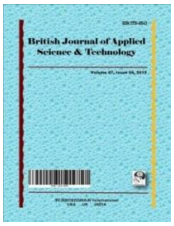

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# Global Optimisation of Gasoline Pool Blending Using Constraint Partitioning

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***Authors' contributions***

*This work was carried out in collaboration between all authors. Author AMA designed the study and performed simulations; author BYD meticulously collected the secondary data. Author AE and SMM managed the literature, authors MU and IAM made technical input on the structure of the algorithm used. Authors OA and SA proofread all drafts. All authors read and approved the final manuscript.*

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## ABSTRACT

**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

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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.

*Keywords: Gasoline blending; simulated annealing; constraint partitioning; stochastic optimisation.*

## 1. INTRODUCTION

Refineries are continuously faced with increasingly tighter constraints. Governments are enforcing more stringent legislation in order to ameliorate climatic change concerns and curtail environmental damage as a result of human activity. Be it emissions reduction targets or large demand for high octane rated fuels at reasonable prices, society is seemingly apathetic to the fact that these refineries are businesses that must turn out profits. Refiners, under the stated limitations, must optimise in order to thrive.

A refinery is a vast petrochemical facility with thousands of interconnected units and processes. Realistic modelling for design and operation therefore gives rise to highly non-linear models. These are difficult problems and can be time-consuming to solve as a whole. Optimising one or several key processes such as the Crude Distillation and Fluid Catalytic Cracking Units, unfortunately do not automatically translate to optimal values for the whole complex [1]. Overall refinery optimisation is a difficult endeavour, nevertheless, this is done based on the major subdivisions as shown in Fig. 1. Product blending and recipe optimisation, the last of the subdivisions, is the closest to the consumer. Therefore, careful monitoring to meet quality and environmental regulations requires proper optimisation. This ensures that the products are “on-spec” and with minimal give-aways.

Linear programming (LP) has been the dominant industry-wide practice. It has the obvious advantages of simplicity, fast convergence, and minimal computational requirements. This has proven satisfactory for long term planning. However, it is unsatisfactory in the short to medium term against the backdrop of tighter profit margins.

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

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

It has been observed that future work in refinery optimisation might focus on how to determine component values and the preferred product recipes, in order to optimize the combined performance of the short-term blending and product shipments and how to incorporate the scheduling decisions with long-term planning decisions [6]. Therefore, in the short-term, another recipe may be more profitable than the long-term optimal recipe, and the deviations from the long-term recipe may indicate that other blending recipes should be used. Ideally, it would

be possible to detect the values of components, and in order to more closely approximate the values of these components, there must be integration between short-term and long-term decision. Problem partitioning can be used to achieve these.

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

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

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

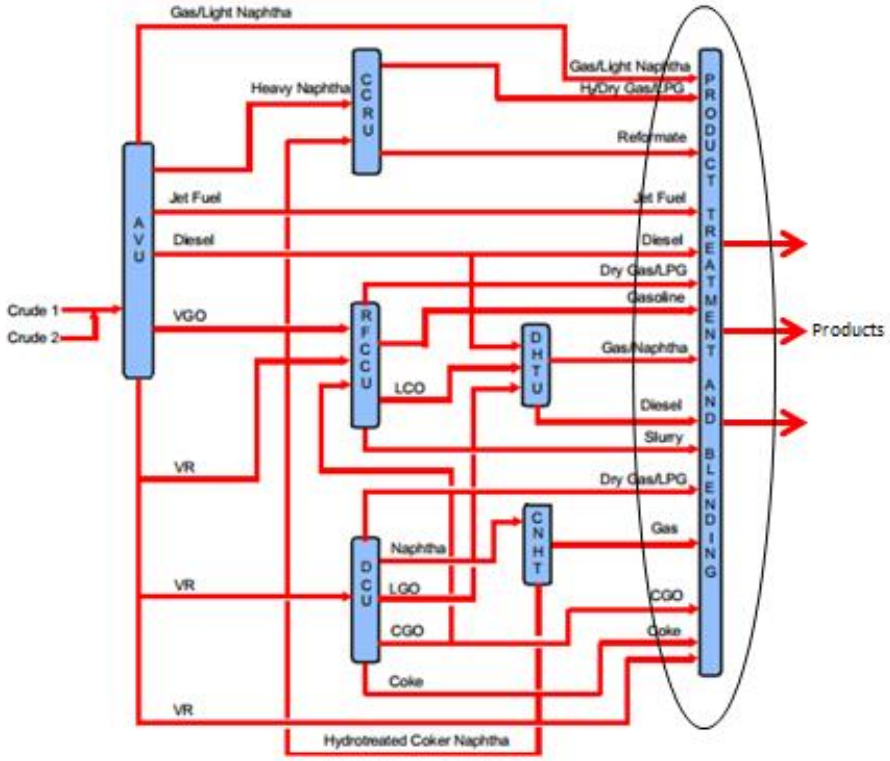


**Fig. 1. A simplified refinery flow sheet from crude oil to gasoline showing the position of product blending**

## 2. METHODOLOGY: OPTIMISATION BY PROBLEM PARTITIONING

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

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

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

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

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

$$g_N(x_1, x_2, ..., x_n) \ge 0 \quad (1d)$$

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

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

Sub-problem 1:

$$\text{Maximise } h(y) \quad (2a)$$

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

Sub-problem 2:

$$\text{Maximise } f(x_1, x_2, ..., x_n) \quad (3a)$$

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

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

$$g_N(x_1, x_2, ..., x_n) \ge 0 \quad (3d)$$

$$x_1 \ge k_1, \ x_2 \ge k_2, \ ..., \ x_n \ge k_n \quad (3e)$$

Here, the link variable chosen reduces sub-problem 2 from *n+1* variables to n and is constrained between a lower and upper bound interval in sub-problem 1. It is instructive to note that this link variable in sub-problem 1 whose generated value (random or otherwise) in each iterative run is passed on to sub-problem 2 and is hence not included as one of the constraints in equations (3e). Sub-problem 1 is such that a stochastic global optimisation method (Tabu Search, Genetic Algorithm, Simulated Annealing, etc.) can be applied while in sub-problem 2 is solved for each sampled y∈ [*l, u*] using NLP until convergence based on the criteria set in sub-problem 1. Fig. 2 illustrates this solution structure. The method is formally described in [10] and they note its ability to handle non-convex problems. [11] used the method to solve an operations research air transport problem, observing its remarkable efficacy in simplifying large-scale problems to simple continuous and mixed integer NLPs.

A general Simulated Annealing pseudo-code is as follows as described by [12]:

- Choose an initial solution x, an initial temperature T, a lower limit on temperature TLOW, and an inner iteration limit L
- While (T > TLOW), do
- For k = 1, 2, …, L, do (Markov Chain Length)
- Make a random choice of an element x' ∈ N(x).
- MoveValue = f(x') – f(x)
- If MoveValue ≤ 0 (downhill move), set x = x'
- If MoveValue > 0 (uphill move), set x = x' with probability
- exp(−MoveValue/T)
- End inner (Markov Chain Length) loop

- Reduce temperature according to an annealing schedule. An example is new T = cT, where 0 < c < 1.
- End temperature loop

Fig. 3 is a flowchart showing the SA programme structure for the case study which is based on the Metropolis algorithm:

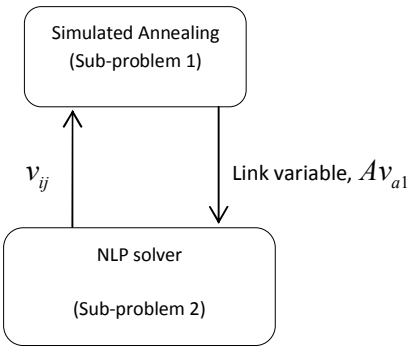


**Fig. 2. Partitioned problem solution structure**

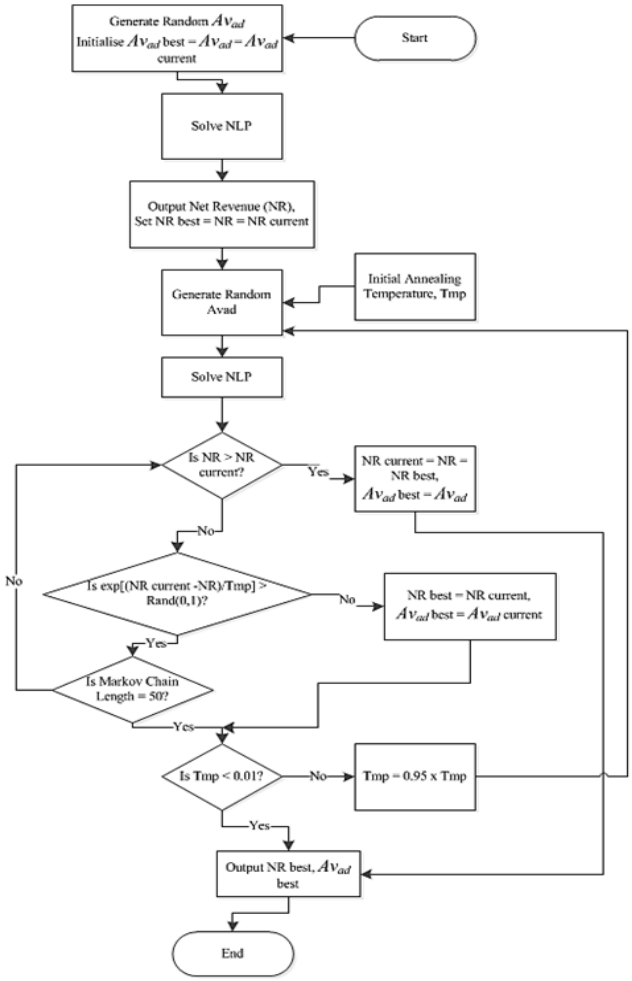


**Fig. 3. Flowchart of hybrid SA-NLP solution procedure**

## 3. RESULTS AND DISCUSSION

### 3.1 Case Study

To demonstrate the proposed method, unpublished refinery data (Tables 1, 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 as shown in Fig. 4). For both gasolines, their RVP and aromatics content must be within the restrictions defined earlier.

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

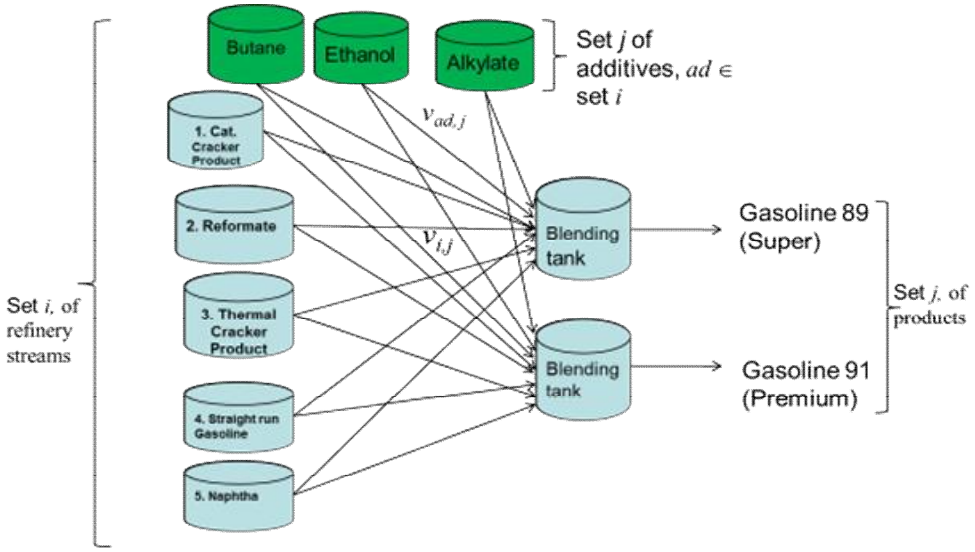


**Fig. 4. Gasoline pool blending problem for two grades of gasoline**

**Table 1. Collected data on available feedstock properties and information about additives†**

| | RON | MON | AKI | RVP (psi) | Aromatics (%) | Availability (kbbl) | 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 |

*Kbbl – 1000 barrels, CCP* – Catalytic cracker product, TCP** – Thermal cracker product, SRG†† – Straight run gasoline †Source: [13]*

**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]*

**Table 3. Detailed product distribution**

| | Gasoline 89 (kbbl) | Gasoline 91 (kbbl) |
|---|---|---|
| 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]*

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.

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

## 3.2 Optimisation Problem Formulation

### 3.2.1 Modelling blend properties

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

$$P_j = \sum_{i=1}^{N} x_i P_i \tag{4}$$

Where $x_i$ is the volume/weight/molar fraction of the blending component i, Pi 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.

$$P_j = \frac{\sum_i P_i v_{ij}}{\sum_i v_{ij}} \tag{5}$$

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.

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

Where $SG_i$ is the specific gravity of component $i$.

### 3.2.2 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.

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

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

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.

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

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

With the RVP of the gasoline blend j being:

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

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

### 3.2.4 Objective function

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

$$\sum_j \mathrm{Pr}_j V_j - \sum_a C_a Av_a - \sum_m k_m s_m^2 \quad (10)$$

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

### 3.2.5 Variables

The problem contains a total of eighteen independent variables to be determined by optimisation. These are in two groups. The first group has the volumes of each blending component $i$ that distributes into gasoline product $j$, i.e. $v_{ij}$. The set $i$ of components contains eight elements (Stream 1–Stream 5, alkylate, ethanol and n-butane). The set $j$ of gasoline products contained 2 elements – Gasoline 89 and Gasoline 91. As such the blend volume fractions $v_{ij}$ optimised were sixteen in number. The second group of independent variables is the volume of market additives $v_{ad}$ required to optimise the objective function. Butane is an additive that boosts RVP of gasoline, but it is not included in $v_{ad}$ as it is

already assumed to be produced as an overhead product in refinery crude distillation columns. Hence the set ad contains two elements (alkylate and ethanol). This set however, is a subset of set $i$ the set of blending components.

**3.2.6 Inequality constraints**

*3.2.6.1 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:

94 ≤ RON ≤ 96 for gasoline 89
96 ≤ RON ≤ 98 for gasoline 91
84 ≤ MON ≤ 86 for Gasoline 89
86 ≤ MON ≤ 88 for Gasoline 91

*3.2.6.2 Reid Vapour Pressure (RVP)*

Reid vapour pressure constraints were imposed as being 0 ≤ RVP ≤ 6.9 psi for both gasolines. This is based on the UK's minimum summer gasoline vapour pressure of 6.53 kPa [16].

*3.2.6.3 Aromatics Content*

European Union regulations specify that all gasolines produced in Europe from 2005 onwards must have aromatics content ≤ 35% by volume [17].

*3.2.6.4 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].

**3.2.7 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.

$$Av_r = \sum_j v_{r,j} \tag{11}$$

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

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

$$Av_{ad} = \sum_j v_{ad,j} \tag{12}$$
$$\forall v_{ad,j}, 0 \le v_{ad,j} \le Av_r$$

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.

$$V_j = \sum_r v_{r,j} + \sum_{ad} v_{ad,j} \tag{13}$$

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

$$\sum_j V_j = \sum_r Av_r + \sum_{ad} Av_{ad} \tag{14}$$

## 3.3 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.

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.

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

**Table 4. Independent optimisation variables**

| | Variables $v_{rj}$ | | Variables $v_{ad}$ |
|---|---|---|---|
| | **Gasoline 89** | **Gasoline 91** | **Availability (kbbl*)** |
| CCP | 1 | 9 | |
| Reformate | 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) |

## 3.4 Search for a Global Optimum

### 3.4.1 Solving the problem by constraint partitioning

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

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

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

**Table 5. Detailed NLP solution product distribution (kbbl)**

| | **Gasoline 89** | **Gasoline 91** |
|---|---|---|
| CCP | 0.00 | 190.00 |
| Reformate | 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 NLP model was integrated into a hybrid NLP-Simulated annealing to directly search for a global solution. The NLP solver used was CONOPT in GAMS 23.9. A Metropolis based search algorithm employing the Boltzmann probability as described earlier was used as the move rejection criterion. It should be noted that results are not exactly reproducible as successive iterations proceed based on uniformly distributed random number generation of ethanol additive volume, as shown in Fig. 5.

**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 |

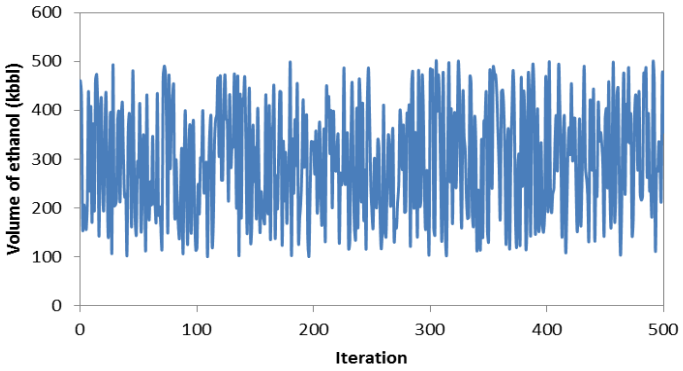


**Fig. 5. Uniform Random number distribution in [100, 500] with iteration for ethanol volume**

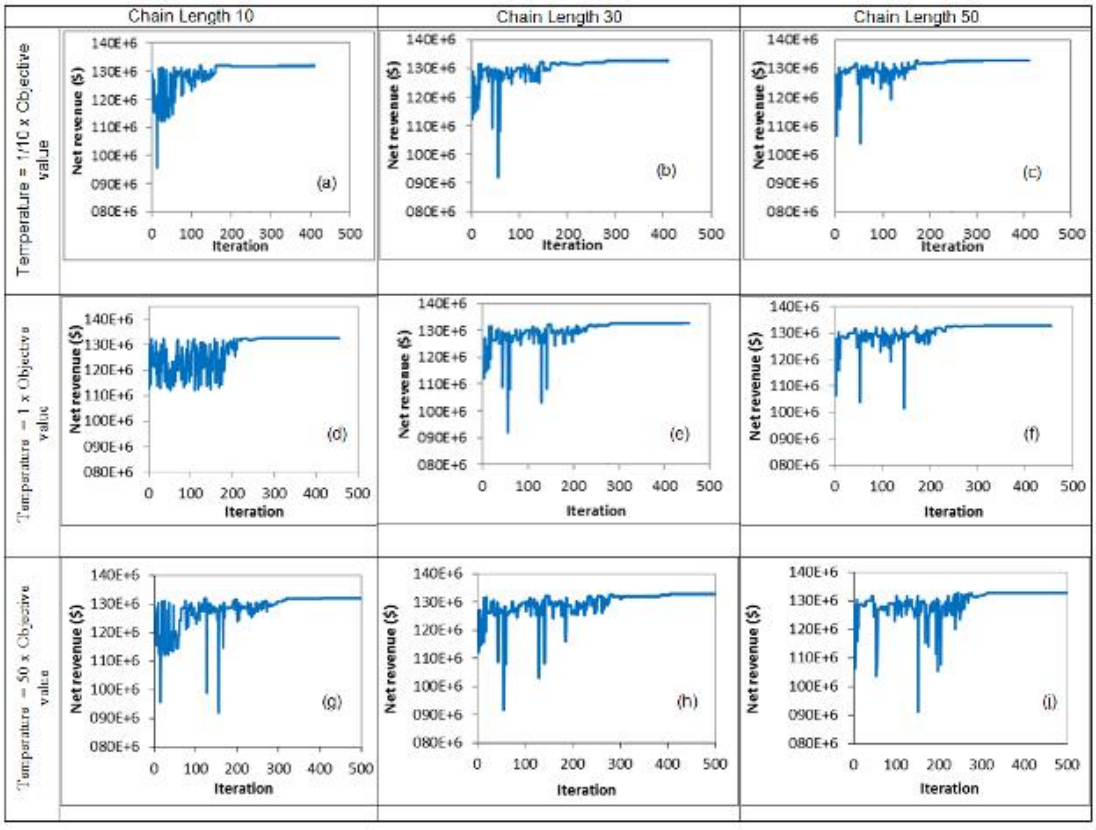


**Fig. 6. Plots of objective value against number of iterations for annealing temperatures of 1/10, 1, and 10 times the objective value and Markov chain lengths of 10, 30, and 50 respectively**

The results obtained as shown in Fig. 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 times the locally optimal objective value). This is to examine the consistency of successive solutions. As is seen in Table 7, computational time is affected by both annealing temperature and Markov chain length. The higher the temperature and the larger the Markov Chain Length the longer the CPU time for a single run. A chain length of 50, which is the largest used, produced the highest best objective value regardless of initial annealing temperature. In theory, infinitely large chain lengths can be used for more refined solutions, but in practice the refinements have to be balanced with solution time which must be realistic for day-to-day plant operations.

Similarly, increasing annealing temperature has an effect on the quality of the best objective found. The Metropolis search algorithm guarantees that the search will yield a good quality result when large annealing temperatures are used as the solution space is properly combed. However, this increases the solution time. Fig. 6 shows the progression of the search with iteration number. They show that lower objective values are also accepted (characterized by peaks as well as troughs). This helps the optimization escape local optima. For an initial temperature of $1.3\times10^{6}$ (approximately one-tenth the objective value) which dropped to $10^{-3}$ by an annealing schedule of 0.95 Temperature, there were 410 iterations (Figs. 6a, b and c). When temperature was increased to exactly the objective value, the number of iterations increased to 455 and to 513 when increased to 50 times the objective (Figs. 6g, h and i).

These confirm that the initial NLP solution of $112,201,183.06 was a local maxima and attempting a basic global search gives an estimated increase of $20,000,000. This was achieved in reasonable time suitable for plant operation (less than 15 minutes, see Table 7 and Fig. 6a). However, a further $700,000 was saved by fine-tuning the SA parameters from those in Fig. 6a to those obtained in Fig. 6i but with a ten-fold increase in computational time at 112 minutes. 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.

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**Table 7. Sensitivity of SA parameters on best objective value**

| | | | |
|---|---|---|---|
| **Annealing Temperature 1/10 × 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 × 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 × 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 |

### 3.4.2 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 |

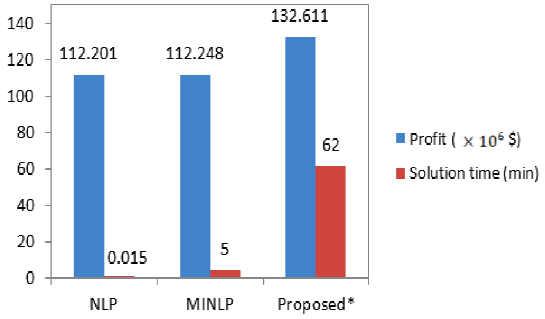


**Fig. 7. Comparison of net revenue obtained and solution times using NLP, MINLP and the proposed partitioned problem method. *Based on average computational times of 3 Markov chain lengths at annealing temperature of 1 x objective function**

## 3.5 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 Fig. 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.

## COMPETING INTERESTS

Authors have declared that no competing interests exist.

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