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:

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

(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:
\[ L_u \leq c p_u^{\text{max}}, \quad \forall u \in U \]  \hspace{1cm} (A2)

where \( L_u \) = load of unit \( u \) and \( c p_u^{\text{max}} \) = maximum capacity of \( u \).

CDU outlet flow rate of cut \( p \) is given by:

\[ Q_{u,p} = L_u W_p, \quad u = \text{CDU}, \quad \forall p \in P \]  \hspace{1cm} (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:

\[ \sum_p W_p = 1 \]  \hspace{1cm} (A4)

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

\[ MW_p = 100 \left( \sum_{p'} W_{p'} + \frac{1}{2} W_p \right), \quad \forall p \in P \setminus \{\text{BR}\}. \]  \hspace{1cm} (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:

\[ Q_{\text{FCC},f} = L_{\text{FCC}} Y_f, \quad \forall f \in F \]  \hspace{1cm} (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:

\[ \Sigma_f Y_f = 1. \]  \hspace{1cm} (A7)

\( Y_f \) is determined using the following regression-based relation:

\[ Y_f = a_f^0 + a_f^1 (\text{conv} - z_f) + a_f^2 (\text{conv} - z_f)^2, \quad \forall f \]  \hspace{1cm} (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 $Q^R_{BR}$) and mixed with total inlet feed ($Q^T_{in}$):

$$Q^T_{FCC} = Q^T_{CDU, BR} + Q^R_{TGO} \quad (A9)$$

where $Q^T_{FCC}$ = total inlet flow rate to FCC, $Q^T_{CDU, BR}$ = flow rate of bottom residue (BR) outlet stream from CDU, and $Q^R_{TGO}$ = flow rate of TGO recycle stream.

FCC load is equal to its inlet flow rate:

$$L_{FCC} = Q^T_{FCC} \quad (A10)$$

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

$$Q^R_{TGO} \leq \frac{1}{2} Q^T_{CDU, BR} \quad (A11)$$

$$Q^R_{TGO} \leq Q^P_{FCC,FHO} \quad (A12)$$

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

$$Q^P_{FCC,FHO} = Q^T_{FCC,TGO} - Q^R_{TGO} \quad (A13)$$

where $Q^P_{FCC,FHO}$ = 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:

$$Q^P_{CDU, p} = \sum_{g \in G} F^P_{p,g}, \quad \forall p \in P_g \quad (A14)$$

where $F^P_{p,g}$ = 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:

\[ Q_p^p = \sum_{g \in G} F_{p,g}^p + \sum_r Q_r^A, \quad \forall p \]  

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

FCC gasoline fraction called \( F_{\text{gas}} \) 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:

\[ Q_{t,f}^{\text{prod}} = \sum_g F_{f,g}^{\text{prod}}, f = F_{\text{gas}} \]  

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

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

\[ Q_{g}^{\text{prod}} = F_{f,g}^{\text{prod}} + \sum_r F_{r,g}^{\text{prod}} + \sum_p F_{p,g}^{\text{prod}}, f = F_{\text{gas}}, p \in P_g, \forall g \]  

where \( Q_{g}^{\text{prod}} \) 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 \( i_{\text{prod}} \), and modelled using equation (A18).
\[ Q_{u,p} = \sum_d f_{p,d}^{i\text{prod}}, u \text{ CDU}, \forall p \in P_d \]  
(A18)

where \( f_{p,d}^{i\text{prod}} \) 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).

\[ Q_{d}^{f\text{prod}} = \sum_p f_{p,d}^{i\text{prod}}, p \in P_d, \forall d \]  
(A19)

where \( Q_{d}^{f\text{prod}} \) 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:

\[ Pr_{j,p} = a_{0,p} + a_{1,p}(MW_{p} - z_{p}) + a_{2,p}(MW_{p} - z_{p})^2, \forall j, \forall p \in (P_g \cup P_d) \]  
(A20)

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

\[ RON_g Q_{g}^{f\text{prod}} \leq Pr_{j,p} F_{p,g}^{i\text{prod}} + Pr_{j,r} F_{r,g}^{i\text{prod}} + Pr_{j,p'} F_{p',g}^{i\text{prod}} + Pr_{j,f} F_{f,g}^{i\text{prod}}, \]  
(A21)

\[ j = ON, p = GO, p' = HN, f = Fgas, \forall g,r \]

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:

\[ Q_{s}^{f\text{prod}} \leq D_{s}^{max}, \forall s \]  
(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).

\[ \text{conv}^{\text{LO}} \leq \text{conv} \leq \text{conv}^{\text{UP}} \]  

(A23)

A.8. Objective Function

The objective function for refinery profit is defined as:

\[
\text{Profit} = \text{Price of valuable products} - \text{crude oil cost} - \text{additive raw materials cost} - \text{operational cost of units}
\]

\[
\text{Profit} = \sum_s Q_{s}^{\text{fprod}} C_{s}^{\text{fprod}} - \sum_{cr} L_{u'} C_{cr} - \sum_{r} F_{r,g}^{\text{iprod}} C_{r} - \sum_{u} L_{u} C_{u}, \forall g \]  

(A24)

where \( C_{s}^{\text{fprod}} \) 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\}
- 𝐇: 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^:\text{Refinery process units}
- 𝑝, 𝑝^:\text{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^\text{max}: Maximum capacity of refinery process unit 𝑢
\( F_{cr} \)  Flow rate of crude oil

\( a_{0p}, a_{1p}, a_{2p}, z_p \)  Correlation coefficients for CDU fractions \( p \)

\( a_{0f}, a_{1f}, a_{2f}, z_f \)  Correlation coefficients for FCC fractions \( f \)

\( C_{f}^{prod} \)  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 \( p \)

\( Q_f^{prod} \)  Flow rate FCC final product \( f \)

\( Y_f \)  Weight transfer ratio of FCC product streams \( f \)

\( \text{conv} \)  FCC conversion level

\( Rcy \)  Recycled stream of FCC product FHO

\( Q_t \)  Sum of flow rates of FCC recycle stream and FCC feed

\( F_{t,f}^{prod} \)  Flow rate of FCC intermediate product stream \( f \), which is produced by total mixed feed stream \( t \) to FCC unit

\( F_{p,g}^{prod} \)  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

\( F_{r,g}^{prod} \)  Flow rate of stream \( g \) (g90, g93) from GB, which is produced by blending additive raw material stream \( r \)

\( Q_g^{prod} \)  Final products flow rate (g90, g93) from GB
\( F_{p,d}^{i\text{prod}} \) Flow rate of intermediate product stream \( d \) from DB, which is produced by blending CDU fraction \( p \)

\( Q_{d}^{f\text{prod}} \) Final products flow rate (\( d0, d10 \)) from DB

\( Q_{s}^{f\text{prod}} \) 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

\( i\text{prod} \) Intermediate product

\( f\text{prod} \) 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