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## A novel MINLP-based representation of the original complex model for predicting gasoline emissions

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### ABSTRACT

The Environmental Protection Agency (EPA) introduced Reformulated Gasoline (RFG) requirements as a measure to reduce emissions from gasoline-powered vehicles in certain geographic areas. As part of this effort, the EPA developed empirical models for predicting emissions as a function of gasoline properties and established statutory baseline emissions from a representative set of gasolines. All reformulated gasoline requires certification via this model, known as the Complex Model, and all refiners and importers calculate emissions performance reductions from the statutory baseline gasoline. The current representation of the Complex Model is extremely difficult to implement within refinery operations models or to use in combination with models for designer gasoline. RFG and boutique fuels are key driving forces in the North American refining industry.

The RFG models introduce increasingly complex constraints with the major limitation that they are implicitly defined through a series of complicated disjunctions assembled by the EPA in the form of spreadsheets. This implicit and cumbersome representation of the emissions predictive models renders rigorous optimization and sensitivity analysis very difficult to address directly. 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. We illustrate the use of this model with two simple example fuel blending problems.

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### 1. Introduction

The Environmental Protection Agency (EPA) introduced Reformulated Gasoline (RFG) requirements (Rhodes, 1998; U.S. Government, 2003) 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 this model, known as 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 current representation of the Complex Model is extremely difficult to implement within refinery operations models or to use in combination with models for designer or specially formulated gasoline. The relevance of the so-called “boutique” fuels is quite significant. The Clean Air Act (CAA) requires certain national standards be met for gasoline quality for the purpose of protecting public health. However, in areas that have special air quality needs, the CAA allows states to adopt unique clean fuel requirements, and to sell gasoline that is specially formulated to meet the air quality needs. As a result many individual oil refiners work locally with city and state air quality officials to create cost-effective fuels programs that meet local specifications. Such locally specific fuel types are referred to as “boutique” fuels. Twelve states have adopted their own clean fuel programs for part or all of the state. Most of these states require gasoline with lower volatility than federal standards, and most are effective for only part of the year. These state fuel programs make up eight different kinds of fuels. The federal programs (Reformulated gasoline and low Reid vapor pressure) make up four different kinds of fuel. The combination of federal fuel programs and the states’ abilities to adopt state fuel controls is intended to reflect a balance that allows areas sufficient flexibility to accomplish air quality needs (EPA, 2007a).

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**Nomenclature***Nomenclature*

$a_{1b}$	normal emitter acetaldehyde term using base fuel properties
$a_{2b}$	high emitter acetaldehyde term using base fuel properties
$ACET_b$	baseline acetaldehyde emissions (mg/mile)
$ARO_b$	aromatics content of baseline fuel (season dependent) (vol%)
$B_{1b}$	normal emitter exhaust benzene term using base fuel properties
$B_{2b}$	high emitter exhaust benzene term using base fuel properties
$BEN_b$	benzene content of baseline fuel (season dependent) (vol%)
$BENZ_b$	exhaust benzene baseline emissions (season dependent) (mg/mile)
$BUTA_b$	baseline 1,3-butadiene emissions (mg/mile)
$d_{1b}$	normal emitter 1,3-butadiene term using base fuel properties
$d_{2b}$	high emitter 1,3-butadiene term using base fuel properties
$E200_b$	200 F distillation fraction of baseline fuel (season dependent) (vol%)
$E300_b$	300 F distillation fraction of baseline fuel (season dependent) (vol%)
$f_{1b}$	normal emitter formaldehyde term using base fuel properties
$f_{2b}$	high emitter formaldehyde term using base fuel properties
$FORM_b$	baseline formaldehyde emissions, mg/mile
$n_{1b}$	normal emitter $NO_x$ term using base fuel properties
$n_{2b}$	high emitter $NO_x$ term using base fuel properties
$NOX_b$	baseline $NO_x$ emissions (season dependent) (mg/mile)
$OLE_b$	olefins content of baseline fuel (season dependent) (vol%)
$OXY_b$	oxygen content of baseline fuel (season dependent) (wt%)
$RVP_b$	Reid vapor pressure of baseline fuel (season dependent) (psi)
$SUL_b$	sulfur content of baseline fuel (season dependent) (ppm)
$TOXIC_b$	baseline total toxic emissions (mg/mile)
$v_{1b}$	normal emitter VOC term using base fuel properties
$v_{2b}$	high emitter VOC term using base fuel properties
$VOC_b$	baseline total VOC emissions (mg/mile)
$VOCE_b$	baseline exhaust VOC emissions for appropriate season
$w_1^{ACET}$	normal emitter weighting for exhaust acetaldehyde
$w_2^{ACET}$	high emitter weighting for acetaldehyde
$w_1^{BUTA}$	normal emitter weighting for 1,3-butadiene mass
$w_2^{BUTA}$	high emitter weighting for 1,3-butadiene mass
$w_1^{EXHBZ}$	normal emitter weighting for exhaust benzene
$w_2^{EXHBZ}$	high emitter weighting for exhaust benzene
$w_1^{FORM}$	normal emitter weighting for formaldehyde
$w_2^{FORM}$	high emitter weighting for formaldehyde
$w_1^{NOX}$	normal emitter weighting for $NO_x$
$w_2^{NOX}$	high emitter weighting for $NO_x$
$w_1^{VOC}$	normal emitter weighting for VOC
$w_2^{VOC}$	high emitter weighting for VOC

*Subscripts*

1	normal emitter index
2	high emitter index
b	baseline fuel index
n	“edge target” fuel index in $NO_x$ constraints
ot	original target (unadjusted) fuel index
t	target fuel index
v	“edge target” fuel index in VOC constraints

*Continuous variables*

$a_{1t}$	normal emitter acetaldehyde term using target fuel properties
$a_{2t}$	high emitter acetaldehyde term using target fuel properties
$ACET_t$	emissions of acetaldehyde of target fuel (mg/mile)
$ARO_n$	aromatics content of edge target fuel in $NO_x$ constraints (vol%)
$ARO_{ot}$	aromatics content of original target fuel (vol%)
$ARO_t$	aromatics content of target fuel (vol%)
$ARO_v$	aromatics content of edge target fuel in VOC constraints (vol%)
$\Delta ARO_n$	aromatics difference in $NO_x$ calculations (vol%)
$\Delta ARO_v$	aromatics content difference in VOC calculations (vol%)

$B_{1t}$	normal emitter benzene term using target fuel properties
$B_{2t}$	high emitter benzene term using target fuel properties
$BEN_{ot}$	benzene content of original target fuel (vol%)
$BEN_t$	benzene content of target fuel (vol%)
$BUTA_t$	emissions of 1,3-butadiene of target fuel (mg/mile)
$d_{1t}$	normal emitter 1,3-butadiene term using target fuel properties
$d_{2t}$	high emitter 1,3-butadiene term using target fuel properties
DIBZ	diurnal emissions of volatile organic compounds (mg/mile)
$E200_{ot}$	200 F distillation fraction of original target fuel (vol%)
$E200_t$	200 F distillation fraction of target fuel (vol%)
$E200_v$	200 F distillation fraction of edge target fuel in VOC constraints (vol%)
$\Delta E200_v$	200 F distillation fraction difference in VOC calculations (vol%)
$E300_*$	$E300_t$ variable upper bound
$E300_{ot}$	300 F distillation fraction of original target fuel (vol%)
$E300_t$	300 F distillation fraction of target fuel (vol%)
$E300_v$	300 F distillation fraction of edge target fuel in VOC constraints (vol%)
$\Delta E300_v$	300 F distillation fraction difference in VOC calculations (vol%)
$ETB_t$	ethyl tertiary butyl ether content of original target fuel (wt% oxygen)
$ETB_t$	ethyl tertiary butyl ether content of target fuel (wt% oxygen)
$ETH_{ot}$	ethanol content of original target fuel (wt% oxygen)
$ETH_t$	ethanol content of target fuel (wt% oxygen)
$EXHBZ_t$	exhaust emissions of benzene of target fuel (mg/mile)
$f_{1t}$	normal emitter formaldehyde term using target fuel properties
$f_{2t}$	high emitter formaldehyde term using target fuel properties
$FORM_t$	emissions of formaldehyde of target fuel (mg/mile)
HSBZ	hot soak emissions of volatile organic compounds (mg/mile)
$MTB_{ot}$	methyl tertiary butyl ether content of original target fuel (wt% oxygen)
$MTB_t$	methyl tertiary butyl ether content of target fuel (wt% oxygen)
$n_{1t}$	normal emitter $NO_x$ term using target fuel properties
$n_{2t}$	high emitter $NO_x$ term using target fuel properties
NEBZ	non-exhaust emissions of benzene of target fuel (mg/mile)
$NOX_t$	$NO_x$ emissions of target fuel (mg/mile)
$NOXS\%$	$\Delta\%$ in $NO_x$ emissions from summer baseline levels
$NOXW\%$	$\Delta\%$ in $NO_x$ emissions from winter baseline levels
$OLE_n$	olefins content of edge target fuel in $NO_x$ constraints (vol%)
$OLE_t$	olefins content of original target fuel (vol%)
$OLE_t$	olefins content of target fuel (vol%)
$\Delta OLE_n$	olefins difference in $NO_x$ calculations (vol%)
$OXY_t$	oxygen content of original target fuel (wt%)
$OXY_t$	oxygen content of target fuel (wt%)
POM	polycyclic organic mass emissions of target fuel (mg/mile)
RFBZ	refueling emissions of volatile organic compounds (mg/mile)
RLBZ	running loss emissions of volatile organic compounds (mg/mile)
$RVP_{ot}$	Reid vapor pressure of original target fuel (psi)
$RVP_t$	Reid vapor pressure of target fuel (psi)
$SUL_n$	sulfur content of edge target fuel in $NO_x$ constraints (ppm)
$SUL_{ot}$	sulfur content of original target fuel (ppm)
$SUL_t$	sulfur content of target fuel (ppm)
$\Delta SUL_n$	sulfur difference in $NO_x$ calculations (ppm)
$TAM_{ot}$	tertiary amyl methyl ether content of original target fuel (wt% oxygen)
$TAM_t$	tertiary amyl methyl ether content of target fuel (wt% oxygen)
$TOXIC_t$	toxics performance of target fuel (mg/mile)
$TOXIC\%$	$\Delta\%$ in toxic emissions from baseline levels
$v_{1t}$	normal emitter VOC term using target fuel properties
$v_{2t}$	high emitter VOC term using target fuel properties
$VOC_t$	total VOC emissions (mg/mile)
$VOC\%$	$\Delta\%$ in VOC emissions from baseline levels
VOCDI	diurnal VOC emissions (g/mile)
$VOCE_t$	exhaust VOC emissions (mg/mile)
VOCHS	hot soak VOC emissions (g/mile)
VOCNE	total non-exhaust VOC emissions (g/mile)
VOCRF	refueling VOC emissions (g/mile)
VOCRL	running loss VOC emissions (g/mile)

$Y_t^{ACET}$	acetaldehyde performance of target fuel in $\Delta\%$ from baseline
$Y_t^{BEN}$	benzene performance of target fuel in $\Delta\%$ from baseline
$Y_t^{BUTA}$	1,3-butadiene performance of target fuel in $\Delta\%$ from baseline
$Y_t^{FORM}$	formaldehyde performance of target fuel in $\Delta\%$ from baseline
$Y_t^{NOX}$	$NO_x$ performance of target fuel in $\Delta\%$ from baseline
$Y_t^{VOC}$	exhaust VOC performance of target fuel, $\Delta\%$ from baseline

#### Binary variables

$Y_{ARO}$	for general ARO disjunctive constraint
$Y_n^{ARO}$	for NOX ARO disjunctive constraint
$Y_n^{ARO'}$	for NOX ARO disjunctive constraint
$Y_n^{ARO''}$	for NOX ARO disjunctive constraint
$Y_v^{ARO}$	for VOC ARO disjunctive constraint
$Y_v^{ARO'}$	for VOC ARO disjunctive constraint
$Y_v^{ARO''}$	for VOC ARO disjunctive constraint
$Y_v^{E200}$	for VOC E200 disjunctive constraint
$Y_v^{E200'}$	for VOC E200 disjunctive constraint
$Y_v^{E200''}$	for VOC E200 disjunctive constraint
$Y^{E300}$	for general E300 disjunctive constraint
$Y^{E300*}$	for VOC E300* disjunctive constraint
$Y_v^{E300}$	for VOC E300 disjunctive constraint
$Y_v^{E300'}$	for VOC E300 disjunctive constraint
$Y_v^{E300''}$	for VOC E300 disjunctive constraint
$Y_n^{OLE}$	for NOX OLE disjunctive constraint
$Y_n^{OLE'}$	for NOX OLE disjunctive constraint
$Y_n^{OLE''}$	for NOX OLE disjunctive constraint
$Y_n^{SUL}$	for NOX SUL disjunctive constraint
$Y_n^{SUL'}$	for NOX SUL disjunctive constraint
$Y_n^{SUL''}$	for NOX SUL disjunctive constraint

The RFG models introduce increasingly complex constraints that are placed on potential technical approaches for determining acceptable product blends. The Complex Model introduces incredibly interactive (i.e., there is high degree of variable overlap) 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 by the EPA in the form of spreadsheets. The EPA Complex Model spreadsheet allows refiners to compute satisfactory limits for properties such as Reid vapor pressure (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 have involved iterative schemes to incorporate simulation and optimization (Treiber, McLeod, Faitakis, & Hutchings, 1998). This complicated representation of the predictive emissions 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 are 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 generalized disjunctive programming techniques (Raman & Grossmann, 1993). In the following sections we provide a novel representation of the Complex Model by translating the rule descriptions to an 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.

Disjunctive programming was developed by Balas in his seminal report (Balas, 1974, 1998) as a unifying framework for the generation of polyhedral facets for use in the solution of mixed-integer programming. Generalized disjunctive programming, originally developed by Raman and Grossmann (Raman & Grossmann, 1994), was conceived in the chemical engineering community as an alternative modeling framework in order to translate physical intuition into more formal mathematical expression. In this paper, the disjunctive constraints used are of linear form as follows:

$$\forall i \in D [A_i x \geq b_i]$$

where  $D$  is a set of disjunctions,  $A_i$  an  $m_i \times n$  matrix parameter,  $b_i$  an  $m_i$  vector parameter, and  $x$  is an  $m_i$  vector variable. These disjunctive constraints are transformed into mixed-integer linear constraints as described in Appendix A.

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) (see Fig. 1 for example pages), however due to discrepancies between the printed model and the spreadsheet model (see Fig. 2 for an example worksheet) provided on the EPA website (EPA, 2007b), the spreadsheet has been chosen as the basis for this study as it is the source for the printed model and is in general use in the refining industry for emissions calculations. There are different regulations based on season and geographic regions as illustrated in Fig. 3.

This paper is organized as follows. Section 2 presents general and linkage constraints for fuel properties. Section 3 describes the constraints related to volatile organic compounds (VOC) emissions. Section 4 presents the constraints related to  $NO_x$  emissions. Various other toxic emissions constraints are modeled in Section 5. The general variable bounds and EPA limits are listed in Section 6. Section 7

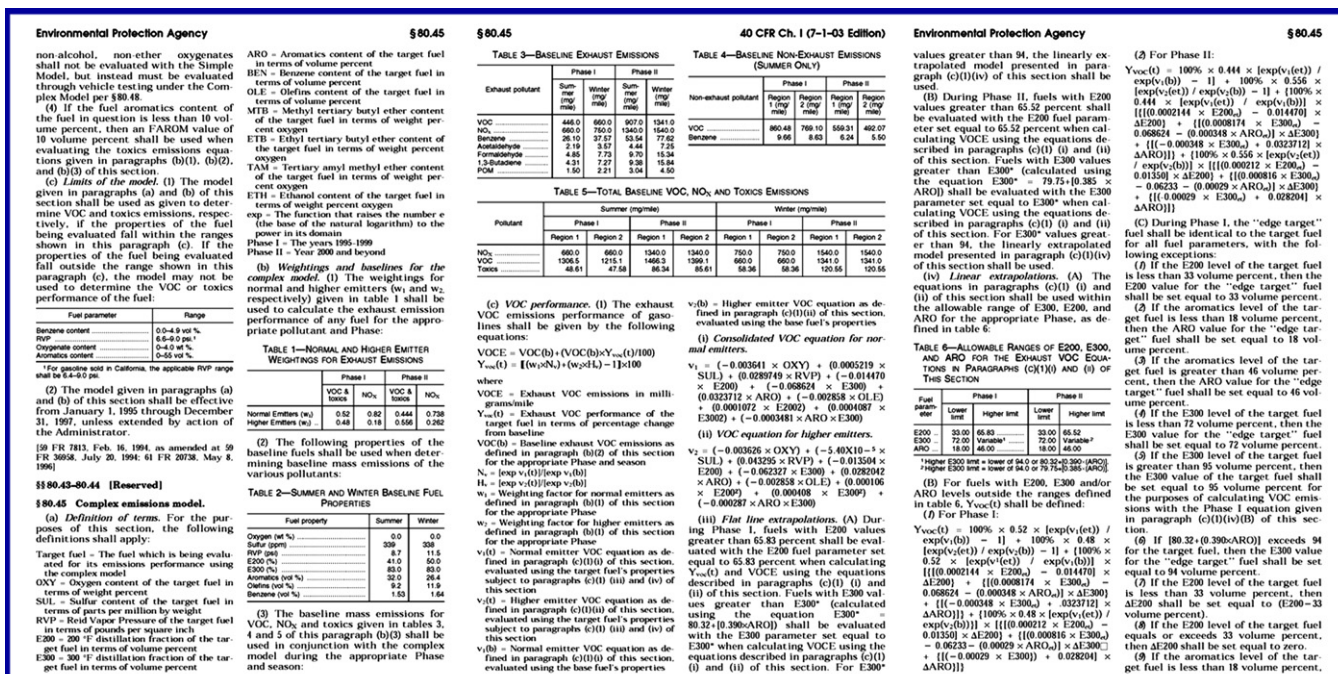


Fig. 1. Example pages from the CFR.

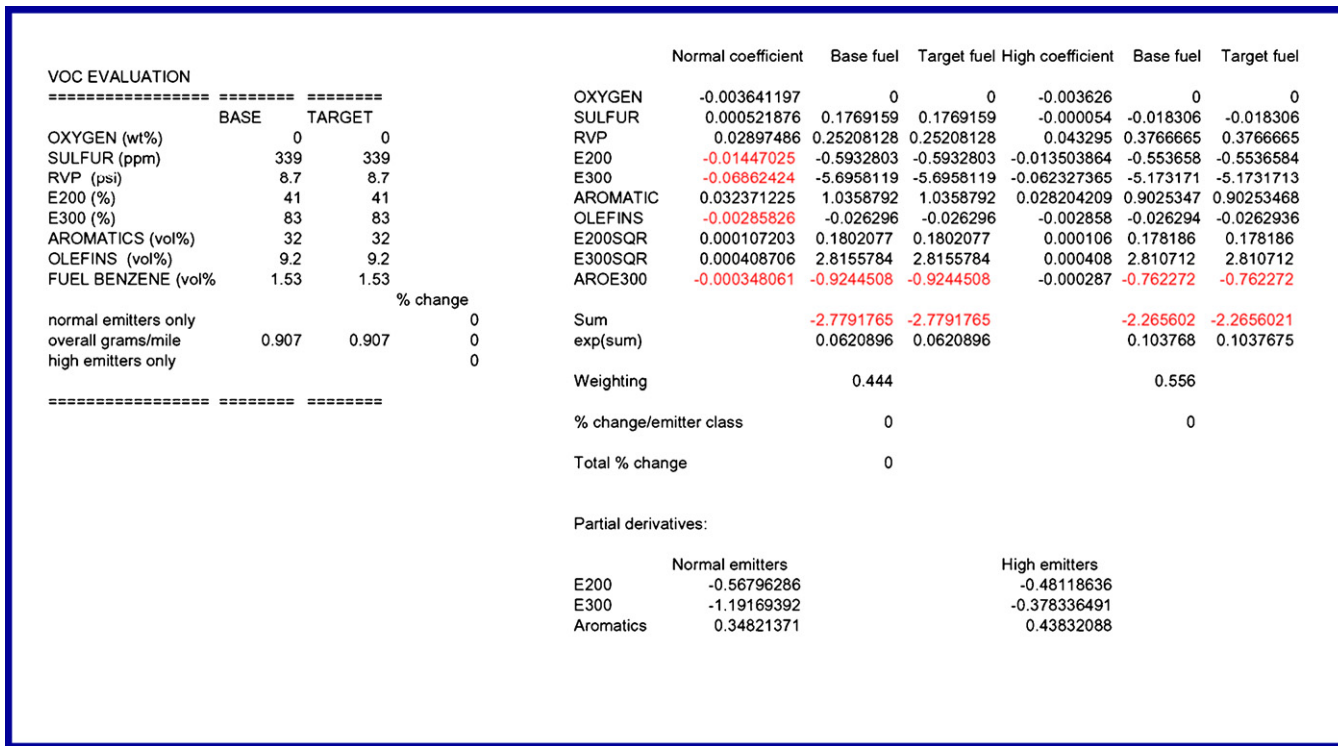


Fig. 2. Example worksheet of the EPA spreadsheet.

discusses some computational results for the use of this model on some simple illustrative examples. Section 8 discusses conclusions and future work. Appendix A explicitly details the MINLP reformulation of all generalized disjunctive constraints that are part of the Complex Model.

## 2. General constraints and links

One of the motivations and potential uses of the model presented in this work is the ability to include a set of constraints for the Complex Model into a mathematical programming formulation. In order to achieve that purpose, the properties of some fuel under consideration

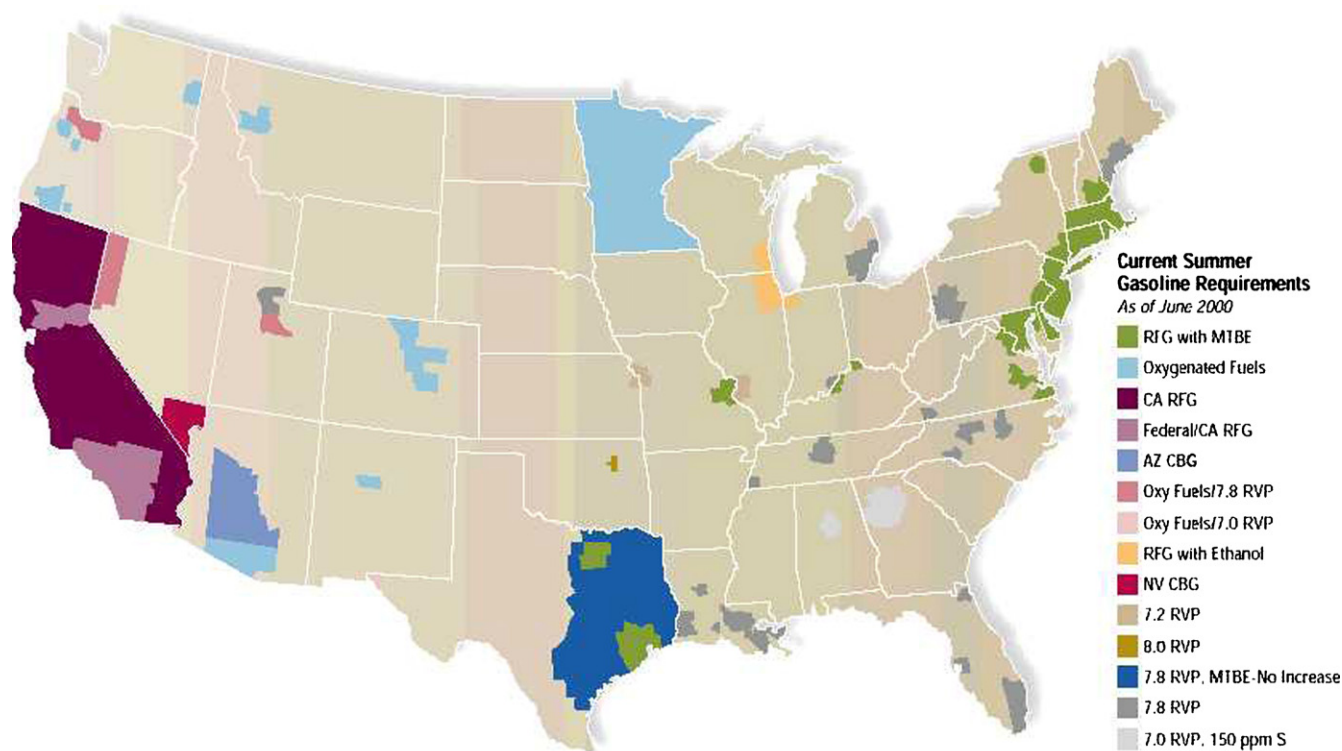


Fig. 3. U.S. regulated areas for summer RFG requirements.

must be linked to the equations of the EPA model presented. The EPA model does not work with the original fuel properties in some cases and requires adjustments.

This section documents the transformations made to original properties of a target fuel. Eqs. (1)–(14) link the original properties of the target fuel with the property values used for target fuel in the Complex Model. The original target fuel properties are indicated with the subscript *ot*, and the adjusted target fuel by *t*.

$$\begin{bmatrix} E300_{ot} \geq 95 \\ E300_t = 95 \end{bmatrix} \vee \begin{bmatrix} E300_{ot} \leq 95 \\ E300_t = E300_{ot} \end{bmatrix} \quad (1)$$

$$\begin{bmatrix} ARO_{ot} \leq 10 \\ ARO_t = 10 \end{bmatrix} \vee \begin{bmatrix} ARO_{ot} \geq 10 \\ ARO_t = ARO_{ot} \end{bmatrix} \quad (2)$$

Aromatics content (ARO) and the distillation fraction of the fuel at 300 F (*E300*) require disjunctions to make their adjustments.

$$SUL_t = SUL_{ot} \quad (3)$$

$$E200_t = E200_{ot} \quad (4)$$

$$OLE_t = OLE_{ot} \quad (5)$$

$$BEN_t = BEN_{ot} \quad (6)$$

$$MTB_t = MTB_{ot} \quad (7)$$

$$ETB_t = ETB_{ot} \quad (8)$$

$$TAM_t = TAM_{ot} \quad (9)$$

$$ETH_t = ETH_{ot} \quad (10)$$

$$OXY_t = OXY_{ot} \quad (11)$$

Sulfur (SUL), olefins (OLE), methyl tertiary butyl ether (MTB), ethyl tertiary butyl ether (ETB), tertiary amyl methyl ether (TAM), ethanol (ETH) and oxygen (OXY) contents and the distillation fraction of the fuel at 200 F (*E300*) do not require an adjustment to their value. In the summer season Reid vapor pressure does not require an adjustment.

$$RVP_t = RVP_{ot} \quad (12)$$

However, in the winter season it is fixed to 8.7 psi.

$$RVP_t = 8.7 \quad (13)$$

The total oxygen content is the sum of the concentrations of several compounds.

$$\text{OXY}_{\text{ot}} = \text{MTB}_{\text{ot}} + \text{ETB}_{\text{ot}} + \text{TAM}_{\text{ot}} + \text{ETH}_{\text{ot}} \quad (14)$$

Note that when calculating formaldehyde and acetaldehyde performance:

- Oxygen in the form of alcohols that are more complex or have higher molecular weights than ethanol is to be evaluated as if it is in the form of ethanol.
- Oxygen in the form of methyl ethers other than TAME and MTBE is to be evaluated as if it is in the form of MTBE.
- Oxygen in the form of ethyl ethers other than ETBE is to be evaluated as if it is in the form of ETBE.
- Oxygen in the form of non-methyl, non-ethyl ethers is to be evaluated as if it is in the form of ETBE.
- Oxygen in the form of methanol or non-alcohol, non-ether oxygenates is not to be evaluated with the Complex Model, but instead evaluated through vehicle testing of CFR Title 40 Part 80.48 (U.S. Government, 2003).

In January 1998, the EPA introduced the so-called Complex Model for refineries to calculate the expected emissions of volatile organic compounds, toxic air pollutants (TOX), and nitrogen oxides ( $\text{NO}_x$ ) from motor gasoline. The Complex Model contains explicit constraints, such as those for percent aromatics, sulfur content and E300, and implicit equations that effectively predict VOC, TOX and  $\text{NO}_x$  as a function of blend properties such as Reid vapor pressure and component composition. The Complex Model was effectively derived from empirical measurements on typical engines and as such the predicted emissions are provided through convoluted rules and if/then statements that make direct incorporation into algebraic optimization models essentially impossible. In the following four sections we are basically translating the set of rules that compose the emissions equations into closed-form mathematical expression through the use of disjunctive constraints.

### 3. VOC performance constraints

Volatile organic compounds are released from gasoline when is it burned as fuel. VOC include a variety of chemicals, some of which may have short-term and long-term adverse health effects. This section develops the constraints of the Complex Model related to volatile organic compounds based on the EPA empirical models. There are different EPA standards based on season (summer/winter).

#### 3.1. Summer exhaust VOC emissions performance of gasoline

The summer exhaust VOC emissions (mg/mile) are calculated based on a percent change from the baseline emissions.

$$\text{VOCE}_t = \text{VOCE}_b + \left( \text{VOCE}_b \frac{Y_t^{\text{VOC}}}{100} \right) \quad (15)$$

The change from baseline of exhaust VOC emissions is calculated based on an EPA correlation that is a function of normal and high emitter VOC terms as well as the VOC calculation differences in E200, E300, and aromatics.

$$\begin{aligned} Y_t^{\text{VOC}} = & 100w_1^{\text{VOC}} \left( \frac{\exp(v_{1v})}{\exp(v_{1b})} - 1 \right) + 100w_2^{\text{VOC}} \left( \frac{\exp(v_{2v})}{\exp(v_{2b})} - 1 \right) + 100w_1^{\text{VOC}} \left( \frac{\exp(v_{1v})}{\exp(v_{1b})} \right) \\ & \times [(2\alpha_8^{\text{V}}E200_v + \alpha_4^{\text{V}})\Delta E200_v + (2\alpha_9^{\text{V}}E300_v + \alpha_5^{\text{V}} + \alpha_{10}^{\text{V}}\text{ARO}_v)\Delta E300_v + (\alpha_{10}^{\text{V}}E300_v + \alpha_6^{\text{V}})\Delta \text{ARO}_v] + 100w_2^{\text{VOC}} \left( \frac{\exp(v_{2v})}{\exp(v_{2b})} \right) \\ & \times [(2\beta_8^{\text{V}}E200_v + \beta_4^{\text{V}})\Delta E200_v + (2\beta_9^{\text{V}}E300_v + \beta_5^{\text{V}} + \beta_{10}^{\text{V}}\text{ARO}_v)\Delta E300_v + (\beta_{10}^{\text{V}}E300_v + \beta_6^{\text{V}})\Delta \text{ARO}_v] \end{aligned} \quad (16)$$

Both the normal and high emitter VOC terms are a function of VOC adjusted E200, E300, and aromatics as well as the target oxygen, sulfur, and olefins contents as well as RVP.

$$v_{1v} = \alpha_1^{\text{V}}\text{OXY}_t + \alpha_2^{\text{V}}\text{SUL}_t + \alpha_3^{\text{V}}\text{RVP}_t + \alpha_4^{\text{V}}E200_v + \alpha_5^{\text{V}}E300_v + \alpha_6^{\text{V}}\text{ARO}_v + \alpha_7^{\text{V}}\text{OLE}_t + \alpha_8^{\text{V}}(E200_v)^2 + \alpha_9^{\text{V}}(E300_v)^2 + \alpha_{10}^{\text{V}}\text{ARO}_vE300_v \quad (17)$$

where

$$\begin{aligned} \alpha_1^{\text{V}} &= -0.003641197, & \alpha_2^{\text{V}} &= +0.0005218758, & \alpha_3^{\text{V}} &= +0.02897486, & \alpha_4^{\text{V}} &= -0.01447025, & \alpha_5^{\text{V}} &= -0.06862424, \\ \alpha_6^{\text{V}} &= +0.032371225, & \alpha_7^{\text{V}} &= -0.00285826, & \alpha_8^{\text{V}} &= +0.0001072027, & \alpha_9^{\text{V}} &= +0.0004087064, & \alpha_{10}^{\text{V}} &= -0.0003480613 \end{aligned}$$

$$v_{2v} = \beta_1^{\text{V}}\text{OXY}_t + \beta_2^{\text{V}}\text{SUL}_t + \beta_3^{\text{V}}\text{RVP}_t + \beta_4^{\text{V}}E200_v + \beta_5^{\text{V}}E300_v + \beta_6^{\text{V}}\text{ARO}_v + \beta_7^{\text{V}}\text{OLE}_t + \beta_8^{\text{V}}(E200_v)^2 + \beta_9^{\text{V}}(E300_v)^2 + \beta_{10}^{\text{V}}\text{ARO}_vE300_v \quad (18)$$

where

$$\begin{aligned} \beta_1^{\text{V}} &= -0.003626, & \beta_2^{\text{V}} &= -5.40 \times 10^{-5}, & \beta_3^{\text{V}} &= +0.043295, & \beta_4^{\text{V}} &= -0.0135038636004, & \beta_5^{\text{V}} &= -0.0623273649147, \\ \beta_6^{\text{V}} &= +0.0282042087973, & \beta_7^{\text{V}} &= -0.002858, & \beta_8^{\text{V}} &= +0.000106, & \beta_9^{\text{V}} &= +0.000408, & \beta_{10}^{\text{V}} &= -0.000287 \end{aligned}$$

The indices t and v can be exchanged with b in Eqs. (17) and (18) to calculate the baseline emitter VOC parameters  $v_{1b}$  and  $v_{2b}$ .

A set of disjunctive constraints is necessary for the determination of both the evaporative and aromatic content specifications adjusted for the VOC calculations.

$$\left[ \begin{array}{l} 79.75 + 0.38465\text{ARO}_t \leq 94 \\ E300_* = 79.75 + 0.38465\text{ARO}_t \end{array} \right] \vee \left[ \begin{array}{l} 79.75 + 0.38465\text{ARO}_t \geq 94 \\ E300_* = 94 \end{array} \right] \quad (19)$$

$$\left[ \begin{array}{l} E200_t \leq 33 \\ E200_v = 33 \\ \Delta E200_v = E200_t - 33 \end{array} \right] \vee \left[ \begin{array}{l} E200_t \geq 33 \\ E200_t \leq 65.52 \\ E200_v = E200_t \\ \Delta E200_v = 0 \end{array} \right] \vee \left[ \begin{array}{l} E200_t \geq 65.52 \\ E200_v = 65.52 \\ \Delta E200_v = E200_t - 65.52 \end{array} \right] \quad (20)$$

$$\left[ \begin{array}{l} E300_t \leq 72 \\ E300_v = 72 \\ \Delta E300_v = E300_t - 72 \end{array} \right] \vee \left[ \begin{array}{l} E300_t \geq 72 \\ E300_t \leq E300_* \\ E300_v = E300_t \\ \Delta E300_v = 0 \end{array} \right] \vee \left[ \begin{array}{l} E300_t \geq E300_* \\ E300_v = E300_* \\ \Delta E300_v = E300_t - E300_* \end{array} \right] \quad (21)$$

$$\left[ \begin{array}{l} \text{ARO}_t \leq 18 \\ \text{ARO}_v = 18 \\ \Delta \text{ARO}_v = \text{ARO}_t - 18 \end{array} \right] \vee \left[ \begin{array}{l} \text{ARO}_t \geq 18 \\ \text{ARO}_t \leq 46 \\ \text{ARO}_v = \text{ARO}_t \\ \Delta \text{ARO}_v = 0 \end{array} \right] \vee \left[ \begin{array}{l} \text{ARO}_t \geq 46 \\ \text{ARO}_v = 46 \\ \Delta \text{ARO}_v = \text{ARO}_t - 46 \end{array} \right] \quad (22)$$

### 3.2. 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  $\text{RVP}_b = \text{RVP}_t = 8.7$  psi.

### 3.3. Summer non-exhaust VOC emissions performance of gasoline

The total non-exhaust VOC emissions (g/mile) are a combination of diurnal (VOCDI), hot soak (VOCHS), running loss (VOCRL) and refueling (VOCRF) VOC emissions.

$$\text{VOCNE} = \text{VOCDI} + \text{VOCHS} + \text{VOCRL} + \text{VOCRF} \quad (23)$$

#### 3.3.1. VOC control region 1

The following set of constraints calculate the components for total non-exhaust VOC emissions as a function of RVP for VOC control region 1.

$$\text{VOCDI} = 0.007384514(\text{RVP}_t)^2 - 0.0898145\text{RVP}_t + 0.35179462 \quad (24)$$

$$\text{VOCHS} = 0.006654486(\text{RVP}_t)^2 - 0.0809355\text{RVP}_t + 0.28457538 \quad (25)$$

$$\text{VOCRL} = 0.017768(\text{RVP}_t)^2 - 0.18746\text{RVP}_t + 0.614567 \quad (26)$$

$$\text{VOCRF} = 0.004767\text{RVP}_t + 0.011859 \quad (27)$$

#### 3.3.2. VOC control region 2

The following set of constraints calculate the components for total non-exhaust VOC emissions as a function of RVP for VOC control region 2.

$$\text{VOCDI} = 0.00477532(\text{RVP}_t)^2 - 0.0587224\text{RVP}_t + 0.213059 \quad (28)$$

$$\text{VOCHS} = 0.00607768(\text{RVP}_t)^2 - 0.0747376\text{RVP}_t + 0.271166 \quad (29)$$

$$\text{VOCRL} = 0.016169(\text{RVP}_t)^2 - 0.17206\text{RVP}_t + 0.56724 \quad (30)$$

$$\text{VOCRF} = 0.004767\text{RVP}_t + 0.011859 \quad (31)$$

### 3.4. Non-exhaust winter VOC emissions performance of gasoline

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

$$\text{VOCNE} = 0 \quad (32)$$

### 3.5. Total VOC emissions

Total summer VOC emissions (mg/mile) for VOC control regions 1 or 2 are calculated by the following equation:

$$\text{VOC}_t = \text{VOCE}_t + 1000\text{VOCNE} \quad (33)$$

Total winter VOC emissions are calculated with the following:

$$\text{VOC}_t = \text{VOCE}_t \quad (34)$$

### 3.6. Total VOC emissions performance

$$\text{VOC}\% = \frac{100\%}{\text{VOC}_b}(\text{VOC}_t - \text{VOC}_b) \quad (35)$$

## 4. NO<sub>x</sub> performance constraints

Nitrogen oxides are the group of gases that are composed of nitrogen and oxygen. Two common nitrogen oxides are nitric oxide and nitrogen dioxide. When combined with volatile organic compounds, nitrogen oxides form ground-level ozone (smog). This section develops the constraints of the Complex Model related to Nitrogen Oxides NO<sub>x</sub> based on the EPA empirical models. There are different EPA standards based on season (summer/winter).

### 4.1. Summer NO<sub>x</sub> emissions performance of gasolines

The summer NO<sub>x</sub> emissions (mg/mile) are calculated based on a percent change from the baseline emissions.

$$\text{NOX}_t = \text{NOX}_b + \text{NOX}_b \frac{Y_t^{\text{NOX}}}{100} \quad (36)$$

The change from baseline of NO<sub>x</sub> emissions is calculated based on a correlation that is a function of normal and high emitter NO<sub>x</sub> terms as well as the NO<sub>x</sub> calculation differences in sulfur, olefins and aromatics.

$$\begin{aligned} Y_t^{\text{NOX}} = & 100w_1^{\text{NOX}} \left( \frac{\exp(n_{1n})}{\exp(n_{1b})} - 1 \right) + 100w_2^{\text{NOX}} \left( \frac{\exp(n_{2n})}{\exp(n_{2b})} - 1 \right) + 100w_1^{\text{NOX}} \left( \frac{\exp(n_{1n})}{\exp(n_{1b})} \right) \\ & \times [(2\alpha_8^N \text{SUL}_n + \alpha_2^N) \Delta \text{SUL}_n + (2\alpha_9^N \text{ARO}_n + \alpha_6^N) \Delta \text{ARO}_n + (2\alpha_{10}^N \text{OLE}_n + \alpha_7^N) \Delta \text{OLE}_n] + 100w_2^{\text{NOX}} \left( \frac{\exp(n_{2n})}{\exp(n_{2b})} \right) \\ & \times [(2\beta_8^N \text{ARO}_n + \beta_6^N) \Delta \text{ARO}_n + (2\beta_9^N \text{OLE}_n + \beta_7^N) \Delta \text{OLE}_n] \end{aligned} \quad (37)$$

$$n_{1n} = \alpha_1^N \text{OXY}_t + \alpha_2^N \text{SUL}_n + \alpha_3^N \text{RVP}_t + \alpha_4^N \text{E200}_t + \alpha_5^N \text{E300}_t + \alpha_6^N \text{ARO}_n + \alpha_7^N \text{OLE}_n + \alpha_8^N (\text{SUL}_n)^2 + \alpha_9^N (\text{ARO}_n)^2 + \alpha_{10}^N (\text{OLE}_n)^2 \quad (38)$$

where

$$\begin{aligned} \alpha_1^N &= 0.0018571, & \alpha_2^N &= +0.00069205, & \alpha_3^N &= +0.0090744, & \alpha_4^N &= +0.00093065, & \alpha_5^N &= +0.00084596, \\ \alpha_6^N &= +0.0083632, & \alpha_7^N &= -0.0027735, & \alpha_8^N &= -6.6263^{-7}, & \alpha_9^N &= -0.00011905, & \alpha_{10}^N &= +0.00036652 \end{aligned}$$

$$n_{2n} = \beta_1^N \text{OXY}_t + \beta_2^N \text{SUL}_n + \beta_3^N \text{RVP}_t + \beta_4^N \text{E200}_t + \beta_5^N \text{E300}_t + \beta_6^N \text{ARO}_n + \beta_7^N \text{OLE}_n + \beta_8^N (\text{ARO}_n)^2 + \beta_9^N (\text{OLE}_n)^2 \quad (39)$$

where

$$\begin{aligned} \beta_1^N &= -0.00913, & \beta_2^N &= +0.000252, & \beta_3^N &= -0.013973, & \beta_4^N &= +0.000931, & \beta_5^N &= -0.004009, \\ \beta_6^N &= +0.0070970046692682, & \beta_7^N &= -0.0027603002584, & \beta_8^N &= -7.9951^{-5}, & \beta_9^N &= +0.000366 \end{aligned}$$

The indices t and n can be exchanged with b in Eqs. (38) and (39) to calculate parameters  $n_{1b}$  and  $n_{2b}$ .

A set of disjunctive constraints is necessary for the determination of the sulfur, aromatics and olefins content specifications adjusted for the NO<sub>x</sub> calculations.

$$\begin{bmatrix} \text{SUL}_t \leq 10 \\ \text{SUL}_n = 10 \\ \Delta \text{SUL}_n = \text{SUL}_t - 10 \end{bmatrix} \vee \begin{bmatrix} \text{SUL}_t \geq 10 \\ \text{SUL}_t \leq 450 \\ \text{SUL}_n = \text{SUL}_t \\ \Delta \text{SUL}_n = 0 \end{bmatrix} \vee \begin{bmatrix} \text{SUL}_t \geq 450 \\ \text{SUL}_n = 450 \\ \Delta \text{SUL}_n = \text{SUL}_t - 450 \end{bmatrix} \quad (40)$$

$$\begin{bmatrix} \text{ARO}_t \leq 18 \\ \text{ARO}_n = 18 \\ \Delta \text{ARO}_n = \text{ARO}_t - 18 \end{bmatrix} \vee \begin{bmatrix} \text{ARO}_t \geq 18 \\ \text{ARO}_t \leq 36.8 \\ \text{ARO}_n = \text{ARO}_t \\ \Delta \text{ARO}_n = 0 \end{bmatrix} \vee \begin{bmatrix} \text{ARO}_t \geq 36.8 \\ \text{ARO}_n = 36.8 \\ \Delta \text{ARO}_n = \text{ARO}_t - 36.8 \end{bmatrix} \quad (41)$$

$$\begin{bmatrix} \text{OLE}_t \leq 3.77 \\ \text{OLE}_n = 3.77 \\ \Delta \text{OLE}_n = \text{OLE}_t - 3.77 \end{bmatrix} \vee \begin{bmatrix} \text{OLE}_t \geq 3.77 \\ \text{OLE}_t \leq 19 \\ \text{OLE}_n = \text{OLE}_t \\ \Delta \text{OLE}_v = 0 \end{bmatrix} \vee \begin{bmatrix} \text{OLE}_t \geq 19 \\ \text{OLE}_n = 19 \\ \Delta \text{OLE}_v = \text{OLE}_t - 19 \end{bmatrix} \quad (42)$$

### 4.2. Winter NO<sub>x</sub> emissions performance of gasolines

For the winter calculations, the same equations as Section 4.1 for the summer are used, however fixing  $\text{RVP}_b = \text{RVP}_t = 8.7$  psi.

### 4.3. NO<sub>x</sub> emissions performance

$$\text{NOX}\% = \frac{100\%}{\text{NOX}_b}(\text{NOX}_t - \text{NOX}_b) \quad (43)$$

## 5. Toxics performance

In addition to VOC and NO<sub>x</sub>, the Complex Model seeks to limit the emissions of other particular toxic compounds. This section develops the constraints of the Complex Model related to toxic air pollutants based on the EPA empirical analysis. The summer toxics emissions performance (mg/mile) is calculated based on a combination of the emissions based on exhaust benzene, formaldehyde, acetaldehyde, 1,3-butadiene, polycyclic organic matter and non-exhaust benzene.

$$\text{TOXIC}_t = \text{EXHBZ}_t + \text{FORM}_t + \text{ACET}_t + \text{BUTA}_t + \text{POM} + \text{NEBZ} \quad (44)$$

The winter toxics emissions performance does not include a term for non-exhaust benzene.

$$\text{TOXIC}_t = \text{EXHBZ}_t + \text{FORM}_t + \text{ACET}_t + \text{BUTA}_t + \text{POM} \quad (45)$$

The percent change in emissions in toxics is calculated based on a difference from the baseline emissions performance.

$$\text{TOXIC}\% = \frac{100\%}{\text{TOXIC}_b}(\text{TOXIC}_t - \text{TOXIC}_b) \quad (46)$$

### 5.1. Year-round toxics performance

Year-round toxics performance in VOC control regions 1 and 2 are derived from volume-weighted performances of individual batches of fuel as described in CFR Title 40 Part 80.67 (U.S. Government, 2003).

### 5.2. Exhaust benzene emissions

Analogous to other emissions calculations, exhaust benzene emissions (mg/mile) are calculated based on a percent change from the baseline benzene content.

$$\text{EXHBZ}_t = \text{BENZ}_b + \text{BENZ}_b \frac{Y_t^{\text{BEN}}}{100} \quad (47)$$

The change from baseline of benzene content is calculated based on a correlation that is a function of normal and high emitter benzene terms, which are in turn a function of sulfur, aromatics and benzene content as well as E200.

$$Y_t^{\text{BEN}} = 100w_1^{\text{BEN}} \left( \frac{\exp(B_{1t})}{\exp(B_{1b})} - 1 \right) + 100w_2^{\text{BEN}} \left( \frac{\exp(B_{2t})}{\exp(B_{2b})} - 1 \right) \quad (48)$$

$$B_{1t} = 0.00061965\text{SUL}_t - 0.003372E200_t + 0.0265500\text{ARO}_t + 0.2223900\text{BEN}_t \quad (49)$$

$$B_{2t} = -0.096047\text{OXY}_t + 0.0003370\text{SUL}_t + 0.0112510E300_t + 0.00118820\text{ARO}_t + 0.2223180\text{BEN}_t \quad (50)$$

The index t can be exchanged with b in Eqs. (49) and (50) to calculate parameters B<sub>1b</sub> and B<sub>2b</sub>.

### 5.3. Formaldehyde mass emissions

Formaldehyde emissions (mg/mile) are calculated based on a percent change from the baseline formaldehyde content.

$$\text{FORM}_t = \text{FORM}_b + \text{FORM}_b \frac{Y_t^{\text{FORM}}}{100} \quad (51)$$

The change from baseline of formaldehyde content is calculated based on a correlation that is a function of normal and high emitter formaldehyde terms, which are in turn a function of aromatics, olefins and MTBE content as well as E300.

$$Y_t^{\text{FORM}} = 100w_1^{\text{FORM}} \left( \frac{\exp(f_{1t})}{\exp(f_{1b})} - 1 \right) + 100w_2^{\text{FORM}} \left( \frac{\exp(f_{2t})}{\exp(f_{2b})} - 1 \right) \quad (52)$$

$$f_{1t} = -0.010226E300_t - 0.007166\text{ARO}_t + 0.046213\text{MTB}_t \quad (53)$$

$$f_{2t} = -0.01022621E300_t - 0.00716603\text{ARO}_t - 0.03135193\text{OLE}_t + 0.04621306\text{MTB}_t \quad (54)$$

The index t can be exchanged with b in Eqs. (53) and (54) to calculate parameters f<sub>1b</sub> and f<sub>2b</sub>.

### 5.4. Acetaldehyde mass emissions

Acetaldehyde emissions (mg/mile) are calculated based on a percent change from the baseline acetaldehyde content.

$$\text{ACET}_t = \text{ACET}_b + \text{ACET}_b \frac{Y_t^{\text{ACET}}}{100} \quad (55)$$

The change from baseline of acetaldehyde content is calculated based on a correlation that is a function of normal and high emitter acetaldehyde terms, which are in turn a function of sulfur, aromatics, MTBE, ETBE, and ethanol content as well as E300 and RVP.

$$Y_t^{ACET} = 100w_1^{ACET} \left( \frac{\exp(a_{1t})}{\exp(a_{1b})} - 1 \right) + 100w_2^{ACET} \left( \frac{\exp(a_{2t})}{\exp(a_{2b})} - 1 \right) \quad (56)$$

$$a_{1t} = 0.00026308SUL_t + 0.0397860RVP_t - 0.012172E300_t - 0.0055252ARO_t - 0.0095944MTB_t + 0.3165800ETB_t + 0.2492500ETH_t \quad (57)$$

$$a_{2t} = 0.00026265SUL_t - 0.01215727E300_t - 0.00554762ARO_t - 0.05598039MTB_t + 0.3164665ETB_t + 0.2493259ETH_t \quad (58)$$

The index t can be exchanged with b in Eqs. (57) and (58) to calculate parameters  $a_{1b}$  and  $a_{2b}$ .

### 5.5. 1,3-Butadiene mass emissions

1,3-Butadiene emissions (mg/mile) are calculated based on a percent change from the baseline 1,3-butadiene content.

$$BUTA_t = BUTA_b + BUTA_b \frac{Y_t^{BUTA}}{100} \quad (59)$$

The change from baseline of 1,3-butadiene content is calculated based on a correlation that is a function of normal and high emitter 1,3-butadiene terms, which are in turn a function of sulfur, aromatics, oxygen and olefins content as well as E200 and E300.

$$Y_t^{BUTA} = 100w_1^{BUTA} \left( \frac{\exp(d_{1t})}{\exp(d_{1b})} - 1 \right) + 100w_2^{BUTA} \left( \frac{\exp(d_{2t})}{\exp(d_{2b})} - 1 \right) \quad (60)$$

$$d_{1t} = 0.0001552SUL_t - 0.00072532E200_t - 0.014866E300_t - 0.0040002ARO_t + 0.028235OLE_t \quad (61)$$

$$d_{2t} = -0.060771OXY_t - 0.007311E200_t - 0.008058E300_t - 0.004005ARO_t + 0.0436960OLE_t \quad (62)$$

The index t can be exchanged with b in Eqs. (61) and (62) to calculate parameters  $d_{1b}$  and  $d_{2b}$ .

### 5.6. Polycyclic organic mass emissions

Polycyclic organic mass emissions are estimated based on the exhaust VOC emissions.

$$POM = 0.003355VOCE_t \quad (63)$$

### 5.7. Non-exhaust benzene emissions

The total non-exhaust benzene emissions are a combination of diurnal (DIBZ), hot soak (HSBZ), running loss (RLBZ) and refueling (RFBZ) benzene emissions.

$$NEBZ = DIBZ + HSBZ + RLBZ + RFBZ \quad (64)$$

### 5.8. Non-exhaust benzene emissions in VOC control region 1

The following set of constraints calculate the components for total non-exhaust benzene emissions as a function of MTBE content and RVP for VOC control region 1.

$$HSBZ = 10BEN_t VOCHS(-0.0342MTB_t - 0.080274RVP_t + 1.4448) \quad (65)$$

$$DIBZ = 10BEN_t VOCDI(-0.02895MTB_t - 0.080274RVP_t + 1.3758) \quad (66)$$

$$RLBZ = 10BEN_t VOCRL(-0.0342MTB_t - 0.080274RVP_t + 1.4448) \quad (67)$$

$$RFBZ = 10BEN_t VOCRF(-0.02955MTB_t - 0.081507RVP_t + 1.3972) \quad (68)$$

### 5.9. Non-exhaust benzene emissions in VOC control region 2

The following set of constraints calculate the components for total non-exhaust benzene emissions as a function of MTBE content and RVP for VOC control region 2.

$$HSBZ = 10BEN_t VOCHS(-0.0342MTB_t - 0.080274RVP_t + 1.4448) \quad (69)$$

$$DIBZ = 10BEN_t VOCDI(-0.02895MTB_t - 0.080274RVP_t + 1.3758) \quad (70)$$

$$RLBZ = 10BEN_t VOCRL(-0.0342MTB_t - 0.080274RVP_t + 1.4448) \quad (71)$$

$$RFBZ = 10BEN_t VOCRF(-0.02955MTB_t - 0.081507RVP_t + 1.3972) \quad (72)$$

## 6. 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 these specifications are as follows:

$$0.0 \leq \text{OXY}_{\text{ot}} \leq 3.7, \quad 0.0 \leq \text{SUL}_{\text{ot}} \leq 500.0, \quad 6.4 \leq \text{RVP}_{\text{ot}} \leq 10.0, \quad 30.0 \leq \text{E200}_{\text{ot}} \leq 70.0, \quad 70.0 \leq \text{E300}_{\text{ot}} \leq 100.0,$$

$$0.0 \leq \text{ARO}_{\text{ot}} \leq 50.0, \quad 0.0 \leq \text{OLE}_{\text{ot}} \leq 25.0, \quad 0.0 \leq \text{BEN}_{\text{ot}} \leq 2.0$$

For conventional gasolines the specifications are as follows:

$$0.0 \leq \text{OXY}_{\text{ot}} \leq 3.7, \quad 0.0 \leq \text{SUL}_{\text{ot}} \leq 1000.0, \quad 6.4 \leq \text{RVP}_{\text{ot}} \leq 11.0, \quad 30.0 \leq \text{E200}_{\text{ot}} \leq 70.0, \quad 70.0 \leq \text{E300}_{\text{ot}} \leq 100.0,$$

$$0.0 \leq \text{ARO}_{\text{ot}} \leq 55.0, \quad 0.0 \leq \text{OLE}_{\text{ot}} \leq 30.0, \quad 0.0 \leq \text{BEN}_{\text{ot}} \leq 4.9$$

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 formulations meeting those standards are deemed certified.

$$\text{VOC}\% \geq V^{\min}, \quad \text{NOX}\% \geq N^{\min}, \quad \text{TOXIC}\% \geq T^{\min}, \quad \text{OXY}_{\text{ot}} \geq O^{\min}, \quad \text{BEN}_{\text{ot}} \leq B^{\max}$$

Actual values for the above limits depend on several factors including the VOC control region. Fig. 3 illustrates the regions of the United States regulated by the RFG model.

### 6.1. Notes on EPA documentation

After a careful examination of the EPA's documentation of the Complex Model in the CFR, it became clear that:

- Apparently baseline non-exhaust benzene, baseline POM exhaust and total baseline toxics are not used even though included in CFR tables.
- There are several typographical errors in the CFR document. A double check of equations and validation through comparison with the original spreadsheet was required.

## 7. Application in blending problem example

The methodology is demonstrated through the analysis of illustrative examples. 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  $\text{NO}_x$  with respect to the baseline fuel is zero. We define a general optimization problem in which we minimize the scaled deviation from the baseline while meeting stricter requirements.

Two simple illustrative component blending examples were created in order to illustrate the use of the mathematical programming representation of the Complex Model. For these examples some additional variables and constraints were required to be added to the RFG Complex Model in order to propose an optimization. The examples consider the design of a gasoline formulation created by the mixture of several components with known properties with the objective of designing a gasoline minimizing its difference from the baseline specifications while remaining within the guidelines and requirements of the EPA as per the CFR. There are also constraints for gasoline specifications (i.e., octane, volatility and distillation fraction properties) added to ensure the design of useful blends.

Variable  $F(i)$  is introduced to represent the fraction of some component  $i$  in the blend.  $P(j)$  is the value of property  $j$  in the blend. RM represents the octane value calculated via

$$\frac{\text{RON} + \text{MON}}{2}$$

Table 1 includes the EPA baseline data for the fuel property parameters used throughout the model. Table 2 includes the EPA baseline emissions data for the various tracked compounds and performance indicators. This data refers to those parameters with the subscript  $b$ .

**Table 1**  
Baseline fuel indices

Index	Summer	Winter
$\text{OXY}_b$	0	0
$\text{SUL}_b$	339	338
$\text{RVP}_b$	8.7	8.7
$\text{E200}_b$	41	50
$\text{E300}_b$	83	83
$\text{ARO}_b$	32	26.4
$\text{OLE}_b$	9.2	11.9
$\text{BEN}_b$	1.53	1.64

**Table 2**  
Baseline emissions (mg/mile)

Pollutant	Summer		Winter	
	Region 1	Region 2	Region 1	Region 2
Exhaust VOC (VOCE <sub>b</sub> )	907.00	907.00	1341.00	1341.00
Non-exhaust VOC	559.31	492.07	0.00	0.00
Total VOC (VOC <sub>b</sub> )	1466.31	1399.07	1341.00	1341.00
Exhaust benzene(BENZ <sub>b</sub> )	53.5400	53.5400	77.6200	77.6200
Non-exhaust benzene	6.2413	5.5047	0.0000	0.0000
Total benzene	59.7813	59.0447	77.6200	77.6200
Acetaldehyde (ACET <sub>b</sub> )	4.4400	4.4400	7.2500	7.2500
Formaldehyde (FORM <sub>b</sub> )	9.7000	9.7000	15.3400	15.3400
Butadiene (BUTA <sub>b</sub> )	9.3800	9.3800	15.8400	15.8400
POM	3.0430	3.0430	4.4991	4.4991
Exhaust toxics	80.1030	80.1030	120.5491	120.5491
Total toxics (TOXIC <sub>b</sub> )	86.3443	85.6077	120.5491	120.5491
NO <sub>x</sub> (NOX <sub>b</sub> )	1340.000	1340.0000	1540.0000	1540.0000

**Table 3**  
Example 1 data

Comp.	ARO%	OLE%	BEN%	SUL	RVP	RON	MON	E158	E200	E240	E300	E360
C4	0.0	0.0	0.0	0	59.5	94.5	90.3	110	101	97	96	97
FCC	26.9	33.7	0.7	420	9.2	95.6	80.8	26	43	56	74	90
Ref	61.0	0.5	3.3	8	7.4	99.0	87.9	17	28	46	78	96
Alky	0.0	0.0	0.0	15	7.1	91.4	89.3	12	33	71	90	96
LSR	1.2	6.9	1.1	325	12.9	74.2	72.7	80	104	105	101	101
Naphtha	8.9	0.2	0.5	500	2.8	61.0	63.4	-13	24	65	94	103
MTBE	0.0	0.0	0.0	0	8.8	118	102	70	113	101	100	99
ETBE	0.0	0.0	0.0	0	5.7	121	105	29	99	117	103	98
TAME	0.0	0.0	0.0	0	2.7	113	100	-2	51	111	107	103
ETOH	0.0	0.0	0.0	0	23.0	130	104	185	120	95	100	97

325 **Tables 3 and 4** include the component and property ( $A(i, j)$ ) data for Examples 1 and 2 over the index sets  $I$  and  $J$  where

$$326 \quad I = \{C4, FCC, Ref, Alky, LSR, Naphtha, MTBE, ETBE, TAME, ETOH\}$$

$$327 \quad J = \{ARO\%, OLE\%, BEN\%, SUL, RVP, RON, MON, E158, E200, E240, E300, E360\}$$

328 Reported values for RVP, RON, MON, E158, E200, E240, E300 and E360 are blend values to be used in linear blending formulas. For each  
329 component, RVP is reported in psi and sulfur (SUL) is reported in ppm.

330 For the sake of simplicity, a linear blending model is used to calculate gasoline properties based on the component properties. In our  
331 model we are using “blend numbers” for octane and volatility which are empirically estimated and widely used in the petroleum industry

**Table 4**  
Example 2 data

Comp.	ARO%	OLE%	BEN%	SUL	RVP	RON	MON	E158	E200	E300	E360
nButane	0	0	0	0	79	98	98	130	100	100	100
iButane	0	0	0	0	60	92	88	130	100	100	100
Butene	0	100	0	0	71	97	85	130	100	100	100
iPentane	0	0	0	0	21	90.3	104	110	105	100	100
nPentane	0	0	0	0	15	62.0	84.5	100	115	100	100
Pentene	0	100	0	0	16	82.0	83.8	110	110	100	100
cPentane	0	0	0	0	5	81.0	93.4	45	99	100	100
iHexane	0	0	0	0	6	73.5	91.0	60	115	100	100
nHexane	0	0	0	0	5	26.0	65.0	20	105	100	100
Hexene	0	100	0	0	6	100	86.0	40	110	100	100
cHexane	0	0	0	0	3	83	77	5	50	100	100
Benzene	100	0	100	0	4	106	106	0	100	100	100
iHeptane	0	0	0	0	2	46.5	74.5	-5	105	100	100
nHeptane	0	0	0	0	2	0	47.0	-5	90	100	100
C7OLE	0	100	0	0	2	99	85	-5	90	100	100
C7Naph	0	0	0	0	2	75	71	-10	45	100	100
Toluene	100	0	0	0	1	107	107	-10	10	100	100
iOctane	0	0	0	0	2	100	100	-10	40	100	100
nOctane	0	0	0	0	1	26	65	-15	-20	100	100
c8OLE	0	100	0	0	1	100	86	-15	-20	100	100
Xylene	100	0	0	0	1	102.5	102.5	-15	0	100	100
MTBE	0	0	0	0	8.8	118	102	70	113	100	99
ETBE	0	0	0	0	5.7	121	105	29	99	103	98
TAME	0	0	0	0	2.7	113	100	-2	51	107	103
ETOH	0	0	0	0	23	130	104	185	120	100	97

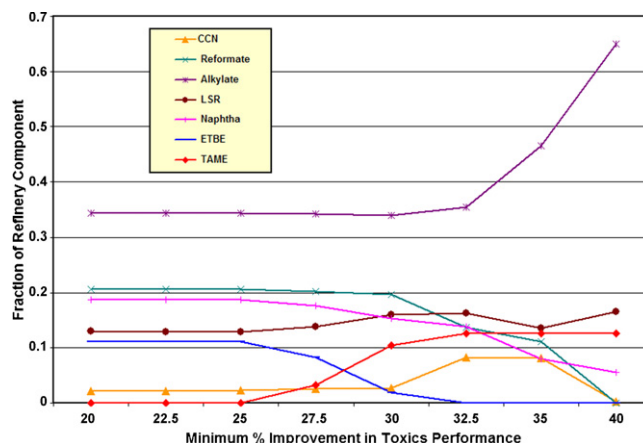


Fig. 4. Example 1: fraction changes with tighter toxics standards.

in order to allow for linear blend models. Several linking constraints are added to map the gasoline blend properties to the corresponding constraints in the Complex Model.

$$\sum_{i \in I} F(i) = 1.0, \quad P(j) = \sum_{i \in I} F(i)A(i, j), \quad ARO_{ot} = P(ARO\%), \quad OLE_{ot} = P(OLE\%), \quad BEN_{ot} = P(BEN\%), \quad RVP_{ot} = P(RVP),$$

$$SUL_{ot} = P(SUL), \quad E200_{ot} = P(E200), \quad E300_{ot} = P(E300), \quad MTB_{ot} = P(MTBE), \quad ETB_{ot} = P(ETBE), \quad TAM_{ot} = P(TAME),$$

$$ETH_{ot} = P(ETOH), \quad RM = \frac{1}{2}P(ROn) + \frac{1}{2}P(MON)$$

Gasoline specifications include the following:

$$86 \leq RM \leq 88, \quad 7 \leq P(RVP_{bl}) \leq 15, \quad 50 \leq P(E158_{bl}), \quad 90 \leq P(E360_{bl})$$

General bounds on variables are:

$$0 \leq F(i) \leq 1$$

$$\min\{0, \min_i A(i, j)\} \leq P(j) \leq \max_i A(i, j)$$

The objective function used in the tests involves a minimization of the change in the mixture's properties as compared to the baseline values established by the EPA.

$$\min \frac{(OXY_{ot} - OXY_b)^2}{(OXY_{ot}^U - OXY_{ot}^L)^2} + \frac{(SUL_{ot} - SUL_b)^2}{(SUL_{ot}^U - SUL_{ot}^L)^2} + \frac{(RVP_{ot} - RVP_b)^2}{(RVP_{ot}^U - RVP_{ot}^L)^2} + \frac{(E200_{ot} - E200_b)^2}{(E200_{ot}^U - E200_{ot}^L)^2} + \frac{(E300_{ot} - E300_b)^2}{(E300_{ot}^U - E300_{ot}^L)^2} + \frac{(ARO_{ot} - ARO_b)^2}{(ARO_{ot}^U - ARO_{ot}^L)^2}$$

$$+ \frac{(OLE_{ot} - OLE_b)^2}{(OLE_{ot}^U - OLE_{ot}^L)^2} + \frac{(BEN_{ot} - BEN_b)^2}{(BEN_{ot}^U - BEN_{ot}^L)^2}$$

There are a small number of variables and constraints in both examples.

- about 20 binary variables,
- about 100 continuous variables,
- about 200 constraint equations.

The model is reformulated into an MINLP and implemented in the GAMS modeling system (Brooke, Kendrick, Meeraus, Raman, & Rosenthal, 2005). See Appendix A for the conversion of the generalized disjunctive constraints into mixed-integer constraints. Since many of the nonlinear constraints in the model are clearly nonconvex, we require the use of a global optimization solver in order to establish a global optimum for our sensitivity analysis. The deterministic global optimization package BARON (Tawarmalani & Sahinidis, 2004) is used for the solver. In real-world situations with large-scale problems, where the run-time for global optimization may be impractical, other MINLP solvers could potentially be used to generate good or locally optimal solutions. All computations were performed on a machine with a 2.4 GHz AMD Athlon processor with 2 GB of memory. Sensitivity case studies of composition with respect to increasingly tighter toxics standards are performed as the proof-of-concept.

Example 1 is a simplified refinery blending problem using generic refinery data for refinery blendstocks and oxygenate additives. The data set is an artificial amalgam of data from multiple gasoline blending studies. There are 10 potential blending components and additional gasoline specifications for the following properties: RVP, E158, E240, E360, and octane number RM. Run times for each instances was no more than 10 min. The results for this example are illustrated in Figs. 4-6.

Fig. 4 shows the changes in refinery component fractions chosen by the optimization model for Example 1. The results seem to indicate that there is no need to change the fuel design for several tightenings of the toxics standards. Fig. 5 shows a similar behavior with respect to

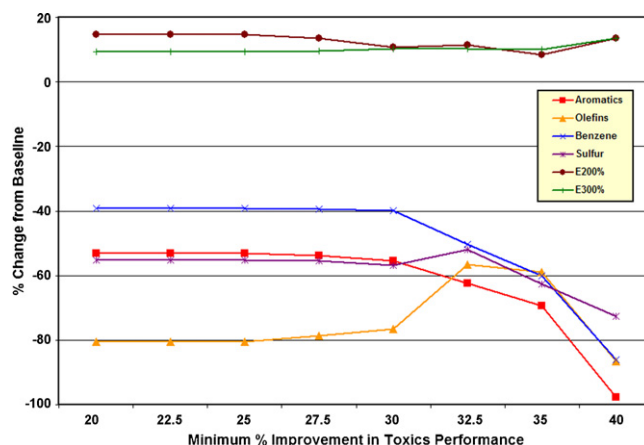


Fig. 5. Example 1: property changes with tighter toxics standards.

the fuel properties. Fig. 6 displays the changes in VOC and NO<sub>x</sub> performance as toxics standards are tightened. The results seem to indicate that there is no effect on VOC performance as a result, while there is only a small effect on improving the NO<sub>x</sub> performance which might indicate that these indicators are not heavily correlated for this example. Further, there are no changes in the performance of any of the indicators with several increasing standards on toxics performance. This appears to indicate that the fuel blends designed by the model are actually performing better than the minimum requirements set by the EPA.

Example 2 is an artificial problem using “pure” chemical components for gasoline design, therefore sulfur is not considered. The data set is partially derived from an Engelhard report (Anonymous, 2008). There are 25 potential blending components and additional gasoline specifications for the following properties: RVP, E158, E360, and octane number RM. E240 is not considered in this example as it was difficult to find the data for pure components. Run times for each instance was typically 3 min or less. The results for this example are illustrated in Figs. 7–9.

Fig. 7 shows the changes in pure component fractions chosen by the optimization model for Example 2. The results show wide changes in the component fractions with increasing tightening of the toxics standards. For example, the C7NAPH component jumps from nearly 50% down to zero and back to above 50% in one instance of three consecutive tightenings of the toxics standards. This might indicate that there are multiple globally optimal solutions to this example. However, it should be noted that BARON is not 100% accurate for all global optimization problems and could have possibly converged to a local solution. Fig. 8 shows a similar behavior as Example 1 with respect to the fuel properties, however the changes in properties is ultimately of a greater magnitude. Fig. 9 also shows a similar pattern to Example 1 in the changes in VOC and NO<sub>x</sub> performance as toxics standards are tightened in that there is no effect on VOC performance and only a small effect on improving the NO<sub>x</sub> performance. This would seem to lend further evidence to the idea that the fuel blends designed by this model are actually performing better than the minimum EPA requirements for toxics. However, it should be noted that the same pattern may not be seen when analyzing changes to the VOC or NO<sub>x</sub> standards for performance improvement.

Although these example problems are posed in a simple manner, they address the very critical concern of meeting more stringent composition requirements while imposing the minimum number of changes in processing. These examples demonstrate the versatility of the new mathematical programming formulation and its potential for accurate refinery optimization. This framework could be expanded to incorporate detailed physical models, as well as blending tools, to derive detailed fuel compositions.

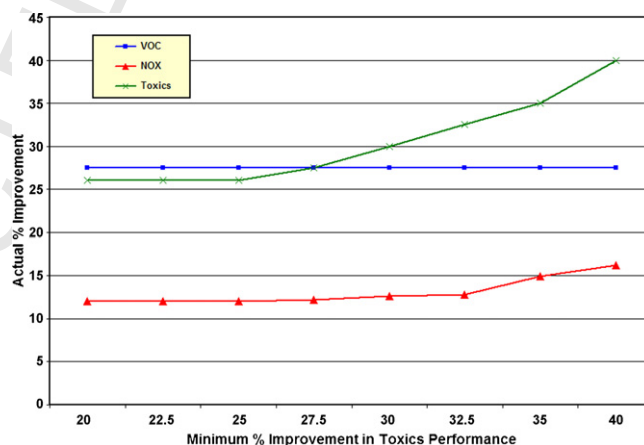


Fig. 6. Example 1: VOC and NO<sub>x</sub> changes with tighter toxics standards.

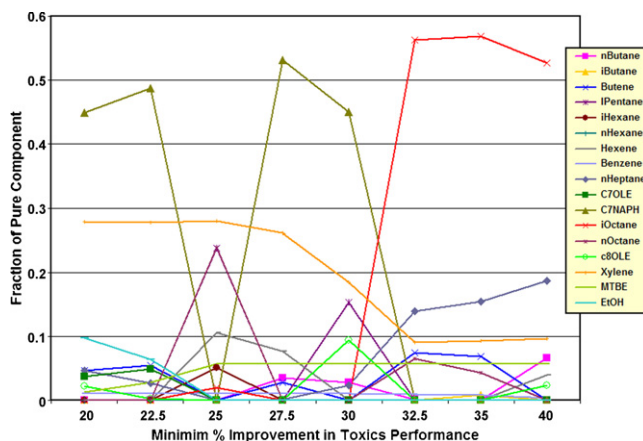


Fig. 7. Example 2: fractions changes with tighter toxics standards.

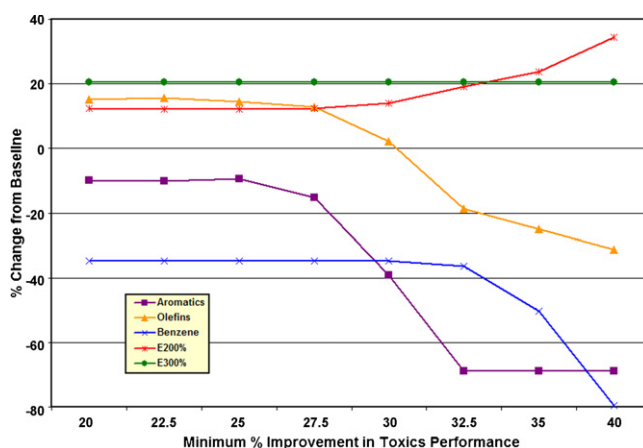


Fig. 8. Example 2: property changes with tighter toxics standards.

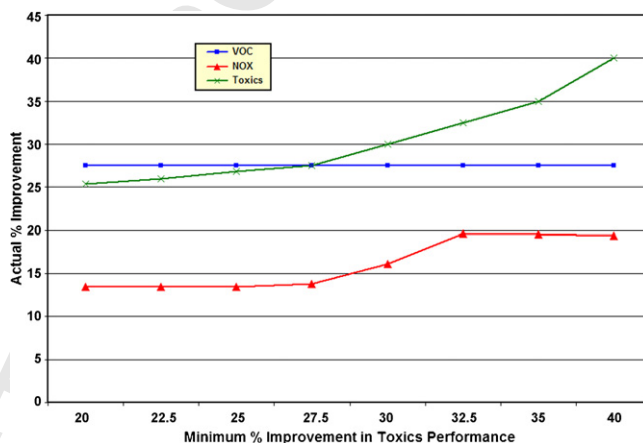


Fig. 9. Example 2: VOC and NOX changes with tighter toxics standards.

8. Conclusions

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

The illustrative examples demonstrate the feasibility of casting the Complex Model in terms of disjunctive programming. The disjunctive programming model is recast as an MINLP model, and the examples were solved using a global optimizer within reasonable run-times considering changes with respect to increasing requirements on toxic exhaust emissions with respect to composition, aggregate fuel properties and other exhaust emissions metrics. Having a mathematical programming representation of the Complex Model allows for simplified incorporation into refinery operations models or use in combination with models for boutique/designer gasoline.

#### Appendix A. Mixed-integer reformulation of disjunctive constraints

In this appendix, the disjunctive constraints of the paper are reformulated into mixed-integer linear constraints. A disjunctive constraint of the form:

$$\forall i \in D [A_i x \geq b_i]$$

is transformed into the following mixed-integer form:

$$\begin{aligned} -A_i x + b_i &\leq M_i(1 - y_i) \quad \forall i \in D \\ \sum_{i \in D} y_i &= 1 \end{aligned}$$

where  $D$  is the set of disjunctions,  $A_i$  an  $m_i \times n$  matrix parameter,  $b_i$  an  $m_i$  vector parameter,  $x$  an  $m_i$  vector variable,  $M_i$  an  $m_i$  “big- $M$ ” bound vector, and  $y_i$  is an  $m_i$  vector binary variable. In the constraints of this appendix, the “big- $M$ ” terms are set to be at the tightest bound determined by the upper and lower bounds of the variables in the disjunctions.

Reformulation of disjunctive constraint (1):

$$\begin{aligned} 95 - E300_{ot} &\leq (95 - E300^L)Y^{E300} \\ 95 - E300_t &\leq (95 - E300^L)Y^{E300} \\ E300_t - 95 &\leq (E300^U - 95)Y^{E300} \\ E300_{ot} - 95 &\leq (E300^U - 95)(1 - Y^{E300}) \\ E300_{ot} - E300_t &\leq (E300^U - E300^L)(1 - Y^{E300}) \\ E300_t - E300_{ot} &\leq (E300^U - E300^L)(1 - Y^{E300}) \\ Y^{E300} &\in \{0, 1\} \end{aligned}$$

Reformulation of disjunctive constraint (2):

$$\begin{aligned} ARO_{ot} - 10 &\leq (ARO^U - 10)Y^{ARO} \\ ARO_t - 10 &\leq (ARO^U - 10)Y^{ARO} \\ 10 - ARO_t &\leq (10 - ARO^L)Y^{ARO} \\ 10 - ARO_{ot} &\leq (10 - ARO^L)(1 - Y^{ARO}) \\ ARO_{ot} - ARO_t &\leq (ARO^U - ARO^L)(1 - Y^{ARO}) \\ ARO_t - ARO_{ot} &\leq (ARO^U - ARO^L)(1 - Y^{ARO}) \\ Y^{ARO} &\in \{0, 1\} \end{aligned}$$

Reformulation of disjunctive constraint (19):

$$\begin{aligned} 0.38465ARO_t - 14.25 &\leq (0.38465ARO^U - 14.25)Y^{E300*} \\ E300^* - 79.75 - 0.38465ARO_t &\leq (14.25 - 0.38465ARO^L)Y^{E300*} \\ 79.75 + 0.38465ARO_t - E300^* &\leq (0.38465ARO^U - 0.38465ARO^L)Y^{E300*} \\ 14.25 - 0.38465ARO_t &\leq (14.25 - 0.38465ARO^L)(1 - Y^{E300*}) \\ E300^* - 94 &\leq (0.38465ARO^U - 0.38465ARO^L)(1 - Y^{E300*}) \\ 94 - E300^* &\leq (14.25 - 0.38465ARO^L)(1 - Y^{E300*}) \\ Y^{E300*} &\in \{0, 1\} \end{aligned}$$

416 Reformulation of disjunctive constraint (20):

$$\begin{aligned}
 E200_t - 33 &\leq (E200^U - 33)(1 - Y_V^{E200}) \\
 E200_v - 33 &\leq (E200^U - 33)(1 - Y_V^{E200}) \\
 33 - E200_v &\leq (33 - E200^L)(1 - Y_V^{E200}) \\
 \Delta E200_v - E200_t + 33 &\leq (\Delta E200^U - E200^L + 33)(1 - Y_V^{E200}) \\
 E200_t - 33 - \Delta E200_v &\leq (E200^U - 33 - \Delta E200^L)(1 - Y_V^{E200}) \\
 33 - E200_t &\leq (33 - E200^L)(1 - Y_V^{E200'}) \\
 E200_t - 65.52 &\leq (E200^U - 65.52)(1 - Y_V^{E200'}) \\
 E200_v - E200_t &\leq (E200^U - E200^L)(1 - Y_V^{E200'}) \\
 E200_t - E200_v &\leq (E200^U - E200^L)(1 - Y_V^{E200'}) \\
 \Delta E200_v &\leq \Delta E200^U(1 - Y_V^{E200'}) \\
 -\Delta E200_v &\leq -\Delta E200^L(1 - Y_V^{E200'}) \\
 65.52 - E200_t &\leq (65.52 - E200^L)(1 - Y_V^{E200''}) \\
 E200_v - 65.52 &\leq (E200^U - 65.52)(1 - Y_V^{E200''}) \\
 65.52 - E200_v &\leq (65.52 - E200^L)(1 - Y_V^{E200''}) \\
 \Delta E200_v - E200_t + 65.52 &\leq (\Delta E200^U - E200^L + 65.52)(1 - Y_V^{E200''}) \\
 E200_t - 65.52 - \Delta E200_v &\leq (E200^U - 65.52 - \Delta E200^L)(1 - Y_V^{E200''}) \\
 Y_V^{E200} + Y_V^{E200'} + Y_V^{E200''} &\geq 1 \\
 Y_V^{E200} &\in \{0, 1\} \\
 Y_V^{E200'} &\in \{0, 1\} \\
 Y_V^{E200''} &\in \{0, 1\}
 \end{aligned}$$

418 Reformulation of disjunctive constraint (21):

$$\begin{aligned}
 E300_t - 72 &\leq (E300^U - 72)(1 - Y_V^{E300}) \\
 E300_v - 72 &\leq (E300^U - 72)(1 - Y_V^{E300}) \\
 72 - E300_v &\leq (72 - E300^L)(1 - Y_V^{E300}) \\
 \Delta E300_v - E300_t + 72 &\leq (\Delta E300^U - E300^L + 72)(1 - Y_V^{E300}) \\
 E300_t - 72 - \Delta E300_v &\leq (E300^U - 72 - \Delta E300^L)(1 - Y_V^{E300}) \\
 72 - E300_t &\leq (72 - E300^L)(1 - Y_V^{E300'}) \\
 E300_t - E300^* &\leq (E300^U - 79.75 - 0.38465ARO^L)(1 - Y_V^{E300'}) \\
 E300_v - E300_t &\leq (E300^U - E300^L)(1 - Y_V^{E300'}) \\
 E300_t - E300_v &\leq (E300^U - E300^L)(1 - Y_V^{E300'}) \\
 \Delta E300_v &\leq \Delta E300^U(1 - Y_V^{E300'}) \\
 -\Delta E300_v &\leq -\Delta E300^L(1 - Y_V^{E300'}) \\
 E300^* - E300_t &\leq (94 - E300^L)(1 - Y_V^{E300''}) \\
 E300_v - E300^* &\leq (E300^U - 79.75 - 0.38465ARO^L)(1 - Y_V^{E300''}) \\
 E300^* - E300_v &\leq (94 - E300^L)(1 - Y_V^{E300''}) \\
 \Delta E300_v - E300_t + E300^* &\leq (\Delta E300^U - E300^L + 94)(1 - Y_V^{E300''}) \\
 E300_t - E300^* - \Delta E300_v &\leq (E300^U - 79.75 - 0.38465ARO^L - \Delta E300^L)(1 - Y_V^{E300''}) \\
 Y_V^{E300} + Y_V^{E300'} + Y_V^{E300''} &\geq 1 \\
 Y_V^{E300} &\in \{0, 1\} \\
 Y_V^{E300'} &\in \{0, 1\} \\
 Y_V^{E300''} &\in \{0, 1\}
 \end{aligned}$$

420 Reformulation of disjunctive constraint (22):

$$\begin{aligned}
 & ARO_t - 18 \leq (ARO^U - 18)(1 - Y_v^{ARO}) \\
 & ARO_v - 18 \leq (ARO^U - 18)(1 - Y_v^{ARO}) \\
 & 18 - ARO_v \leq (18 - ARO^L)(1 - Y_v^{ARO}) \\
 & \Delta ARO_v - ARO_t + 18 \leq (\Delta ARO^U - ARO^L + 18)(1 - Y_v^{ARO}) \\
 & ARO_t - 18 - \Delta ARO_v \leq (ARO^U - 18 - \Delta ARO^L)(1 - Y_v^{ARO}) \\
 & 18 - ARO_t \leq (18 - ARO^L)(1 - Y_v^{ARO'}) \\
 & ARO_t - 46 \leq (ARO^U - 46)(1 - Y_v^{ARO'}) \\
 & ARO_v - ARO_t \leq (ARO^U - ARO^L)(1 - Y_v^{ARO'}) \\
 & ARO_t - ARO_v \leq (ARO^U - ARO^L)(1 - Y_v^{ARO'}) \\
 & \Delta ARO_v \leq \Delta ARO^U(1 - Y_v^{ARO'}) \\
 & -\Delta ARO_v \leq -\Delta ARO^L(1 - Y_v^{ARO'}) \\
 & 46 - ARO_t \leq (46 - ARO^L)(1 - Y_v^{ARO''}) \\
 & ARO_v - 46 \leq (ARO^U - 46)(1 - Y_v^{ARO''}) \\
 & 46 - ARO_v \leq (46 - ARO^L)(1 - Y_v^{ARO''}) \\
 & \Delta ARO_v - ARO_t + 46 \leq (\Delta ARO^U - ARO^L + 46)(1 - Y_v^{ARO''}) \\
 & ARO_t - 46 - \Delta ARO_v \leq (ARO^U - 46 - \Delta ARO^L)(1 - Y_v^{ARO''}) \\
 & Y_v^{ARO} + Y_v^{ARO'} + Y_v^{ARO''} \geq 1 \\
 & Y_v^{ARO} \in \{0, 1\} \\
 & Y_v^{ARO'} \in \{0, 1\} \\
 & Y_v^{ARO''} \in \{0, 1\}
 \end{aligned}$$

422 Reformulation of disjunctive constraint (40):

$$\begin{aligned}
 & SUL_t - 10 \leq (SUL^U - 10)(1 - Y_n^{SUL}) \\
 & SUL_n - 10 \leq (SUL^U - 10)(1 - Y_n^{SUL}) \\
 & 10 - SUL_n \leq (10 - SUL^L)(1 - Y_n^{SUL}) \\
 & \Delta SUL_n - SUL_t + 10 \leq (\Delta SUL^U - SUL^L + 10)(1 - Y_n^{SUL}) \\
 & SUL_t - 10 - \Delta SUL_n \leq (SUL^U - 10 - \Delta SUL^L)(1 - Y_n^{SUL}) \\
 & 10 - SUL_t \leq (10 - SUL^L)(1 - Y_n^{SUL'}) \\
 & SUL_t - 450 \leq (SUL^U - 450)(1 - Y_n^{SUL'}) \\
 & SUL_n - SUL_t \leq (SUL^U - SUL^L)(1 - Y_n^{SUL'}) \\
 & SUL_t - SUL_n \leq (SUL^U - SUL^L)(1 - Y_n^{SUL'}) \\
 & \Delta SUL_n \leq \Delta SUL^U(1 - Y_n^{SUL'}) \\
 & -\Delta SUL_n \leq -\Delta SUL^L(1 - Y_n^{SUL'}) \\
 & 450 - SUL_t \leq (450 - SUL^L)(1 - Y_n^{SUL''}) \\
 & SUL_n - 450 \leq (SUL^U - 450)(1 - Y_n^{SUL''}) \\
 & 450 - SUL_n \leq (450 - SUL^L)(1 - Y_n^{SUL''}) \\
 & \Delta SUL_n - SUL_t + 450 \leq (\Delta SUL^U - SUL^L + 450)(1 - Y_n^{SUL''}) \\
 & SUL_t - 450 - \Delta SUL_n \leq (SUL^U - 450 - \Delta SUL^L)(1 - Y_n^{SUL''}) \\
 & Y_n^{SUL} + Y_n^{SUL'} + Y_n^{SUL''} \geq 1 \\
 & Y_n^{SUL} \in \{0, 1\} \\
 & Y_n^{SUL'} \in \{0, 1\} \\
 & Y_n^{SUL''} \in \{0, 1\}
 \end{aligned}$$

423

424 Reformulation of disjunctive constraint (41):

$$\begin{aligned}
 \text{ARO}_t - 18 &\leq (\text{ARO}^U - 18)(1 - Y_n^{\text{ARO}}) \\
 \text{ARO}_n - 18 &\leq (\text{ARO}^U - 18)(1 - Y_n^{\text{ARO}}) \\
 18 - \text{ARO}_n &\leq (18 - \text{ARO}^L)(1 - Y_n^{\text{ARO}}) \\
 \Delta \text{ARO}_n - \text{ARO}_t + 18 &\leq (\Delta \text{ARO}^U - \text{ARO}^L + 18)(1 - Y_n^{\text{ARO}}) \\
 \text{ARO}_t - 18 - \Delta \text{ARO}_n &\leq (\text{ARO}^U - 18 - \Delta \text{ARO}^L)(1 - Y_n^{\text{ARO}}) \\
 18 - \text{ARO}_t &\leq (18 - \text{ARO}^L)(1 - Y_n^{\text{ARO}'}) \\
 \text{ARO}_t - 36.8 &\leq (\text{ARO}^U - 36.8)(1 - Y_n^{\text{ARO}'}) \\
 \text{ARO}_n - \text{ARO}_t &\leq (\text{ARO}^U - \text{ARO}^L)(1 - Y_n^{\text{ARO}'}) \\
 \text{ARO}_t - \text{ARO}_n &\leq (\text{ARO}^U - \text{ARO}^L)(1 - Y_n^{\text{ARO}'}) \\
 \Delta \text{ARO}_n &\leq \Delta \text{ARO}^U(1 - Y_n^{\text{ARO}'}) \\
 -\Delta \text{ARO}_n &\leq -\Delta \text{ARO}^L(1 - Y_n^{\text{ARO}'}) \\
 36.8 - \text{ARO}_t &\leq (36.8 - \text{ARO}^L)(1 - Y_n^{\text{ARO}''}) \\
 \text{ARO}_n - 36.8 &\leq (\text{ARO}^U - 36.8)(1 - Y_n^{\text{ARO}''}) \\
 36.8 - \text{ARO}_n &\leq (36.8 - \text{ARO}^L)(1 - Y_n^{\text{ARO}''}) \\
 \Delta \text{ARO}_n - \text{ARO}_t + 36.8 &\leq (\Delta \text{ARO}^U - \text{ARO}^L + 36.8)(1 - Y_n^{\text{ARO}''}) \\
 \text{ARO}_t - 36.8 - \Delta \text{ARO}_n &\leq (\text{ARO}^U - 36.8 - \Delta \text{ARO}^L)(1 - Y_n^{\text{ARO}''}) \\
 Y_n^{\text{ARO}} + Y_n^{\text{ARO}'} + Y_n^{\text{ARO}''} &\geq 1 \\
 Y_n^{\text{ARO}} &\in \{0, 1\} \\
 Y_n^{\text{ARO}'} &\in \{0, 1\} \\
 Y_n^{\text{ARO}''} &\in \{0, 1\}
 \end{aligned}$$

425  
426 Reformulation of disjunctive constraint (42):

$$\begin{aligned}
 \text{OLE}_t - 3.77 &\leq (\text{OLE}^U - 3.77)(1 - Y_n^{\text{OLE}}) \\
 \text{OLE}_n - 3.77 &\leq (\text{OLE}^U - 3.77)(1 - Y_n^{\text{OLE}}) \\
 3.77 - \text{OLE}_n &\leq (3.77 - \text{OLE}^L)(1 - Y_n^{\text{OLE}}) \\
 \Delta \text{OLE}_n - \text{OLE}_t + 3.77 &\leq (\Delta \text{OLE}^U - \text{OLE}^L + 3.77)(1 - Y_n) \\
 \text{OLE}_t - 3.77 - \Delta \text{OLE}_n &\leq (\text{OLE}^U - 3.77 - \Delta \text{OLE}^L)(1 - Y_n^{\text{OLE}}) \\
 3.77 - \text{OLE}_t &\leq (3.77 - \text{OLE}^L)(1 - Y_n^{\text{OLE}'}) \\
 \text{OLE}_t - 19 &\leq (\text{OLE}^U - 19)(1 - Y_n^{\text{OLE}'}) \\
 \text{OLE}_n - \text{OLE}_t &\leq (\text{OLE}^U - \text{OLE}^L)(1 - Y_n^{\text{OLE}'}) \\
 \text{OLE}_t - \text{OLE}_n &\leq (\text{OLE}^U - \text{OLE}^L)(1 - Y_n^{\text{OLE}'}) \\
 \Delta \text{OLE}_n &\leq \Delta \text{OLE}^U(1 - Y_n^{\text{OLE}'}) \\
 -\Delta \text{OLE}_n &\leq -\Delta \text{OLE}^L(1 - Y_n^{\text{OLE}'}) \\
 19 - \text{OLE}_t &\leq (19 - \text{OLE}^L)(1 - Y_n^{\text{OLE}''}) \\
 \text{OLE}_n - 19 &\leq (\text{OLE}^U - 19)(1 - Y_n^{\text{OLE}''}) \\
 19 - \text{OLE}_n &\leq (19 - \text{OLE}^L)(1 - Y_n^{\text{OLE}''}) \\
 \Delta \text{OLE}_n - \text{OLE}_t + 19 &\leq (\Delta \text{OLE}^U - \text{OLE}^L + 19)(1 - Y_n^{\text{OLE}''}) \\
 \text{OLE}_t - 19 - \Delta \text{OLE}_n &\leq (\text{OLE}^U - 19 - \Delta \text{OLE}^L)(1 - Y_n^{\text{OLE}''}) \\
 Y_n^{\text{OLE}} + Y_n^{\text{OLE}'} + Y_n^{\text{OLE}''} &\geq 1 \\
 Y_n^{\text{OLE}} &\in \{0, 1\} \\
 Y_n^{\text{OLE}'} &\in \{0, 1\} \\
 Y_n^{\text{OLE}''} &\in \{0, 1\}
 \end{aligned}$$

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