EPAct/V2/E-89: Assessing the Effect of Five Gasoline Properties on Exhaust Emissions from Light-Duty Vehicles Certified to Tier 2 Standards

Final Report on Program Design and Data Collection

Appendix A
Re-Design of Fuel Matrices for EPAct Program

Assessment and Standards Division
Office of Transportation and Air Quality
U.S. Environmental Protection Agency

National Renewable Energy Laboratory
U.S. Department of Energy

Coordinating Research Council

NOTICE

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United States Environmental Protection Agency

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RE-DESIGN OF FUEL MATRICES FOR EPACT PROGRAM

(Work Assignment WA 1-08 for Contract EP-C-07-028)

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1.0 Introduction

The objective of this project was to re-design the test fuel matrices previously provided to the EPA in February and August 2008 for its EPAct Program. The experimental designs were to be used to construct prediction equations for light-duty gasoline vehicle emissions. Five fuel properties were chosen as the experimental factors. These included ethanol (ETOH), T50, T90, aromatics (AROMATICS) and DVPE. The number of levels for each factor was 4 for ETOH, 5 for T50, 2 for T90, 2 for aromatics and 2 for DVPE.

Due to the desire to minimize the number of exhaust emissions test fuels, statistical designs were selected using a computer algorithm that generated optimal designs. In optimal designs, unlike in standard factorial and fractional factorial experiments, the factors are selected to be nearly orthogonal rather than exactly orthogonal, and the estimates of the factor effects are correlated rather than uncorrelated with one another. Computer-generated optimal designs are labeled non-orthogonal designs.

The process of generating an optimal design requires specification of the linear model that is to be estimated as well as a list of candidate design points from which to choose the design points. The candidate design points are usually located at the vertices of the space generated by the chosen levels of the factors to be included in the experiment, but may include any points within the ranges of the chosen factors.

An optimal design is generated by choosing design points from the candidate design point list that maximize or minimize a chosen optimality criterion that is related to the specified linear model. There are several different optimality criteria for generating optimal designs, and the one chosen for this study was G-optimality. Optimal designs are judged by their efficiency, which is usually expressed as a percentage. The efficiency value is a function of the number of points in the design, the number and types of factors in the model, and the maximum standard error for model prediction over the design points. The G-optimality criterion seeks to minimize the maximum standard error for prediction over the design points. Since a standard fractional factorial design will have an efficiency of 100%, a large G-efficiency value indicates the design is good. Generally, a design with a G-efficiency greater than 50-60% is considered adequate for prediction purposes.

Different types of search algorithms are available for finding an optimal design. These algorithms are based on adding and deleting candidate points to a design and stopping when the chosen criterion ceases to improve the design. The search method used in this project was the simple exchange algorithm. The initialization of the search process is started by specifying a random number.

Given below is a brief description of the process used in selecting the design requested by EPA for studying fuel effects on tailpipe emissions in light-duty vehicles.

2.0 Original Experimental Design #1: 16-Fuel Matrix

Factors and Model

Five experimental factors were used in this matrix development. The factors and their levels are listed in Table 1.

TABLE 1. EXPERIMENTAL FACTORS AND LEVELS FOR DESIGN #1

Factor	Low Level	Mid Levels	High Level
T50, ^{o}F	150	190, 220	240
T90, ^{o}F	300	-	340
ETOH, %	0	-	10
DVPE, psi	7	-	10
Aromatics, %	15	-	40

All combinations of the above values would yield 4x2x2x2x2=64 candidate test fuels. However, due to problems in blending some of the fuels, EPA eliminated (1) the 8 candidate fuels with T50=240^{o}F and ETOH=10%, (2) the 8 candidate fuels with T50=150^{o}F and ETOH=0% and (3) the 4 candidate fuels with T50=150^{o}F, ETOH=10% and DVPE=7. This left n = 64-20 = 44 candidate fuels available for usage in generating the model.

EPA requested that the experimental design should generate data to estimate the coefficients (labeled b_1 to b_{10}) for the following polynomial-type model:

$$\begin{aligned} Response \;=\; & b_0 + b_1*T50 + b_2*T90 + b_3*ETOH + b_4*DVPE + b_5*Aromatics + \\ & b_6*T50*T50 + b_7*ETOH*T50 + b_8*ETOH*T90 + \\ & b_9*ETOH*DVPE + b_{10}*ETOH*Aromatics + Error \end{aligned}$$

where *Response* indicates the emissions or engine property of interest, and *Error* denotes the random error in the experiment.

Design Results

An experimental design software package, ECHIP Version 7.01, was used to generate the experimental design matrix to meet the above conditions. Several design attempts were

made with varying starting random seeds for the algorithmic process in ECHIP. The 'best' design resulted in a G-efficiency equal to 72.6%. Table 2 lists the experimental design fuel matrix, consisting of 16 unique factor-level combinations, that was produced using ECHIP.

TABLE 2. FUEL MATRIX DESIGN #1

Fuel No.	T50, °F	T90, °F	ETOH, %	DVPE, psi	AROMATICS, %
1	150	300	10	10	15
2	240	340	0	10	15
3	220	300	10	7	15
4	220	340	10	10	15
5	240	300	0	7	40
6	190	340	10	7	15
7	190	300	0	7	15
8	220	300	0	10	15
9	190	340	0	10	40
10	220	340	10	7	40
11	190	300	10	10	40
12	150	340	10	10	40
13	220	340	0	7	40
14	190	340	0	7	15
15	190	300	0	10	40
16	220	300	10	7	40

3.0 Original Experimental Design #2: 25-Fuel Matrix

After the 16-fuel experimental design given in Table 2 was developed, EPA requested that additional fuels be added to include an area of the design space that extended the ethanol content (ETOH) to 20%, but included points at 15%. An additional criterion was that the original 16-fuel design be kept intact and that the additional fuels would be used to augment this design. There was also a request to keep the number of additional test fuels to 9 so that the total number of fuels was 25.

Factors and Model

The factors and their levels are listed in Table 3.

TABLE 3. EXPERIMENTAL FACTORS AND LEVELS FOR DESIGN #2

Factor	Low Level	Mid Levels	High Level
T50, ^{o}F	150	160	190
T90, ^{o}F	300	-	340
ETOH, %	15	-	20
DVPE, psi	7	-	10
Aromatics, %	15	-	40

All combinations of the above values would yield 3x2x2x2x2=48 candidate test fuels. However, due to problems in blending some of the fuels, EPA chose to (1) eliminate the 4 candidate fuels with T50=150^{o}F, ETOH=15% and DVPE=7, (2) eliminate the 16 candidate fuels at ETOH=20% and T50=150^{o}F and 190^{o}F by restricting the candidate fuels at ETOH=20% to have only T50=160^{o}F and (3) eliminate the 8 candidate fuels with T50=160^{o}F and ETOH=15%. This left a candidate set of n = 48-28 = 20 fuels for usage in augmenting the design given in Table 2.

EPA also requested that the experimental design should generate data to estimate the coefficients (labeled b_1 to b_{11}) for the following polynomial-type model (which now includes a squared term for ETOH):

$$\begin{aligned} Response = {} & b_0 + b_1*T50 + b_2*T90 + b_3*ETOH + b_4*DVPE + b_5*Aromatics + \\ & b_6*T50*T50 + b_7*ETOH*T50 + b_8*ETOH*T90 + \\ & b_9*ETOH*DVPE + b_{10}*ETOH*Aromatics + b_{11}*ETOH*ETOH + \\ & Error \end{aligned}$$

where *Response* indicates the emissions or engine property of interest, and *Error* denotes the random error in the experiment.

Design Results

An experimental design software package, ECHIP Version 7.01, was used to generate the experimental design matrix to meet the above conditions. Several design attempts were made with varying starting random seeds for the algorithmic process in ECHIP. The chosen design resulted in a G-efficiency equal to 68.1% and is listed in Table 4 as Design #2. The experimental design consists of 25 unique factor-level combinations.

TABLE 4. FUEL MATRIX DESIGN #2

(WITH G-EFFICIENCY = 68.1%)

Fuel No.	T50, °F	T90, °F	ETOH, %	DVPE, psi	AROMATICS, %
1	150	300	10	10	15
2	240	340	0	10	15
3	220	300	10	7	15
4	220	340	10	10	15
5	240	300	0	7	40
6	190	340	10	7	15
7	190	300	0	7	15
8	220	300	0	10	15
9	190	340	0	10	40
10	220	340	10	7	40
11	190	300	10	10	40
12	150	340	10	10	40
13	220	340	0	7	40
14	190	340	0	7	15
15	190	300	0	10	40
16	220	300	10	7	40
17	160	300	20	7	40
18	160	300	20	10	15
19	160	340	20	10	40
20	160	340	20	7	15
21	150	340	15	10	15
22	150	300	15	10	40
23	190	300	15	7	40
24	190	340	15	10	40
25	190	300	15	10	15

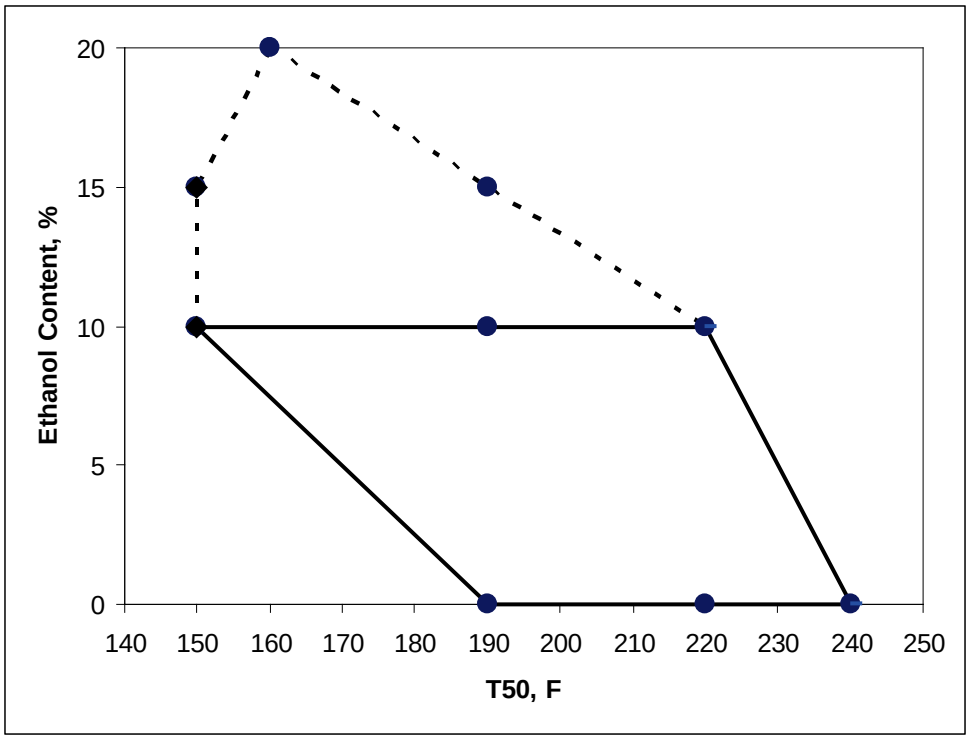

FIGURE 1. ETOH AND T50 DOMAIN FOR DESIGNS #2 AND #3 (DVPE=7 AND 10 PSI; T90=300 AND 340^{O}F; AROMATICS=15 AND 40 %)

4.0 Revised Experimental Design #3: 25-Fuel Matrix

After the 25-fuel experimental design given in Table 4 was developed, EPA, due to a problem in blending the fuels at ETOH=15%, requested that the test fuel matrix be redesigned. The revised design was to include the 16 original fuels listed in Table 2 in addition to 9 new fuels so that the total number of fuels was 25. The additional fuels were to include six fuels with the ethanol content (ETOH) set at 20%, and three fuels with ETOH set at 15%. The candidate factors and levels for these fuels are listed in Table 3 and the proposed model is the same as the model described in Section 3.0.

Design Results

An experimental design software package, ECHIP Version 7.01, was used to generate the experimental design matrix to meet the above conditions. Because of the complexity in needing to include six fuels with ETOH=20% and three fuels with ETOH=15%, the algorithmic approach was not used. Instead, all combinations of fuels meeting the above criteria were individually augmented to the 16-fuel matrix Design #1 given in Table 2 and the resulting G-efficiency was computed. The design with the highest G-efficiency was selected. The chosen design resulted in a G-efficiency equal to

68.7% and is listed in Table 5 as Design #3. The experimental design consists of 25 unique factor-level combinations.

TABLE 5. FUEL MATRIX DESIGN #3

(WITH G-EFFICIENCY = 68.7%)

Fuel No.	T50, °F	T90, °F	ETOH, %	DVPE, psi	AROMATICS, %
1	150	300	10	10	15
2	240	340	0	10	15
3	220	300	10	7	15
4	220	340	10	10	15
5	240	300	0	7	40
6	190	340	10	7	15
7	190	300	0	7	15
8	220	300	0	10	15
9	190	340	0	10	40
10	220	340	10	7	40
11	190	300	10	10	40
12	150	340	10	10	40
13	220	340	0	7	40
14	190	340	0	7	15
15	190	300	0	10	40
16	220	300	10	7	40
17	160	300	20	7	15
18	160	300	20	7	40
19	160	300	20	10	15
20	160	340	20	7	15
21	160	340	20	10	15
22	160	340	20	10	40
23	150	340	15	10	40
24	190	340	15	7	15
25	190	300	15	7	40

5.0 Revised CRC Experimental Design #4: 30-Fuel Matrix

At the completion of the above design work, EPA requested that SwRI work with Mr. Jim Uihlein from Chevron to prepare a 30-fuel experimental design for the Coordinating Research Council. The steps followed in this process are described below.

1. The response surface model had the same form as the one used in developing EPA's original 25-fuel matrix (i.e., described in Section 3.0), but also included a squared term for T90.

2. Three fuels were added to the EPA's revised 25-fuel matrix given in Table 5 to obtain a 28-fuel matrix, and the G-efficiency of this design was determined. The three additional fuels had the properties listed in Table 6.

TABLE 6. ADDITIONAL CRC FUELS

Factor	Fuel 1	Fuel 2	Fuel 3
T50, ^{o}F	215	202	195
T90, ^{o}F	325	325	325
ETOH, %	0	9.5	14.5
DVPE, psi	9	9	9
AROMATICS, %	29.5	24.9	22.6

3. The 28 fuels were forced into the model described in Step 1 above, and then a single additional fuel was selected that maximized the G-efficiency of the design. The candidate fuels for the additional fuel were restricted to the following two regions.

   Region 1:

T50, ETOH	(150, 10) (150, 15) (160, 10) (160, 15)
T90	300, 325, 340
DVPE	10
ARO	15, 40

   Region 2:

T50, ETOH	(160, 20)
T90	300, 325, 340
DVPE	7, 10
ARO	15, 40

   Taken together there were 4x3x1x2=24 candidate fuels in Region 1 and 1x3x2x2=12 candidate fuels in Region 2 for a total of 36 candidate fuels. These fuels are listed in Table 7.

4. A second model was fit using the same criteria as given in Step 3 above, but two additional fuels (rather than one additional fuel) were selected to yield a 30-fuel matrix. This was determined by selecting the best pair of fuels to add to the 28-fuel matrix.

Many different experimental designs were generated in this process. Included for each were the G-efficiencies of the designs using the new response surface model described in Step 1, as well as the G-efficiencies of these same fuel matrices using the original response surface model (i.e., without the squared T90 term). CRC preferred the experimental design given in Table 8 with G-efficiency = 64.1% for the model with the squared T90 term and G-efficiency = 59.4% for the model without the squared T90 term (i.e., see model in Section 2).

TABLE 7. CANDIDATE FUELS FOR CRC AUGMENTED EXPERIMENTAL DESIGNS

Fuel No.	T50, °F	T90, °F	ETOH, %	DVPE, psi	AROMATICS, %
1	150	300	10	10	15
2	150	300	10	10	40
3	150	325	10	10	15
4	150	325	10	10	40
5	150	340	10	10	15
6	150	340	10	10	40
7	150	300	15	10	15
8	150	300	15	10	40
9	150	325	15	10	15
10	150	325	15	10	40
11	150	340	15	10	15
12	150	340	15	10	40
13	160	300	10	10	15
14	160	300	10	10	40
15	160	325	10	10	15
16	160	325	10	10	40
17	160	340	10	10	15
18	160	340	10	10	40
19	160	300	15	10	15
20	160	300	15	10	40
21	160	325	15	10	15
22	160	325	15	10	40
23	160	340	15	10	15
24	160	340	15	10	40
25	160	300	20	7	15
26	160	300	20	7	40
27	160	325	20	7	15
28	160	325	20	7	40
29	160	340	20	7	15
30	160	340	20	7	40
31	160	300	20	10	15
32	160	300	20	10	40
33	160	325	20	10	15
34	160	325	20	10	40
35	160	340	20	10	15
36	160	340	20	10	40

After observing the alternative generated experimental designs, CRC noted that a very similar design, with similar G-efficiency values, could be obtained by replacing the test fuel No. 29 in Table 6 with the following fuel:

T50	T90	Ethanol	DVPE	Aromatics
°F	°F	%	psi	%
150	325	10	10	15

CRC decided that, if EPA believed that this E10 fuel was considerably easier to blend than E10 fuel No. 29 in Table 8, then this could be used as an acceptable alternative.

TABLE 8. FUEL MATRIX DESIGN #4

(WITH G-EFFICIENCY = 64.1% FOR MODEL WITH $T90^2$ TERM)

Fuel No.	T50, °F	T90, °F	ETOH, %	DVPE, psi	AROMATICS, %
1	150	300	10	10	15
2	240	340	0	10	15
3	220	300	10	7	15
4	220	340	10	10	15
5	240	300	0	7	40
6	190	340	10	7	15
7	190	300	0	7	15
8	220	300	0	10	15
9	190	340	0	10	40
10	220	340	10	7	40
11	190	300	10	10	40
12	150	340	10	10	40
13	220	340	0	7	40
14	190	340	0	7	15
15	190	300	0	10	40
16	220	300	10	7	40
17	160	300	20	7	15
18	160	300	20	7	40
19	160	300	20	10	15
20	160	340	20	7	15
21	160	340	20	10	15
22	160	340	20	10	40
23	150	340	15	10	40
24	190	340	15	7	15
25	190	300	15	7	40
26	215	325	0	9	29.5
27	202	325	9.5	9	24.9
28	195	325	14.5	9	22.6
29	150	325	10	10	40
30	160	325	20	7	40

***** THE FOLLOWING SECTION WAS ADDED TO THE ABOVE REPORT AND WAS NOT PART OF WORK ASSIGNMENT 1-08, EPA CONTRACT EP-C-07-028. IT IS BASED ON WORK ASSIGNMENT 3-02, EPA CONTRACT EP-C-07-028. *****

6.0 Final Fuel Matrix Design Tested in Phase 3 of the EPAct/V2/E-89 Program

The fuel matrix design #5 which was tested in Phase 3 of the EPAct/V2/E-89 Program is shown in Table 9. It was derived by the EPA from the design #4 shown in Table 8 in the following manner:

- Fuels 26, 27 and 28 were removed from the matrix design #4
- Fuels 17 through 25 and 29 through 30 in fuel matrix design #4 were renumbered in design #5 to match designations which were already being used in the blend development process
- Some nominal levels of T50, T90 and aromatic content were adjusted in fuel matrix #5 to match levels achievable with the available blending components. Specifically,
    - T50 of E15 fuel 26 and all E20 fuels (Table 9) was changed to 165 ^{o}F from 150 ^{o}F and 160 ^{o}F, respectively
    - T50 of E15 fuels 27 and 28 was changed from 190 ^{o}F to 220 ^{o}F
    - High level of aromatic content was changed from 40 vol.% to 35 vol.%

The G-efficiency of this 27-fuel matrix #5 was computed to equal 51.6 % for the model without the squared T90 term.

TABLE 9. FUEL MATRIX DESIGN #5

(WITH G-EFFICIENCY = 51.6% FOR MODEL WITHOUT $T90^2$ TERM)

Fuel No.	T50, °F	T90, °F	ETOH, %	DVPE, psi	AROMATICS, %
1	150	300	10	10	15
2	240	340	0	10	15
3	220	300	10	7	15
4	220	340	10	10	15
5	240	300	0	7	35
6	190	340	10	7	15
7	190	300	0	7	15
8	220	300	0	10	15
9	190	340	0	10	35
10	220	340	10	7	35
11	190	300	10	10	35
12	150	340	10	10	35
13	220	340	0	7	35
14	190	340	0	7	15
15	190	300	0	10	35
16	220	300	10	7	35
20	165	300	20	7	15
21	165	300	20	7	35
22	165	300	20	10	15
23	165	340	20	7	15
24	165	340	20	10	15
25	165	340	20	10	35
26	165	340	15	10	35
27	220	340	15	7	15
28	220	300	15	7	35
30	150	325	10	10	35
31	165	325	20	7	35