{FCC}^T = total inlet flow rate to FCC, $Q_{\mathrm{CDU,BR}}$ = flow rate of bottom residue (BR) outlet stream from CDU, and Q_{TGO}^R = flow rate of TGO recycle stream.

FCC load is equal to its inlet flow rate:

$$L_{\mathrm{FCC}} = Q_{\mathrm{FCC}}^T \quad \text{(A10)}$$

TGO recycle stream flow rate are bounded (from above) by the following constraints:

$$Q_{\mathrm{TGO}}^R \leq \frac{1}{2} Q_{\mathrm{CDU,BR}} \quad \text{(A11)}$$

$$Q_{\mathrm{TGO}}^R \leq Q_{\mathrm{FCC,FHO}}^P \quad \text{(A12)}$$

Remaining TGO stream (after split for recycle) is sold as heavy oil (FHO):

$$Q_{\mathrm{FCC,FHO}} = Q_{\mathrm{FCC,TGO}} - Q_{\mathrm{TGO}}^R \quad \text{(A13)}$$

where $Q_{\mathrm{FCC,FHO}}$ = flow rate of FHO product from FCC.

A.3. Gasoline Blending Unit

Lighter CDU fractions of GO and HN are processed further to improve their for gasoline blending to meet required research octane number (RON) specifications:

$$Q_{\mathrm{CDU},p} = \sum_{g \in G} F_{p,g}^P, \quad \forall p \in P_g \quad \text{(A14)}$$

where $F_{p,g}^P$ = flow rate of gasoline product grade g, G = set of gasoline product grades with RON of 90 (g_{90}) and 93 (g_{93}), and P_g = set of CDU fractions for gasoline blending.

To improve product quality, additives (e.g., MTBE) are mixed with blended CDU fractions according to the following relation:

$$Q_p^P = \sum_{g \in G} F_{p,g}^P + \sum_r Q_r^A, \quad \forall p \tag{A15}$$

where Q_r^A = flow rate of additive r and Q_p^P = flow rate of final product p.

FCC gasoline fraction called $Fgas$ is blended to improve its quality. The flow rate of FCC blended fraction equals the sum of flow rates of its respective blended products, as follows:

$$Q_{t,f}^{iprod} = \sum_g F_{f,g}^{iprod}, f = \text{Fgas} \tag{A16}$$

where $Q_{t,f}^{fprod}$ is the flow rate of final product fraction f (Fgas), $F_{f,g}^{iprod}$ is the flow rate of intermediate blended product g, which is produced by blending flow stream Fgas from FCC.

The gasoline final products g90 and g93 are sold to customers. Their flow rates are calculated using equation (A17).

$$Q_g^{fprod} = F_{f,g}^{iprod} + \sum_r F_{r,g}^{iprod} + \sum_p F_{p,g}^{iprod}, f = \text{Fgas}, p \in P_g, \forall g \tag{A17}$$

where Q_g^{fprod} represents flow of final product g.

A.4. Diesel Blending Unit

Heavier CDU fractions LD and HD are blended in the DB to improve their properties such as, pour point. Flow rate of each CDU fraction p to DB equals the sum of flow rates of its respective diesel blended products (d0 and d10). These blended products are called as $iprod$, and modelled using equation (A18).

$$Q_{u,p} = \sum_{d} F_{p,d}^{iprod}, u = \text{CDU}, \forall p \in P_d \tag{A18}$$

where $F_{p,d}^{iprod}$ is the flow rate of intermediate product d from the DB, which is produced by blending feed p (LD, HD) from the CDU.

The final products d10 and d0, from the DB are sold to customers. Their flow rates are calculated using equation (A19).

$$Q_{d}^{fprod} = \sum_{p} F_{p,d}^{iprod}, p \in P_d, \forall d \tag{A19}$$

where Q_{d}^{fprod} represents flow rate of final product d from DB.

A.5. Quality Specifications

Octane numbers of light CDU fractions GO and HN and pour points of CDU heavy fractions LD and HD are calculated using property correlations from the literature:

$$Pr_{j,p} = a0_p + a1_p\left(MW_p - z_p\right) + a2_p\left(MW_p - z_p\right)^2, \forall j, \forall p \in (P_g \cup P_d) \tag{A20}$$

Minimum octane number specifications for gasoline blended product g90 and g93 are given by:

$$\text{RON}_g Q_{g}^{fprod} \leq Pr_{j,p} F_{p,g}^{iprod} + Pr_{j,r} F_{r,g}^{iprod} + Pr_{j,p'} F_{p',g}^{iprod} + Pr_{j,f} F_{f,g}^{iprod}, \tag{A21}$$

$$j = \text{ON}, p = \text{GO}, p' = \text{HN}, f = \text{Fgas}, \forall g, r$$

where RON_g is the research octane number of gasoline blended products g90 and g93.

A.6. Demand Requirement

Market demand of final products s (g90, g93, d0, d10, FHO, C24) is written as:

$$Q_{s}^{fprod} \leq D_{s}^{max}, \forall s \tag{A22}$$

where D_{s}^{max} is the maximum demand of final product *s*.

A.7. Variable Bounds

FCC conversion level is bounded by equation (A23).

$$conv^{\mathrm{LO}} \leq conv \leq conv^{\mathrm{UP}} \quad \text{(A23)}$$

A.8. Objective Function

The objective function for refinery profit is defined as:

$$Profit = Price\ of\ valuable\ products - crude\ oil\ cost - additive\ raw\ materials\ cost - opertional\ cost\ of\ units$$

$$Profit = \sum_s Q_s^{fprod} C_s^{fprod} - \sum_{cr} L_{u'} C_{cr} - \sum_r F_{r,g}^{iprod} C_r - \sum_u L_u C_u , u' = \mathrm{CDU}, \forall g \quad \text{(A24)}$$

where C_s^{fprod} is the price of sellable products, C_{cr} is the cost of crude oil, C_r is the cost of additive raw materials, $C_u$is the operating cost of process unit u.

Nomenclature

Sets

CR	Crude oils
U	Process units {CDU, FCC}
P	CDU fractions {GO, HN, LD, HD, BR}
P_g	Feed to GB {GO, HN}
P_d	Feed to DB {LD, HD}
F	FCC fractions {Fgas, C24, FHO, Coke}
G	Products of GB {g90, g93}
D	Products of DB {d0, d10}
R	Additive raw materials {MTBE}
S	Sellable products {g90, g93, d0, d10, C24, FHO}
J	Quality properties, octane number and pour point {ON, PP}
N	Set containing grid-points/number of partitions{1,2,3,…,N}
RON_g	Research octane number of GB products {90,93}

Indices

u, u'	Refinery process units
p, p'	Material stream from CDU unit
f	Material stream from FCC unit
g	Material stream from gasoline blending unit
d	Material stream from diesel oil blending unit
r	Additive raw material stream for improving product quality
s	Sellable products
j	Property

Parameters

cp_u^{max}	Maximum capacity of refinery process unit u

F_{cr}	Flow rate of crude oil
$a0_p, a1_p, a2_p, z_p$	Correlation coefficients for CDU fractions p
$a0_f, a1_f, a2_f, z_f$	Correlation coefficients for FCC fractions f
C_s^{fprod}	Price of sellable product s
C_r	Cost of additive raw materials r
C_u	Operating cost of refinery units
C_{cr}	Cost of crude oil
D_s^{max}	Maximum demand of sellable product s
$Pr_{j,r}$, $Pr_{j,f}$	Property specification j of material streams r and f

Continuous Variables

L_u	Load of process unit u
$Q_{u,p}$	Flow rate of CDU fraction p from process unit u
W_p	Weight transfer ratio of CDU fraction p
Q_f^{fprod}	Flow rate FCC final product f
Y_f	Weight transfer ratio of FCC product streams f
conv	FCC conversion level
Rcy	Recycled stream of FCC product FHO
Q_t	Sum of flow rates of FCC recycle stream and FCC feed
$F_{t,f}^{iprod}$	Flow rate of FCC intermediate product stream f, which is produced by total mixed feed stream t to FCC unit
$F_{p,g}^{iprod}$	Flow rate of intermediate product stream g (g90, g93) from GB, which is produced by blending CDU fraction p
Q_r	Flow rate of additive raw material r to GB to improve blended products quality
$F_{r,g}^{iprod}$	Flow rate of stream g (g90, g93) from GB, which is produced by blending additive raw material stream r
Q_g^{fprod}	Final products flow rate (g90, g93) from GB

$F_{p,d}^{iprod}$	Flow rate of intermediate product stream d from DB, which is produced by blending CDU fraction p
Q_d^{fprod}	Final products flow rate (d0, d10) from DB
Q_s^{fprod}	Flow of final sellable products s
MW_p	Mid-point weight transfer ratio of CDU fraction p
$Pr_{j,p}$	Property specification j of CDU fraction p
Profit	Total profit of the refinery

Other – Subscripts and Superscripts

$iprod$	Intermediate product
$fprod$	Final product

Abbreviations

CDU	Crude Distillation Unit
FCC	Fluid Catalytic Cracking Unit
GB	Gasoline Blending Unit
DB	Diesel Oil Blending Unit
GO	Gross Overhead
HN	Heavy Naphtha
LD	Light Distillate
HD	Heavy Distillate
BR	Bottom Residue