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Global Optimization of Gasoline Blending Model using Bound Contraction Technique

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Abstract

We present the performance of recently developed techniques on domain and image partitioning (part of the global optimizer, RYSIA) to obtain a good lower bound for the gasoline blending problem. We show that without good initial values, this model cannot be solved using local solvers and we show the need for bound contraction.

Keywords: Global optimization, Optimization, MINLP

1. Introduction

Quality specification and environmental regulations for petroleum products are a challenging problem in the petroleum and petrochemical fields because when not properly done, they limit profit (Jia *et al.*, 2003). Of all the products of a refinery (gasoline, diesel, and naphtha), gasoline is one of the most important because it constitutes 60 to 70% of a refinery's total revenue (Gao, 2014). Only a small fraction of the products from distillation are suitable for blending directly into gasoline: light virgin naphtha or light straight run (LSP) naphtha. Other fractions have to be further processed through reforming, isomerization, etc. Thus the blending process of gasoline combines a number of feed stocks with small amount of some additives to make a blended fuel that meets quality specifications such as octane number, volatility, and sulfur content, among others, to make sure that the blended gasoline products are acceptable in terms of engine performance and environmental regulations (Singh *et al.*, 2000).

Blending equations for gasoline properties are nonlinear and non-convex (Pinto *et al.*, 2000) and the problem is NLP. There are several methods of global optimization used to solve these NLP problems such as Outer- Approximation, Generalized Benders Decomposition, Bound Contraction, and Branch and Bound. Almost all methods require reformulation. Our Bound contraction (RYSIA) is an efficient technique for solving the MINLP by eliminating intervals that do not contain the solution and bound contract each variable until the global optimum is obtained (Faria and Bagajewicz, 2011; Faria *et al.*, 2012) without using branch and bound, the usual technique of a lot of global optimizers.

An upper bound model was constructed by reformulating and linearizing the original NLP problem, resulting in an MILP (the problem requires profit maximization). Then, the lower and upper bound models are solved iteratively, performing bound contraction.

2. Model

The objective function and the blending equation of each property are shown next.

Objective Function: Profit of blending process is equal the difference between all product price and all used stream cost.

$$Max\ \ \sum_p \left(pr_p \times V_p\right) - \sum_{ip}(ct_i \times V_{ip}) \quad (1)$$

s.t.

$$X_{ip} = \frac{V_{ip}}{V_T} \quad (2)$$

$$RVP_p = \left[\sum_{i=1}^{n}\left(X_{ip} \times RVP_i^{1,25}\right)\right]^{0.8} \quad \textit{RVP blending} \quad (3)$$

$$SUL_p = \sum_{i=1}^{n} m_{ip} SUL_i \quad \textit{Sulfur content blending} \quad (4)$$

$$DEN_p = \sum_{i=1}^{n} X_{ip} DEN_i \quad \textit{Density blending} \quad (5)$$

$$ARO_p = \sum_{i=1}^{n} X_{ip} ARO_i \quad \textit{Aromatic content blending} \quad (6)$$

Ethyl RT-70 model: Instead of using linear blending for octane we use the following equations (Singh *et al.*, 2000) for RON (*R*) and MON (*M*)

$$R_p = \sum\left(X_{ip}\bar{R}_\iota\right) + a_1\left\{\left[\sum\left(X_{ip}\bar{R}_\iota\bar{S}_\iota\right)\right] - \left[\sum\left(X_{ip}\bar{R}_\iota\right) \cdot \sum\left(X_{ip}\bar{S}_\iota\right)\right]\right\} + a_2\left[\sum\left(X_{ip}\bar{O}_\iota^{\,2}\right) - \left(\sum X_{ip}\bar{O}_\iota\right)^2\right] \quad (7)$$

$$M_p = \sum\left(X_{ip}\bar{M}_i\right) + a_4\left\{\left[\sum\left(X_{ip}\overline{M_\iota}\bar{S}_\iota\right)\right] - \left[\sum\left(X_{ip}\bar{M}_i\right) \cdot \sum\left(X_{ip}\bar{S}_i\right)\right]\right\} + a_5\left[\sum\left(X_{ip}\bar{O}_i^{\,2}\right) - \left(\sum X_{ip}\bar{O}_i\right)^2\right] + a_6\left[\frac{\sum\left(X_{ip}\bar{A}_i^{\,2}\right) - \left(\sum X_{ip}\bar{A}_i\right)^2}{100}\right]^2 \quad (8)$$

$$\bar{S}_i = \bar{R}_i - \bar{M}_i \quad (9)$$

3. Global Optimization

To perform global optimization of this maximization problem one needs an upper bound, normally a relaxation of the original NLP problem, which is used as a lower bound. Our methodology is RYSIA (Faria *et al.*, 2011 a, 2012) and its algorithm is shown in Figure 1. Of this algorithm, we only show the performance of the bounds when domain and image partitioning is used for an increasing number of partitions is used.

3.1 Upper bound model

We first partition the variable X_{ip}

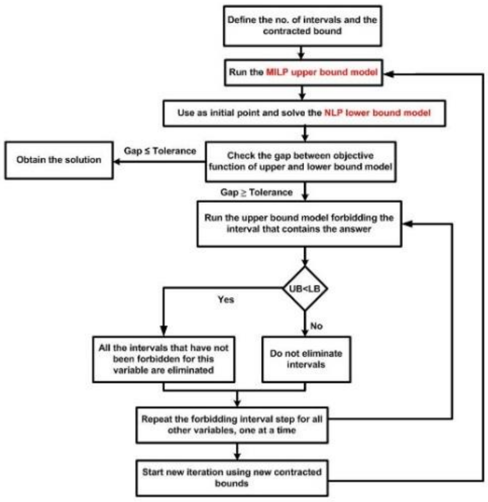
$$\sum_{fi}\left(yX_{ipf} \times \overline{X\iota at}_f\right) \le X_{ip} \le \sum_{fi}\left(yX_{ipf} \times \overline{X\iota at}_{p(f+1)}\right) \quad (10)$$

$$\sum_f\ yX_{ipf} = 1 \quad (11)$$

This allows us to rewrite equation (2) as $X_{ip}V_p = V_{ip}$ and linearize it as follows:

$$\sum_{fi}\left(yX_{ipf}\times V_p\times\overline{X\iota at}_f\right) \le V_{ip} \le \sum_{fi}\left(yX_{ipf}\times V_p\overline{\times X\iota at}_{p(f+1)}\right) \qquad (12)$$

Figure 1. Flowchart for



RYSIA

Equation 912) is linearized as follows:

$$\sum_{fi}\left(VyX_{ipf}\times\overline{X\iota at}_f\right) \le V_{ip} \le \sum_{fi}\left(VyX_{ipf}\overline{\times X\iota at}_{p(f+1)}\right) \qquad (13)$$

$$VyX_{ipf} - \Omega\cdot yX_{ipf} \le 0 \qquad (14)$$

$$\left(V_p - VyX_{ipf}\right) - \Omega\left(1 - yX_{ipf}\right) \le 0 \qquad (15)$$

$$\left(V_p - VyX_{ipf}\right) \ge 0 \qquad (16)$$

We now relax the RVP equation by rewriting equation (3) as follows.

$$\left(RVP_p\right)^{1.25} = \sum_i \left(X_{ip}\overline{RVP_\iota}^{1.25}\right) \qquad (17)$$

Next, we introduce a new variable Q_p and rewrite equation (17) as follows:

$$Q_p = \sum\left(X_{ip}\overline{RVP_\iota}^{1.25}\right) \qquad (18)$$

$$Q_p = \left(RVP_b\right)^{1.25} \qquad (19)$$

Eq. (18) is linear, but equation (19) needs relaxation. Then, we partition RVP_b as follows

$$\sum_f \left(yr_f\times\overline{Rat}_f\right) \le RVP_b \le \sum_f \left(yr_f\times\overline{Rat}_{f+1}\right) \qquad (20)$$

$$\sum_f yr_f = 1 \qquad (21)$$

and we follow by relaxing equation (12) as follows:

$$\sum_f \left(yr_f \times \overline{Rat_f}^{1.25}\right) \le Q_p \le \sum_f \left(yr_f \times \overline{Rat}_{f+1}^{1.25}\right) \quad (22)$$

In turn, equation (7) is rewritten as follows:

$$R_p = \sum_i X_{ip}\overline{R_\iota} + a_1\{[\sum_i X_{ip}\overline{R_\iota}\overline{S_\iota}] - ZRS_p\} + a_2\left[\sum_i X_{ip}\overline{O_\iota}^2 - O2_p\right] \quad (23)$$

where

$$ZRS_p = \sum_{ij} X_{ip}X_{jp}\,\overline{R_\iota}\overline{S_J} \quad (24)$$

$$O2_p = \sum_i (X_{ip}\overline{O_\iota})^2 \quad = \sum_{ij} X_{ip}X_{jp}\overline{O_\iota}\overline{O_J} \quad (25)$$

Next, we introduce a new variable $Z_{ijp} = X_{ip}X_{jp}$ and rewrite equation (24) and (25):

$$ZRS_p = \sum_{ij} Z_{ijp}\,\overline{R_\iota}\overline{S_J} \quad (26)$$

$$O2_p = \sum_{ij} Z_{ijp}\overline{O_\iota}\overline{O_J} \quad (27)$$

and we relax $Z_{ijp} = X_{ip}X_{jp}$ as follows:

$$\sum\left(yX_{ipf} \times X_{jp} \times \overline{X\iota at_f}\right) \le Z_{ijp} \le \sum\left(yX_{ipf} \times X_{jp} \times \overline{X\iota at}_{f+1}\right) \quad (28)$$

which is linearized as follows

$$\sum\left(WX_{ipf} \times \overline{X\iota at_f}\right) \le Z_{ijp} \le \sum\left(WX_{ipf} \times \overline{X\iota at}_{f+1}\right) \quad (29)$$

$$WX_{ipf} - \Omega \cdot yX_{ipf} \le 0 \quad (30)$$

$$\left(X_{jp} - WX_f\right) - \Omega\left(1 - yX_{ipf}\right) \le 0 \quad (31)$$

$$(X_{jp} - WX_f) \ge 0 \quad (32)$$

4. Example

We use five feedstock streams (reformate: RF, LSR naphtha: LSR, n-butane: BT, catalytic gas: CTG, and alkylate: ALK) to blend into two product streams: Regular Gasoline and Premium Gasoline shown as Figure 2. And we leave the values of V_p variable, so they achieve their maximum. An example where they are fixed is simpler.

Table 1 Information and properties of the feedstock stream.

Streams	RVP (psi)	DEN (lb/bbl)	ARO (%vol)	SUL (ppmw)	RON	MON	Max. capacity (bbl/day)
RF	3.8	282.00	61.1	9	94.1	80.5	12000
LSR	12	232.29	2.2	325	70.7	68.7	6500
BT	138	210.74	0	0	93.8	90	3000
CTG	5.3	270.16	35.9	522	92.9	80.8	4500
ALK	6.6	264.53	0.5	15	95	91.7	7000

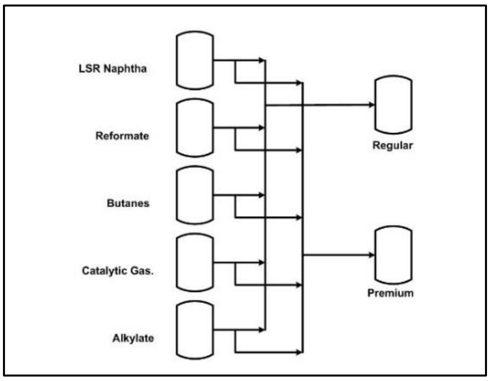


Figure 2. The flow diagram of gasoline blending.

We first run only the lower bound model, the original NLP, using CONOPT and we found that if the initial value is not given, the solver says the problem is infeasible. When, we set the initial values of volumetric flowrate of each stream to 10000 bbl/day, we obtained the total profit to $14976.5/day, much lower than the global optimum.

To solve the problem, we use different amounts of intervals for each partitioning. Results are shown in Table 2. The profit of this process will increase depending on the total volumetric flowrate of blending but not exceed the maximum capacity of each feedstock as shown in table 1.

Table 2. The solution of the model for blending in six properties.

No. of intervals	Objective from UB model	Objective from LB model	CPU time		Gap
			UB model	LB model	
10	$89400	$36073.547	1s	0.31s	147.83%
100	$42155.56	$36073.547	14s	0.31s	16.86%
200	$39520.603	$36073.547	1m58s	0.36s	9.56%
300	$38706.355	$36073.547	16m42s	0.24s	7.30%
500	$38392.184	$36073.547	1h3m41s	0.8s	6.43%

Quite clearly, the domain/image partitioning that RYSIA uses provides a) good gaps, and b) good initial points for the lower bound, which then performs very quickly.

4. Conclusions

We used the domain/image partitioning methodology from RYSIA (Faria and Bagajewicz, 2011) to show the performance of the relaxed problem in the gasoline blending problem. Future work will include bound contraction and more complex equation for blending.

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Nomenclature

RVP	RVP
SUL	sulfur content
DEN	density
ARO	aromatic content
R	Research Octane Number,
M	Motor Octane Number,
S	component sensitivity (RON-MON),
O	olefin content (percent by volume),
a	correlation coefficient.
pr	price of each product
ct	cost of each feedstock stream
V	volumetric flow rate of each product.

Subscript

i	feedstock stream
p	product stream
T	Total stream

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