DRIVING RESEARCH AND INNOVATION FOR VEHICLE EFFICIENCY AND ENERGY SUSTAINABILITY

Well-to-Wheels Energy and Greenhouse Gas Emission Analysis of Bio-Blended High-Octane Fuels for High-Efficiency Engines

Appendix 2 – Refinery Gasoline Components and Octane Numbers

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Appendix 2 – Refinery Gasoline Components and Octane Numbers

Contents

Figures

Tables

Part 1 The Component of E Set Finished Gasolines Produced in Configuration Refineries

Table A2-1. BAU and HOF Finished Gasoline Components for E Set Fuels Produced in CRK Configuration in 2022

			2022 CRK		
BAU	F10	F14	F18	F19	F20
C4s	2.0%	1.3%	1.9%	2.1%	2.0%
Naphtha	3.0%	8.6%	10.6%	5.8%	3.3%
Isomerate	9.7%	15.4%	15.3%	14.5%	15.0%
Alkylate	7.9%	4.0%	4.6%	5.3%	6.4%
Reformate	38.4%	57.6%	57.6%	50.5%	52.8%
FCC	29.1%	3.1%	0.0%	11.9%	10.5%
EtOH	10.0%	10.0%	10.0%	10.0%	10.0%
Total	100.0%	100.0%	100.0%	100.0%	100.0%
HOF	F10	F14	F18	F19	F20
C4s	2.9%	2.0%	0.3%	1.0%	0.6%
Naphtha	8.3%	0.0%	0.0%	19.3%	11.0%
Isomerate	5.2%	0.0%	0.0%	0.0%	0.0%
Alkylate	8.8%	13.5%	11.7%	9.3%	9.6%
Reformate	36.4%	21.7%	20.1%	8.0%	22.1%
FCC	28.5%	52.8%	47.9%	32.5%	36.6%
EtOH	10.0%	10.0%	20.0%	30.0%	20.0%
Total	100.0%	100.0%	100.0%	100.0%	100.0%

Table A2-2. BAU and HOF Finished Gasoline Components for E Set Fuels Produced in LtCOK Configuration in 2022

2022 LtCOK					
BAU	F10	F14	F18	F19	F20
C4s	3.7%	0.8%	2.0%	2.0%	2.0%
Naphtha	7.4%	8.0%	6.6%	4.4%	3.0%
Isomerate	0.3%	14.3%	14.2%	11.0%	14.1%
Alkylate	14.8%	4.1%	6.4%	8.3%	6.5%
Reformate	34.4%	45.4%	57.1%	43.3%	50.0%
FCC	29.5%	17.3%	3.7%	20.9%	14.4%
EtOH	10.0%	10.0%	10.0%	10.0%	10.0%
Total	100.0%	100.0%	100.0%	100.0%	100.0%
HOF	F10	F14	F18	F19	F20
C4s	1.4%	2.5%	0.0%	1.0%	0.5%
Naphtha	5.1%	0.0%	0.0%	21.5%	14.6%
Isomerate	13.1%	0.0%	0.0%	0.0%	0.0%
Alklate	5.0%	16.5%	13.6%	9.6%	13.1%
Reformate	30.8%	23.8%	14.3%	8.4%	11.8%
FCC	34.7%	47.1%	52.1%	29.6%	40.0%
EtOH	10.0%	10.0%	20.0%	30.0%	20.0%
Total	100.0%	100.0%	100.0%	100.0%	100.0%

Table A2-3. BAU and HOF Finished Gasoline Components for E Set Fuels Produced in HvyCOK Configuration in 2022

2022 HvyCOK					
BAU	F10	F14	F18	F19	F20
C4s	2.7%	0.5%	1.4%	2.6%	2.0%
Naphtha	8.2%	20.9%	13.7%	5.0%	3.5%
Isomerate	4.9%	14.3%	14.2%	5.2%	14.2%
Alkylate	6.5%	4.2%	6.5%	7.7%	6.5%
Reformate	39.8%	50.2%	50.6%	53.1%	56.4%
FCC	28.0%	0.0%	3.6%	16.5%	7.4%
EtOH	10.0%	10.0%	10.0%	10.0%	10.0%
Total	100.0%	100.0%	100.0%	100.0%	100.0%
HOF	F10	F14	F18	F19	F20
C4s	0.8%	2.0%	0.0%	0.0%	0.0%
Naphtha	22.4%	0.0%	3.1%	31.4%	21.4%
Isomerate	8.7%	0.0%	0.0%	0.1%	0.0%
Alkylate	10.7%	14.1%	11.5%	9.1%	12.5%
Reformate	20.4%	19.5%	18.9%	0.3%	0.0%
FCC	27.0%	54.4%	46.5%	29.2%	46.0%
EtOH	EtOH	EtOH	EtOH	EtOH	EtOH
Total	100.0%	100.0%	100.0%	100.0%	100.0%

Table A2-4. BAU and HOF Finished Gasoline Components for E Set Fuels Produced in COKHCK Configuration in 2022

			2022 HvyCOK		
BAU	F10	F14	F18	F19	F20
C4s	0.1%	NF	0.2%	0.4%	0.5%
Naphtha	19.2%	NF	8.5%	11.9%	19.7%
Isomerate	3.5%	NF	2.3%	1.8%	1.6%
Alkylate	31.1%	NF	17.3%	31.8%	31.2%
Reformate	18.5%	NF	44.0%	27.6%	20.0%
FCC	17.6%	NF	17.7%	16.5%	17.1%
EtOH	10.0%	NF	10.0%	10.0%	10.0%
Total	100.0%	NF	100.0%	100.0%	100.0%
HOF	F10	F14	F18	F19	F20
C4s	0.0%	NF	0.0%	0.0%	0.0%
Naphtha	29.8%	NF	11.2%	24.6%	21.3%
Isomerate	0.0%	NF	1.9%	8.1%	0.5%
Alkylate	29.4%	NF	31.4%	11.2%	16.6%
Reformate	17.0%	NF	16.0%	9.3%	22.3%
FCC	13.8%	NF	19.5%	16.9%	19.4%
EtOH	10.0%	NF	20.0%	30.0%	20.0%
Total	100.0%	NF	100.0%	100.0%	100.0%

Table A2-5. Components of the E Set Fuels Produced in Configuration Refineries in 2040 (all HOF gasoline)

CRK	F10	F14	F18	F19	F20
C4s	2%	2%	1%	1%	1%
Naphtha	7%	2%	0%	9%	6%
Isomerate	8%	8%	8%	8%	8%
Alkylate	8%	9%	8%	6%	8%
Reformate	40%	42%	39%	27%	36%
FCC	25%	27%	24%	19%	22%
EtOH	10%	10%	20%	30%	20%

LtCOK	F10	F14	F18	F19	F20
C4s	2%	1%	1%	1%	1%
Naphtha	7%	3%	0%	11%	5%
Isomerate	8%	8%	7%	4%	7%
Alkylate	9%	11%	10%	6%	8%
Reformate	36%	37%	34%	20%	31%
FCC	28%	30%	28%	27%	27%
EtOH	10%	10%	20%	30%	20%

HvyCOK	F10	F14	F18	F19	F20
C4s	1%	1%	1%	1%	1%
Naphtha	13%	5%	0%	14%	9%
Isomerate	8%	8%	8%	7%	8%
Alkylate	9%	10%	10%	6%	8%
Reformate	33%	37%	36%	22%	29%
FCC	26%	28%	26%	21%	25%
EtOH	10%	10%	20%	30%	20%

COKHCK	F10	F14	F18	F19	F20
C4s	0%	0%	0%	0%	0%
Naphtha	28%	0%	9%	27%	25%
Isomerate	0%	0%	6%	0%	4%
Alkylate	28%	0%	27%	16%	23%
Reformate	16%	0%	20%	11%	12%
FCC	17%	0%	17%	15%	16%
EtOH	10%	0%	20%	30%	20%

Part 2 The Comparisons of RONs and MONs of E Set HOF Gasolines BOBs from LP Modeling to the Measured Values

Table A2-6. The E Set HOF Gasoline BOB RONs and MONs Resultant from Aggregate Refinery LP Modeling and that from Lab Measured Values

		F1	F7	F10	F14	F15	F16	F18	F19	F20
Measured	HOF RON	85.6	94.2	86.4	91.8	76.8	97.8	92.3	83.1	86.4
	HOF MON	81.2	90.3	79.3	83.8	71.0	87.6	86.1	80.7	82.2
2022 PADD 3	CBOB HOF RON	85.4	97.5	85.8	91.5	76.4	98.7	88.5	77.5	83.8
	RBOB HOF RON	85.2	93.7	89.4	90.8	80.0	97.3	89.3	76.8	82.8
	CBOB HOF MON	78.5	94.3	80.5	81.8	70.5	90.3	81.9	73.4	77.6
	RBOB HOF MON	78.9	94.3	80.4	83.7	73.3	90.3	81.8	73.1	78.0
2022 CA	CBOB HOF RON	85.9	95.3	86.0	91.1	70.2	--	89.2	78.5	83.9
	RBOB HOF RON	85.7	95.3	85.6	91.1	70.2	--	88.0	78.4	84.0
	CBOB HOF MON	78.5	90.4	80.5	84.5	67.2	--	83.8	73.8	78.3
	RBOB HOF MON	79.2	90.0	80.4	84.5	67.2	--	83.0	74.3	78.6
2040 PADD 3	CBOB HOF RON	86.3	--	87.0	92.6	82.3	--	91.1	81.0	85.5
	RBOB HOF RON	87.1	--	88.9	90.6	79.3	--	93.1	85.7	88.1
	CBOB HOF MON	79.0	--	80.5	83.4	75.2	--	82.7	75.3	78.1
	RBOB HOF MON	79.5	--	80.4	84.4	72.7	--	84.2	78.4	80.0
2040 CA	CBOB HOF RON	86.8	--	85.9	92.0	88.3	--	89.8	85.4	86.9
	RBOB HOF RON	85.7	--	86.4	91.3	77.6	--	90.2	79.4	84.9
	CBOB HOF MON	80.2	--	80.5	84.9	82.1	--	83.9	78.5	80.6
	RBOB HOF MON	79.8	--	80.4	84.6	72.7	--	83.2	74.2	78.9

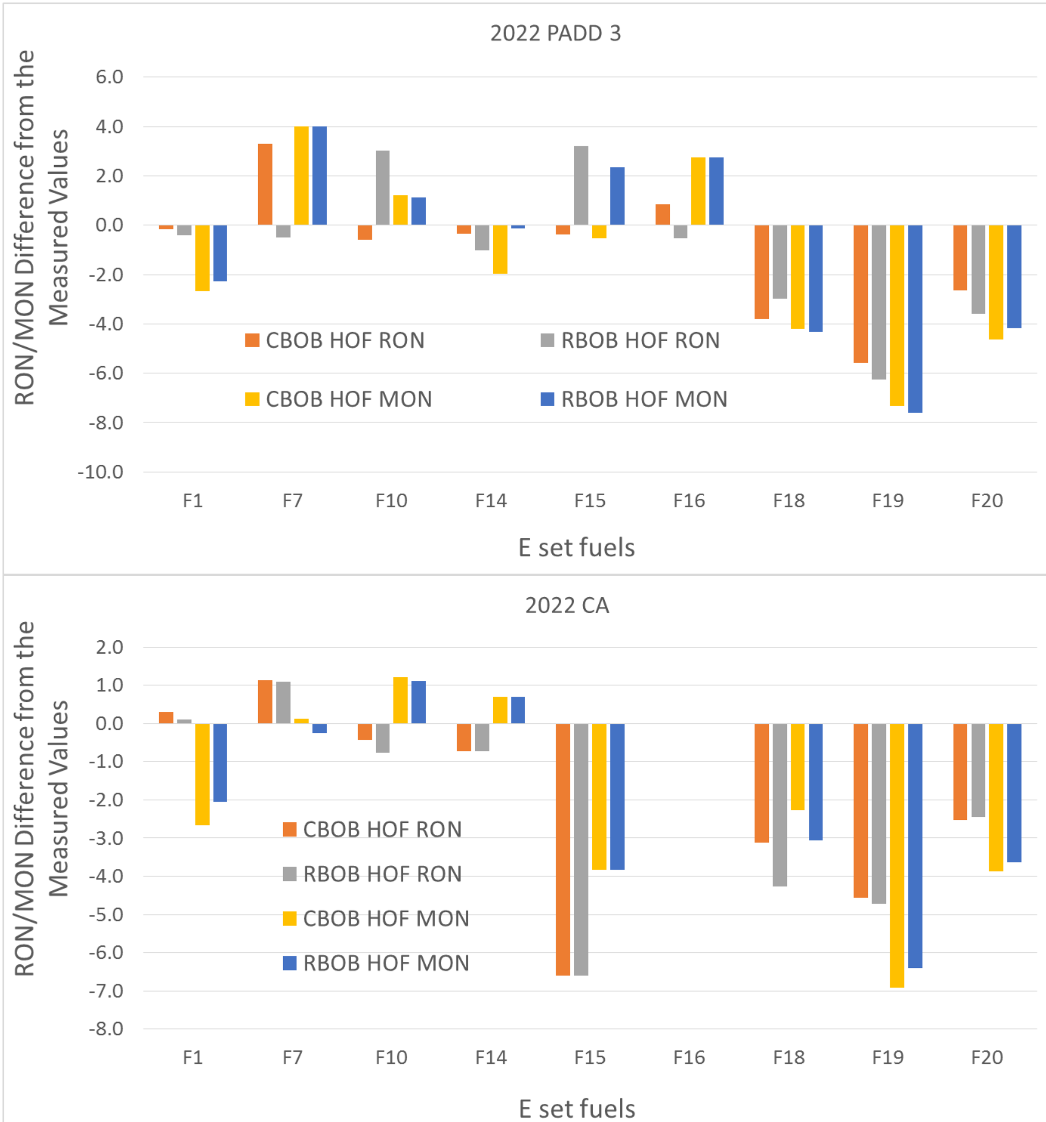

Figure A2-1. The Comparison of 2022 PADD 3 and CA Refinery LP Modeling Resultant HOF Gasoline BOB RONs and MONs with the Measured Values for the Lab Prepared BOBs

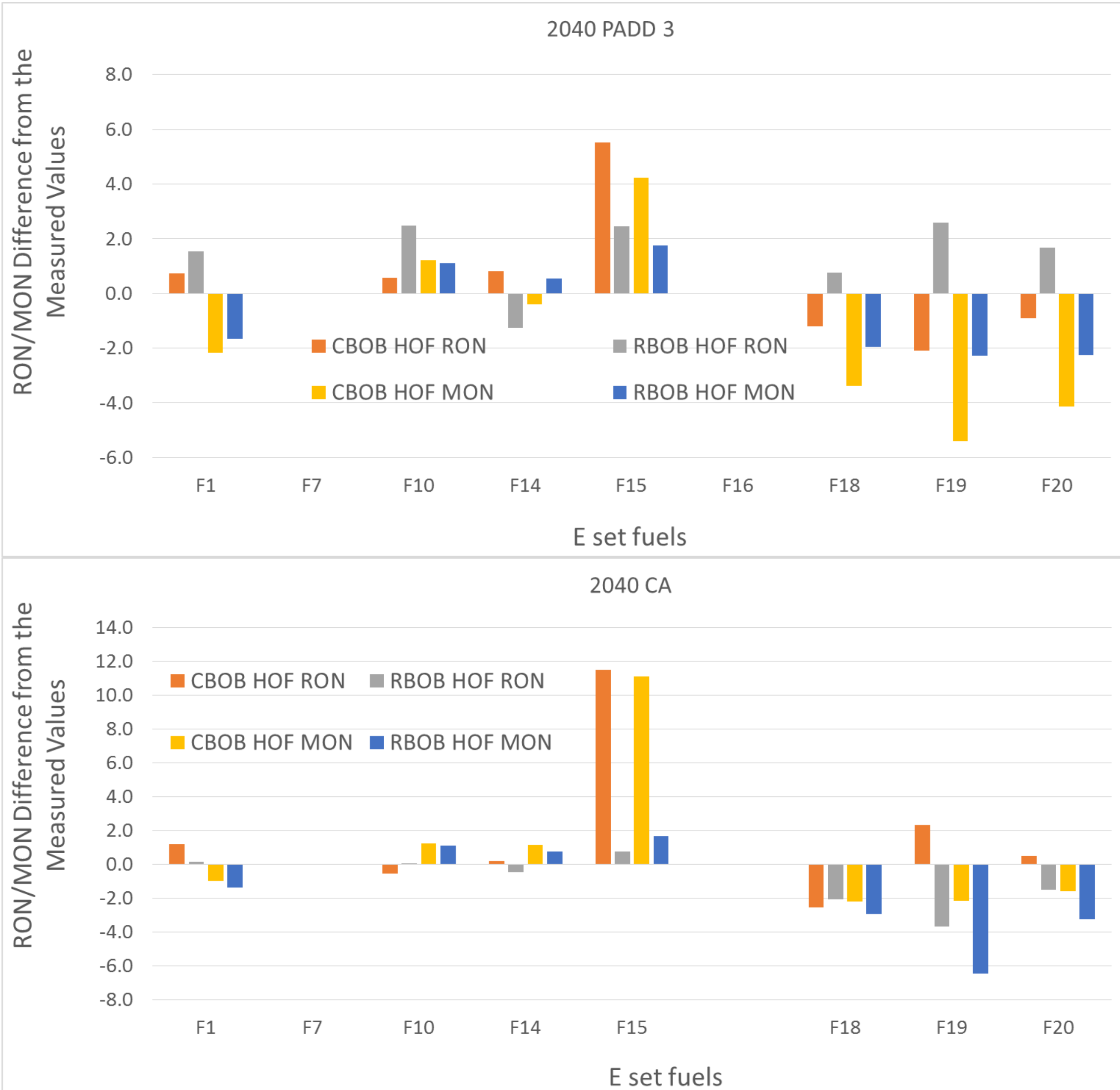

Figure A2-2. The Comparison of 2040 PADD 3 and CA Refinery LP Modeling Resultant HOF Gasoline BOB RONs and MONs with the Measured Values for the Lab Prepared BOBs

Overall, for the HOF BOB gasolines, the comparison trends of LP modeling resultant RONs and MONs with the lab measured values are approximately consistent with the HOF finished gasolines, but with greater divergence. By and large, the divergence (the LP modeling resultant RONs and MONs minus the lab measured values) for the E10 (F1, F7, F10, F14, F16) gasolines BOBs are relatively small, while the divergence for E20 (F18 and F20) and E30 (F15 and F19) gasoline BOBs are noticeable or sizeable. Especially, the F15 and F19 HOF BOBs show large divergence that reached 11 number in 2040 cases. This is related to the non-linear blending behavior of ethanol and its blending octanes calculated in LP modeling. In the LP modeling, with the regression approach described in the main report, the ethanol blending RON is a function of aromatic content. For F15 and F19, the regressed ethanol blending RONs reach 140–150 numbers, bringing significant octanes to the finished gasoline pool with high blending level of 30 vol% ethanol. With 97 and 101 RON requirements for the finished gasoline of F15 and F19 (while keeping MON values float), the LP modeling optimized to produce BOBs to maximize refinery margins with much greater variations (or leeway) than for the cases for E10 blending. For 2022 cases, the LP modeling achieved maximum margins by producing BOBs with low RONs or MONs (with eased operation, indicated by reformer severity) to take advantage of the large octanes introduced by ethanol blending. For 2040 cases, with the HOF share increasing from 50% to 100%, the significant octanes brought by 30% ethanol blending "flushed" the octane pool of the F15 and F19 domestic finished gasolines. The abundant octanes could be distributed via the three outlets below.

1. Diverting the "flushed" octanes to gasoline export by expanding export volume. This is observed for E20 and E30 fuels in Section 5 of the main report.

2. Diverting some BOB "swing" streams from gasoline pool to distillate pool. This is observed for E20 and E30 gasoline cases which have lower G/D ratios than the E10 cases and base cases. See Appendix 1.

3. Providing BOBs with higher RON/MON than requirements) and leading to undesired octane giveaways. For F15, noticeable RON giveaway was observed.

It is worth noting that the divergence of LP modeling resultant gasoline BOB RONs and MONs from the lab-measured values are also indicated by the difference of gasoline components, especially by the aromatic content, shown in the report from Jacobs Consultancy [1].

Table A2-7. The E Set HOF Gasoline BOB RONs and MONs Resultant from Configuration Refinery LP Modeling and that from Lab Measured Values

		F10	F14	F18	F19	F20	F10	F14	F18	F19	F20
Measured	HOF RON	86.4	91.8	92.3	83.1	86.4	86.4	91.8	92.3	83.1	86.4
	HOF MON	79.3	83.8	86.1	80.7	82.2	79.3	83.8	86.1	80.7	82.2
		CRK					LtCOK				
2022	CBOB HOF RON	88.2	92.5	91.0	81.4	86.2	88.4	92.6	90.8	81.0	85.4
	RBOB HOF RON	87.3	92.8	92.7	86.7	87.8	87.3	92.7	92.1	86.3	87.9
	CBOB HOF MON	80.5	83.2	81.8	74.8	78.4	80.5	83.6	81.6	74.6	78.0
	RBOB HOF MON	80.4	83.8	83.9	78.5	80.2	80.4	83.9	83.8	78.3	79.8
		HvyCOK					COKHCK				
	CBOB HOF RON	86.8	92.2	90.3	80.6	85.1	86.3	--	90.1	80.7	86.3
	RBOB HOF RON	88.2	92.7	89.7	76.4	83.1	85.7	--	90.1	82.0	85.7
	CBOB HOF MON	80.5	83.1	81.5	73.7	77.1	80.5	--	84.1	76.4	78.9
	RBOB HOF MON	80.4	83.8	81.6	73.3	77.9	80.4	--	84.1	76.0	79.4
		CRK					LtCOK				
2040	CBOB HOF RON	88.3	92.7	93.8	86.3	87.7	88.4	93.1	93.6	86.5	88.1
	RBOB HOF RON	86.0	93.4	94.0	85.5	88.8	86.6	90.8	93.4	81.3	87.0
	CBOB HOF MON	80.5	84.3	84.9	79.1	80.6	80.5	84.1	84.7	78.7	80.2
	RBOB HOF MON	80.4	83.3	84.6	78.8	79.7	80.4	83.7	84.3	75.3	80.0
		HvyCOK					COKHCK				
	CBOB HOF RON	87.5	92.3	93.0	84.7	87.5	86.5	--	90.0	84.2	84.4
	RBOB HOF RON	88.5	93.3	93.7	85.0	87.3	86.1	--	90.1	82.6	85.0
	CBOB HOF MON	80.5	84.2	84.1	77.7	80.0	80.5	--	84.0	78.3	80.1
	RBOB HOF MON	80.4	83.3	86.0	79.1	80.4	80.4	--	83.9	77.1	79.4

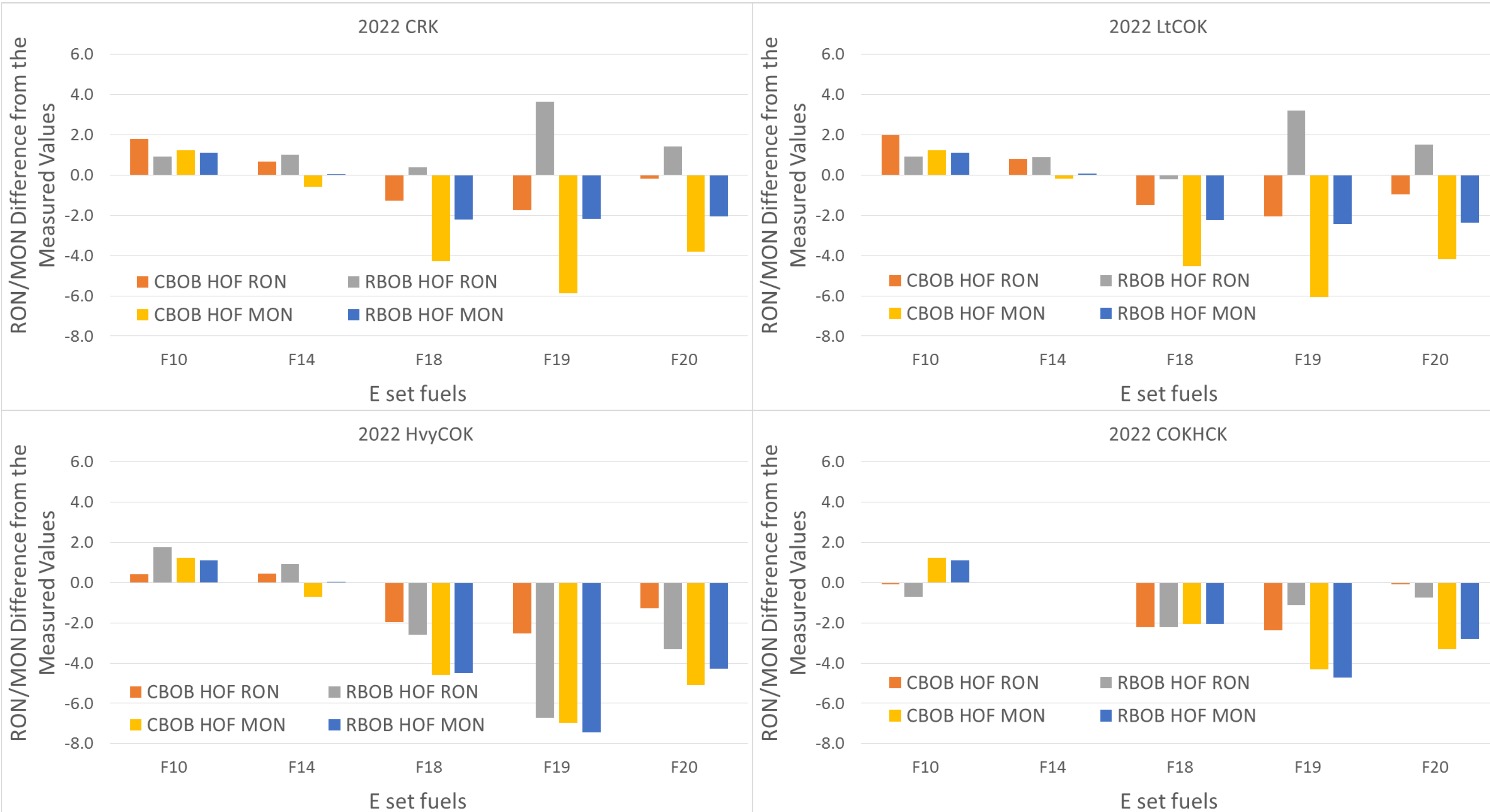

Figure A2-3. The Comparison of 2022 Configuration Refinery LP Modeling Resultant HOF Gasoline BOB RONs and MONs with the Measured Values for the Lab Prepared BOBs

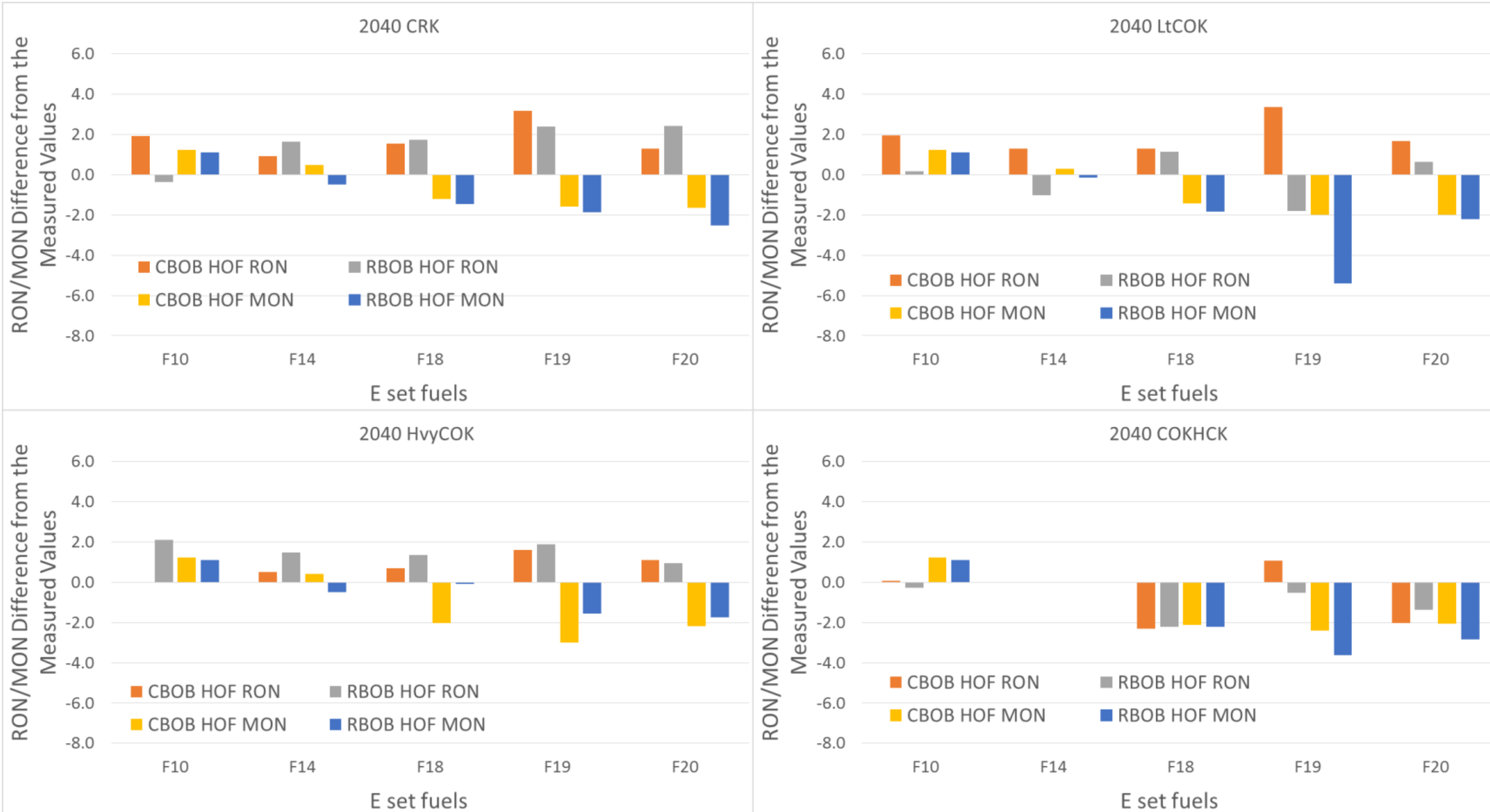

Figure A2-4. The Comparison of 2040 Configuration Refinery LP Modeling Resultant HOF Gasoline BOB RONs and MONs with the Measured Values for the Lab Prepared BOBs

Similar with the aggregate refinery cases, for the configuration refinery cases, the divergence of LP modeling resultant RONs and MONs of the E set HOF gasoline BOBs from the measured values are more pronounced for E20 (F18 and F20) and E30 (F19) fuels than for E10 fuels (F10 and F14). From 2022 to 2040, the divergence is somewhat alleviated. The configuration refineries do not produce export gasolines (all BOB), thus, the abundant octanes are likely distributed by the other two outlets: diverting swing streams to distillate pool and octane giveaway. Especially, for the more complex and distillate–oriented refineries, HvyCOK refinery, from 2022 to 2040, the G/D ratios of E20 and E30 gasoline BOBs decrease from 1.02-1.10 to 0.66-0.75, diverting significant gasoline streams to distillate pool. The octane giveaway is observed for F19 BOB, which is to be blended with 30% ethanol for E30 production.

Reference

[1] Jenkins, J. (Jacobs Consultancy), and V. DiVita (Jacobs Consultancy). Refinery Modeling for Argonne National Laboratory. (November 2017). https://greet.es.anl.gov/publication-refinery_anl.