A NOVEL MINLP-BASED REPRESENTATION OF THE ORIGINAL COMPLEX MODEL FOR PREDICTING GASOLINE EMISSIONS

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Abstract

The Environmental Protection Agency introduced Reformulated Gasoline (RFG) requirements as a measure to reduce emissions from gasoline-powered vehicles in certain geographic areas. The EPA developed models for predicting emissions as a function of gasoline properties and established statutory baseline emissions from a representative set of gasolines. RFG is a key driving force for investment in the North American refining industry. All reformulated gasoline requires certification via the complex model, and all refiners and importers calculate emissions performance reductions from the statutory baseline gasoline.

The RFG models introduce increasing complex constraints with the major limitation that it is implicitly defined through a series of complicated disjunctions assembled in the form of spreadsheets by the EPA. This implicit and cumbersome representation of the emissions predictive models renders rigorous optimization and sensitivity analysis very difficult. In this paper, we discuss how the federal government requirements for reformulated gasoline can be restated as a set of mixed-integer nonlinear programming (MINLP) constraints with the aid of disjunctive programming techniques.

Keywords

Generalized disjunctive programming, Gasoline emissions.

Introduction

The Environmental Protection Agency (EPA) introduced Reformulated Gasoline (RFG) requirements (U.S. Government, 2003; Rhodes, 1998) as a measure to reduce emissions from gasoline-powered vehicles in certain geographic areas. The EPA developed models for predicting emissions as a function of gasoline properties and established statutory baseline emissions from a representative set of gasolines produced in the United States in 1990. RFG is a key driving force for investment in the North American refining industry. Beginning in 1998, all reformulated gasoline required certification via the complex model, which is a refinement of the original simple model introduced in 1995. All refiners and importers calculate emissions performance reductions from the statutory baseline gasoline.

The RFG models introduce increasing complex constraints that are placed on the product blending problems and their possible technological solutions. The complex model introduces incredibly interactive and nonlinear equations for predicting emissions. One of the major limitations of the current state of the complex model is that it is implicitly defined through a series of complicated disjunctions assembled in the form of spreadsheets by the EPA. The EPA complex model spreadsheet allows refiners to compute satisfactory limits for properties such as RVP, Sulfur, Benzene, etc. which permit the gasoline to meet the complex model requirements. The implicit definition of the constraints through the spreadsheet and their convoluted logic makes their incorporation to design and blending studies cumbersome. Previous attempts involve iterative schemes to incorporate simulation and optimization (Treiber et al., 1998). This complicated representation of the emissions predictive models renders rigorous optimization and sensitivity analysis very difficult.

In this paper, we discuss how the federal government requirements for reformulated gasoline, which at present is published as a set of discontinuous and nonlinear equations, can be restated as a set of mixed-integer nonlinear programming (MINLP) constraints with the aid of disjunctive programming techniques (Raman and Grossmann, 1994; Türkay and Grossmann, 1996; Vecchietti and Grossmann, 2000). In the following section we provide a novel representation of part of the complex model by translating the rule descriptions to exact mathematical formulation using the principles of disjunctive programming. We demonstrate how the implicit spreadsheet formalism is translated to a compact generalized disjunctive programming formulation amenable to incorporation in complex decision making problems involving optimal refinery operations.

VOC Performance GDP Formulation

The EPA Phase II Complex Emissions Model is stated in the Code of Federal Regulations (CFR) Title 40 Part 80.45 (U.S. Government, 2003), however due to discrepancies between the printed model and the spreadsheet model provided on the EPA website (Environmental Protection

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Agency, 2003)), the spreadsheet has been chosen as the basis for this study as it is the source for the printed model and in general use in the refining industry for emissions calculations. For the purposes of preserving space, we shall only present the generalized disjunctive programming (Raman and Grossmann, 1994) formulation for volatile organic compounds (VOC) emissions performance. There are different regulations based on season and geographic location.

Exhaust VOC Emissions Performance of Gasoline (Summer)

$$VOCE = VOC_b + \left(VOC_b \frac{Y_{VOC}}{100} \right) \tag{1}$$

$$\begin{aligned} & Y_{VOC,t} = \\ & 100 w_1^{VOC} \left(\frac{\exp(v_{1et})}{\exp(v_{1b})} - 1 \right) + \\ & 100 w_2^{VOC} \left(\frac{\exp(v_{2et})}{\exp(v_{2b})} - 1 \right) + \\ & 100 w_1^{VOC} \left(\frac{\exp(v_{1et})}{\exp(v_{1b})} \right) \times \\ & \quad \left[\begin{array}{l} (2\alpha_8 E200_{et} + \alpha_4)\, \Delta E200_v + \\ (2\alpha_9 E300_{et} + \alpha_5 + \alpha_{10} ARO_{et})\, \Delta E300_v + \\ (\alpha_{10} E300_{et} + \alpha_6)\, \Delta ARO_v \end{array} \right] \\ & 100 w_2^{VOC} \left(\frac{\exp(v_{2et})}{\exp(v_{2b})} \right) \times \\ & \quad \left[\begin{array}{l} (2\beta_8 E200_{et} + \beta_4)\, \Delta E200_v + \\ (2\beta_9 E300_{et} + \beta_5 + \beta_{10} ARO_{et})\, \Delta E300_v + \\ (\beta_{10} E300_{et} + \beta_6)\, \Delta ARO_v \end{array} \right] \end{aligned} \tag{2}$$

$$\begin{aligned} v_{1et} = \; & \alpha_1\, OXY_{et} + \alpha_2\, SUL_{et} + \\ & \alpha_3\, RVP_{et} + \alpha_4\, E200_{et} + \\ & \alpha_5\, E300_{et} + \alpha_6\, ARO_{et} + \\ & \alpha_7\, OLE_{et} + \alpha_8\, (E200_{et})^2 + \\ & \alpha_9\, (E300_{et})^2 + \alpha_{10}\, ARO_{et} E300_{et} \end{aligned} \tag{3}$$

$$\begin{aligned} v_{2t} = \; & \beta_1\, OXY_{et} + \beta_2\, SUL_{et} + \\ & \beta_3\, RVP_{et} + \beta_4\, E200_{et} + \\ & \beta_5\, E300_{et} + \beta_6\, ARO_{et} + \\ & \beta_7\, OLE_{et} + \beta_8\, (E200_{et})^2 + \\ & \beta_9\, (E300_{et})^2 + \beta_{10}\, ARO_{et} E300_{et} \end{aligned} \tag{4}$$

The index et can be exchanged with b in the above equations (3) and (4) to calculate parameters v_{1b} and v_{2b}.

$$\left[\begin{array}{rcl} E300_{ot} & \geq & 95 \\ E300_t & = & 95 \end{array} \right] \vee \left[\begin{array}{rcl} E300_{ot} & \leq & 95 \\ E300_t & = & E300_{ot} \end{array} \right] \tag{5}$$

$$\left[\begin{array}{rcl} ARO_{ot} & \leq & 10 \\ ARO_t & = & 10 \end{array} \right] \vee \left[\begin{array}{rcl} ARO_{ot} & \geq & 10 \\ ARO_t & = & ARO_{ot} \end{array} \right] \tag{6}$$

It should be noted that equations (5) and (6) are actually common to the entire complex model and not limited to the VOC calculations.

$$\begin{array}{l} \left[\begin{array}{rcl} 79.75 + 0.385 ARO_t & \leq & 94 \\ E300* & = & 79.75 + 0.385 ARO_t \end{array} \right] \\ \vee \left[\begin{array}{rcl} 79.75 + 0.385 ARO_t & \geq & 94 \\ E300* & = & 94 \end{array} \right] \end{array} \tag{7}$$

$$\begin{array}{l} \left[\begin{array}{rcl} E200_t & \leq & 33 \\ E200_{et} & = & 33 \\ \Delta E200_v & = & E200_t - 33 \end{array} \right] \\ \vee \left[\begin{array}{rcl} E200_t & \geq & 33 \\ E200_t & \leq & 65.52 \\ E200_{et} & = & E200_t \\ \Delta E200_v & = & 0 \end{array} \right] \\ \vee \left[\begin{array}{rcl} E200_t & \geq & 65.52 \\ E200_{et} & = & 65.52 \\ \Delta E200_v & = & E200_t - 65.52 \end{array} \right] \end{array} \tag{8}$$

$$\begin{array}{l} \left[\begin{array}{rcl} E300_t & \leq & 72 \\ E300_{et} & = & 72 \\ \Delta E300_v & = & E300_t - 72 \end{array} \right] \\ \vee \left[\begin{array}{rcl} E300_t & \geq & 72 \\ E300_t & \leq & E300* \\ E300_{et} & = & E300_t \\ \Delta E300_v & = & 0 \end{array} \right] \\ \vee \left[\begin{array}{rcl} E300_t & \geq & E300* \\ E300_{et} & = & E300* \\ \Delta E300_v & = & E300_t - E300* \end{array} \right] \end{array} \tag{9}$$

$$\begin{array}{l} \left[\begin{array}{rcl} ARO_t & \leq & 18 \\ ARO_{et} & = & 18 \\ \Delta ARO_v & = & ARO_t - 18 \end{array} \right] \\ \vee \left[\begin{array}{rcl} ARO_t & \geq & 18 \\ ARO_t & \leq & 46 \\ ARO_{et} & = & ARO_t \\ \Delta ARO_v & = & 0 \end{array} \right] \\ \vee \left[\begin{array}{rcl} ARO_t & \geq & 46 \\ ARO_{et} & = & 46 \\ \Delta ARO_v & = & ARO_t - 46 \end{array} \right] \end{array} \tag{10}$$

Winter Exhaust VOC Emissions Performance of Gasoline

For the winter exhaust VOC emissions performance constraints, the same equations as the previous section are to be used, however substituting for the values of RVP such that $RVP_b = RVP_t = 8.7$ psi.

Non-Exhaust VOC Emissions Performance of Gasoline in VOC Control Region 1

$$VOCNE1 = DI1 + HS1 + RL1 + RF1 \tag{11}$$

$$DI1 = 0.007385(RVP_t)^2 - 0.08981 RVP_t + 0.3518 \tag{12}$$

$$HS1 = 0.006654(RVP_t)^2 - 0.08094 RVP_t + 0.2846 \tag{13}$$

$$RL1 = 0.017768(RVP_t)^2 - 0.18746 RVP_t + 0.6146 \tag{14}$$

$$RF1 = 0.004767 RVP_t + 0.011859 \tag{15}$$

Non-Exhaust VOC Emissions Performance of Gasoline in VOC Control Region 2

$$VOCNE2 = DI2 + HS2 + RL2 + RF2 \tag{16}$$

$$DI2 = 0.004775(RVP_t)^2 - 0.05872RVP_t + 0.21306 \tag{17}$$

$$HS2 = 0.006078(RVP_t)^2 - 0.07474RVP_t + 0.27117 \tag{18}$$

$$RL2 = 0.016169(RVP_t)^2 - 0.17206RVP_t + 0.56724 \tag{19}$$

$$RF2 = 0.0.004767RVP_t + 0.011859 \tag{20}$$

Non-exhaust Winter VOC Emissions Performance of Gasoline

Winter non-exhaust VOC emissions are set equal to zero.

Total VOC Emissions

Total summer VOC emissions for VOC control regions 1 and 2 is calculated by the following equations:

$$VOCS1 = \frac{VOCE}{1000} + VOCNE1 \tag{21}$$

$$VOCS2 = \frac{VOCE}{1000} + VOCNE2 \tag{22}$$

Total winter VOC emissions are calculated with the following:

$$VOCW = \frac{VOCE}{1000} \tag{23}$$

Total VOC Emissions Performance

Total summer VOC emissions performance of gasoline for VOC control regions 1 and 2 are calculated with the following:

$$VOCS1\% = \frac{100\%}{1.4663}(VOCS1 - 1.4663) \tag{24}$$

$$VOCS2\% = \frac{100\%}{1.3991}(VOCS1 - 1.3991) \tag{25}$$

Total winter VOC emissions performance of gasoline is calculated by the following equation:

$$VOCW\% = \frac{100\%}{1.341}(VOCW - 1.341) \tag{26}$$

Limits of the Model and Standards of Compliance

The equations for the complex model are only valid when the fuel properties are within certain ranges for reformulated and conventional gasolines. For reformulated gasolines:

$$0.0 \leq OXY_t \leq 3.7 \tag{27}$$

$$0.0 \leq SUL_t \leq 500.0 \tag{28}$$

$$6.4 \leq RVP_t \leq 10.0 \tag{29}$$

$$30.0 \leq E200_t \leq 70.0 \tag{30}$$

$$70.0 \leq E300_t \leq 100.0 \tag{31}$$

$$0.0 \leq ARO_t \leq 50.0 \tag{32}$$

$$0.0 \leq OLE_t \leq 25.0 \tag{33}$$

$$0.0 \leq BEN_t \leq 2.0 \tag{34}$$

For conventional gasolines:

$$0.0 \leq OXY_t \leq 3.7 \tag{35}$$

$$0.0 \leq SUL_t \leq 1000.0 \tag{36}$$

$$6.4 \leq RVP_t \leq 11.0 \tag{37}$$

$$30.0 \leq E200_t \leq 70.0 \tag{38}$$

$$70.0 \leq E300_t \leq 100.0 \tag{39}$$

$$0.0 \leq ARO_t \leq 55.0 \tag{40}$$

$$0.0 \leq OLE_t \leq 30.0 \tag{41}$$

$$0.0 \leq BEN_t \leq 4.9 \tag{42}$$

Fuels with one or more properties that do not fall within the ranges described above are not certified or evaluated for their emissions performance using the complex emissions model.

The EPA standards of compliance for reformulated gasoline are stated in the CFR Title 40 Part 80.41 (U.S. Government, 2003). Gasoline meeting those standards are deemed certified.

$$VOC\% \geq -V^{\min} \tag{43}$$

$$NOX\% \geq -N^{\min} \tag{44}$$

$$TOXIC\% \geq -T^{\min} \tag{45}$$

$$OXY_t \geq O^{\min} \tag{46}$$

$$BEN_t \leq B^{\max} \tag{47}$$

where $VOC\%$ is either $VOCS1\%$, $VOCS2\%$, or $VOCW\%$ depending on the season and the VOC control region. The constraints in the model related to NO_x and toxics emissions performance ($NOX\%$ and $TOXIC\%$) have not been presented in this paper, but are developed in a manner similar to that of the previous section. Figure 1 illustrates the regions of the United States regulted by the RFG model.

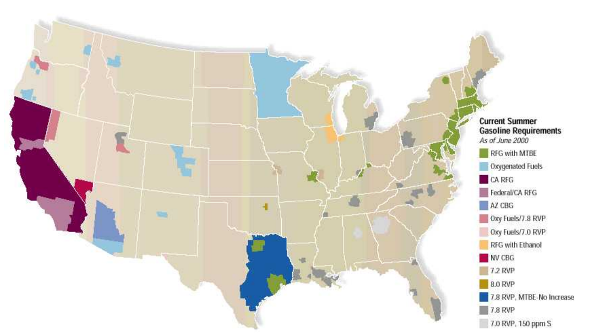

Figure 1: U.S. Regulated Areas for RFG Requirements

Motivating Results

The methodology is demonstrated through the analysis of an illustrative example. We wish to identify fuel compositions that remain as close as possible to a reference composition after imposing additional restrictions. We define the reference composition state as the baseline fuel defined by the EPA. The model has been calibrated against this composition and therefore the relative change in VOC, Toxics and NO_x with respect to the baseline fuel are zero. We define a general optimization problem in which we minimize the scaled deviation from the baseline while meeting stricter requirements. Namely, we define five case studies such that the VOC requirement is raised to a 30% reduction and the maximum Sulfur levels are gradually reduced (500ppm, 150ppm, 100ppm, 50ppm, and 10ppm). The resulting non-convex MINLP is formulated within the GAMS (Brooke et al., 2003) modeling environment and is solved to global optimality using BARON (Tawarmalani and Sahinidis, 2004). Figure 2 summarizes the percent change in fuel composition properties, relative to the base case, that is required in order to meet the tighter VOC regulations. It should be pointed out that all fuel compositions achieve a 30% VOC reduction while significantly reducing the Sulfur levels. The formulation also takes into account the explicit bounds on RFG fuel properties, as defined in constraints (27) and (29)-(34). Although this problem is posed in a simple manner, it addresses the very critical concern of meeting more stringent composition requirements while imposing the minimum number of changes in processing. This example demonstrates the versatility of the new formulation and its potential for accurate refinery optimization. In future efforts, this framework could be expanded to incorporate detailed physical models, as well as blending tools, to derive detailed fuel compositions.

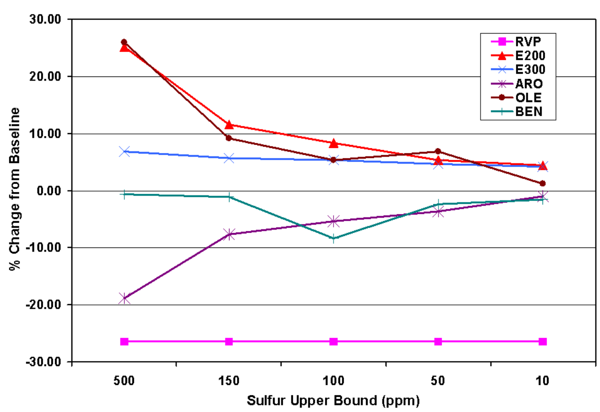

Figure 2: Sensitivity of Fuel Properties to Sulfur Bounds

Conclusions

A set of mathematical programming constraints is developed for the EPA RFG complex model that is simplified and easier to understand, yet remains fully compliant with the model and specifications of the EPA. The generalized disjunctive programming constraints developed could be easily included in a refining industry optimization problem. Such a problem could be posed as a GDP problem, reformulated as MINLP, or cast as some hybrid form and solved using one of several potential solution algorithms (Vecchietti and Grossmann, 2000). This form of the RFG model is much more convenient than the EPA spreadsheet for implementation in computational problems. The implementation of the model has been illustrated through a sensitivity study.

Indices

1	Normal emitter index
2	High emitter index
b	Baseline fuel index
et	"Edge target" fuel index
t	Target fuel index
ot	Original target (unadjusted) fuel index
v	VOC index

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