

1 Original Research Article

2 **Global Optimisation of Gasoline Pool Blending**

3 **Using Constraint Partitioning**

4 **ABSTRACT**

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Aims: A hybrid Nonlinear Programming–Simulated Annealing method has been applied to solving the constrained offline gasoline recipe optimisation problem using constraint partitioning.

Methodology: The method was demonstrated by applying it to a small blending case study with eighteen independent variables where one of the variables was used as a link variable between the two sub-problems of the partitioned non-convex problem. It is noted that this can in theory be extended to larger tightly constrained problems with more link variables e.g. whole refineries where the models involve huge numbers of nonlinear equations and many process units.

Results: The approach exhibited good performance representing significant savings against both a derivative-based NLP method used alone and a Mixed Integer Non-Linear Programming method. This performance was examined by way of a sensitivity analysis of the simulated annealing parameters.

Conclusion: The convergence times were in minutes and are realistic for short-term recipe optimisation.

7

8 *Keywords: Gasoline blending, simulated annealing, constraint partitioning, stochastic*

9 *optimisation.*

10 **1. INTRODUCTION**

11

12 Refineries are continuously faced with increasingly tighter constraints. Governments are

13 enforcing more stringent legislation in order to ameliorate climatic change concerns and

14 curtail environmental damage as a result of human activity. Be it emissions reduction targets

15 or large demand for high octane rated fuels at reasonable prices, society is seemingly

16 apathetic to the fact that these refineries are businesses that must turn out profits. Refiners,

17 under the stated limitations, must optimise in order to thrive.

18 A refinery is a vast petrochemical facility with thousands of interconnected units and

19 processes. Realistic modelling for design and operation therefore gives rise to highly non-

20 linear models. These are difficult problems and can be time-consuming to solve as a whole.

21 Optimising one or several key processes such as the Crude Distillation and Fluid Catalytic

22 Cracking Units, unfortunately do not automatically translate to optimal values for the whole

23 complex (1). Overall refinery optimisation is a difficult endeavour, nevertheless, this is done

24 based on the major subdivisions as shown in Figure 1. Product blending and recipe

25 optimisation, the last of the subdivisions, is the closest to the consumer. Therefore, careful

26 monitoring to meet quality and environmental regulations requires proper optimisation. This

27 ensures that the products are “on-spec” and with minimal give-aways.

28 Linear programming (LP) has been the dominant industry-wide practice. It has the obvious

29 advantages of simplicity, fast convergence, and minimal computational requirements. This

30 has proven satisfactory for long term planning. However, it is unsatisfactory in the short to

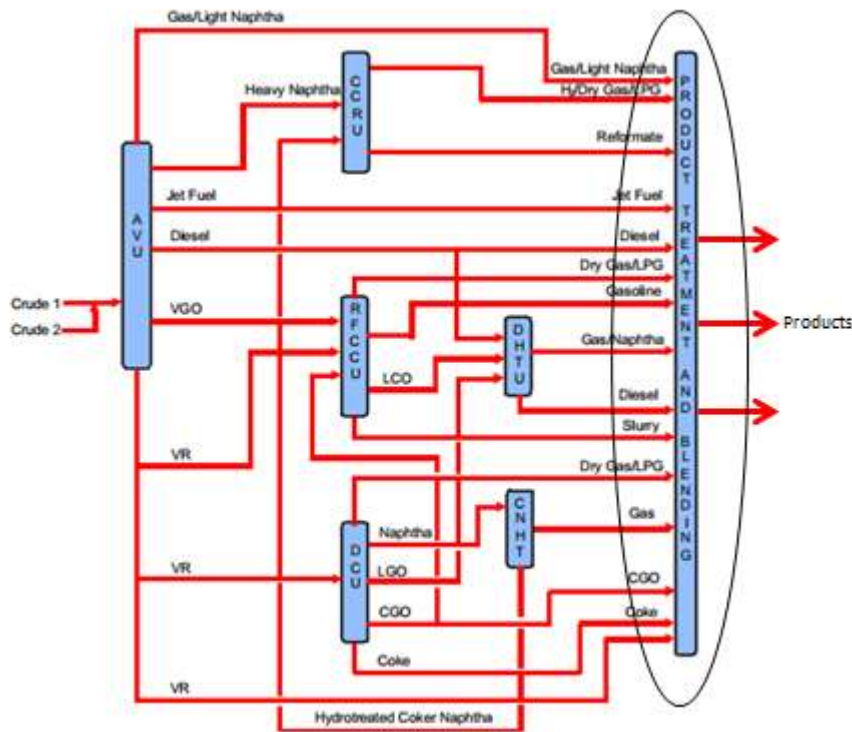
31 medium term against the backdrop of tighter profit margins.

32 Several techniques that approximate nonlinear behaviour have been used including
33 Successive Quadratic Programming (SQP) and piecewise linearization (2–4). These give
34 rise to Mixed Integer Linear and Nonlinear Programs (MILPs and MINLPs). Mixed integer
35 programs can result in huge models with large numbers of variables and constraints,
36 therefore requiring long converging times. These may not be suitable for the day-to-day
37 operations of a refinery. Commercial applications such as Aspen BlendTM and AspenPIMS-
38 MBOTM from AspenTech are available for treating online and offline blending optimization
39 problems. These are based on black box models that reduce the required intelligence by the
40 engineer; the so-called engineering judgement and as such; they offer less in terms of
41 flexibility.

42 An approach was developed by (5) to coordinate non-linear recipe optimization and short-
43 term scheduling of blending processes. They propose a two-level optimization approach that
44 sets up a large scale NLP model to determine product quantities and recipes. Given the
45 result from the NLP model, a MILP model based on a resource task network is used for the
46 scheduling problem to optimize resource and temporal aspects. Both models are discrete
47 time models. Whereas the NLP model maximizes profit, the MILP model minimizes
48 deviations from given tank volume goals. Alternative strategies were also presented in (5) to
49 handle situations where a given goal cannot be met.

50 It has been observed that future work in refinery optimisation might focus on how to
51 determine component values and the preferred product recipes, in order to optimize the
52 combined performance of the short-term blending and product shipments and how to
53 incorporate the scheduling decisions with long-term planning decisions (6). Therefore, in the
54 short-term, another recipe may be more profitable than the long-term optimal recipe, and the
55 deviations from the long-term recipe may indicate that other blending recipes should be
56 used. Ideally, it would be possible to detect the values of components, and in order to more
57 closely approximate the values of these components, there must be integration between

58 short-term and long-term decision. Problem partitioning can be used to achieve these.



59
60 **Figure 1: A simplified refinery flow sheet from crude oil to gasoline showing the**
61 **position of product blending**

62 Problem Partitioning has been used to solve problems in economics and logistics and has
63 been proposed for efficiently solving large-scale planning and engineering nonlinear
64 problems by exploiting the problem structure and partitioning the constraints (7–9). The sub-
65 problems become much more relaxed since they involve a smaller number of constraints,
66 thus, the total time to solve all the sub-problems is greatly reduced. However, since there are
67 global constraints which may be violated when multiple sub-problems are combined, the
68 efficiency in resolving inconsistent global constraints is a key factor for the overall
69 performance of the proposed constraint partitioning approach.

70 In recent years, the use of stochastic optimisation methods has gained prominence because
71 hybrid algorithms permit the use of complete NLP models. Simulated annealing (SA) and
72 Genetic Algorithms (GA) are examples of stochastic methods that produce high quality
73 globally or near-globally optimal results. Their success however, hinges on high
74 computational requirements but then this is becoming less and less of an issue with the
75 rapid increase in computer memory capacity. Nevertheless, exploring the entire solution
76 space can take impracticably long periods of time and there has to be a compromise in
77 solution quality.

78 In this paper, we present a constraint partitioning approach applied to tightly constrained
79 offline optimisation of the refinery blend pool problem by combining simulated annealing with
80 standard nonlinear programming. Secondly, after solving the problem, a sensitivity analysis
81 is done on the simulated annealing parameters in order to give more insight on solution
82 times. Finally, the solution a simple conventional MINLP formulation of the same problem is
83 compared with the new method.

84
85

2. METHODOLOGY

2.1 Optimisation by Problem Partitioning

87 Highly constrained problems require conditioning before optimisation can be used to obtain
88 acceptable solutions to them. A commonly used technique is using penalty functions
89 whereby the constrained problem is converted to a problem with penalty terms to the
90 objective function for violating the constraints.

91 Using Problem partitioning, optimization problems can be converted to two sub-problems
92 linked by one or more variables. These variable(s) are the decision variables for one sub-
93 problem and parameters for the other sub-problem. One of the sub-problems is an
94 unconstrained problem with simple bounds and the other is a more complicated one with its
95 normal constraints. Consider the following maximisation problem:

$$\text{Maximise } f(x_1, x_2, \dots, x_n) \quad (1a)$$

$$\text{Subject to: } g_1(x_1, x_2, \dots, x_{n+1}) \leq 0 \quad (1b)$$

$$g_2(x_1, x_2, \dots, x_{n+1}) = 0 \quad (1c)$$

$$g_N(x_1, x_2, \dots, x_n) \geq 0 \quad (1d)$$

$$x_1 \geq k_1, x_2 \geq k_2, \dots, x_{n+1} \geq k_{n+1} \quad (1e)$$

96 This is a general nonlinear problem in the objective function and the constraints with $n+1$
97 variables. The solution, although easy to obtain with common NLP solvers, can
98 unfortunately be locked up in local maxima. To escape the localisation issues, however, the
99 problem can be reformulated so that it is partitioned into two optimisation problems. The
100 variables are $x_1, x_2, \dots, x_{n+1}$, making a total of $n+1$ variables so that any one of them can in
101 theory be selected as the link variable between the two sub-problems. In selecting the link
102 variable $x_i \in g_i$ a rule of thumb is that the variable be of the lowest order present and that it
103 appears in as few constraints as possible. This contributes to ease of convergence and
104 convergence to acceptable solutions. Suppose the link variable x_i chosen using the rule of
105 thumb is y , the problem is now partitioned as follows:

106 Sub-problem 1:
Maximise $h(y)$ (2a)

$$l \leq y \leq u \quad (2b)$$

107

108 Sub-problem 2:
Maximise $f(x_1, x_2, \dots, x_n) \quad x_2 \geq k_2$ (3a)

$$\text{Subject to: } g_1(x_1, x_2, \dots, x_n, y) \leq 0 \quad (3b)$$

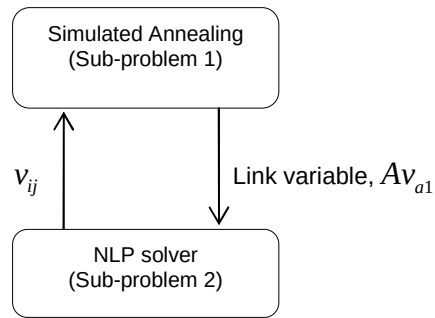
$$g_2(x_1, x_2, \dots, x_n) = 0 \quad (3c)$$

$$g_N(x_1, x_2, \dots, x_n) \geq 0 \quad (3d)$$

$$x_1 \geq k_1, x_2 \geq k_2, \dots, x_n \geq k_n \quad (3e)$$

109 Here, the link variable chosen reduces sub-problem 2 from $n+1$ variables to n and is
110 constrained between a lower and upper bound interval in sub-problem 1. It is instructive to

111 note that this link variable in sub-problem 1 whose generated value (random or otherwise) in
 112 each iterative run is passed on to sub-problem 2 and is hence not included as one of the
 113 constraints in equations (3e). Sub-problem 1 is such that a stochastic global optimisation
 114 method (Tabu Search, Genetic Algorithm, Simulated Annealing, etc.) can be applied while in
 115 sub-problem 2 is solved for each sampled $y \in [l, u]$ using NLP until convergence based on
 116 the criteria set in sub-problem 1. Figure 2 illustrates this solution structure. The method is
 117 formally described in (10) and they note its ability to handle non-convex problems. (11) used
 118 the method to solve an operations research air transport problem, observing its remarkable
 119 efficacy in simplifying large-scale problems to simple continuous and mixed integer NLPs.



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 121

Figure 2: Partitioned problem solution structure

122 A general Simulated Annealing pseudo-code is as follows as described by (12):

- 123
- Choose an initial solution x , an initial temperature T , a lower limit on temperature $TLOW$, and an inner iteration limit L
 - 124
 - 125 • While ($T > TLOW$), do
 - 126 • For $k = 1, 2, \dots, L$, do (Markov Chain Length)
 - 127 • Make a random choice of an element $x' \in N(x)$.
 - 128 • $MoveValue = f(x') - f(x)$
 - 129 • If $MoveValue \leq 0$ (downhill move), set $x = x'$
 - 130 • If $MoveValue > 0$ (uphill move), set $x = x'$ with probability
 - 131 • $\exp(-MoveValue/T)$
 - 132 • End inner (Markov Chain Length) loop
 - 133 • Reduce temperature according to an annealing schedule. An example is new $T = cT$, where $0 < c < 1$.
 - 134
 - 135 • End temperature loop

136 Figure 3 below is a flowchart showing the SA programme structure for the case study which
 137 is based on the Metropolis algorithm:

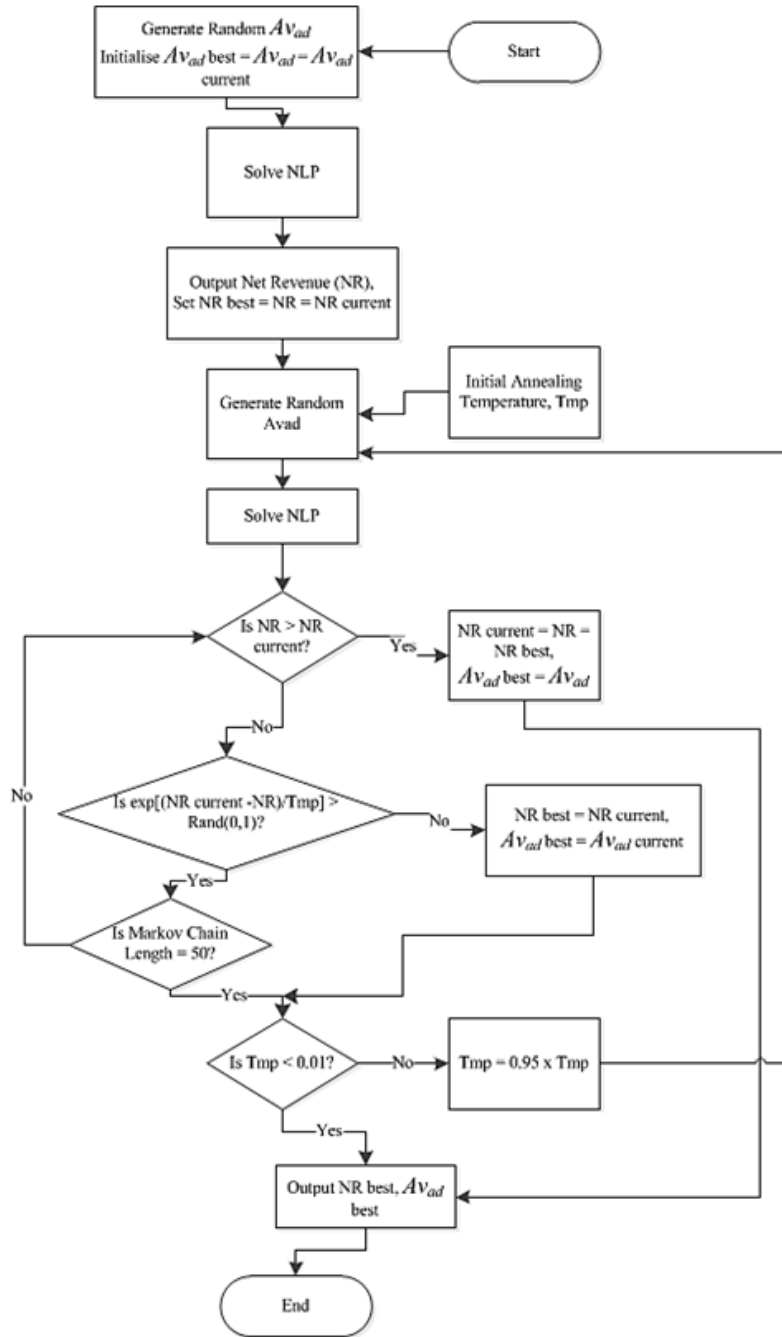


Figure 3: Flowchart of hybrid SA-NLP solution procedure

3. RESULTS AND DISCUSSION

3.1 Case Study

To demonstrate the proposed method, unpublished refinery data (Tables 2, 3, 4 and 5) collected by (13) was used. The system consists of refinery products from the crude

distillation unit (Straight run gasoline, SRG and naphtha), catalytic cracker, thermal cracker, steam reforming, and naphtha hydro-treating units. Clearly, this is a refinery without an alkylation unit as alkylate has to be externally procured as an additive as it has high octane number relative to SRG. Butane, obtained from overhead refinery gases, is also blend component. It possesses good Octane Number (ON) rating; however it has exceptionally high Reid Vapour Pressure (RVP) responsible for vapour lock in vehicles and this is controlled so that the gasolines only contain optimal amounts. The product specification is based on two grades of unleaded premium grade gasolines with RON 94 and 96 respectively (here termed Gasoline 89 and Gasoline 91 named after their Anti-knock Index). For both gasolines, their RVP and aromatics content must be within the restrictions defined earlier.

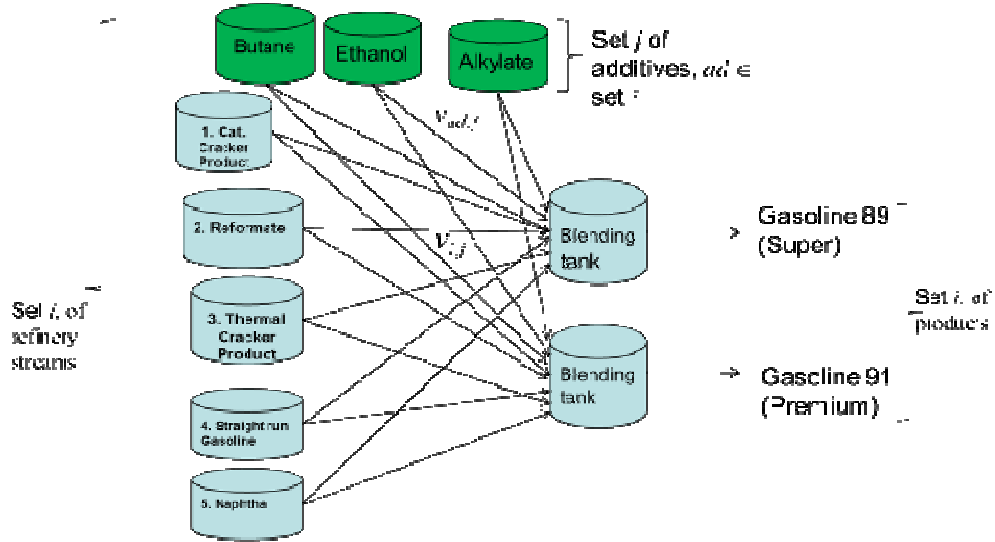


Figure 4: Gasoline pool blending problem for two grades of gasoline

Table 2 shows the RON, MON, RVP and aromatics content of refinery streams 1 to 5, n-butane obtained as overhead distillate gas, ethanol, and alkylate. Collected data also include the open market cost of ethanol and alkylate externally procured for use as additives.

Table 1: Collected data on available feedstock properties and information about additives[†]

	RON	MON	AKI	RVP (psi)	Aromatics (%)	Availability (kbbbl)	Price(\$)
CCP*	97.2	86.6	91.9	1.1	78.1	190	-
Reformate	93.8	84.4	89.1	1.4	64.3	100	-
TCP**	100.7	89	94.9	0.92	89.9	125	-
SRG ^{††}	97.6	86.6	92.1	1.28	85.5	90	-
Naphtha	89.3	81.9	85.6	2.7	15.2	600	-
n-Butane	93	92	92.5	52	-	70	-
Ethanol	107	89	98	9.6	-	-	4.50/gal
Alkylate	93	90	91.5	5	-	-	2.95/gal

Kbbbl – 1000 barrels, CCP* – Catalytic cracker product, TCP** – Thermal cracker product, SRG^{††} – Straight run gasoline [†]Source: (13)

Table 2 displays data collected for product specifications and market price of two grades of gasoline with AKI 89 and 91 respectively.

Table 2: Product specifications for different grades of gasoline

	RON	MON	AKI	RVP (psi)	Aromatics (%)	Price
Gasoline 89	94	84	89	6.9	35	\$2.75/Gallon
Gasoline 91	96	86	91	6.9	35	\$2.90/Gallon

[†]Source: (13)

Gupta's optimisation results of maximising product sales revenue are as presented in Table 3. It shows the optimal product distribution of each component in each product and the predicted product properties based on the Ethyl RT-70 model for MON and RON, Chevron RVPI model and linear blending for Aromatics.

Table 3: Detailed product distribution

	Gasoline 89 (kbbbl)	Gasoline 91 (kbbbl)
CCP	147.7	42.3
Reformate	100	-
TCP	-	125
SRG	90	-
Naphtha	467.3	132.7
n-Butane	53.9	16.1
Ethanol	115.5	47.3
Alkylate	180.2	109.5
Total	1154.6	472.9

[†]Source: (13)

The information in Table 3 above was then used to verify the model developed for this work.

3.2 Optimisation Problem Formulation

3.1.1 Modelling Blend Properties

Blending blend properties is mixing rule-based. The simplest and practical mixing rule applicable to most physical properties is linear (14):

$$P_j = \sum_{i=1}^N x_i P_i \quad (4)$$

Where x_i is the volume/weight/molar fraction of the blending component i , P_i is a property for the blending component i and P_j is property of the product with N blending components. The application of Equation 4 can be made for any property so that the volumetric fraction x_i can be more explicitly expressed with v_{ij} which is the volume of blend component i in gasoline blend j which is a fraction of the total available feedstock.

$$P_j = \frac{\sum_i P_i v_{ij}}{\sum_i v_{ij}} \quad (5)$$

Where P_i is the property under consideration of gasoline blend j and P_i is the property of blend component of stream i . Equation (2) was applied for the blend calculation of ethanol (oxygenate) content, aromatics, and butane content. Some properties however, such as sulphur content, density, that are usually quoted in wt% or ppm are modelled gravimetrically, using a revised form of Equation 2.

$$P_j = \frac{\sum_i (P_i v_{ij} SG_i)}{\sum_i (v_{ij} SG_i)} \quad (6)$$

Where SG_i is the specific gravity of component i .

3.1.2 Modelling Octane Number

Octane number does not blend linearly. Several non-linear models are widely available in open literature for octane number modelling with varying degrees of accuracy. While the Blending Octane number method is easy to use, its accuracy is impaired by its range of application as "Blending Octane Numbers" are obtained by regressing a limited number of data; the Interaction and Transformation methods have issues of complexity of use without commensurate increase in accuracy. As a result, the Ethyl RT-70 model, proposed by Healy et al. (1959) was used. Despite its age, it has the advantage of relative ease of use while maintaining a great deal of accuracy. Non-linearity in blending is explicitly accounted for as a function of component sensitivity (RON minus MON), aromatic and olefin content.

$$R = \bar{r} + a_1 (\bar{rS} - \bar{r}\bar{S}) + a_2 (\bar{O}^2 - \bar{O}^2) + a_3 (\bar{A}^2 - \bar{A}^2) \quad (7a)$$

$$M = \bar{m} + a_1 (\bar{mS} - \bar{m}\bar{S}) + b_2 (\bar{O}^2 - \bar{O}^2) + b_3 \left(\frac{\bar{A}^2 - \bar{A}^2}{100} \right)^2 \quad (7b)$$

Where $\bar{r}$ and $\bar{m}$ are volumetric average RON and MON respectively, S is the ON sensitivity (RON–MON), O is olefin content (% by volume) and A is the aromatic content (% by volume). The Equations contain a total of six parameters ($a_1, a_2, a_3, b_1, b_2, b_3$) given in Healy (1959). All quantities denoted with an over bar represent volumetric averages.

3.1.3 Modelling Reid Vapour Pressure (RVP)

RVP is defined by the ASTM D-323-56 and gives an indication of the volatility of a gasoline blend. RVP may be considered as the vapour pressure of the gasoline (or blend component) at 100 °F (38 °C). The RVP of a gasoline blend affects the gasoline performance in internal combustion engines' ease of starting, engine warm-up, and rate of acceleration. Many attempts exist to accurately model RVP of blends. One of them is the interaction method. The method is identical to that for octane numbers. Singh (1997) and Gupta (2007) noted however that many of such methods have huge computational requirements with large

214 numbers of parameters to be determined. For the present study, the method used is the
 215 enduring Chevron Blending Index method where the RVP blending index was estimated for
 216 each stream using the non-linear mixing rule (15):

$$RVPI = (RVP)^{1.25} \quad (8)$$

217 With the RVP of the gasoline blend j being:

$$RVP_j = \left[\sum v_{ij} (RVPI)_i \right]^{0.8} \quad (9)$$

218 Where v_{ij} is the available volume of stream i , distributed to blend j .

219 **3.1.4 Objective Function**

220 Here we formulate the objective function as an economic potential of sales revenue less
 221 additive costs. In this case the net revenue is obtained from the sale of the two gasoline
 222 products, less the costs of required amount of additives, is to be maximised and takes no
 223 account of capital or other costs.

$$\sum_j Pr_j V_j - \sum_a C_a A v_a - \sum_m k_m s_m^2 \quad (10)$$

224 Where $A v_a$ is the volume of additive that is required to maximise profit, Pr_j is the market
 225 price of each gasoline, C_a is the cost of market additive. The third term is the penalty term
 226 comprising of slack variables s_m and a penalty factor k_m usually a large number. The penalty
 227 term is subtracted from the objective function to minimise violations in certain equality
 228 constraints of interest. Slack variable s_m is squared to accelerate convergence since for this
 229 problem it is observed that the slack variables are rather small and of order less than one. It
 230 should be noted that if the direction of optimisation is to minimise, the penalty term will be
 231 added to the objective function. For this problem, four slack variables were used each added
 232 to the constraints for RVP, ethanol content, and blend tank material balances. An alternative
 233 method for penalising given tank volume goal deviations is an MINLP approach as
 234 presented by (5).

235 **3.1.5 Variables**

236 The problem contains a total of eighteen independent variables to be determined by
 237 optimisation. These are in two groups. The first group has the volumes of each blending
 238 component i that distributes into gasoline product j , v_{ij} . The set i of components
 239 contains eight elements (Stream 1–Stream 5, alkylate, ethanol and n-butane). The set j of
 240 gasoline products contained 2 elements – Gasoline 89 and Gasoline 91. As such the blend
 241 volume fractions v_{ij} optimised were sixteen in number. The second group of independent
 242 variables is the volume of market additives v_{ad} required to optimise the objective function.
 243 Butane is an additive that boosts RVP of gasoline, but it is not included in v_{ad} as it is already
 244 assumed to be produced as an overhead product in refinery crude distillation columns.
 245 Hence the set ad contains two elements (alkylate and ethanol). This set however, is a subset
 246 of set i the set of blending components.

Table 4: Independent optimisation variables

	Variables v_{ij}		Variables v_{ad}
	Gasoline 89	Gasoline 91	Availability (kbbbl*)
CCP	1	9	
Reformat	2	10	
TCP	3	11	
SRG	4	12	
Naphtha	5	13	
n-Butane	6	14	
Ethanol	7	15	17. v_{ad1} (ethanol)
Alkylate	8	16	18. v_{ad2} (alkylate)

3.1.6 Inequality Constraints**3.1.6.1 Research and Motor Octane Number (RON & MON)**

The lower bounds for octane numbers were included to ensure that minimum market specifications were met, while the upper bounds ensured that octane number giveaway is curtailed. These are:

$$\begin{aligned}
 &94 \leq \text{RON} \leq 96 \text{ for gasoline 89} \\
 &96 \leq \text{RON} \leq 98 \text{ for gasoline 91} \\
 &84 \leq \text{MON} \leq 86 \text{ for Gasoline 89} \\
 &86 \leq \text{MON} \leq 88 \text{ for Gasoline 91}
 \end{aligned}$$

3.1.6.2 Reid Vapour Pressure (RVP)

Reid vapour pressure constraints were imposed as being $0 \leq \text{RVP} \leq 6.9$ psi for both gasolines. This is based on the UK's minimum summer gasoline vapour pressure of 6.53 kPa (16).

3.1.6.3 Aromatics Content

European Union regulations specify that all gasolines produced in Europe from 2005 onwards must have aromatics content $\leq 35\%$ by volume (17).

3.1.6.4 Ethanol Content

Ethanol is added as an oxygenate in gasoline as it is a cleaner burning fuel. It acts as an octane enhancer and EU regulations stipulate that there must be at most 10% ethanol by volume in gasoline (18, 19).

3.1.7 Equality Constraints

These are the material (volume) balances over blend and component tanks. Equation (12) imposes that the availability of all blend components (without additives) must equal their respective distribution to the gasolines.

$$Av_r = \sum_j v_{r,j} \quad (11)$$

$$\forall v_{rj}, 0 \leq v_{rj} \leq Av_r$$

Similarly, the availability of all additives must be equal to their respective distribution to the gasolines.

$$Av_{ad} = \sum_j v_{ad,j} \quad (12)$$

$$\forall v_{ad,j}, 0 \leq v_{ad,j} \leq Av_r$$

Both Av_{ad} and $v_{ad,j}$ are positive variables and are constrained appropriately. The volume of each gasoline produced is the sum of component streams and additives distributed to it as shown in constraint below.

$$V_j = \sum_r v_{r,j} + \sum_{ad} v_{ad,j} \quad (13)$$

The total volume of gasolines produced must equal the available components fed to the blend tanks

$$\sum_j V_j = \sum_r Av_r + \sum_{ad} Av_{ad} \quad (14)$$

3.2 NLP Solution of Blending Model

An NLP solution was obtained of the blending model described. This was done in GAMS 23.9 and solved with the CONOPT solver. The solution time was 0.881 seconds. For a minimum production of 500 kbbl of Gasoline 89 from the available feed stock, Table 5 shows the product distribution after optimisation.

Table 5: Detailed NLP solution product distribution (kbbl)

	Gasoline 89	Gasoline 91
CCP	0.00	190.00
Reformat	0.00	100.00
TCP	0.00	125.00
SRG	20.40	69.60
Naphtha	196.13	403.87
n-Butane	0.00	70.00
Ethanol	73.43	306.73
Alkylate	210.03	823.26
Total	500.00	2088.46

The objective was to maximise net revenue and the optimal value was \$112,248,183.06. Without putting a lower bound of 500 kbbl on Gasoline 89, the optimisation results give a product distribution as shown in Table 6.

Table 6: Results of gasoline product specifications from NLP

	RON	MON	AKI	RVP	Aromatics (vol%)	Ethanol (vol%)
Gasoline 89	94	86	90	4.763	9.451	306.73
Gasoline 91	96	88	92	6.836	21.354	73.43

291 The value of the objective (Net revenue) maximised was \$112,248,183.06. In Table 6, both
 292 gasoline blends were on specification. It should however be noted that this is only a locally
 293 optimal NLP solution and this was used as a base case for obtaining a globally optimal
 294 solution using simulated annealing in the next section.

295 **3.3 Search for a global optimum**

296 **3.3.1 Solving the problem by constraint partitioning**

297 The method outlined in Section 2.1 is demonstrated here to solve the formulated problem in
 298 Section 3.2 above. The problem was split in two so that it forms a hybrid deterministic–
 299 stochastic problem. Each of these forms the partitioned sub-problems. While NLP was used
 300 to solve the first sub-problem to obtain a solution from which the second sub-problem was
 301 initialised and proceeds iteratively (as earlier shown in Figure 3). The second sub-problem
 302 was solved using Simulated Annealing with successive results compared until the final
 303 annealing temperature is reached according to an annealing schedule of 0.95.

304 In this work, the overall blending model contains eighteen independent variables and the link
 305 variable between the SA and NLP model is the volume of the additive ethanol required to
 306 maximise the net revenue of the blending process. This was a made parameter in the NLP
 307 model and a univariate search was conducted by randomly choosing from the uniform
 308 distribution [100, 500]. The choice of interval was informed by the NLP solution of the system
 309 previously obtained gave values ethanol additive volume of 380.162 kbbl respectively, and
 310 the SA was given a reasonably large search space which makes the search for a globally
 311 optimal value more probable.

312 Initial annealing temperature was set at 1.3×10^8 . This value is an estimate chosen to be
 313 approximately the value of the objective function obtained in the local solution which was
 314 \$112,248,183.06. Subsequent values of 2.6×10^9 , 3.9×10^9 were allocated to the
 315 temperatures to gauge the computational performance of the procedure. These
 316 temperatures were allowed to drop to a final value of 0.01 according to an annealing
 317 schedule of 0.95 of the annealing temperature (i.e. for each iteration, $T = 0.95T$). For the
 318 Markov chain length (inner while loop), values of 10, 40, and 60 were used. The Boltzmann
 319 probability was employed as the bad move acceptance probability and is a function of the
 320 annealing temperature.

321 The NLP model was integrated into a hybrid NLP-Simulated annealing to directly search for
 322 a global solution. The NLP solver used was CONOPT in GAMS 23.9. A Metropolis based
 323 search algorithm employing the Boltzmann probability as described earlier was used as the
 324 move rejection criterion. It should be noted that results are not exactly reproducible as
 325 successive iterations proceed based on uniformly distributed random number generation of
 326 ethanol additive volume, as shown in Figure 5.

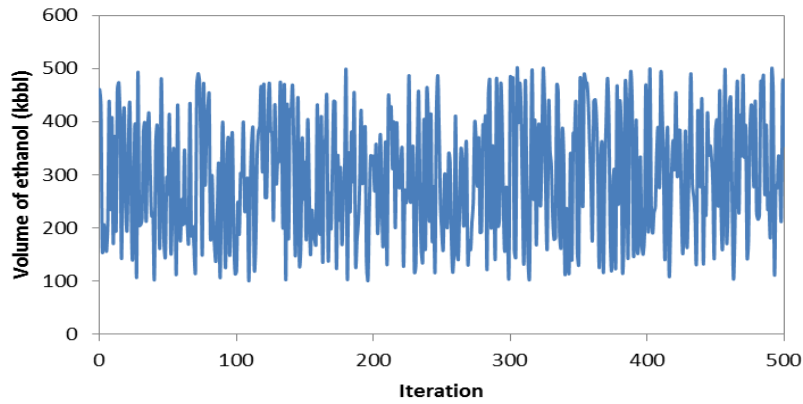


Figure 5: Uniform Random number distribution in [100, 500] with iteration for ethanol volume

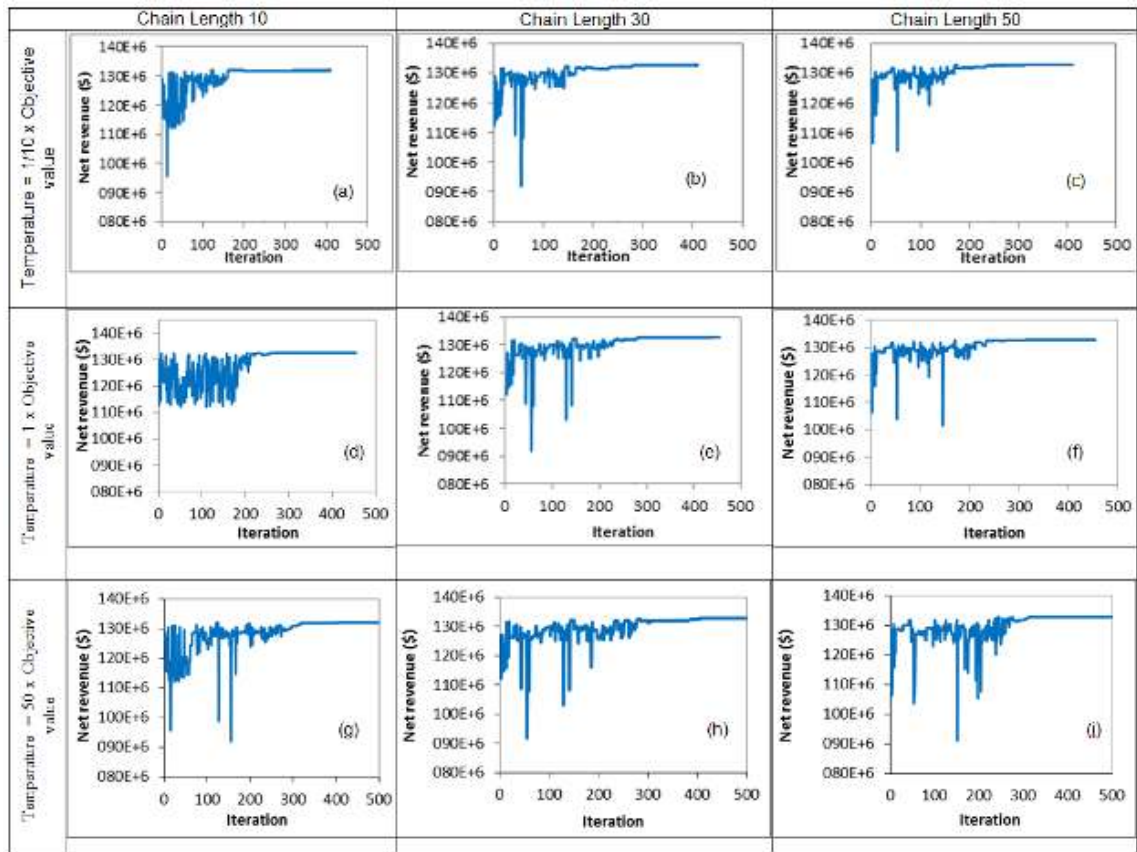


Figure 6: Plots of objective value against number of iterations for annealing temperatures of 1/10, 1, and 10 times the objective value and Markov chain lengths of 10, 30, and 50 respectively

The results obtained as shown in Figure 6 reveal how the optimisation proceeds by varying the Markov chain length for each of three initial annealing temperatures (i.e. 1/10, 1 and 20

336 times the locally optimal objective value). This is to examine the consistency of successive
337 solutions.

338 As is seen in Table 7, computational time is affected by both annealing temperature and
339 Markov chain length. The higher the temperature and the larger the Markov Chain Length
340 the longer the CPU time for a single run. A chain length of 50, which is the largest used,
341 produced the highest best objective value regardless of initial annealing temperature. In
342 theory, infinitely large chain lengths can be used for more refined solutions, but in practice
343 the refinements have to be balanced with solution time which must be realistic for day-to-day
344 plant operations.

345 **Table 7: Sensitivity of SA parameters on best objective value**

Annealing Temperature $1/10 \times$ Objective value			
Markov Chain Length	10	30	50
Av_{ad} , best (ethanol volume)	382.1	386.78	390.5
Best Objective (\$)	132,076,648	132,786,104	132,786,103
CPU Time (minutes)	14.43	44.19	90.36
Annealing Temperature $1 \times$ Objective value			
Markov Chain Length	10	30	50
Av_{ad} , best (ethanol volume)	383.16	386.78	390.5
Best Objective (\$)	132,550,889	132,786,103	132,786,103
CPU Time (minutes)	31.58	55.33	91.51
Annealing Temperature $20 \times$ Objective value			
Markov Chain Length	10	30	50
Av_{ad} , best (ethanol volume)	382.1	386.8	390.5
Best Objective (\$)	132,076,649	132,825,104	132,825,103
CPU Time (minutes)	39.04	79.08	112.02

346 Similarly, increasing annealing temperature has an effect on the quality of the best objective
347 found. The Metropolis search algorithm guarantees that the search will yield a good quality
348 result when large annealing temperatures are used as the solution space is properly
349 combed. However, this increases the solution time. Figure 6 shows the progression of the
350 search with iteration number. They show that lower objective values are also accepted
351 (characterized by peaks as well as troughs). This helps the optimization escape local optima.
352 For an initial temperature of 1.3×10^6 (approximately one-tenth the objective value) which
353 dropped to 10^{-3} by an annealing schedule of 0.95 Temperature, there were 410 iterations
354 (Figures 6a, b and c). When temperature was increased to exactly the objective value, the
355 number of iterations increased to 455 and to 513 when increased to 50 times the objective
356 (Figures 6g, h and i).

357 These confirm that the initial NLP solution of \$112,201,183.06 was a local maxima and
358 attempting a basic global search gives an estimated increase of \$20,000,000. This was
359 achieved in reasonable time suitable for plant operation (less than 15 minutes, see Table 7
360 and Figure 6a). However, a further \$700,000 was saved by fine-tuning the SA parameters
361 from those in Figure 6a to those obtained in Figure 6i but with a ten-fold increase in
362 computational time at 112 minutes. The flat sections of the profiles indicate lack of
363 improvement in the search within the given interval. It is instructive to note that the values of

best objectives may not necessarily be the true optimum and there is no way to tell an optimal solution has been found unless it is known in advance (20). Also, since each run yields a slightly different best objective, an advantage is that the engineer is provided with a solution space rather than a single point solution and various options can be explored.

The flat sections of the profiles indicate lack of improvement in the search within the given interval. It is instructive to note that the values of best objectives may not necessarily be the true optimum and there is no way to tell an optimal solution has been found unless it is known in advance (20). Also, since each run yields a slightly different best objective, an advantage is that the engineer is provided with a solution space rather than a single point solution and various options can be explored.

3.3.2 MINLP Solution of the problem

An MINLP solution of the problem (Table 8) was obtained in GAMS 23.9 with the AlphaECP solver. The formulation differs from that of the NLP except that the variable Av_{ad1} (ethanol volume) was used as an integer variable here rather than a continuous one. This can be a disadvantage in that good solutions may hide within the decimal places. It is noted that the objective value of \$112,201,400.00 obtained is remarkably close to the NLP solution and generally inferior to that obtained by the hybrid procedure. However, the solution time was better (just over 5 minutes) even though it was obtained at the expense of a reduced economic potential. Again, the proposed method ensures that huge financial savings can be made.

Table 8: Product distribution obtained by an MINLP solution of the problem

	Gasoline 89	Gasoline 91
CCP	0.00	190.00
Reformate	0.00	100.00
TCP	0.00	125.00
SRG	20.33	69.67
Naphtha	195.11	404.89
n-Butane	0.00	70.00
Ethanol	73.70	307.30
Alkylate	210.87	817.89
Total	500.00	2084.76

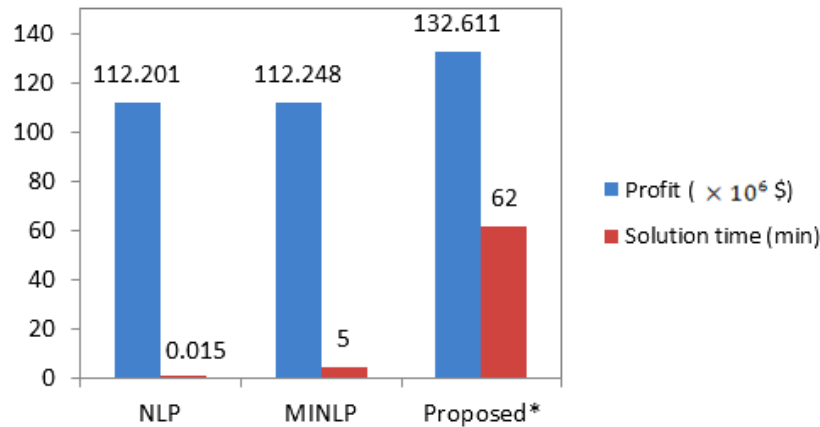


Figure 7: Comparison of net revenue obtained and solution times using NLP, MINLP and the proposed partitioned problem method. *Based on average computational times of 3 Markov chain lengths at annealing temperature of 1 x objective function

3.4 Discussion

Are the savings worth it? This has to be answered within the context of the whole plant operations. Marginal savings in product blending may only pale in comparison to losses elsewhere that may be accrued as a result of the additional time required by fine-tuned optimisation parameters. One way around it is the use of larger CPU memory. On the other hand, this may be integrated in a wider recipe–scheduling or recipe–production unit optimisation as suggested by (5). In a nutshell, as shown in Figure 7, trade-offs are involved between solution quality, which in this case are characterized by large annealing temperatures; and computational time.

A possible area of enhancing our method is the use of sequential quadratic programming SQP to improve the solution within the neighborhood of the feasible region identified. Even though this results in the loss of some control by way of eliminating the use of the engineering judgment, it has however been used by other investigators. Such a hybrid method has been used by (21) on a set of constrained nonlinear optimisation problems from the open literature. Genetic algorithm was used to locate feasible domains after which SQP was used to converge to the exact solution. Comparing with other approaches, for short-term recipe optimisation, they reported good solution times, improved profit, and satisfactory quality indicators were obtained including when uncertainty is considered.

On the issue of computational time, refinery wide optimisation performed by (22) focused on model reduction. Their approach entailed the use of novel artificial neural network/integer programming estimation of the nonlinear models describing the refinery. Solution times were in the order of 0.2 seconds. This was done against the backdrop of industry practice where large LP models which require tedious formulation and collection of large amounts of data are used. However, it is noted that this low solution time comes at a huge cost of utilizing a reduced model where the possibility of missing some nonlinear features inherent in the system.

4. CONCLUSION

Constraint or problem partitioning is an effective method that resolves large-scale highly constrained nonlinear optimisation problems into smaller and simpler partitioned problems. A

variant of this method was used here where hybrid Nonlinear Programming–Simulated Annealing procedure was applied to solve the offline gasoline recipe optimisation problem. The case study had eighteen independent variables where one of the variables (ethanol volume) was used a link variable between the two sub-problems of the partitioned non-convex problem. (10) noted that this can in theory be extended to larger highly constrained problems with more link variables such as refineries where the models involve huge number of nonlinear equations and many process units. The method exhibited good performance with little computational resources. This represented significant savings as against a derivative-based NLP method used alone. The performance was examined using a sensitivity analysis of the simulated annealing parameters. Convergence times were in minutes and are realistic for short term recipe optimisation. With computing power becoming less of an issue these days, indeed the scope of the problem can be extended to handle larger scale refinery optimisation.

Definitions, Acronyms, Abbreviations

1. Abbreviations

AKI	anti-knock index
kbbl	1000 barrels
LP	Linear Programming
MILP	Mixed Integer Linear Programming
MINLP	Mixed Integer Non-Linear Programming
MON	Motor Octane Number
NLP	Non-Linear Programming
CCP	Catalytic Cracking Product
RON	Research Octane Number
SQP	Successive Quadratic Programming
SRG	straight run gasoline
TCP	Thermal Cracking Product

2. Variables/parameters

Symbol	Description	Unit
A	Aromatics content	vol %
Av	Availability of feedstock	kbbl
$\bar{m}$	Volumetric average MON	-
O	Olefin Content	vol %
P	generic gasoline Property	-
RVP	Reid Vapour Pressure	psia
$\bar{r}$	Volumetric average RON	-
S	Octane Number Sensitivity (RON - MON)	-
v	Volume fraction of component	vol %
x	volume/weight/molar fraction	-

3. Subscripts

a	Set of additives
j	Set of gasoline blends
r	Set of refinery blending feedstock

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