CRC PROJECT RW-107-2: Emerging PMI Methodologies

Final PMI and PMI-A Values

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Standardization of BP/VP Values

- The past emission studies used somewhat different slates of BP/VP values for the hydrocarbon compounds:
  - A few differences are large (suggesting errors) while the others are small (suggesting different data sources).
- All calculations are now “standardized” meaning:
  - Done using BP/VP values derived from the SSI Enhanced DHAs, adopted as the more current and authoritative values.
  - All oxygenates are assigned their empirical BP and VP.
  - For all other compounds, the VP=f(BP) equation from Aikawa is used to estimate VP.
- Standardization introduces only minor differences in the PMI values.

Standardization of Oxygenate Vapor Pressures

Vapor Pressure for Oxygenates in Gasoline kPA @ 443°K					
Adopted for RW-107-2		ASTM DHAs			SSI Master List and DHAs
Oxygenate	Standard Value (NIST)	E-94-2/3	E-129	EPAct	
Ethanol	1,475	1,581	1,581	1,581	853
i-Butanol	403		442	481	352
2-methyl-1-propanol	403				403
MTBE	1,075		1,440		1,075

PMI Calculations using ASTM DHAs

PMI-A

ASTM DHAs	DHAs Conducted	DHA Lab	BP or VP Reported	VP Values Used in Replicating Study's PMI Calculation ‡	PMI Comparison: Δ = Published - Replicated
EPAct Study	c. 2010	SwRI	NO	Adopted from E-94-2/3	-0.03 to +0.01
E-94-2 (Reprocessed)					
E10 Fuels (A,B,E,F)	mid-2017	SwRI	NO	E-94-2/3 (inferred †)	-0.01 to +0.02
E0 Fuels (C,D,G,H) *	mid-2017	SwRI	NO	E-94-2/3 (inferred †)	-0.01 to +0.04
E-94-3 (Reprocessed)					
C/D/G/H – E10	mid-2017	SwRI	NO	E-94-2/3 (inferred †)	-0.01 to +0.00
E-129	2018-19	CRC Member Company	NO	E-129 (inferred †)	-0.00 to +0.01

‡ Empirical vapor pressures used for ethanol and other oxygenates (i-Butanol and MTBE).

† Inferred by back-calculating VP from the i-term from each compound for DHAs where the PMI calculations are available.

* DHAs conducted at start of E-94-3 for the E0 base fuels before they were splash-blended with ethanol to create E-10 fuels.

EPAct Fuels		RW-107 (Published)	RW-107-2 (Final)
Study	Fuel	PMI	PMI (standardized)
EPAct	Fuel 1	0.93	0.93
	Fuel 2	1.32	1.30
	Fuel 3	0.93	0.93
	Fuel 4	1.31	1.30
	Fuel 5	1.37	1.37
	Fuel 6	1.29	1.28
	Fuel 7	1.01	1.00
	Fuel 8	1.00	1.00
	Fuel 9	1.97	1.94
	Fuel 10	2.01	2.00
	Fuel 11	1.34	1.34
	Fuel 12	2.10	2.08
	Fuel 13	1.89	1.87
	Fuel 14	1.30	1.28

EPAct Fuels		RW-107 (Published)	RW-107-2 (Final)
Study	Fuel	PMI	PMI (standardized)
EPAct	Fuel 15	1.25	1.24
	Fuel 16	1.28	1.27
	Fuel 20	0.87	0.87
	Fuel 21	1.30	1.30
	Fuel 22	0.85	0.86
	Fuel 23	1.27	1.27
	Fuel 24	1.16	1.17
	Fuel 25	1.83	1.82
	Fuel 26	1.98	1.97
	Fuel 27	1.20	1.20
	Fuel 28	1.27	1.27
	Fuel 30	1.59	1.58
	Fuel 31	1.61	1.61

E-94-2/3 Fuels		RW-107 (Published)	RW-107-2 (Final)	
Study	Fuel	PMI	FLRD	PMI (standardized)
E-94-2	A	1.42	771	1.42
	B	2.65	772	2.62
	C	1.40	1365*	1.42
	D	2.61	1382*	2.63
	E	1.28	775	1.32
	F	2.54	776	2.55
	G	1.26	1376*	1.30
	H	2.49	1368*	2.50
E-94-3	C-E10	1.28	1367	1.29
	D-E10	2.45	1383	2.44
	G-E10	1.17	1378	1.20
	H-E10	2.32	1372	2.33

* DHAs conducted at start of E-94-3 for the E0 base fuels before they were splash-blended with ethanol to create the E-10 fuels.

E-129 Fuels		RW-107 (Published)	RW-107-2 (Final)	
Study	Fuel	PMI	Source	PMI (standardized)
E-129	Fuel C	1.30	E-129 results (PMI).xlsx	1.28
	EtOH10	1.16	E-129 results (PMI).xlsx	1.15
	EtOH15	1.08	E-129 results (PMI).xlsx	1.08
	MTBE19	1.07	E-129 results (PMI).xlsx	1.06
	MTBE29	1.09	E-129 results (PMI).xlsx	1.09
	iBut16	1.04	E-129 results (PMI).xlsx	1.03
	iBut24	0.92	Final iBut24 Copy of ODDB-46661.xlsx	0.91

PMI Calculations using Enhanced DHAs

PMI-B

Enhanced DHAs	Enhanced DHAs Conducted	DHA Lab	BP Reported	VP Values Used in Replicating Study's PMI ‡	PMI Comparison: Δ = Published - Replicated
EPAct Study	Cannot be done because fuel samples are no longer available				
E-94-2					
E10 Fuels (A,B,E,F)	Jul-2019	SSI	YES	Aikawa Eq.	-0.02 to +0.00
E0 Fuels (C,D,G,H)	Jul-2019	SSI	YES	Aikawa Eq.	-0.01 to +0.01
E-94-3					
C/D/G/H – E10	Jul-2019	SSI	YES	Aikawa Eq.	±0.00
E-129	Mid-2018	SSI	YES	Aikawa Eq.	TBD

‡ Empirical vapor pressures are used for ethanol and other oxygenates (i-Butanol and MTBE).

For the E-94-2/3 fuels, the differences between published and replicated PMI-As are minor, stemming most likely from differences between the VPs we calculated from the Aikawa Eq. and the ones used by SSI in their PMI calculations.

E-94-2/3 Fuels		RW-107 (Published)	RW-107-2 (Final)	
Study	Fuel	PMI-A	Enhanced DHA Dated	PMI-A (Standardized)
E-94-2	A	1.43	20-Jul-19	1.43
	B	3.01	20-Jul-19	3.01
	C	1.32	20-Jul-19	1.34
	D	2.97	20-Jul-19	2.97
	E	1.25	20-Jul-19	1.25
	F	2.83	20-Jul-19	2.83
	G	1.23	20-Jul-19	1.23
	H	2.78	20-Jul-19	2.77
E-94-3	C-E10	1.30	25-Jul-19	1.32
	D-E10	2.75	20-Jul-19	2.75
	G-E10	1.15	20-Jul-19	1.15
	H-E10	2.46	20-Jul-19	2.45

E-129 Fuels		RW-107 (Unpublished)	RW-107-2 (Final)	
Study	Fuel	PMI-B	SSI ID	PMI-B (standardized)
E-129	Fuel C	1.22	11744700	1.24
	EtOH10	1.10	11745000	1.12
	EtOH15	1.04	11745300	1.05
	iBut16	1.02	11745600	1.04
	iBut24	0.94	11745900	0.95
	MTBE19	0.97	11746200	0.97
	MTBE29	0.87	11746500	0.86