Supporting Information

Criteria Air Pollutant and Greenhouse Gases Emissions from U.S. Refineries Allocated to Refinery Products

Pingping Sun,[a] Ben Young,[b] Amgad Elgowainy,[a] * Zifeng Lu,[a] Michael Wang,[a] Ben Morelli,[b] Troy Hawkins[a]

[a] Energy Systems Division, Argonne National Laboratory, 9700 S. Cass Avenue, Lemont, Illinois 60439, USA.
[b] Eastern Research Group, Inc. (ERG), 110 Hartwell Avenue #1, Lexington, Massachusetts 02421, USA.

* Email: aelgowainy@anl.gov

Contents

1. Refinery Fuels Combustion Emission Factor

1.1 Refinery Fuels Consumption

Table S1. Count of Facilities Reporting Combustion Emissions by Fuel Type.

Combustion Fuel	Facilities Reporting NEI		GHGRP	
Coal	3	(2%)	1	(1%)
Coke	74	(58%)	93	(72%)
Distillate	89	(70%)	50	(39%)
Liquefied petroleum gases (LPG)	10	(8%)	3	(2%)
Residual Oil	29	(23%)	9	(7%)
Natural Gas	95	(74%)	113	(88%)
Refinery Gas	98	(77%)	124	(96%)
Other	32	(25%)	51	(40%)
Any Combustion Type	123	(96%)	129	(100%)
Total Facility Count	128		129	

Table S2. Fuel Consumption at U.S. Refineries, 2014.

EIA Fuel Type	Fuel Consumption	Unit	Fuel Consumption (mmBTU)	Percent of Total Consumption
Catalyst petcoke[1]	15,402,363,953	kg	457,552,791	17%
Coal	14,514,956	kg	362,229	<0.1%
Distillate fuel oil	49,126	m^3	1,666,974	0.1%
Electricity, purchased	47,224,000,000	kwh	161,134,977	5.9%
Liquefied petroleum gases (LPG)	366,455	m^3	8,223,762	0.3%
Marketable petcoke	115,393,899	kg	3,427,967	0.1%
Natural gas, fuel	20,025,588,959	m^3	695,174,651	25%
Other products [2]	183,307	m^3	5,767,654	0.2%
Residual fuel oil	65,660	m^3	2,434,482	0.1%
Steam, purchased	59,196,023,960	kg	156,538,544	5.7%
Still gas [3]	36,552,941	m^3 fuel oil eq.	1,241,669,179	45%

[1] Petcoke is converted from volume to mass using the EIA conversion factor of 5 barrels per short tons.
[2] Other products includes pentanes plus, other hydrocarbons, oxygenates, hydrogen, unfinished oils, gasoline, special naphthas, jet fuel, lubricants, asphalt and road oil, and miscellaneous products.
[3] Still gas energy basis uses a LHV conversion of 128,950 btu/gal fuel oil eq. based on liquid still gas reported in GREET 2016. EIA reports HHV only for still gas as 142,857 btu/gal fuel oil eq.[16].

Table S3. Adjusted Fuel Consumption at Refineries for NEI Emissions Dataset by PADD, 2014.

	Adjusted Fuel Consumption (million MJ)				
EIA Fuel Type	**PADD 1**	**PADD 2**	**PADD 3**	**PADD 4**	**PADD 5**
Catalyst petcoke	45,766	95,610	253,348	16,533	68,690
Coal	382	--	--	--	--
Distillate fuel oil	--	188	989		562
Electricity, purchased	9,637	45,630	90,113	7,482	16,392
LPG	--	5,067	1,583	86	1,869
Marketable petcoke	--	--	--	2,787	787
Natural gas, fuel	40,736	116,039	428,212	15,937	127,554
Other products	42	285	1,887	--	3,744
Residual fuel oil	19	143	174	80	2,082
Steam, purchased	6,202	16,484	123,506	1,878	16,374
Still gas	86,461	278,643	631,561	49,551	254,008

Table S4. U.S. Refinery Fuels Combustions GHG Emissions in 2014 (MT).

Fuel	**PADD 1**	**PADD 2**	**PADD 3**	**PADD 4**	**PADD 5**	**U. S.**
			CO_2 (MT)			
Coal	53,960	-	-	-	-	53,960
Distillate	81,052	28,640	26,478	6,802	64,511	207,483
LPG	-	-	-	17	37,508	37,524
Residual Oil	391	4,298	-	11,578	159,432	175,698
Other	4,043	13,156	37,784	2,598	215,241	272,821
Coke	4,492,413	9,550,592	22,292,446	1,644,402	7,416,416	45,396,268
Combined gas	7,228,477	22,355,839	60,411,372	4,207,371	22,177,307	116,380,367
			CH_4 (MT)			
Coal	6.4	-	-	-	-	6.4
Distillate	3.3	1.2	1.1	0.3	2.6	8.4
LPG	-	-	-	-	1.7	1.7
Residual Oil	0.0	0.2	-	0.5	6.4	7.0
Other	0.1	0.7	29.6	0.0	9.6	40.0
Coke	167.1	292.9	679.1	57.7	213.3	1,410.1
Combined gas	374.8	1,244.5	3,598.0	247.6	992.7	6,457.5
N_2O (MT)						
Coal	0.93	-	-	-	-	0.93
Distillate	0.66	0.23	0.22	0.06	0.52	1.68
LPG	-	-	-	-	0.35	0.35
Residual Oil	0.00	0.03	-	0.09	1.28	1.41
Other	0.02	0.15	5.94	0.01	1.91	8.02
Coke	30.84	59.54	134.63	10.15	43.04	278.19
Combined gas	71.73	244.32	699.65	48.00	186.99	1,250.69

Table S5. U.S. Refinery Fuels Combustions CAP Emissions in 2014 (kg).

Fuel	PADD 1	PADD 2	PADD 3	PADD 4	PADD 5	U. S.
			VOC (kg)			
Coal	653	429	3,250	-	-	4,333
Coke	17,807	253,859	562,832	79,730	169,901	1,084,130
Distillate	27,763	33,402	111,309	10,625	8,806	191,905
LPG	-	1,867	757	-	1,573	4,197
Other	7,367	94,730	389,496	18,749	336,104	846,446
Residual Oil	423	10,683	148,372	491	13,267	173,236
Combined Gas	148,302	796,359	1,907,109	170,812	938,866	3,961,447
			CO (kg)			
Coal	46,784	5,776	5	-	-	52,564
Coke	139,583	1,566,166	3,256,214	147,773	1,059,406	6,169,142
Distillate	74,225	83,228	199,532	51,267	26,915	435,167
LPG	-	534	1,245	-	6,076	7,855
Other	68,006	1,134,391	2,653,719	791,358	993,059	5,640,534
Residual Oil	1,625	35,866	609,438	290	123,520	770,738
Combined Gas	2,489,789	9,098,178	10,678,673	1,802,065	5,014,344	29,083,049
			NO_X (kg)			
Coal	134,336	626	39	-	-	135,001
Coke	931,172	1,716,169	2,580,207	229,947	519,231	5,976,726
Distillate	86,202	342,879	498,337	146,771	130,316	1,204,505
LPG	-	263	1,481	-	28,235	29,980
Other	142,983	1,447,820	5,024,883	298,085	1,853,680	8,767,450
Residual Oil	1,240	57,977	934,448	694	242,806	1,237,165
Combined Gas	4,071,115	13,439,312	25,592,406	2,455,940	9,730,526	55,289,299
			SO_2 (kg)			
Coal	589,743	2,485	7	-	-	592,235
Coke	1,079,595	1,510,994	2,852,891	496,517	520,074	6,460,072
Distillate	2,044	9,571	40,625	70,457	32,744	155,440
LPG	-	8	360	-	171	538
Other	20,785	93,291	689,473	187,970	72,830	1,064,349
Residual Oil	14	222	158,921	59	68,841	228,057
Combined Gas	406,502	2,528,260	5,146,416	587,247	3,132,889	11,801,314
			PM_{10} (kg)			
Coal	10,659	231	1	-	-	10,892
Coke	515,781	1,810,673	2,540,200	603,018	279,329	5,749,001
Distillate	7,767	39,783	37,542	26,091	8,338	119,521
LPG	-	9	65	-	1,350	1,424
Other	18,725	152,373	915,391	35,967	178,171	1,300,628
Residual Oil	56	913	137,649	114	14,110	152,842
Combined Gas	769,728	2,147,602	3,253,191	271,671	1,364,501	7,806,692

Fuel	PADD 1	PADD 2	PADD 3	PADD 4	PADD 5	U. S.
			$PM_{2.5}$ (kg)			
Coal	10,278	93	0	489,371	-	10,372
Coke	477,178	1,638,704	2,295,442	10,560	228,336	5,129,030
Distillate	7,349	38,158	37,517	-	7,041	100,624
LPG	-	9	65	35,961	1,348	1,422
Other	15,531	152,359	906,425	114	176,466	1,286,742
Residual Oil	56	913	137,648	244,592	13,702	152,433
Combined Gas	652,368	2,000,415	3,189,008	69	1,336,410	7,422,793

1.2 Refinery Fuels Combustion Emission Factors

Table S6. Emission Factors of Distillate Oil Combusted in U.S. Refineries in Various PADDs in 2014.

Pollutant	Distillate Emission Factor (g/MJ for CO_2 and mg/MJ for Other Pollutants)					
	PADD 1	PADD 2	PADD 3	PADD 4	PADD 5	U.S.
CO_2	–	152.5	27.5	–	111.1	119.7
CH_4	–	6.2	1.1	–	4.4	4.8
N_2O	–	1.2	0.2	–	0.9	1.0
VOC	–	178.1	112.5	–	15.7	110.4
CO	–	443.7	201.7	–	47.9	250.3
NO_x	–	1,828.1	503.7	–	232.0	692.8
SO_2	–	51.0	41.1	–	58.3	89.4
PM_{10}	–	212.1	37.9	–	14.8	68.7
$PM_{2.5}$	–	203.4	37.9	–	12.5	57.9

Table S7. Emission Factors of Other Fuel Combusted in U.S. Refineries in Various PADDs in 2014.

Pollutant	Other Fuel Emission Factor (g/MJ for CO_2 and mg/MJ for Other Pollutants)					
	PADD 1	**PADD 2**	**PADD 3**	**PADD 4**	**PADD 5**	**U.S.**
CO_2	95.8	46.2	20.5	–	55.6	45.2
CH_4	1.9	2.6	16.1	–	2.5	6.6
N_2O	0.4	0.5	3.2	–	0.5	1.3
VOC	10.0	37.5	78.6	–	3.5	29.1
CO	38.5	126.0	322.9	–	33.0	129.4
NO_x	29.4	203.7	495.1	–	64.9	207.6
SO_2	0.3	0.8	84.2	–	18.4	38.3
PM_{10}	1.3	3.2	72.9	–	3.8	25.7
$PM_{2.5}$	1.3	3.2	72.9	–	3.7	25.6

Table S8. Emission Factors of Residual Oil Combusted in U.S. Refineries in Various PADDs in 2014.

Pollutant	Residual Oil Emission Factor (g/MJ for CO_2 and mg/MJ for Other Pollutants)					
	PADD 1	**PADD 2**	**PADD 3**	**PADD 4**	**PADD 5**	**U.S.**
CO_2	20.9	30.0	–	143.2	74.1	68.5
CH_4	1.1	1.2	–	5.7	3.0	2.7
N_2O	0.1	0.2	–	1.2	0.6	0.5
VOC	0.3	2.5	78.0	0.1	11.6	15.2
CO	8.1	22.6	351.6	2.2	62.9	78.3
NO_x	88.6	248.2	938.2	24.0	427.0	436.9
SO_2	1,183.7	457.5	56.5	3.0	429.6	397.1
PM_{10}	8,990.1	32.9	100.8	4.7	78.1	141.3
$PM_{2.5}$	6,103.3	28.8	100.1	0.9	68.5	111.3

Table S9. Emission Factors of LPG Fuel Combusted in U.S. Refineries in Various PADDs in 2014.

Pollutant	LPG Emission Factor (g/MJ for CO_2 and mg/MJ for Other Pollutants)					
	PADD 1	PADD 2	PADD 3	PADD 4	PADD 5	U.S.
CO_2	–	–	–	0.2	19.4	4.3
CH_4	–	–	–	0.2	19.4	4.3
N_2O	–	–	–	–	0.2	0.0
VOC	–	0.4	0.5	–	0.8	0.5
CO	–	0.1	0.8	–	3.3	0.9
NO_x	–	0.1	0.9	–	15.1	3.5
SO_2	–	0.001	0.2	–	0.1	0.1
PM_{10}	–	0.002	0.0	–	0.7	0.2
$PM_{2.5}$	–	0.002	0.0	–	0.7	0.2

Emissions from coal combustion are reported in PADD 1, PADD 2, and PADD 3. However, coal consumption data is only reported in PADD 1. Thus, the coal combustion emission factor can only be derived based on a single facility in PADD 1. Using a single facility to generate emission factors for coal combustion is likely not representative. Emission factors from less common fuel types, such as LPG, are also more susceptible to reporting errors such as fuel mis-categorization at the facility. However, because fuel consumption data is only available at the PADD level, it is not possible to compare combustion emission factors across refineries. As a result, emission factors for both coal and LPG are less reliable than those of catalyst coke and combined gas (natural gas and refinery still gas). Note that PADD 4 and PADD 5 reported marketable pet coke consumption; however, the NEI database did not report corresponding combustion emissions. Thus, the emission factors for marketable pet coke cannot be derived.

Table S10. Comparison of Catalyst Coke Emission Factors of the Present Study with Those of AP-42.

		AP42-uncontrolled			AP42-controlled		
Pollutant (kg/m^3)	**Present Study**	**Average**	**Low**	**High**	**Average**	**Low**	**High**
VOC	0.004	NA	NA	NA	NA	NA	NA
CO	0.023	39.2	NA	NA	Neg	NA	NA
NOx	0.022	0.204	0.107	0.416	0.204	0.107	0.416
SO_2	0.024	1.413	0.286	1.505	1.413	0.286	1.505
PM_{10}	0.021	0.695	0.267	0.976	0.128	0.02	0.428
$PM_{2.5}$	0.019	NA	NA	NA	NA	NA	NA

2. U.S. Refinery Emissions per Crude Throughput

Table S11. U.S. PADD Refinery Emissions per Crude Throughput for 2014.

Pollutant	PADD 1	PADD 2	PADD 3	PADD 4	PADD 5	U.S.
CO_2 (g/m^3 crude)	204,636	179,037	189,913	216,239	256,805	200,401
CH_4 (g/m^3 crude)	15.79	30.74	30.94	66.12	30.19	31.0
N_2O (g/m^3 crude)	1.71	1.53	1.80	1.83	1.58	1.70
GHG (g $CO_{2,eq}$ /m^3 crude)	205,563	180,363	191,317	218,706	258,131	201,781
CO_2 (g/MJcrude[1])	5.66	4.95	5.25	5.98	7.11	5.54
CH_4 (mg/MJ crude)	0.44	0.85	0.86	1.83	0.84	0.86
N_2O (mg/MJ crude)	0.05	0.04	0.05	0.05	0.04	0.05
GHG (g $CO_{2,eq}$/MJ crude)	5.69	4.99	5.29	6.05	7.14	5.58
VOC (mg/MJ crude)	1.03	1.83	1.67	3.51	2.02	1.78
CO (mg/MJ crude)	1.42	1.93	1.26	2.86	1.63	1.53
NO_x (mg/MJ crude)	2.42	2.49	2.06	3.05	2.77	2.32
SO_2 (mg/MJ crude)	1.00	1.13	0.72	2.17	1.11	0.94
PM_{10} (mg/MJ crude)	0.70	0.77	0.53	1.25	0.62	0.63

Pollutant	PADD 1	PADD 2	PADD 3	PADD 4	PADD 5	U.S.
$PM_{2.5}$ (mg/MJ crude)	0.61	0.65	0.47	0.73	0.56	0.55

1. The crude volume was converted to energy using 36,141 MJ/m^3 (129,670 btu/gal) lower heating value, from GREET 2016 [18].

Table S12. U.S. PADD Refinery Shares in National Capacity for 2014.

Dataset	PADD 1	PADD 2	PADD 3	PADD 4	PADD 5	U.S.
GHGRP	6.9%	22.0%	51.1%	3.6%	16.3%	100%
NEI	6.9%	21.8%	52.1%	3.5%	15.7%	100%

Note that GHGRP and NEI are two independent data systems, and thus have slightly different facility coverage.

The U.S. averaged CAP emissions per national crude input can be itemized as the PADD contributions weighted by PADD refinery capacity (see Table S12). Figure S1 shows the U.S. weighted average CAP emissions per crude input.

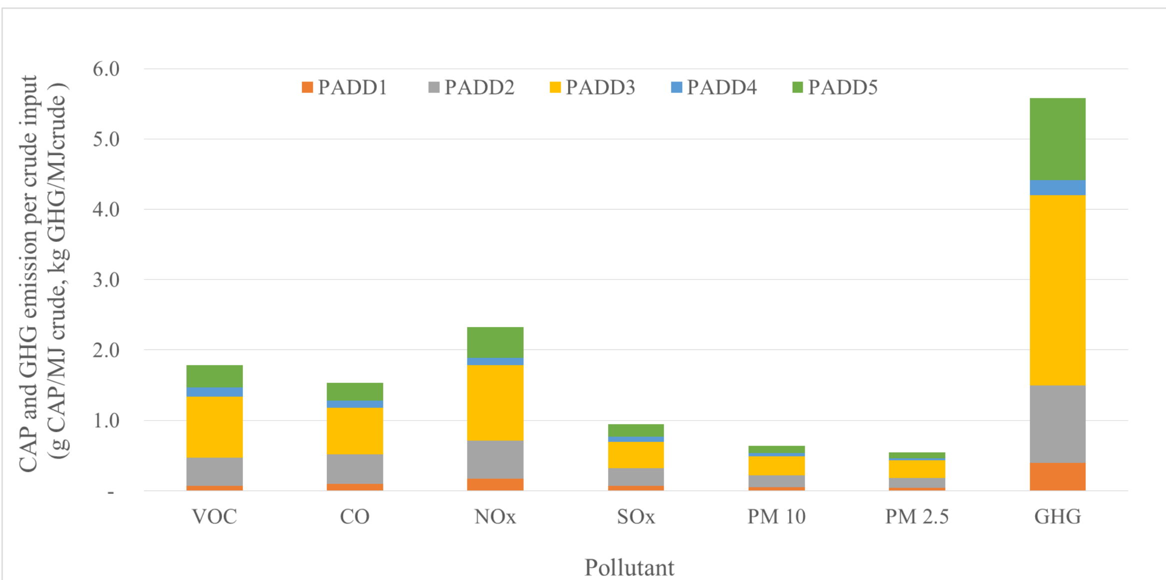


Figure S1. U.S. Refinery CAP and GHG Emissions per MJ Crude Processed in 2014, with Capacity Weighted Contribution from Each PADD.

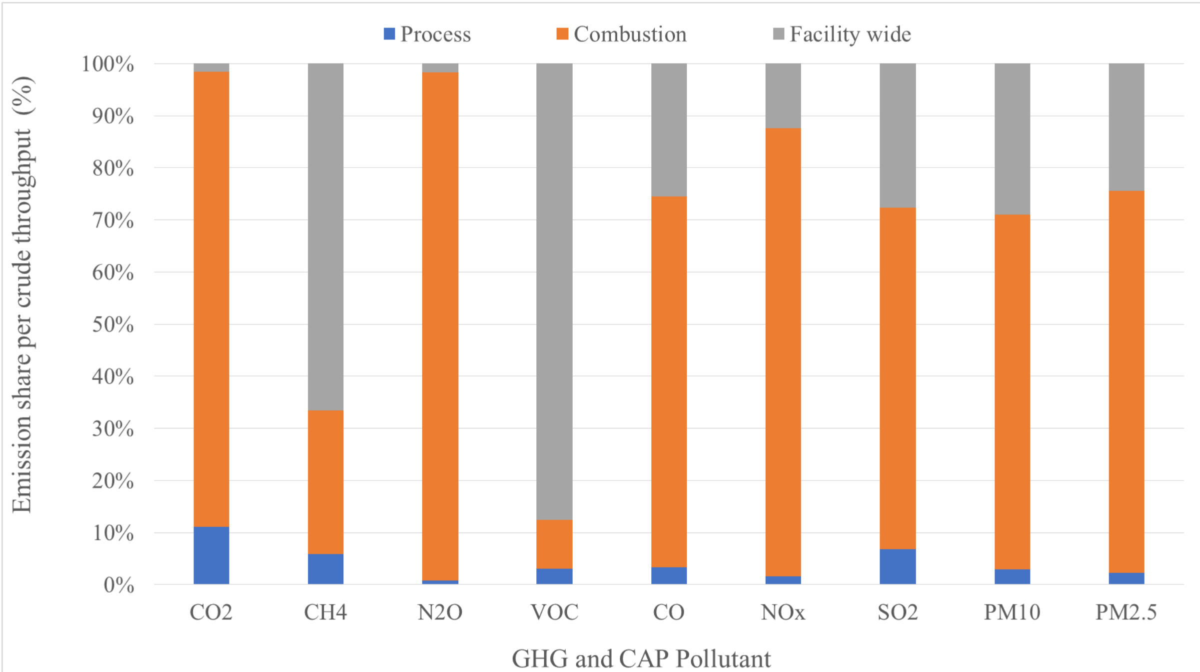
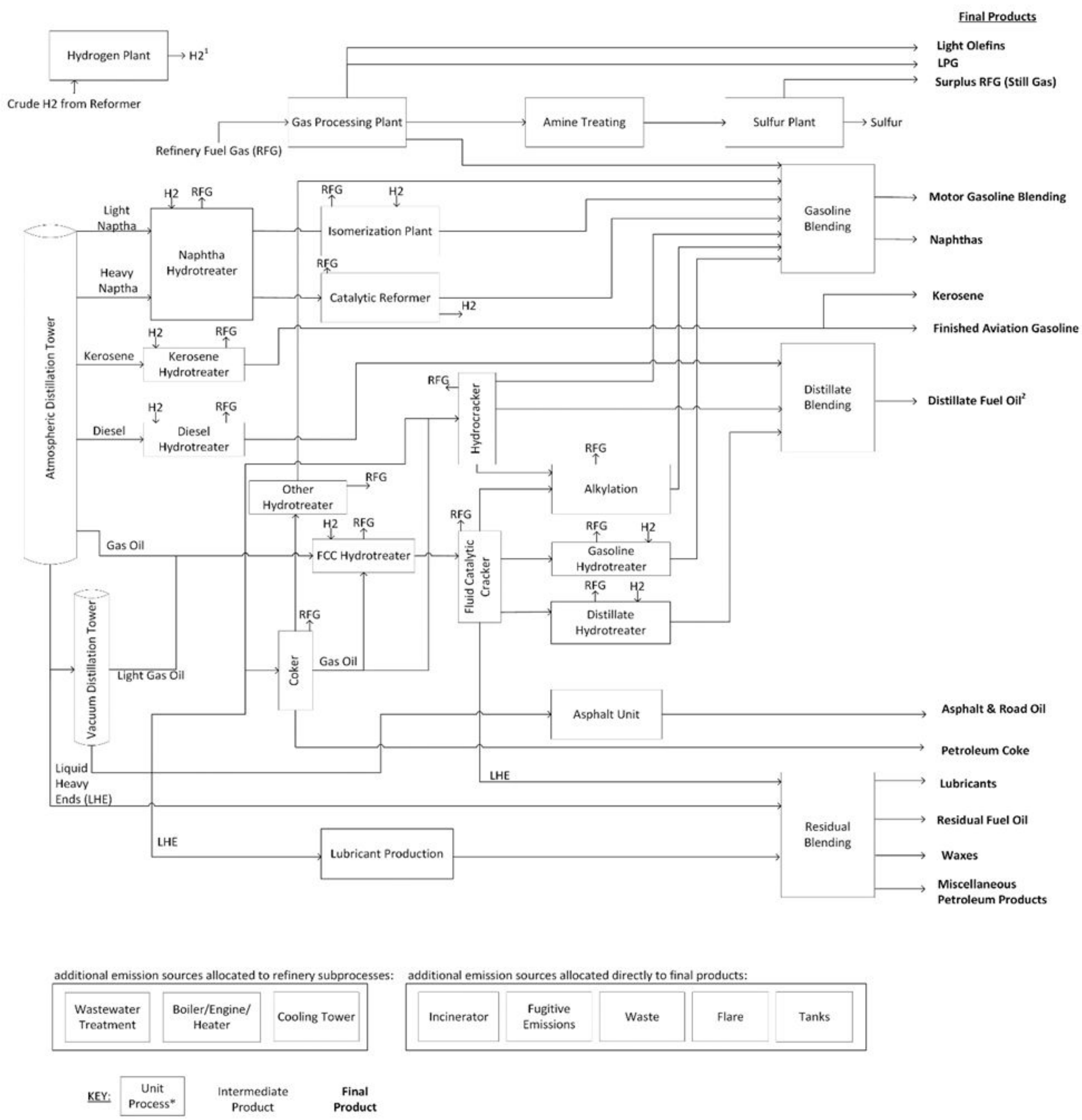


Figure S2. Shares of Process Emissions, Combustion Emissions, and Facility-wide Emissions for U.S. Refinery Total Emissions per Crude Throughput.

3. U.S. Refinery Process Unit Capacity and Energy Use

A typical refinery process diagram was created using previous research effort as a starting point.[8,9] The original process diagram was modified to reflect unit process designations to which emission factors are associated, and unit throughput capacity as reported in the EIA refinery capacity dataset.



[1] It is assumed that no surplus H_2 is produced for sale. All H_2 is used internally, primarily for desulfurization.
[2] Distillate fuel oil includes both diesel and the lighter fuel oils.
* Residual hydrocracker, thermal cracking (other), and residual hydrotreating are not included in the figure as they are present at very few U.S. refining facilities.
LHE: Liquid heavy ends
RFG: Refinery fuel gas or refinery still gas

Figure S3. Process Diagram of a General U.S. Refinery.

Table S13. PADD-Level Refinery Unit Throughput (in Millions), 2014.

Refinery Unit	Units	Dataset[2]	PADD 1	PADD 2	PADD 3	PADD 4	PADD 5	National
Alkylation	m^3 alkylate product	P	4.0	14	32	2.3	12	64
Asphalt Unit	m^3 asphalt and road oil	P	4.1	13	11	3.8	2.7	34
Atmospheric Distillation Tower	m^3	C	64	200	490	33	150	940
Catalytic Reformer	m^3	C	12	45	91	6.2	27	180
Coker	m^3	C	3.8	28	79	4.3	28	140
Diesel Hydrotreater	m^3	C	14	53	110	7.7	25	210
Distillate Hydrotreater	m^3	C	8.7	3.9	6.3	2.6	6.1	28
Fluid Catalytic Cracker	m^3	C	24	66	160	10	44	300
Gas/Oil Hydrotreater	m^3	C	0.31	33	73	4.9	36	150
Gasoline Hydrotreater	m^3	C	7.9	21	85	2.2	16	130
Hydrocracker	m^3	C	2.1	17	60	1.5	28	110
Hydrogen Plant	m^3 hydrogen gas at stp	P	600	4,800	9,400	1,600	11,000	28,000
Isomerization Plant	m^3 liquid isomers[1]	P	1.3	8.1	17	0.82	9.8	37
Kerosene Hydrotreater	m^3	C	2.5	15	45	2.1	11	76
Lubricant Production	m^3 lubricants	P	1.0	0.48	8.3	-	1.9	12
Naphtha Hydrotreater	m^3	C	17	60	110	7.4	31	230
Other Hydrotreater	m^3	C	-	2.2	11	0.75	3.0	17
Residual Hydrotreater	m^3	C	-	-	13	-	-	13
Sulfur Plant	kg sulfur	P	310	2,400	7,100	280	1,700	12,000
Thermal Cracking	m^3	C	-	-	0.54	-	0.72	1.3
Vacuum Distillation	m^3	C	28	87	240	12	80	450

[1] Isomers include isobutane, isopentane, isohexane, and isooctane.
[2] Unit throughputs are calculated from EIA datasets of charge capacity (C) or production capacity (P). Charge capacity represents the input capacity in liquid volume to the process unit. Production capacity represents product output from a process unit.

Table S14. Refinery Unit Energy Intensity Estimates per Barrel of Utilized Charge Capacity.

Refinery Unit	Throughput (T_U) (million bbl)	Energy Use (MJ / bbl)*			Energy Use (billion MJ)		
		Heat ($I_{U,h}$)	Steam ($I_{U,b}$)	Electricity ($I_{U,e}$)	Heater	Boiler[1]	Electricity
Alkylation	401	0	227	0	–	113.5	–
Asphalt Unit [2]	215	0	0	0	–	–	–
Atmospheric Tower	5,932	96	8	3	571.2	61.9	19.2
Catalytic Reformer	1,141	293	38	11	334.4	54.1	12.3
Coker. Delayed	849	154	4	5	130.7	4.4	4.0
Coker, Fluid[2]	48	0	0	0	–	–	–
Diesel Hydrotreater	1,339	126	10	14	168.9	17.0	19.3
Distillate Hydrotreater	173	126	10	14	21.9	2.2	2.5
Fluid Catalytic Cracker [3]	1,902	0	0	0	–	–	–
Gasoil Hydrotreater	926	126	10	14	116.7	11.7	13.3
Gasoline Hydrotreater	832	126	10	14	104.9	10.5	12.0
Hydrocracker (Distillate)	212	157	2	20	33.3	0.5	4.2
Hydrocracker (Gas Oil)	433	139	95	47	60.2	51.4	20.4
Hydrocracker (Residual)	35	157	2	20	5.5	0.1	0.7
Isomerization Plant	235	271	0	4	63.6	–	0.8
Kerosene Hydrotreater	480	126	10	14	60.5	6.1	6.9
Lubricant Production	73	695	695	0	51.0	63.8	(0.0)
Naphtha Hydrotreater	1,438	126	10	14	181.3	18.2	20.7
Other Hydrotreater	108	126	10	14	13.7	1.4	1.6
Residual Hydrotreater	79	126	10	14	10.0	1.0	1.1
Thermal Cracking	8	159	4	5	1.3	0.0	0.0
Vacuum Distillation	2,809	57	7	1	160.1	24.6	2.8
Hydrogen Plant[4] (mil kg)	2,479	154	-34	1	382.5	(105.9)	2.4
Sulfur Plant[4] (mil short tons)	13	0	-1538	1010	–	-24.9	13.1
Total					2,473.1	312.8	157.5

[1] Energy use at boiler accounts for an 80% boiler efficiency rating

[2] PRELIM shows zero heat intensity and steam intensity for asphalt unit.

[3] Fluid coking and the FCC are treated as self-sustained; no additional facility heat is supplied outside of catalyst coke combustion

[4] Hydrogen and sulfur energy use reported in MJ per kg and short ton, respectively

Table S15. Refinery Process Unit Shares of Heaters and Boilers Energy Uses, Aggregated Nationally.

Refinery Unit	Heater	Boiler	Combined
Alkylation	-	26%	4.0%
Asphalt Unit	-	-	-
Atmospheric Distillation Tower	23%	14%	23%
Catalytic Reformer	14%	12%	14%
Coker, Delayed	5.3%	1.0%	4.8%
Coker, Fluid	-	-	-
Diesel Hydrotreater	6.8%	3.8%	6.6%
Distillate Hydrotreater	0.9%	0.5%	0.9%
Fluid Catalytic Cracker	-	-	-
Gas/Oil Hydrotreater	4.7%	2.6%	4.6%
Gasoline Hydrotreater	4.2%	2.4%	4.1%
Hydrocracker	4.0%	12%	5.4%
Isomerization Plant	2.6%	-	2.3%
Kerosene Hydrotreater	2.4%	1.4%	2.4%
Lubricant Production	2.1%	14%	4.1%
Naphtha Hydrotreater	7.3%	4.1%	7.1%
Other Hydrotreater	0.6%	0.3%	0.5%
Residual Hydrotreater	0.4%	0.2%	0.4%
Thermal Cracking	< 0.1%	< 0.1%	< 0.1%
Vacuum Distillation	6.5%	5.8%	6.7%
Hydrogen Plant	15%	-	9.8%
Sulfur Plant	-	-	-

Table S16. Calculated PADD Refineries Energy Uses (Heater, Boiler and Electricity) by Refinery Unit, in Billion MJ.

Refinery Unit	PADD 1	PADD 2	PADD 3	PADD 4	PADD 5	National
Alkylation	7.2	24.2	57.4	4.0	20.7	113.5
Asphalt Unit[1]	–	–	–	–	–	–
Atmospheric Tower	44.6	141.8	338.0	22.9	105.1	652.4
Catalytic Reformer	27.0	99.8	201.0	13.7	59.3	400.9
Coker, Delayed	1.4	28.7	79.0	4.0	26.0	139.1
Coker, Fluid[2]	–	–	–	–	–	–
Diesel Hydrotreater	13.1	51.3	109.4	7.4	24.0	205.1
Distillate Hydrotreater	8.3	3.8	6.1	2.5	5.9	26.6
Fluid Catalytic Cracker[2]	–	–	–	–	–	–
Gas/Oil Hydrotreater	0.3	31.7	70.7	4.7	34.5	141.8
Gasoline Hydrotreater	7.6	20.3	82.0	2.1	15.5	127.4
Hydrocracker	3.2	26.6	98.0	2.0	46.4	176.3
Hydrogen Plant	6.1	48.7	94.9	16.1	113.3	279.0
Isomerization Plant	2.2	14.1	29.8	1.4	17.0	64.4
Kerosene Hydrotreater	2.4	14.8	43.6	2.0	10.6	73.5
Lubricant Production	10.2	4.8	81.4	–	18.5	114.8
Naphtha Hydrotreater	16.1	58.0	108.6	7.2	30.3	220.2
Other Hydrotreater	–	2.1	10.9	0.7	2.9	16.6
Residual Hydrotreater	–	–	12.1	–	–	12.1
Sulfur Plant	(0.3)	(2.4)	(7.1)	(0.3)	(1.7)	(11.8)

Refinery Unit	PADD 1	PADD 2	PADD 3	PADD 4	PADD 5	National
Thermal Cracking	–	–	0.6	–	0.8	1.3
Vacuum Distillation	12.1	37.2	102.0	5.0	33.9	190.2
Total	161.4	605.5	1,518.2	95.6	562.9	2,943

[1] The asphalt unit energy use is neglected because PRELIM shows zero heat intensity and steam intensity.
[2] Fluid coking and the FCC are treated as self-sustained; no additional facility heat is supplied outside of catalyst coke combustion.

Validating Energy Consumption at Refineries

The total energy use for a specific refinery unit is calculated from unit throughput and energy intensity (heater energy use, boiler energy use, and electricity use). This approach is validated by comparing results with national refinery energy consumption data. Although electricity use is not used to allocate emissions to process units, it is included here to better reflect the granularity of data provided in the EIA fuel consumption dataset:

$$\mathrm{E_U} = \left(\mathrm{I_{U,h}} + \mathrm{I_{U,b}} + \mathrm{I_{U,e}}\right) * \mathrm{T_U}, \quad (1)$$

where E_U represents the total energy used for refinery unit *U*; *I* represents the average energy intensity required from heaters, boilers, and other energy sources for each unit *U* (in MJ/bbl. unit throughput); and *T* represents the estimated unit throughput for each unit *U* at each facility.

Total energy use at refineries, estimated using this method, indicates that approximately 9% of energy embodied in incoming crude is consumed during the refining process (Table S2). Total energy use estimated by each process is compared with the fuel consumption reported by EIA (in Table S2), and shows approximately 2% difference at the national level, validating this estimation approach.

Table S17. Comparison of Total Energy Consumption by PADD (billion MJ).

Refinery Input/Energy Use	PADD 1	PADD 2	PADD 3	PADD 4	PADD 5	National
Sum of Process Unit Energy Use	161	605	1,518	96	563	2,943
Fuel Inputs by PADD (EIA[10])	189	559	1,533	95	509	2,885
Crude Input (EIA[20])	2,330	7,406	17,658	1,197	5,486	34,085

4. Refinery Process Unit Emissions

Table S18. National Refinery Process Unit GHG and CAP emissions (MT/year) from 2014, After Allocations of Combustion Emissions and FWE-1.

Process	CO_2	CH_4	N_2O	VOC	CO	NO_x	SO_2	PM_{10}	$PM_{2.5}$
Alkylation	4,807,119	268	52	608	1,913	4,221	709	900	737
Amine Treating	–	–	–	27	76	47	40	2.5	2.5
Asphalt Unit	111,233	277	–	0.2	–	–	–	–	–

Process	CO_2	CH_4	N_2O	VOC	CO	NO_x	SO_2	PM_{10}	$PM_{2.5}$
Atmospheric Distillation Tower	27,954,360	1,539	297	2,961	7,964	15,035	3,132	3,036	2,634
Catalytic Reformer	16,601,577	1,068	181	1,792	5,058	9,539	1,881	1,881	1,635
Coker	7,074,309	1,611	74	1,152	1,800	3,319	1,101	869	654
Diesel Hydrotreater	7,795,436	446	87	812	2,341	4,186	876	826	694
Distillate Hydrotreater	1,073,568	57	11	157	528	532	55	181	167
Fluid Catalytic Cracker	45,396,268	1,410	278	1,294	7,924	8,204	7,598	6,231	5,525
Gas Processing Plant	–	–	–	–	–	–	–	–	–
Gas/Oil Hydrotreater	5,145,969	278	54	596	1,163	2,458	517	586	528
Gasoline Blending	–	–	–	47	–	–	–	–	–
Gasoline Hydrotreater	5,285,833	301	58	552	1,291	2,709	636	579	522
Hydrocracker	5,752,065	337	66	620	1,340	3,319	669	554	473
Hydrogen Plant	26,893,022	541	105	1,231	2,736	6,276	1,468	1,281	1,122
Isomerization Plant	2,524,132	136	26	236	628	1,279	223	233	217
Kerosene Hydrotreater	3,061,967	166	32	243	555	1,384	314	286	264
Lubricant Production	4,025,718	205	38	614	866	1,610	785	287	270
Naphtha Hydrotreater	8,580,882	478	93	915	2,414	4,714	892	926	802
Other Hydrotreater	662,398	37	7.1	65	182	360	79	58	54
Residual Hydrotreater	438,356	31	6.2	24	40	144	11	38	29
Sulfur Plant	2,470,964	14	0.8	265	1,037	386	1,796	168	159
Thermal Cracking	50,840	2.5	0.5	12	26	67	47	81	54
Vacuum Distillation	7,944,110	441	86	1,036	1,970	4,325	969	867	751
Total	183,650,126	9,643	1,553	15,257	41,851	74,112	23,799	19,869	17,295

Table S19. U.S. Refineries National Aggregated GHG and CAP Unit Emissions Intensity (g/M^3), After Allocations of Combustion Emissions, Facility-wide Emissions FWE-1.

Process	Unit	VOC	CO	NO_x	SO_2	PM_{10}	$PM_{2.5}$	CO_2	CH_4	N_2O
Alkylation	g/m^3	9.5	30.0	66.2	11.1	14.1	11.6	77,792	4.3	0.8
Asphalt Unit	g/m^3	0.0	0.0	0.0	0.0	0.0	0.0	3,278	8.2	0.0
Atmospheric Distillation Tower	g/m^3	3.2	8.5	16.0	3.3	3.2	2.8	30,049	1.7	0.3

Process	Unit	VOC	CO	NO_x	SO_2	PM_{10}	$PM_{2.5}$	CO_2	CH_4	N_2O
Catalytic Reformer	g/m^3	9.9	27.9	52.7	10.4	10.4	9.0	92,647	6.0	1.0
Coker (Delayed)	g/m^3	8.1	12.6	23.3	7.7	6.1	4.6	50,133	11.4	0.5
Diesel Hydrotreater	g/m^3	3.8	11.0	19.7	4.1	3.9	3.3	37,233	2.1	0.4
Distillate Hydrotreater	g/m^3	5.7	19.1	19.3	2.0	6.6	6.1	38,937	2.1	0.4
Fluid Catalytic Cracker	g/m^3	4.3	26.2	27.1	25.1	20.6	18.3	153,135	4.8	0.9
Gas/Oil Hydrotreater	g/m^3	4.0	7.9	16.7	3.5	4.0	3.6	34,960	1.9	0.4
Gasoline Hydrotreater	g/m^3	4.2	9.8	20.5	4.8	4.4	3.9	41,178	2.3	0.5
Hydrocracker	g/m^3	5.9	12.7	31.4	6.3	5.2	4.5	55,515	3.3	0.6
Hydrogen Plant	g/m^3	0.0	0.1	0.2	0.1	0.0	0.0	977	0.0	0.0
Isomerization Plant	g/m^3	6.3	16.8	34.3	6.0	6.2	5.8	67,868	3.7	0.7
Kerosene Hydrotreater	g/m^3	3.2	7.3	18.1	4.1	3.7	3.5	40,132	2.2	0.4
Lubricant Production	g/m^3	62.1	87.5	162.8	79.4	29.1	27.3	398,315	20.3	3.8
Naphtha Hydrotreater	g/m^3	4.0	10.6	20.6	3.9	4.1	3.5	37,927	2.1	0.4
Other Hydrotreater	g/m^3	3.8	10.7	21.2	4.7	3.4	3.1	38,899	2.2	0.4
Residual Hydrotreater	g/m^3	1.9	3.1	11.4	0.9	3.0	2.3	34,755	2.5	0.5
Sulfur Plant	g/kg	0.0	0.1	0.0	0.2	0.0	0.0	212	0.0	0.0
Thermal Cracking	g/m^3	9.2	20.5	52.8	37.3	64.0	42.4	40,185	2.0	0.4
Vacuum Distillation	g/m^3	2.3	4.4	9.7	2.2	2.0	1.7	18,009	1.0	0.2

Table S20. National Refinery Process Unit GHG and CAP emissions (MT/year), After Appropriate Allocations of Combustion Emissions and FWE-1, and After Refinery Still Gas Burdens Allocation upon Iterations.

Process after Still Gas Allocation	CO_2	CH_4	N_2O	VOC	CO	NO_x	SO_2	PM_{10}	$PM_{2.5}$
Alkylation	4,879,541	271	53	615	1,934	4,248	729	907	743
Amine Treating	–	–	–	22	62	38	32	2	2
Asphalt Unit	111,233	277	–	0	–	–	–	–	–
Atmospheric Distillation Tower	28,150,985	1,548	298	2,979	8,026	15,075	3,220	3,055	2,651
Catalytic Reformer	16,552,596	1,062	180	1,785	5,043	9,463	1,916	1,873	1,629
Coker	7,025,828	1,584	74	1,140	1,789	3,288	1,104	861	649
Diesel Hydrotreater	7,911,172	452	88	824	2,376	4,229	908	838	705
Distillate Hydrotreater	1,088,354	58	11	158	533	537	59	182	168
Fluid Catalytic Cracker	45,138,823	1,402	277	1,286	7,879	8,158	7,556	6,196	5,494
Gas Processing Plant	–	–	–	–	–	–	–	–	–
Gas/Oil Hydrotreater	5,214,742	281	54	603	1,183	2,483	539	593	534
Gasoline Blending	–	–	–	47	–	–	–	–	–

Process after Still Gas Allocation	CO_2	CH_4	N_2O	VOC	CO	NO_x	SO_2	PM_{10}	$PM_{2.5}$
Gasoline Hydrotreater	5,285,448	301	58	552	1,294	2,698	646	578	521
Hydrocracker	5,834,737	341	66	628	1,363	3,346	692	562	480
Hydrogen Plant	26,932,750	547	105	1,242	2,770	6,310	1,516	1,292	1,131
Isomerization Plant	2,559,561	138	26	239	638	1,292	234	236	220
Kerosene Hydrotreater	3,103,696	168	32	247	567	1,400	326	290	268
Lubricant Production	4,101,338	209	39	620	886	1,636	802	294	276
Naphtha Hydrotreater	8,586,894	478	92	915	2,418	4,696	914	926	802
Other Hydrotreater	668,015	37	7	65	184	362	81	59	54
Residual Hydrotreater	445,631	32	6	24	41	146	13	38	30
Sulfur Plant	2,020,409	12	1	217	851	316	1,476	137	130
Thermal Cracking	50,679	3	0	12	26	66	47	80	53
Vacuum Distillation	7,987,693	443	86	1,038	1,987	4,328	991	871	755
Total	183,649,628	9,643	1,553	15,257	41,851	74,112	23,799	19,869	17,295

5. U.S. Refinery Final Products

Products reported by EIA are matched to product categories in PRELIM V1.1. Some important variations, shown in Table S21, are discussed here.

- EIA reports gasoline products as either "finished motor gasoline" or "motor gasoline blending components," based on whether or not the blending takes place within the refinery gate. In the present study, the two categories are grouped as motor gasoline blending components or blendstock (BOB), because they are produced from the same pathways. The volume of ethanol included in finished motor gasoline, estimated at 65 vol% for the "Greater than Ed55" pool and 10 vol% for all other finished motor gasoline pools, is excluded from the grouped gasoline BOB pool.
- EIA reports liquefied refinery gas, including both C2-C4 paraffins and C2-C4 olefins, while PRELIM V1.1 categorizes propane and butane as LPG and light olefins (ethylene and propylene) as petrochemical (PC) feedstock. In contrast, in the EIA report, PC feedstock refers to naphtha with a boiling point less than 401°F. In the present study, to avoid the potential confusion of using the term "PC feedstock," the term "light olefins" was used to refer to ethylene and propylene, and LPG includes propane and butane. EIA reports a negative production amount of isobutane, isobutene, and isobutylene, implying they are input (e.g., purchased to feed the alkylation unit), and thus not accounted for as refinery final product. In PRELIM, refinery still gas, LPG, and light olefins are produced at the top of many refinery units and are then sent to a gas plant, amine plant, and sulfur plant to remove sulfur and other impurities.
- In the EIA report, the petrochemical feedstock refers to "naphtha for petrochemical feedstock use" and "other oils for petrochemical feedstock use." This is different from the

petrochemical feedstock term used in PRELIM, which refers to ethylene and propylene. The definition of PC feedstock might be related to whether steam cracking, which cracks refinery naphtha to ethylene and propylene, is within or beyond the refinery boundary. If it is within, ethylene and propylene will be regarded as PC feedstock; if it is beyond the boundary, naphtha will be regarded as the PC feedstock.

Thus, the present study uses the term "light olefins" to present ethylene and propylene, and the generic stream "naphtha" to include the EIA products of both "naphtha for petrochemical feedstock use" and "other oils for petrochemical feedstock use." The EIA product "special naphtha" is also grouped into the current study's naphtha product. PRELIM does not specify the production of naphtha, but the naphtha range products are included in the Jet-A/AVTUR category.

Table S21. Correspondence Between Refinery Products Across EIA and PRELIM.

Product Category (the present study)	PRELIM Product	EIA Product
Asphalt	Asphalt	Asphalt and Road Oil
Diesel/Distillate	ULSD[1]	Distillate Fuel Oil, 0 to 15 ppm Sulfur
Diesel/Distillate	ULSD[1]	Distillate Fuel Oil, Greater than 15 to 500 ppm Sulfur
Diesel/Distillate	ULSD	Distillate Fuel Oil, Greater than 500 ppm Sulfur
Diesel/Distillate	Liquid Heavy Ends	-
Gasoline Blending Components (BOB)[2]	Blended Gasoline	Motor Gasoline, Finished, Conventional, Ed55 and Lower
Gasoline Blending Components (BOB)[2]	Blended Gasoline	Motor Gasoline, Finished, Conventional, Greater Than Ed55
Motor Gasoline Blending Components (BOB)[2]	Blended Gasoline	Other Conventional Motor Gasoline
Motor Gasoline Blending Components (BOB)[2]	Blended Gasoline	Reformulated Motor Gasoline with Fuel Alcohol
Motor Gasoline Blending Components (BOB)[2]	Blended Gasoline	Motor Gasoline Blending Components
Aviation Gasoline	Jet-A/AVTUR[3]	Aviation Gasoline
Jet/Kerosene	Jet-A/AVTUR[3]	Commercial Kerosene-Type Jet Fuel
Jet/Kerosene	Jet-A/AVTUR[3]	Kerosene
Jet/Kerosene	Jet-A/AVTUR[3]	Military Kerosene-Type Jet Fuel
Naphtha	Jet-A/AVTUR[3]	Special Naphthas
Naphtha	Jet-A/AVTUR[3]	Naphtha For Petrochemical Feedstock Use
Naphtha	Jet-A/AVTUR[3]	Other Oils for Petrochemical Feedstock Use
Light olefins	PC Feedstock	Ethylene
Light olefins	PC Feedstock	Propylene
LPG or Liquefied Refinery Gas	LPG	Ethane
LPG	LPG	Propane
LPG	LPG	Normal Butane
Not Final Product	LPG	Isobutane (negative amount in 2014, not accounted in the final product)
Not Final Product	NA	Isobutylene (negative amount in 2014, not product)
Not Final Product	NA	Normal Butylene (negative amount in 2014, not final product)
Lubricants	Liquid Heavy Ends	Naphthenic Lubricants
Lubricants	Liquid Heavy Ends	Paraffinic Lubricants

Product Category (the present study)	PRELIM Product	EIA Product
Miscellaneous Petroleum Products	Liquid Heavy Ends	Miscellaneous Petroleum Products for Fuel Use
Miscellaneous Petroleum Products	Liquid Heavy Ends	Miscellaneous Petroleum Products for Nonfuel Use
Residual Fuel Oil	Liquid Heavy Ends	Residual Fuel Oil, 0.31 to 1.00% Sulfur
Residual Fuel Oil	Liquid Heavy Ends	Residual Fuel Oil, Greater than 1.00% Sulfur
Residual Fuel Oil	Liquid Heavy Ends	Residual Fuel Oil, Less than 0.31% Sulfur
Waxes	Liquid Heavy Ends	Waxes
Petroleum Coke, Catalyst (combusted, not final product)	Catalyst Coke	Petroleum Coke, Catalyst
Petroleum Coke	Coke	Petroleum Coke, Marketable
Still Gas (not final product)	Surplus RFG	Still Gas

[1] ULSD = ultra-low sulfur diesel.
[2] PRELIM produced finished gasoline are converted to gasoline BOB by extracting ethanol amount.
[3] AVTUR = aviation turbine fuel.

6. Comparison of PRELIM Derived Products with EIA Reported Products

Table S22 shows national product output from the EIA report at refineries, and Table S23 shows the comparison of EIA products volume with the PRELIM modeling derived volumes.

Table S22. EIA Reported Final Product Output at Refineries by PADD (Annual), 2014

Product	Unit	PADD1	PADD2	PADD3	PADD4	PADD5	U.S.
Motor Gasoline Blending Components[1]	10^3 m^3	31,740	107,269	228,270	16,098	72,297	455,674
Distillate Fuel Oil	10^3 m^3	19,389	63,033	157,705	11,261	33,337	284,725
Kerosene	10^3 m^3	5,689	13,436	45,522	1,725	24,841	91,213
Finished Aviation Gasoline	10^3 m^3	–	109	488	13	104	714
Special Naphtha[2]	10^3 m^3	37	73	2,266	–	66	2,442
Liquefied Refinery Gases (or LPG)	10^3 m^3	2,314	6,869	24,646	608	3,479	37,916
Lubricants	10^3 m^3	749	462	7,274	–	1,161	9,647
Miscellaneous Petroleum Products[3]	10^3 m^3	179	834	3,106	198	756	5,073
Residual Fuel Oil	10^3 m^3	3,240	3,000	10,867	690	7,425	25,221
Waxes	10^3 m^3	11	64	336	–	–	411
Petrochemical Feedstocks[4]	10^3 m^3	187	1,819	16,107	–	11	18,125
Petroleum Coke	MT	693	8,518	24,834	1,018	7,657	42,720
Asphalt and Road Oil	10^3 m^3	2,927	8,203	4,278	1,936	1,203	18,548
Still Gas[5]	m^3 fuel oil eq.	2,348	7,514	21,876	1,364	7,094	40,196

[1] An estimate of ethanol content has been excluded from the finished motor gasoline pool prior to combining with gasoline blend. See explanation in text.
[2] All finished products within the naphtha boiling range that are used as paint thinners, cleaners, or solvents. These products are refined to a specified flash point. Special naphthas include all commercial hexane and cleaning solvents conforming to ASTM Specification D1836 and D484, respectively. Naphthas to be blended or marketed as motor gasoline or aviation gasoline, or those that are to be used as petrochemical and synthetic natural gas (SNG) feedstocks, are excluded.
[3] "Includes all finished products not classified elsewhere (e.g., petrolatum, lube refining byproducts (aromatic extracts and tars), absorption oils, ram-jet fuel, petroleum rocket fuels, synthetic natural gas feedstocks, and specialty oils)" (U.S. EIA[16]).

[4] "Chemical feedstocks derived from petroleum principally for the manufacture of chemicals, synthetic rubber, and a variety of plastics. The categories reported are "Naphtha Less than 401°F" and "Other Oils Equal to or Greater than 401°F" (U.S. EIA[16]).
[5] Refinery still gas is listed as final product, but is actually mostly consumed inside refineries.

Table S23. Comparison of Refinery Final Products Volume from PRELIM V1.1 and EIA Report in 2014.

Refinery Final Product	PRELIM V1.1 Estimate	EIA[16]	Volume Difference
Gasoline BOB (m^3)	450,802,395	449,700,635	0.2%
Diesel/Distillate (m^3)	294,965,568	280,598,467	5.1%
Jet/Kerosene (m^3)	89,663,636	90,021,921	-0.4%
Aviation Gasoline (m^3)	691,463	701,085	-1.4%
Naphtha (m^3)	20,188,259	20,085,515	0.5%
LPG (m^3)	27,053,545	22,120,294	22.3%
Lubricants (m^3)	9,276,610	9,456,682	-1.9%
Miscellaneous Petroleum Products (m^3)	6,197,781	4,991,526	24.2%
Residual Fuel Oil (m^3)	24,651,068	24,936,919	-1.1%
Waxes (m^3)	440,444	402,660	9.4%
Light olefins (m^3)	13,984,043	15,150,883	-7.7%
Petroleum Coke[1] (kg)	26,094,334	30,401,951	-14.2%
Asphalt and Road Oil[2] (m^3)	17,578,568	18,435,842	-4.7%
Total[a] (m^3)	981,587,714	967,004,381	1.5%

[1] The conversion factor for petroleum coke is 5.0 bbl per short ton, based on EIA Petroleum and Other Liquids, Definitions, Sources and Explanatory Notes (https://www.eia.gov/dnav/pet/TblDefs/pet_pnp_refp2_tbldef2.asp).
[2] The conversion factor for asphalt is 5.5 bbl per short ton, based on EIA Petroleum and Other Liquids, Definitions, Sources and Explanatory Notes (https://www.eia.gov/dnav/pet/TblDefs/pet_pnp_refp2_tbldef2.asp).

For the major refinery products, such as gasoline BOB, diesel, and jet/kerosene, the model-derived product volumes match the EIA-reported volumes very well with 0.2%, 5.1%, and -0.4% differences, respectively. Some other products show higher degrees of deviation. These differences may be due to several factors:

- PRELIM V1.1 features a series of typical refinery configurations. However, it does not represent actual U.S. individual refinery configurations or operations. Fitting a U.S. individual refinery with PRELIM default configurations without modification leads to differences between the modeled products and the actual refinery products.

  For example, in our study, fitting an individual U.S. refinery with existing PRELIM V1.1 models led to an underestimation of the capacity in the vacuum distillation, FCC, coker, and alkylation units, and an overestimation of the catalytic reformer, isomerization, and hydrotreating units.[S1] The presence of specific refinery processes affects total energy use and final product slate. The underestimation of coker unit capacity might be related to the underestimated production of petroleum coke.

- PRELIM V1.1 does not "customize" the refinery operations for individual crude slates; instead, it applies general correlations or calculations [10,24] (e.g., for the properties of intermediate products). In contrast, “real world” refineries optimize operations corresponsive to refinery configurations as well as crude slates. These different approaches might cause differences in operations, in unit product slates, and therefore in final product slates.

- The largest degrees of deviation between PRELIM V1.1 product amount and the EIA-reported product amounts are observed for LPG and olefins. PRELIM V1.1, calculated the production of these two refinery products using a number of simplifications and assumptions.

Light products (refinery still gas, LPG, and light olefins) are often produced from the top of many refinery units. They are then sent to gas plants, amine plants, and sulfur plants to remove sulfur and other impurities (see Figure S3). In contrast to the major refinery products (gasoline BOB, diesel/distillate, jet/kerosene, etc.), which have relatively constant yields from refinery units, the yields of light products can vary significantly with refinery configuration, unit operations, and crude quality. PRELIM V1.1 splits still gas, LPG, and olefins yield with fixed ratios in the refinery modules, which might differ from individual refinery practice. In particular, PRELIM points out that the assumption of fuel gas production amount and composition can have noticeable impacts on energy uses and GHG emissions.[10,24]

7. U.S. Refinery Unit Emission Allocations to Products

Upon establishing the correspondence between PRELIM-derived products and EIA final products, the allocation factors of refinery process units to refinery products can be developed in PRELIM V1.1. These factors are calculated for each refinery facility and aggregated at the PADD or national level based on a production weighted average. The PADD and national unit allocation factors derived from PRELIM V1.1 need some adjustments to better reflect U.S. refinery production.

Splitting Factors

While a single PRELIM V1.1 final product (e.g., Jet-A/AVTUR) is matched to multiple EIA products, further allocation (splitting) is required to complete the allocation to EIA final products.

Splitting factors are developed for each PADD and are calculated as the PADD-level production ratio of the EIA final products to which a given PRELIM V1.1 final product category is matched. For example, emissions allocated to the PRELIM V1.1 product category Jet-A/AVTUR are split between EIA products: finished aviation gasoline, kerosene, and naphtha, based on the relative production volume of these fuel groups reported by EIA. Naphtha includes EIA products “naphtha for petrochemical feedstock use,” “other oils for petrochemical feedstock use,” and special naphtha. Using this approach, the three refinery products, finished aviation gasoline, kerosene, and naphtha will have similar emissions burdens per unit of energy in each product without differentiating between their production pathways. For some other products, such as light products, liquid heavy ends used in PRELIM V1.1 were further split to match the more diverse EIA product slates.

Refinery Still Gas

In the present study, all still gas is assumed to be consumed on site for heat generation within the refinery. Therefore, emissions allocated to still gas in PRELIM V1.1 are reallocated to refinery process units according to the relative heat and steam demand of each process unit within each PADD. These emissions are allocated again to unit final products based on their energy content. This iterative process continues until the results converge (the emissions remaining in the still gas pool are less than 0.00001% of total emissions for each flow) and the emissions attributed to individual unit products are obtained. In the present study, the calculation process required four iterations to attain convergence.

Figures S4 and S5 show the allocation factors of refinery unit emissions to unit products, before and after the emission burdens to refinery still gas are reallocated.

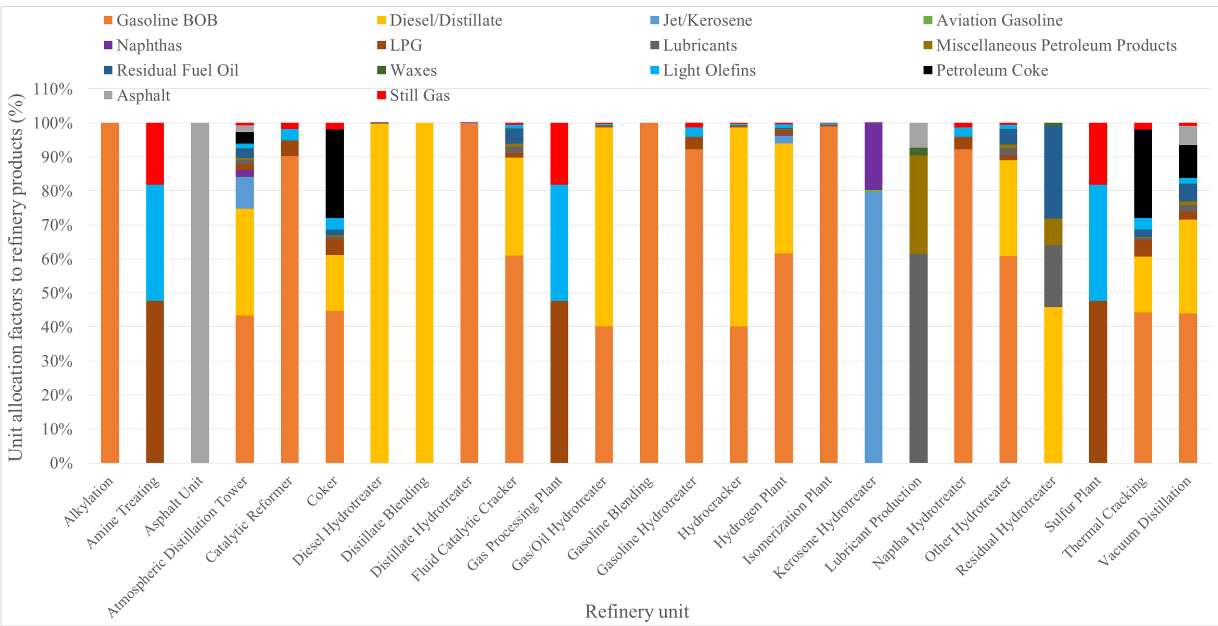


Figure S4. Refinery Process Unit Emissions (Process, Combustion, and FWE-1) Allocation Factors to Unit Products (Including Still Gas), Aggregated Nationally.

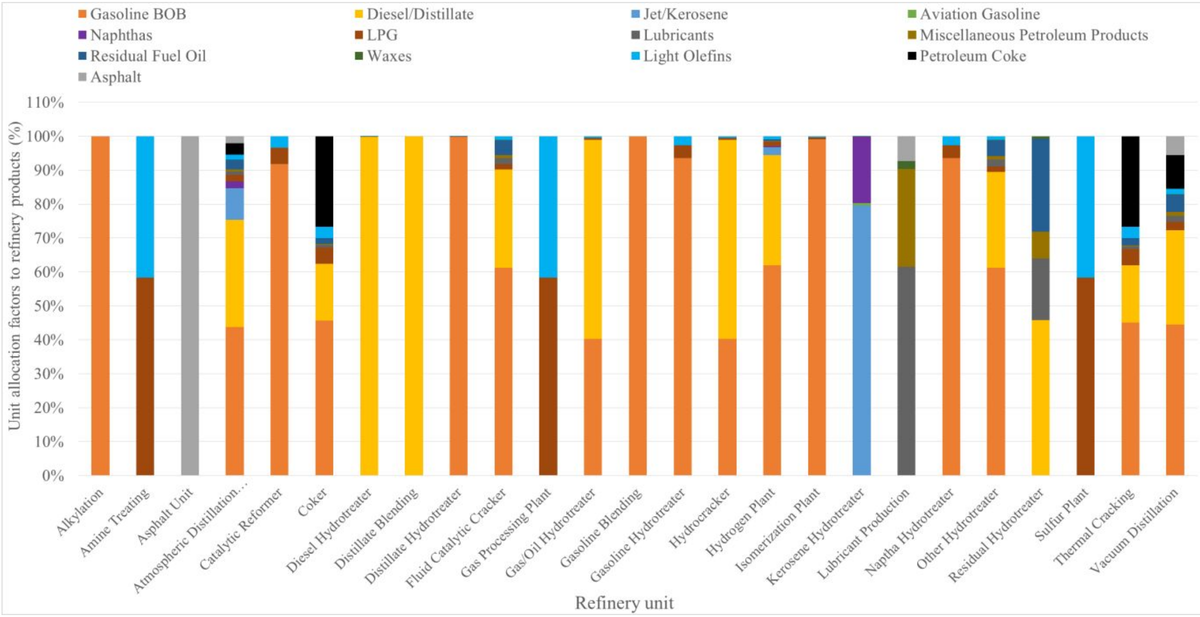


Figure S5. U.S. Refinery Process Unit Allocation Factors for Refinery Final Products, Aggregated Nationally, Following Reallocation of Emissions Attributed to Still Gas Production.

Lubricant Production

Lubricant production includes several complex and energy-intensive (thus emission-intensive) processes converts crude heavy cuts.[27,29] Each process will coproduce some other refinery products,[27,29] as illustrated in Figure S6.

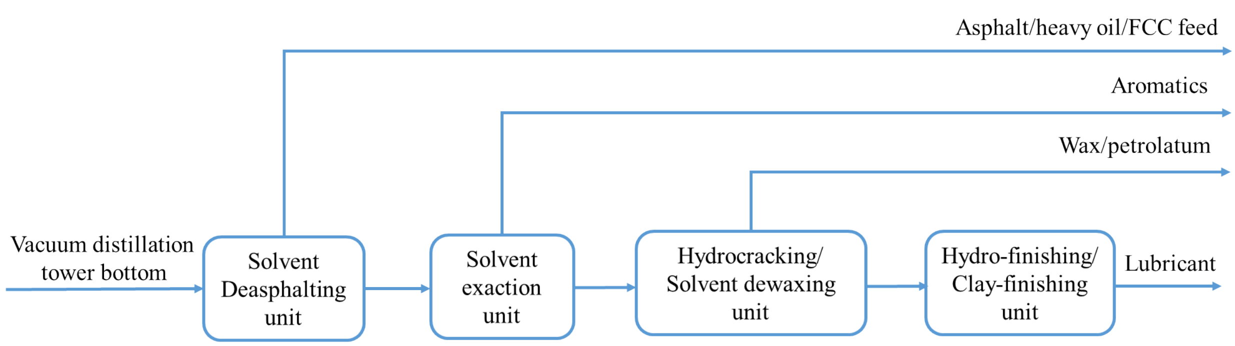


Figure S6. General Process of Lubricant Production.

The types of coproducts from the lubricant production process depend on individual refinery configurations and process technologies. For example, solvent-extracted asphalt/heavy oil can be blended with asphalt, blended with heavy oil, or used as feedstock to an FCC unit.[29] For dewaxing, hydrocracking technology breaks down wax, whereas solvent dewaxing separates wax and coproduces wax. Wax can be fed to the FCC or sold after appropriate treatment. Asphalt can be coproduced from deasphalting unit, but is produced in greater quantity by a separate dedicated asphalt unit, and thus the asphalt reported by the EIA is not mainly associated with lubricant production. These variations in refinery, technology, and categorization, along with the absence of mass/energy flow information among these units, make sub-process-level (solvent de-asphalting, solvent exaction, hydrocracking/dewaxing, finishing) allocation infeasible. Thus, the present study treats the overall lubricant production as a "black box unit." The burdens are split among the products by volume (because they are not energy products). To allocate the lubricant process burdens, one key element is determining the appropriate amount of asphalt product as coproduct of lubricant production, because most asphalts are more often produced from asphalt units. This asphalt coproduced with lubricant is estimated by summing up the asphalt products in the refinery facilities that also have lubricant product. Compared to the total amount of asphalt product in each region, the estimated share of asphalt coproduced with lubricant production is about 18.0%, 6.2%, 7.6%, 0%, and 9.3% for PADDs 1 through 5, respectively. The national average in the United States is about 7.6%.

With this estimated amount of coproduced asphalt, the lubricant production burdens can be allocated to both main product and coproducts. The lubricant unit allocation factors vary from PADD to PADD, and the national level is about 58.3%, 30.6%, 8.6%, and 2.5% for lubricant, aromatics/tar (miscellaneous product), asphalt, and wax, respectively.

8. Emissions of Refinery Final Products

Adding up the unit emissions attributed to refinery products and the FWE-2 attributed to refinery products produces the total emissions attributable to each refinery product. The emissions allocated to each refinery product pool varies, and the shares of total facility emissions are shown emissions are shown in Figure S7.

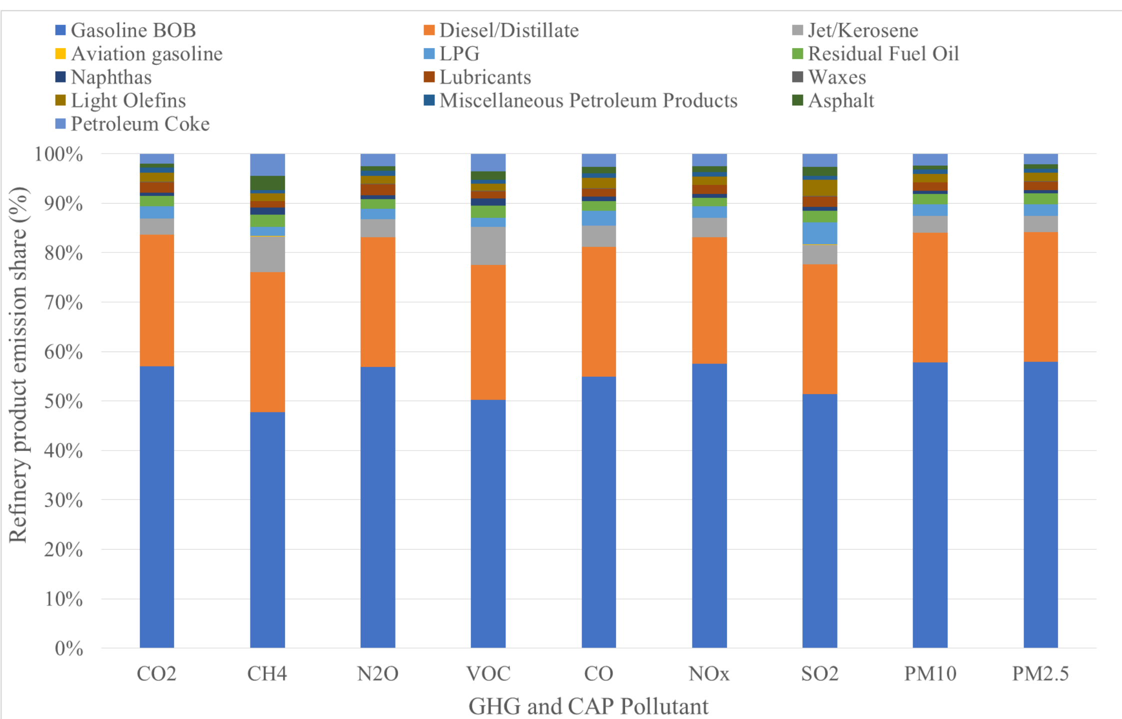


Figure S7. Emission Shares of Refinery Products to Total Refinery Emissions at National Level.

The emissions associated with refinery products vary among PADDs, and the final results are shown in Table S24 below.

Table S24. Refinery GHG and CAP Emissions per MJ of Refinery Final Products in Each PADD.

Final Product	CO_2	CH_4	N_2O	VOC	CO	NO_x	SO_2	PM_{10}	$PM_{2.5}$
Unit	g/MJ	mg/MJ	mg/MJ	mg/MJ	mg/MJ	mg/MJ	mg/MJ	mg/MJ	mg/MJ
PADD 1									
LPG	8.2	0.69	0.07	0.95	3.89	2.63	1.20	0.83	0.72
Gasoline BOB	7.9	0.55	0.07	1.29	2.04	3.50	1.12	1.11	0.96
Aviation gasoline	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Diesel/distillate	4.5	0.37	0.04	0.88	0.92	1.66	0.68	0.50	0.43
Jet/kerosene	1.5	0.20	0.01	0.66	0.29	0.55	0.12	0.13	0.11
Residual Fuel Oil	3.4	0.39	0.03	1.02	0.94	1.46	0.66	0.48	0.42
Petroleum Coke	8.8	0.56	0.07	0.74	0.46	0.83	0.16	0.58	0.51
Asphalt	3.1	0.34	0.03	0.90	0.94	2.13	1.81	0.29	0.26
Light Olefins	8.2	0.72	0.07	1.06	3.93	2.66	1.22	0.83	0.72
Naphtha	1.5	0.19	0.01	0.54	0.29	0.55	0.12	0.12	0.11
Lubricants	13.4	0.88	0.13	1.27	4.02	10.29	11.46	1.02	0.95
Miscellaneous	13.4	0.86	0.13	1.19	4.00	10.27	11.45	1.02	0.95
Waxes	13.4	0.86	0.13	1.20	4.00	10.28	11.45	1.02	0.95
PADD 2									
LPG	7.2	0.83	0.05	1.96	2.78	3.45	2.77	0.91	0.76
Gasoline BOB	6.9	1.01	0.06	2.30	2.61	3.45	1.40	1.09	0.92
Aviation gasoline	1.7	0.48	0.02	0.91	0.82	1.05	0.50	0.25	0.22
Diesel/distillate	4.2	0.77	0.04	1.59	1.61	2.03	0.99	0.65	0.56
Jet/kerosene	1.7	0.48	0.02	1.01	0.82	1.05	0.50	0.25	0.22
Residual Fuel Oil	3.1	0.64	0.03	1.42	1.07	1.22	0.84	0.59	0.51
Petroleum Coke	2.9	1.17	0.03	2.32	1.38	1.97	1.02	0.61	0.39
Asphalt	1.8	0.93	0.02	1.31	1.00	1.12	0.63	0.28	0.23
Light Olefins	7.2	0.77	0.05	1.85	2.76	3.44	2.73	0.91	0.76
Naphtha	1.6	0.46	0.02	0.87	0.81	1.04	0.48	0.25	0.22
Lubricants	6.1	0.81	0.05	2.13	3.60	3.15	1.01	0.96	0.71
Miscellaneous	6.1	0.76	0.05	2.03	3.57	3.14	0.97	0.96	0.71
Waxes	6.1	0.76	0.05	2.04	3.57	3.14	0.97	0.96	0.71
PADD 3									
LPG	7.2	0.86	0.05	1.65	2.09	2.47	1.62	0.67	0.62
Gasoline BOB	6.5	0.88	0.06	1.76	1.46	2.57	0.82	0.66	0.60
Aviation gasoline	2.1	0.72	0.02	1.49	0.69	1.00	0.39	0.21	0.19
Diesel/distillate	4.4	0.80	0.04	1.55	1.09	1.73	0.62	0.44	0.40

Final Product	CO_2	CH_4	N_2O	VOC	CO	NO_x	SO_2	PM_{10}	$PM_{2.5}$
Unit	**g/MJ**	**mg/MJ**	**mg/MJ**	**mg/MJ**	**mg/MJ**	**mg/MJ**	**mg/MJ**	**mg/MJ**	**mg/MJ**
Jet/kerosene	2.1	0.72	0.02	1.61	0.69	1.00	0.39	0.21	0.19
Residual Fuel Oil	4.4	0.81	0.04	1.63	1.12	1.30	0.68	0.50	0.45
Petroleum Coke	2.9	1.11	0.03	1.59	0.90	1.49	0.47	0.31	0.27
Asphalt	2.5	2.12	0.03	1.78	0.83	1.11	0.42	0.24	0.21
Light Olefins	7.3	1.22	0.05	2.45	2.32	2.56	1.75	0.70	0.64
Naphtha	2.1	0.68	0.02	1.41	0.67	0.99	0.38	0.21	0.18
Lubricants	12.0	1.17	0.11	2.58	2.37	3.69	1.25	1.06	0.99
Miscellaneous	10.6	0.97	0.10	2.12	2.04	3.29	1.08	0.93	0.87
Waxes	12.0	1.12	0.11	2.47	2.34	3.68	1.24	1.05	0.99
PADD 4									
LPG	7.7	1.49	0.06	2.70	3.64	3.93	9.52	1.97	1.25
Gasoline BOB	9.2	2.22	0.08	4.97	4.24	4.61	2.71	1.84	1.09
Aviation gasoline	2.0	0.81	0.02	1.23	1.11	1.22	0.58	0.25	0.12
Diesel/distillate	4.6	1.73	0.04	2.77	2.21	2.28	1.66	1.03	0.59
Jet/kerosene	2.0	0.81	0.02	1.60	1.11	1.22	0.58	0.25	0.12
Residual Fuel Oil	2.7	1.49	0.02	2.44	1.30	1.32	1.29	0.75	0.50
Petroleum Coke	4.2	2.33	0.04	3.74	2.75	2.93	3.67	1.52	0.73
Asphalt	1.9	2.75	0.02	3.91	1.78	1.67	1.31	0.32	0.13
Light Olefins	7.7	0.38	0.06	1.24	3.32	3.69	9.17	1.97	1.25
Naphtha	--	--	--	--	--	--	--	--	--
Lubricants	--	--	--	--	--	--	--	--	--
Miscellaneous	2.7	1.23	0.02	1.78	1.22	1.26	1.19	0.75	0.50
Waxes	--	--	--	--	--	--	--	--	--
PADD 5									
LPG	8.1	0.72	0.05	1.52	2.13	3.11	2.65	0.69	0.60
Gasoline BOB	9.6	0.95	0.06	2.52	2.15	3.83	1.42	0.83	0.75
Aviation gasoline	2.1	0.95	0.01	2.05	0.72	1.05	0.40	0.28	0.26
Diesel/distillate	6.4	0.65	0.04	1.46	1.35	2.28	0.89	0.53	0.48
Jet/kerosene	2.1	0.95	0.01	2.11	0.72	1.05	0.40	0.28	0.26
Residual Fuel Oil	3.8	0.72	0.03	1.58	0.98	1.47	0.78	0.36	0.31
Petroleum Coke	4.3	1.15	0.04	2.22	1.89	2.51	1.10	0.58	0.53
Asphalt	2.4	0.86	0.02	1.99	0.77	1.25	0.45	0.30	0.28
Light Olefins	8.1	0.45	0.05	0.95	2.04	3.06	2.63	0.65	0.57
Naphtha	2.1	0.89	0.01	1.94	0.71	1.04	0.39	0.28	0.25
Lubricants	10.5	1.08	0.08	2.92	1.58	3.01	1.02	0.65	0.61
Miscellaneous	10.5	1.01	0.08	2.78	1.56	3.00	1.00	0.64	0.60
Waxes	--	--	--	--	--	--	--	--	--

Figure S8 displays the variations of GHG emissions between gasoline BOB, diesel/distillate, and jet/kerosene in different PADD, and compares them with those from Cooney et al.[11]

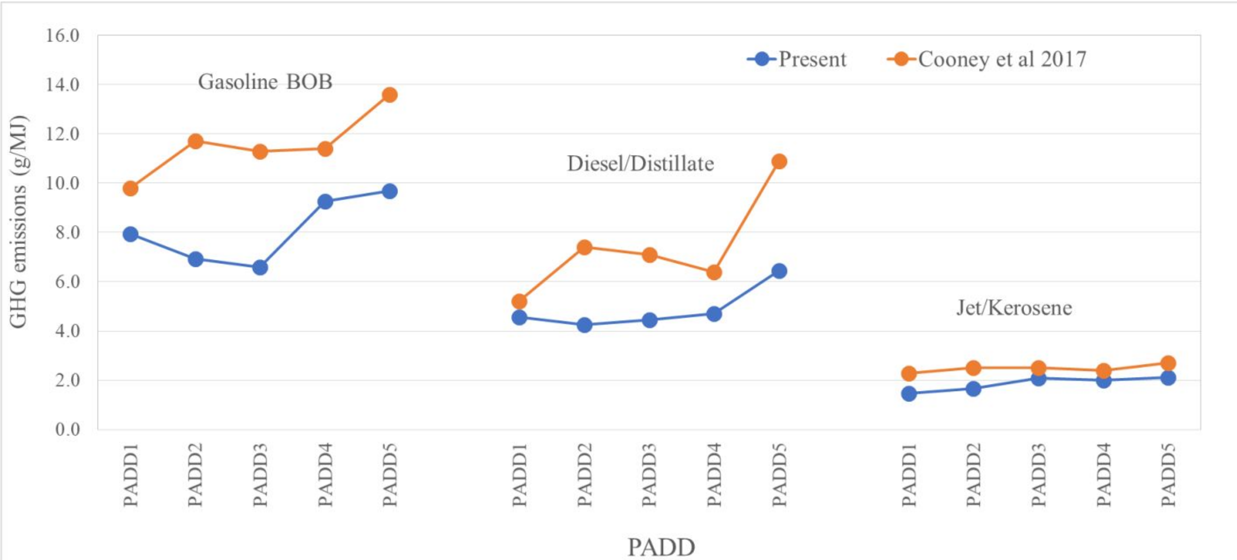


Figure S8. Comparison of the Present Study GHG Emissions (Gasoline, Diesel/Distillate, and Jet/Kerosene Fuels in U.S. PADD Refineries in 2014) with Literature Results.

The breakdown of the emissions associated with refinery products (U.S. average) is shown in Table S25 below.

Table S25. Refinery GHG and CAP Emissions per MJ of Refinery Final Products in Each PADD, from Process, Combustion, and Facility-wide Sources.

Final Product	CO_2 (g/MJ)	CH_4 (mg/MJ)	N_2O (mg/MJ)	VOC (mg/MJ)	CO (mg/MJ)	NO_x (mg/MJ)	SO_2 (mg/MJ)	PM_{10} (mg/MJ)	$PM_{2.5}$ (mg/MJ)
				Process Emissions					
LPG	2.30	0.12	0.00	0.29	0.87	0.38	1.40	0.16	0.14
Gasoline BOB	0.77	0.05	0.00	0.05	0.03	0.03	0.02	0.02	0.01
Aviation gasoline	0.11	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
Diesel/distillate	0.55	0.02	0.00	0.03	0.01	0.02	0.01	0.01	0.01
Jet/kerosene	0.13	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
Residual Fuel Oil	0.10	0.02	0.00	0.03	0.02	0.02	0.02	0.01	0.00
Petroleum Coke	0.32	0.30	0.00	0.18	0.13	0.15	0.14	0.09	0.06
Asphalt	0.16	0.40	0.00	0.03	0.00	0.00	0.00	0.00	0.00
Light Olefins	2.32	0.12	0.00	0.29	0.88	0.38	1.42	0.16	0.14

Naphtha	0.06	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
Lubricants	0.07	0.03	0.00	0.36	0.01	0.01	0.01	0.00	0.00
Miscellaneous	0.13	0.02	0.00	0.28	0.01	0.01	0.01	0.01	0.00
Waxes	0.05	0.03	0.00	0.39	0.01	0.00	0.00	0.00	0.00
Combustion Emissions									
LPG	5.04	0.26	0.05	0.17	1.16	2.16	0.61	0.42	0.39
Gasoline BOB	6.42	0.31	0.06	0.23	1.48	2.70	0.82	0.60	0.55
Aviation gasoline	1.77	0.10	0.02	0.06	0.38	0.82	0.19	0.12	0.11
Diesel/distillate	4.08	0.20	0.04	0.14	0.90	1.63	0.52	0.37	0.34
Jet/kerosene	1.71	0.09	0.02	0.06	0.38	0.78	0.18	0.11	0.11
Residual Fuel Oil	3.70	0.15	0.03	0.12	0.71	1.12	0.53	0.35	0.32
Petroleum Coke	2.88	0.16	0.03	0.10	0.61	1.33	0.29	0.18	0.17
Asphalt	1.95	0.11	0.02	0.07	0.63	1.10	0.45	0.15	0.14
Light Olefins	5.06	0.26	0.05	0.17	1.17	2.17	0.61	0.42	0.39
Naphtha	1.83	0.11	0.02	0.06	0.33	0.82	0.18	0.12	0.11
Lubricants	11.46	0.55	0.10	0.34	2.00	3.60	1.75	0.68	0.64
Miscellaneous	9.37	0.45	0.08	0.29	1.85	2.94	1.13	0.61	0.57
Waxes	10.85	0.53	0.10	0.33	2.15	3.36	1.19	0.70	0.66
Facility-wide Emissions (FWE-1 and FWE-2)									
LPG	0.07	0.47	0.00	1.22	0.35	0.28	0.22	0.20	0.14
Gasoline BOB	0.08	0.58	0.00	1.79	0.43	0.34	0.28	0.23	0.17
Aviation gasoline	0.09	0.59	0.00	1.33	0.36	0.20	0.24	0.11	0.08
Diesel/distillate	0.08	0.56	0.00	1.38	0.37	0.25	0.26	0.15	0.11
Jet/kerosene	0.07	0.57	0.00	1.42	0.34	0.21	0.22	0.12	0.09
Residual Fuel Oil	0.07	0.56	0.00	1.39	0.33	0.22	0.21	0.11	0.09
Petroleum Coke	0.10	0.69	0.00	1.57	0.43	0.27	0.30	0.17	0.12
Asphalt	0.10	0.67	0.00	1.45	0.36	0.24	0.37	0.13	0.08
Light Olefins	0.09	0.57	0.00	1.51	0.45	0.31	0.25	0.20	0.15
Naphtha	0.09	0.53	0.00	1.25	0.36	0.17	0.21	0.10	0.07
Lubricants	0.08	0.53	0.00	1.79	0.45	0.47	0.23	0.31	0.28
Miscellaneous	0.07	0.48	0.00	1.57	0.39	0.40	0.23	0.27	0.21
Waxes	0.08	0.49	0.00	1.64	0.44	0.39	0.26	0.33	0.27

The refinery onsite GHG and CAP emissions allocated to various products are itemized by refinery process units, shown in the figures below.

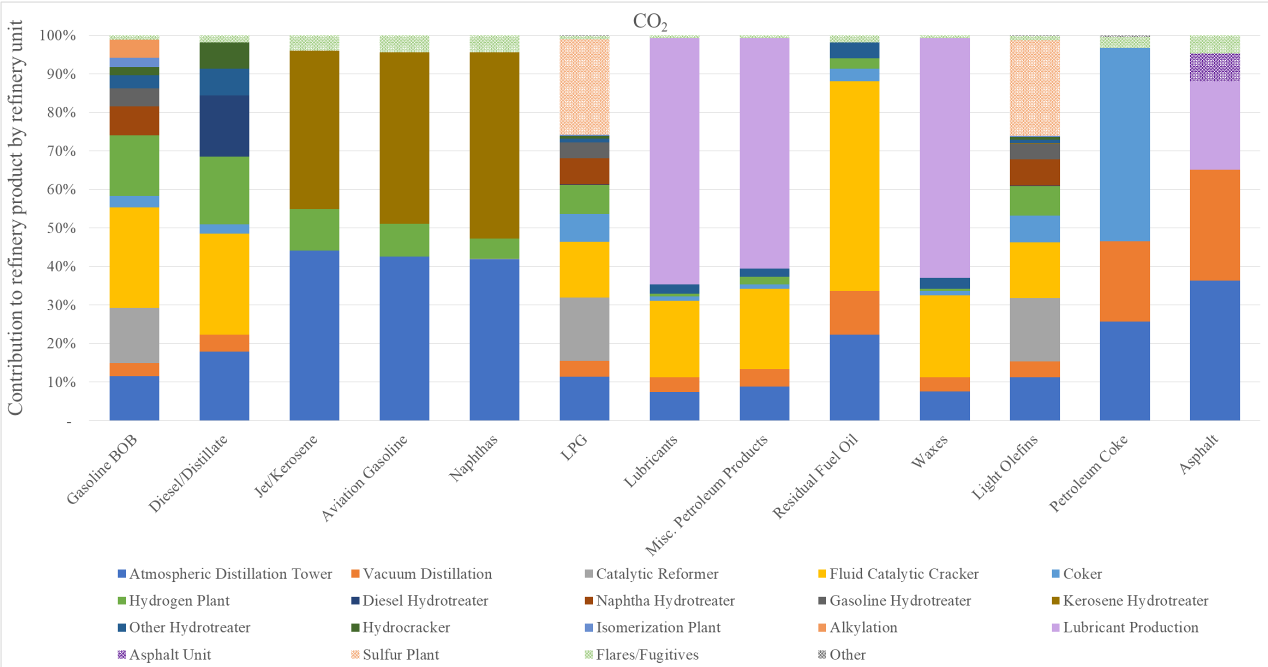


Figure S9. The Refinery Onsite CO_2 Emissions Allocated to Products from Various Refinery Units.

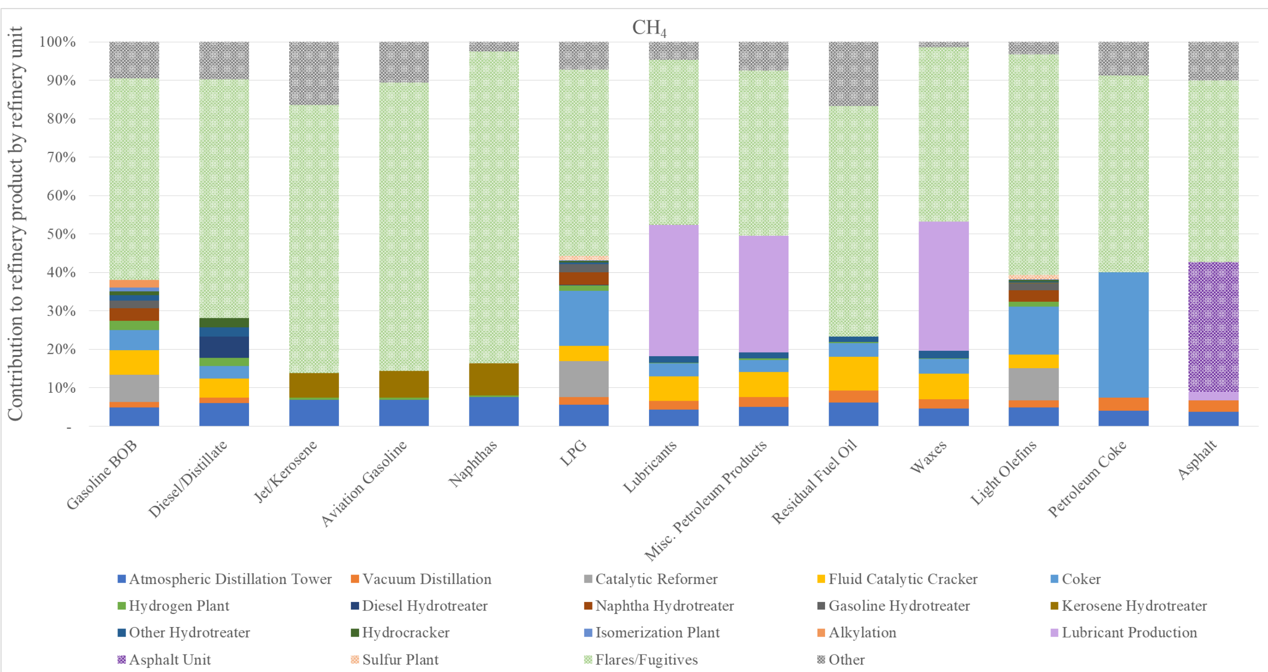


Figure S10. The Refinery Onsite CH_4 Emissions Allocated to Products from Various Refinery Units.

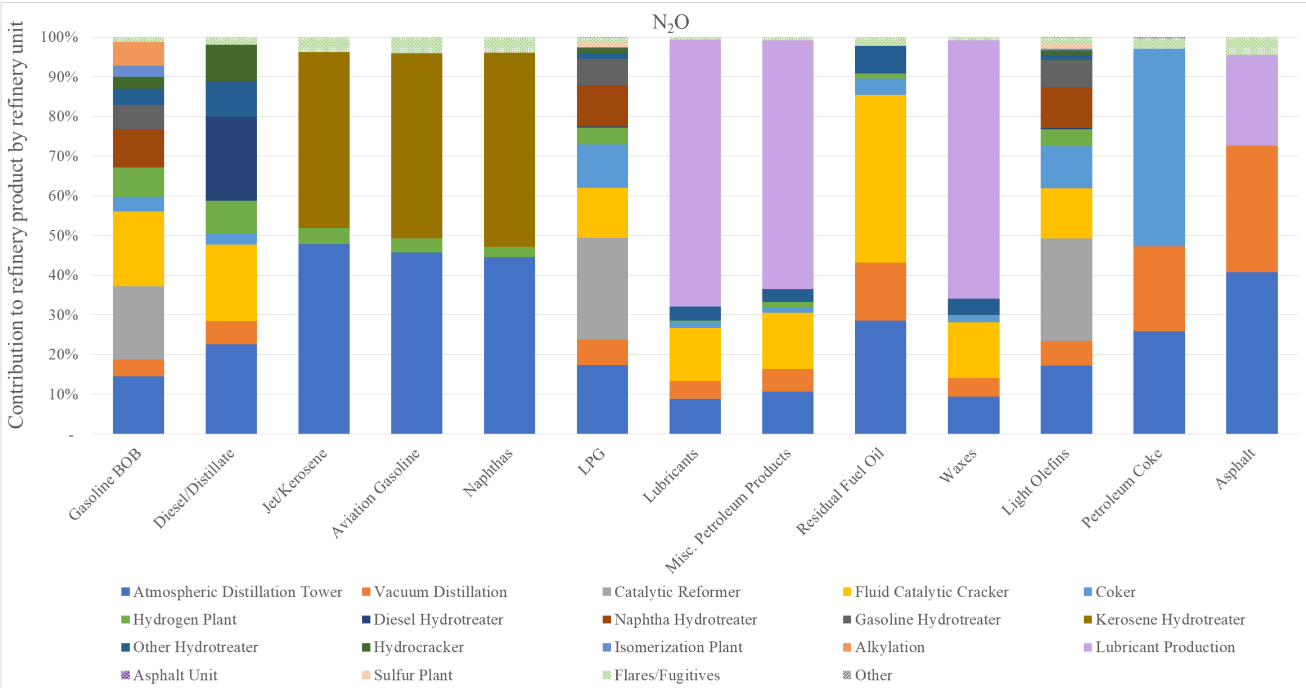


Figure S11. The Refinery Onsite N_2O Emissions Allocated to Products from Various Refinery Units.

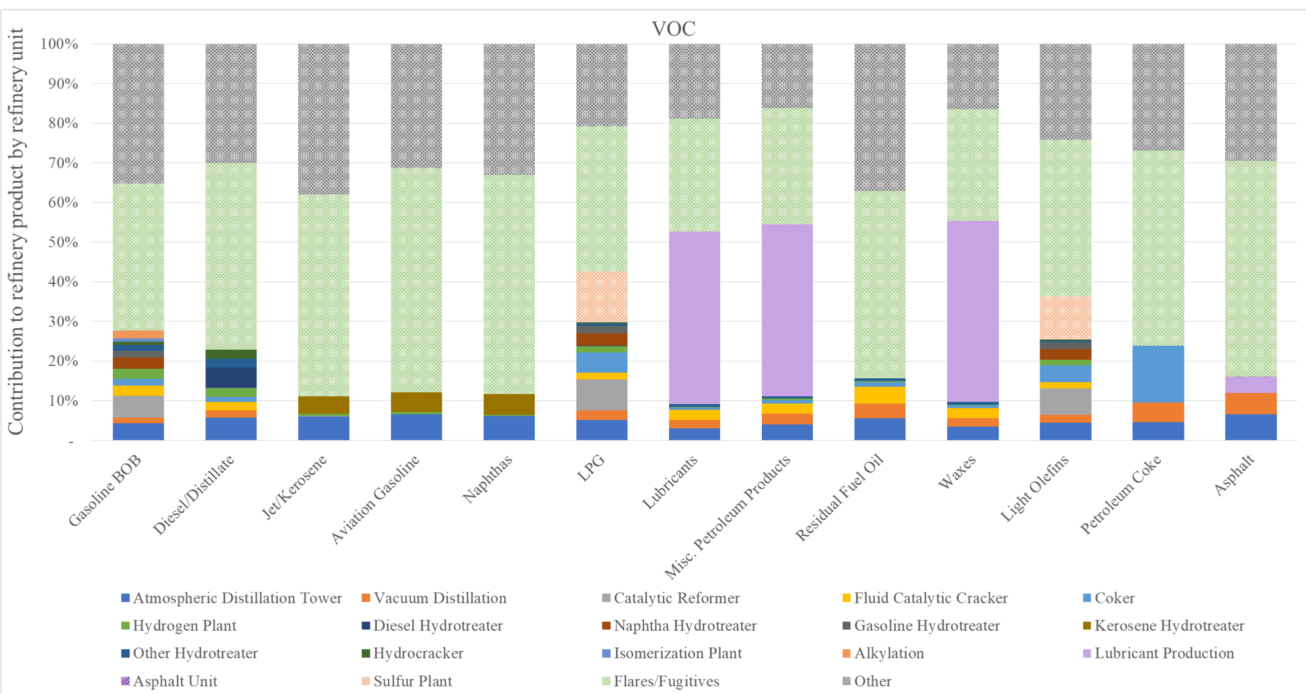


Figure S12. The Refinery Onsite VOC Emissions Allocated to Products from Various Refinery Units.

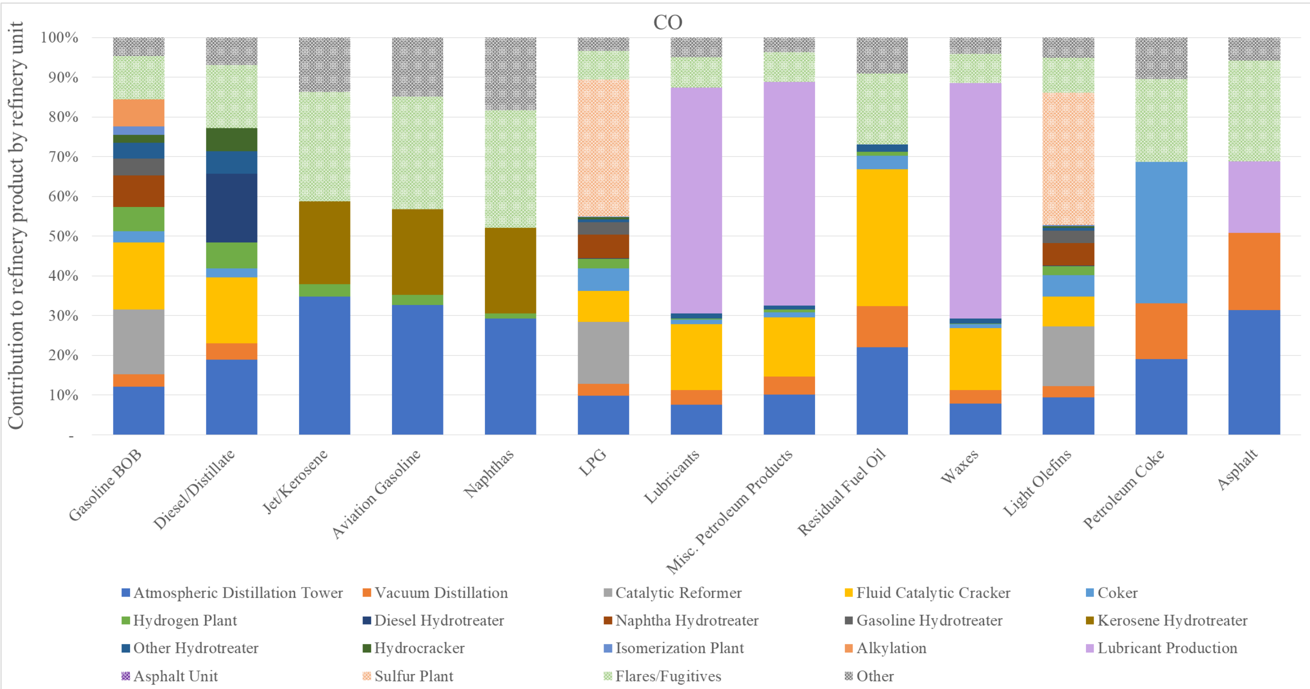


Figure S13. The Refinery Onsite CO Emissions Allocated to Products from Various Refinery Units.

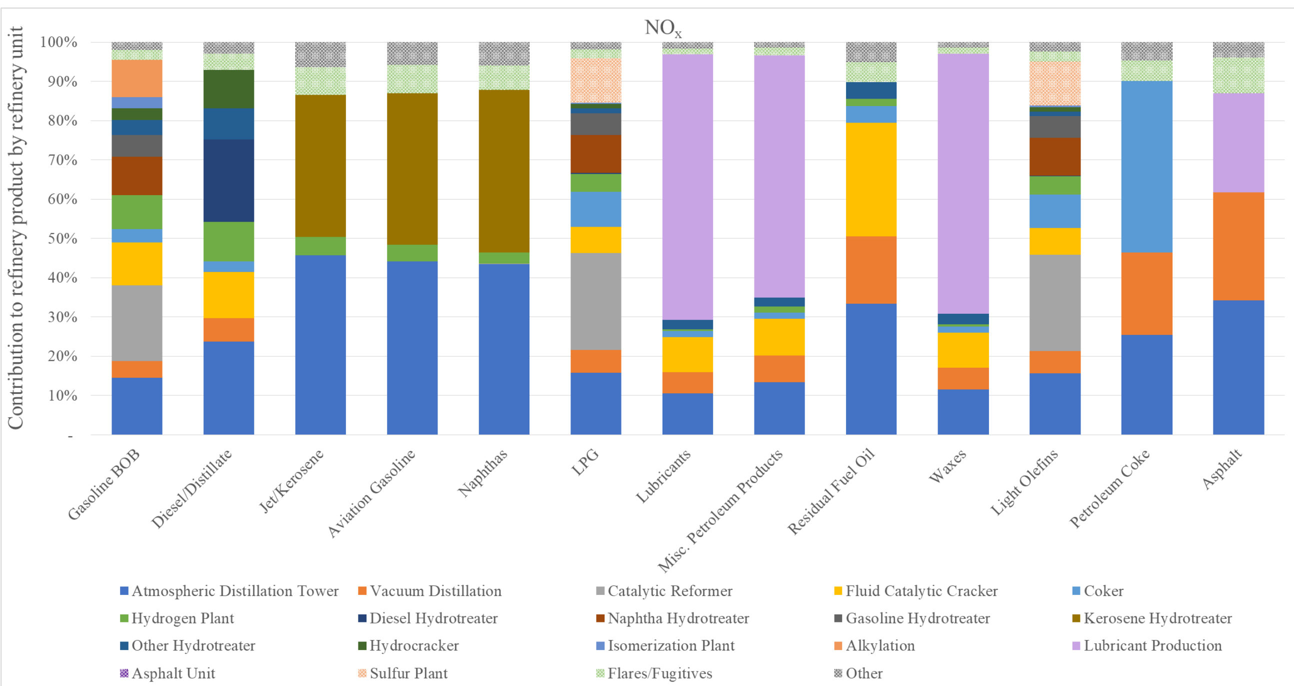


Figure S14. The Refinery Onsite NO_x Emissions Allocated to Products, from Various Refinery Units.

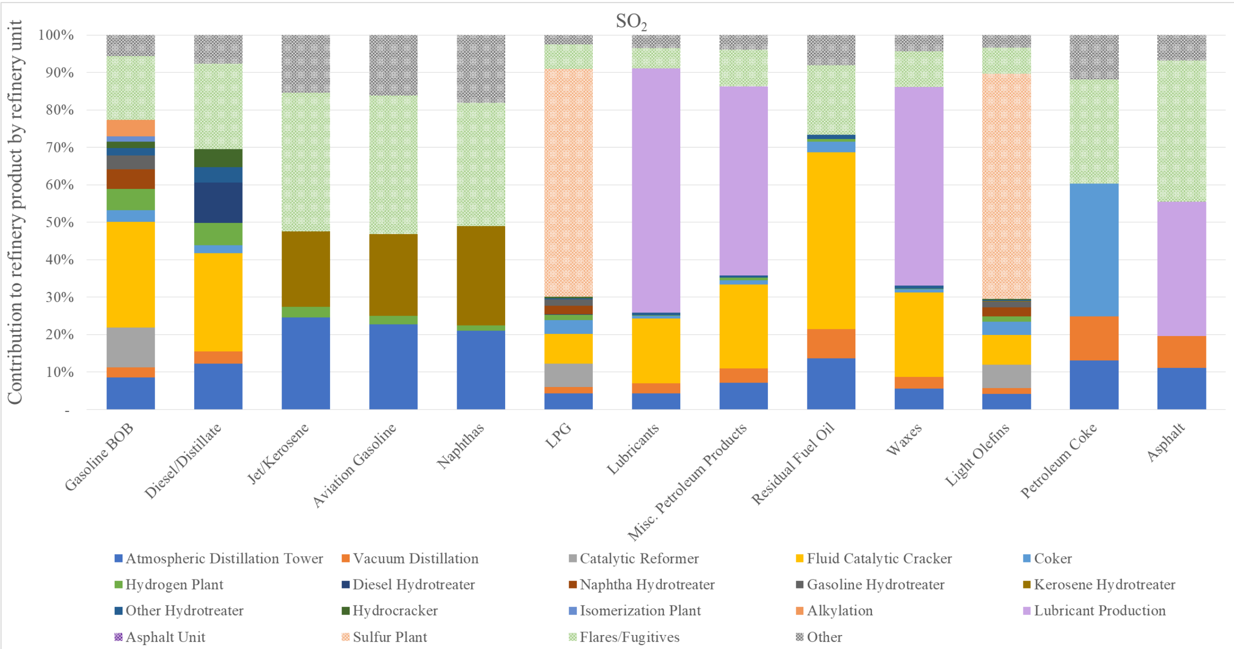


Figure S15. The Refinery Onsite SO_2 Emissions Allocated to Products from Various Refinery Units.

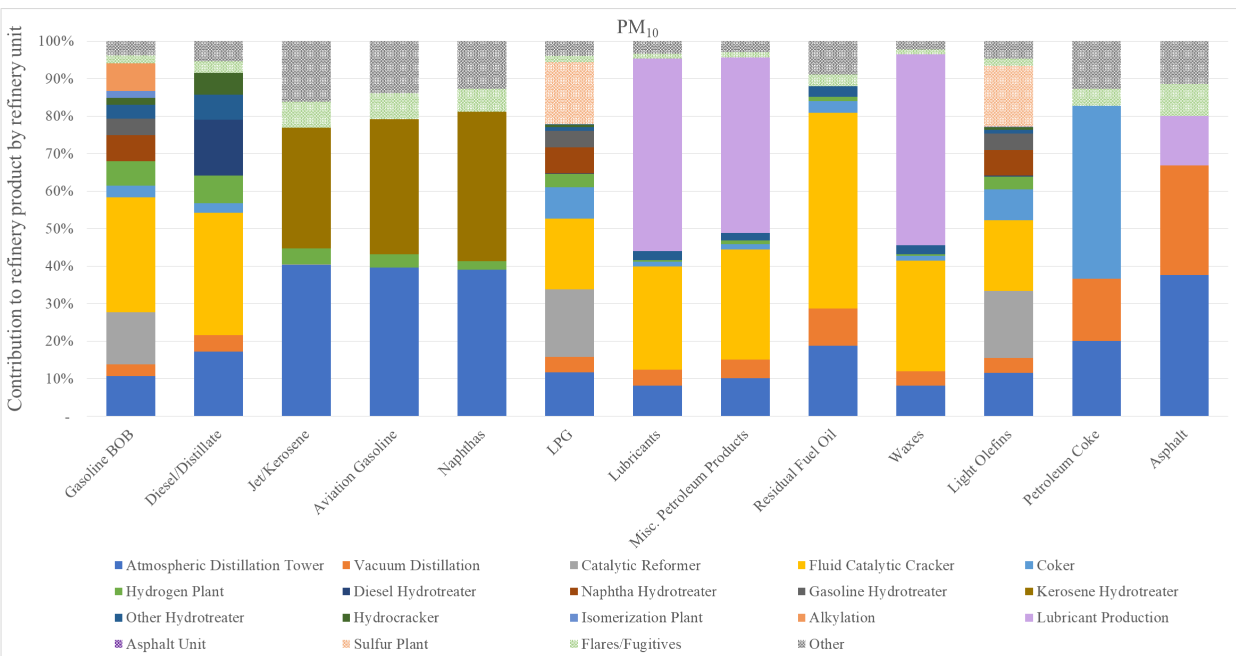


Figure S16. The Refinery Onsite PM_{10} Emissions Allocated to Products from Various Refinery Units.

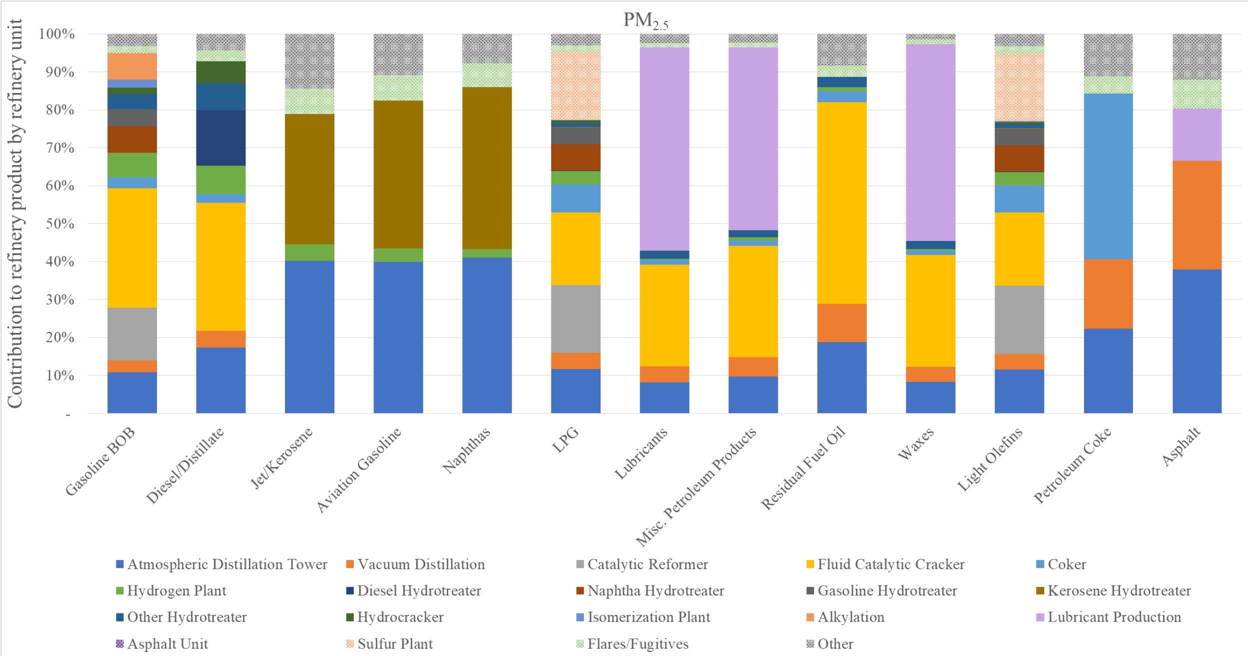


Figure S17. The Refinery Onsite PM_{10} Emissions Allocated to Products from Various Refinery Units.

Reference

[S1] Young, B.; Morelli, B.; Hawkins, T. R.; Creation of Unit Process Data for Life Cycle Assessment of Steam Methane Reforming and Petroleum Refining; Eastern Research Group: https://greet.es.anl.gov/publication-air_pollutants_smr_petroleum.