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TECHNICAL SUPPORT DOCUMENT

Petroleum Products and Natural Gas Liquids: Definitions, Emission Factors, Methods and Assumptions

FINAL RULE FOR MANDATORY REPORTING OF GREENHOUSE GASES

Climate Change Division
Office of Atmospheric Programs
U.S. Environmental Protection Agency

September 15, 2009

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Introduction

On April 10, 2009, EPA published a proposed rule for the reporting of greenhouse gases in the Federal Register (Vol.74, No.68). Subpart MM of that proposed rule provided default CO_2 factors for petroleum products and natural gas liquids (NGLs). It is EPA's intent to allow refiners, importers, and exporters of petroleum products to easily and accurately identify the products that they are supplying and to calculate the CO_2 emissions that would result from the complete combustion or oxidation of the products. Toward that end, we have prepared the document that follows, which includes the following elements:

1) Default emission factors for seventy products covered in Subpart MM of the final rule;

2) Definitions of each product covered in Subpart MM of the final rule;

3) A summary of the overall general methods employed to derive emission factors for each product; and

4) Detailed descriptions of the methods and assumptions used to arrive at each default factor for each product.

Each product in the default factor table has an associated reference number (1 – 70) to facilitate cross referencing with the definitions and methods and assumptions sections.

This document reflects several updates from the proposed rule and its technical supporting documents:

1) EPA has updated product characteristics and default factors for several products based on additional technical research;

2) Density values have been expanded to the fourth significant digit from two significant digits to enhance the precision of the factors;

3) For motor gasolines and blendstocks, EPA has added grade based sub-categories;

4) The diesel and fuel oil categories have been combined into "distillate fuel" categories; and

5) Sulfur-based subcategories of distillate fuel No.1 and No.2 have been added to further distinguish between product categories with potentially different carbon contents.

Table 1. Default Factors for Petroleum Products and Natural Gas Liquids

Reference Number	Products	Column A: Density Metric tons/bbl)	Column B: Carbon Share (% of mass)	Column C: Emission Factor (metric tons CO_2/bbl)]
	Finished Motor Gasoline			
	Conventional—Summer			
1	Regular	0.1181	86.66	0.3753
2	Midgrade	0.1183	86.63	0.3758
3	Premium	0.1185	86.61	0.3763
	Conventional—Winter			
4	Regular	0.1155	86.50	0.3663
5	Midgrade	0.1161	86.55	0.3684
6	Premium	0.1167	86.59	0.3705
	Reformulated—Summer			
7	Regular	0.1167	86.13	0.3686
8	Midgrade	0.1165	86.07	0.3677
9	Premium	0.1164	86.00	0.3670
	Reformulated—Winter			
10	Regular	0.1165	86.05	0.3676
11	Midgrade	0.1165	86.06	0.3676
12	Premium	0.1166	86.06	0.3679
13	Gasoline—Other	0.1185	86.61	0.3763
	Blendstocks			
	CBOB—Summer			
14	Regular	0.1181	86.66	0.3753
15	Midgrade	0.1183	86.63	0.3758
16	Premium	0.1185	86.61	0.3763
	CBOB—Winter			
17	Regular	0.1155	86.50	0.3663
18	Midgrade	0.1161	86.55	0.3684
19	Premium	0.1167	86.59	0.3705
	RBOB—Summer			

20	Regular	0.1167	86.13	0.3686
21	Midgrade	0.1165	86.07	0.3677
22	Premium	0.1164	86.00	0.3670
	RBOB—Winter			
23	Regular	0.1165	86.05	0.3676
24	Midgrade	0.1165	86.06	0.3676
25	Premium	0.1166	86.06	0.3679
26	Blendstocks—Other	0.1185	86.61	0.3763
	Oxygenates			
27	Methanol	0.1268	37.48	0.1743
28	GTBA	0.1257	64.82	0.2988
29	MTBE	0.1181	68.13	0.2950
30	ETBE	0.1182	70.53	0.3057
31	TAME	0.1229	70.53	0.3178
32	DIPE	0.1156	70.53	0.2990
	Distillate Fuel Oil			
	Distillate No. 1			
33	Ultra Low Sulfur	0.1346	86.40	0.4264
34	Low Sulfur	0.1346	86.40	0.4264
35	High Sulfur	0.1346	86.40	0.4264
	Distillate No. 2			
36	Ultra Low Sulfur	0.1342	87.30	0.4296
37	Low Sulfur	0.1342	87.30	0.4296
38	High Sulfur	0.1342	87.30	0.4296
39	Distillate Fuel Oil No. 4	0.1452	86.47	0.4604
40	**Residual Fuel Oil No. 5 (Navy Special)**	0.1365	85.67	0.4288
41	**Residual Fuel Oil No. 6 (a.k.a. Bunker C)**	0.1528	84.67	0.4744
42	**Kerosene-Type Jet Fuel**	0.1294	86.30	0.4095
43	**Kerosene**	0.1346	86.40	0.4264
44	**Diesel—Other**	0.1452	86.47	0.4604
	Petrochemical Feedstocks			
45	Naphthas (< 401 °F)	0.1158	84.11	0.3571
46	Other Oils (> 401 °F)	0.1390	87.30	0.4450
	Unfinished Oils			

47	Heavy Gas Oils	0.1476	85.80	0.4643
48	Residuum	0.1622	85.70	0.5097
	Other Petroleum Products and Natural Gas Liquids			
49	Aviation Gasoline	0.1120	85.00	0.3490
50	Special Naphthas	0.1222	84.76	0.3798
51	Lubricants	0.1428	85.80	0.4492
52	Waxes	0.1285	85.30	0.4019
53	Petroleum Coke	0.1818	92.28	0.6151
54, 55	Asphalt and Road Oil	0.1634	83.47	0.5001
56	Still Gas	0.1405	77.70	0.4003
57	Ethane	0.0866	79.89	0.2537
58	Ethylene	0.0903	85.63	0.2835
59	Propane	0.0784	81.71	0.2349
60	Propylene	0.0803	85.63	0.2521
61	Butane	0.0911	82.66	0.2761
62	Butylene	0.0935	85.63	0.2936
63	Isobutane	0.0876	82.66	0.2655
64	Isobutylene	0.0936	85.63	0.2939
65	Pentanes Plus	0.1055	83.63	0.3235
66	Miscellaneous Products	0.1380	85.49	0.4326
	Biomass-Based Fuel and Biomass			
67	Ethanol (100%)	0.1267	52.14	0.2422
68	Biodiesel (100%, methyl ester)	0.1396	77.30	0.3957
69	Rendered Animal Fat	0.1333	76.19	0.3724
70	Vegetable Oil	0.1460	76.77	0.4110

Revised definitions

1 – 26. Motor gasoline (finished) means a complex mixture of volatile hydrocarbons, with or without additives, suitably blended to be used in spark ignition engines. Motor gasoline includes conventional gasoline, reformulated gasoline, and all types of oxygenated gasoline. Gasoline also has seasonal variations in an effort to control ozone levels. This is achieved by lowering the Reid Vapor Pressure (RVP) of gasoline during the summer driving season. Depending on the region of the country the RVP is lowered to below 9.0 psi or 7.8 psi. The RVP may be further lowered by state regulations.

1 – 3. Conventional—Summer refers to finished gasoline formulated for use in motor vehicles, the composition and properties of which do not meet the requirements of the reformulated gasoline regulations promulgated by the U.S. Environmental Protection Agency under 40 CFR 80.40, but which meet summer RVP standards required under 40 CFR 80.27 or as specified by the state. Note: This category excludes conventional gasoline for oxygenate blending (CBOB) as well as other blendstock.

4 – 6. Conventional—Winter refers to finished gasoline formulated for use in motor vehicles, the composition and properties of which do not meet the requirements of the reformulated gasoline regulations promulgated by the U.S. Environmental Protection Agency under 40 CFR 80.40 or the summer RVP standards required under 40 CFR 80.27 or as specified by the state. Note: This category excludes conventional blendstock for oxygenate blending (CBOB) as well as other blendstock.

7 – 9. Reformulated—Summer refers to finished gasoline formulated for use in motor vehicles, the composition and properties of which meet the requirements of the reformulated gasoline regulations promulgated by the U.S. Environmental Protection Agency under 40 CFR 80.40 and 40 CFR 80.41, and summer RVP standards required under 40 CFR 80.27 or as specified by the state. Reformulated gasoline excludes Reformulated Blendstock for Oxygenate Blending (RBOB) as well as other blendstock.

10 – 12. Reformulated—Winter refers to finished gasoline formulated for use in motor vehicles, the composition and properties of which meet the requirements of the reformulated gasoline regulations promulgated by the U.S. Environmental Protection Agency under 40 CFR 80.40 and 40 CFR 80.41, but which do not meet summer RVP standards required under 40 CFR 80.27 or as specified by the state. Note: This category includes Oxygenated Fuels Program Reformulated Gasoline (OPRG). Reformulated gasoline excludes Reformulated Blendstock for Oxygenate Blending (RBOB) as well as other blendstock.

1, 4, 7, 10, 14, 17, 20, 23. Regular grade gasoline is gasoline having an antiknock index, i.e., octane rating, greater than or equal to 85 and less than 88. This definition applies to the regular grade categories of Conventional-Summer, Conventional-Winter, Reformulated-Summer, and Reformulated-Winter. For regular grade categories of RBOB-Summer, RBOB-Winter, CBOB-Summer, and CBOB-Winter, this definition refers

to the expected octane rating of the finished gasoline after oxygenate has been added to the RBOB or CBOB.

2, 5, 8, 11, 15, 18, 21, 24. Midgrade gasoline has an octane rating greater than or equal to 88 and less than or equal to 90. This definition applies to the midgrade categories of Conventional-Summer, Conventional-Winter, Reformulated-Summer, and Reformulated-Winter. For midgrade categories of RBOB-Summer, RBOB-Winter, CBOB-Summer, and CBOB-Winter, this definition refers to the expected octane rating of the finished gasoline after oxygenate has been added to the RBOB or CBOB.

3, 6, 9, 12, 16, 19, 22, 25. Premium grade gasoline is gasoline having an antiknock index, i.e., octane rating, greater than 90. This definition applies to the premium grade categories of Conventional-Summer, Conventional-Winter, Reformulated-Summer, and Reformulated-Winter. For premium grade categories of RBOB-Summer, RBOB-Winter, CBOB-Summer, and CBOB-Winter, this definition refers to the expected octane rating of the finished gasoline after oxygenate has been added to the RBOB or CBOB.

13. Gasoline – Other is any gasoline that is not defined elsewhere, including GTAB (gasoline treated as blendstock).

14 – 26. Blendstocks are petroleum products used for blending or compounding into finished motor gasoline. These include RBOB (reformulated blendstock for oxygenate blending) and CBOB (conventional blendstock for oxygenate blending), but exclude oxygenates, butane, and pentanes plus.

14 – 16. CBOB-Summer (conventional blendstock for oxygenate blending) means a petroleum product which, when blended with a specified type and percentage of oxygenate, meets the definition of Conventional-Summer.

17 – 19. CBOB-Winter (conventional blendstock for oxygenate blending) means a petroleum product which, when blended with a specified type and percentage of oxygenate, meets the definition of Conventional-Winter.

20 – 22. RBOB-Summer (reformulated blendstock for oxygenate blending) means a petroleum product which, when blended with a specified type and percentage of oxygenate, meets the definition of Reformulated-Summer.

23 – 25. RBOB-Winter (reformulated blendstock for oxygenate blending) means a petroleum product which, when blended with a specified type and percentage of oxygenate, meets the definition of Reformulated-Winter.

26. Blendstocks -- Others are products used for blending or compounding into finished motor gasoline that are not defined elsewhere. Excludes Gasoline Treated as Blendstock (GTAB), Diesel Treated as Blendstock (DTAB), conventional blendstock for oxygenate blending (CBOB), reformulated blendstock for oxygenate blending (RBOB),

oxygenates (e.g. fuel ethanol and methyl tertiary butyl ether), butane, and pentanes plus.

27 – 32. Oxygenates means substances which, when added to gasoline, increase the oxygen content of the gasoline. Common oxygenates are ethanol, methyl tertiary butyl ether (MTBE), ethyl tertiary butyl ether (ETBE), tertiary amyl methyl ether (TAME), diisopropyl ether (DIPE), and methanol.

27. Methanol (CH3OH) is an alcohol as described in "Oxygenates."

28. GTBA (gasoline-grade tertiary butyl alcohol, (CH3)3COH), or t-butanol, is an alcohol as described in "Oxygenates."

29. MTBE (methyl tertiary butyl ether, (CH3)3COCH3) is an ether as described in "Oxygenates."

30. ETBE (ethyl tertiary butyl ether, (CH3)3COC2H) is an ether as described in "Oxygenates."

31. TAME means tertiary amyl methyl ether, (CH3)2(C2H5)COCH3).

32. DIPE (diisopropyl ether, (CH3)2CHOCH(CH3)2) is an ether as described in "Oxygenates."

33 – 39, 44. Distillate Fuel Oil means a classification for one of the petroleum fractions produced in conventional distillation operations and from crackers and hydrotreating process units. The generic term distillate fuel oil includes kerosene, diesel fuels (Diesel Fuels No. 1, No. 2, and No. 4), and fuel oils (Fuel Oils No. 1, No. 2, and No. 4).

33 – 35. Distillate Fuel No. 1 has a maximum distillation temperature of 550 °F at the 90 percent recovery point and a minimum flash point of 100 °F and includes fuels commonly known as Diesel Fuel No. 1 and Fuel Oil No. 1, but excludes kerosene. This fuel is further subdivided into categories of sulfur content: High Sulfur (greater than 500 ppm), Low Sulfur (less than or equal to 500 ppm and greater than 15 ppm), and Ultra Low Sulfur (less than or equal to 15 ppm).

36 – 38. Distillate Fuel No. 2 has a minimum and maximum distillation temperature of 540 °F and 640 °F at the 90 percent recovery point, respectively, and includes fuels commonly known as Diesel Fuel No. 2 and Fuel Oil No. 2. This fuel is further subdivided into categories of sulfur content: High Sulfur (greater than 500 ppm), Low Sulfur (less than or equal to 500 ppm and greater than 15 ppm), and Ultra Low Sulfur (less than or equal to 15 ppm).

39. Distillate Fuel No. 4 is a distillate fuel oil made by blending distillate fuel oil and residual fuel oil, with a minimum flash point of 131 °F.

40. Residual Fuel Oil No. 5 (Navy Special) is a classification for the heavier fuel oil generally used in steam powered vessels in government service and inshore power plants. It has a minimum flash point of 131 °F.

41. Residual Fuel Oil No. 6 (a.k.a. Bunker C) is a classification for the heavier fuel oil generally used for the production of electric power, space heating, vessel bunkering and various industrial purposes. It has a minimum flash point of 140 °F.

42. Kerosene-Type Jet Fuel means a kerosene-based product used in commercial and military turbojet and turboprop aircraft. The product has a maximum distillation temperature of 400 °F at the 10 percent recovery point and a final maximum boiling point of 572 °F. Included are Jet A, Jet A-1, JP-5, and JP-8.

43. Kerosene is a light petroleum distillate with a maximum distillation temperature of 400 °F at the 10-percent recovery point, a final maximum boiling point of 572 °F, a minimum flash point of 100 °F, and a maximum freezing point of -22 °F. Included are No. 1-K and No. 2-K, distinguished by maximum sulfur content (0.04 and 0.30 percent of total mass, respectively), as well as all other grades of kerosene called range or stove oil. Excluded is kerosene-type jet fuel (see definition herein).

44. Diesel–Other is any distillate fuel oil not defined elsewhere, including Diesel Treated as Blendstock (DTAB).

45 – 46. Petrochemical Feedstocks means feedstocks derived from petroleum for the manufacture of chemicals, synthetic rubber, and a variety of plastics. This category is usually divided into naphthas less than 401 °F and other oils greater than 401 °F.

45. Naphthas (< 401 °F) is a generic term applied to a petroleum fraction with an approximate boiling range between 122 °F and 400 °F. The naphtha fraction of crude oil is the raw material for gasoline and is composed largely of paraffinic hydrocarbons.

46. Other Oils (> 401 °F) are oils with a boiling range equal to or greater than 401 °F that are generally intended for use as a petrochemical feedstock and are not defined elsewhere.

47 – 48. Unfinished oils are all oils requiring further processing, except those requiring only mechanical blending.
47. Heavy Gas Oils are petroleum distillates with an approximate boiling range from 651 °F to 1,000 °F.

48. Residuum is residue from crude oil after distilling off all but the heaviest components, with a boiling range greater than 1,000 °F.

49. Aviation Gasoline means a complex mixture of volatile hydrocarbons, with or without additives, suitably blended to be used in aviation reciprocating engines. Specifications can be found in ASTM Specification D910–07a, Standard Specification

for Aviation Gasolines (incorporated by reference, see §98.7).B0 means the maximum CH4 producing capacity of a waste stream, kg CH4/kg COD.

50. Special naphthas means all finished products with the naphtha boiling range (290° to 470 °F) that are generally 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 D1836-07, Standard Specification for Commercial Hexanes, and D235-02(2007), Standard Specification for Mineral Spirits (Petroleum Spirits) (Hydrocarbon Dry Cleaning Solvent), respectively. Naphthas to be blended or marketed as motor gasoline or aviation gasoline, or that are to be used as petrochemical and synthetic natural gas (SNG) feedstocks are excluded.

51. Lubricants include all grades of lubricating oils, from spindle oil to cylinder oil to those used in greases. Petroleum lubricants may be produced from distillates or residues.

52. Waxes means a solid or semi-solid material at 77 °F consisting of a mixture of hydrocarbons obtained or derived from petroleum fractions, or through a Fischer-Tropsch type process, in which the straight chained paraffin series predominates. This includes all marketable wax, whether crude or refined, with a congealing point between 80 (or 85) and 240 °F and a maximum oil content of 50 weight percent.

53. Petroleum coke means a black solid residue, obtained mainly by cracking and carbonizing of petroleum derived feedstocks, vacuum bottoms, tar and pitches in processes such as delayed coking or fluid coking. It consists mainly of carbon (90 to 95 percent), has low ash content, and may be used as a feedstock in coke ovens. This product is also known as marketable coke or catalyst coke.

54. Asphalt means a dark brown-to-black cement-like material obtained by petroleum processing and containing bitumens as the predominant component. It includes crude asphalt as well as the following finished products: cements, fluxes, the asphalt content of emulsions (exclusive of water), and petroleum distillates blended with asphalt to make cutback asphalts.

55. Road Oil is any heavy petroleum oil, including residual asphaltic oil used as a dust palliative and surface treatment on roads and highways. It is generally produced in six grades, from 0, the most liquid, to 5, the most viscous.

56. Still gas, or refinery gas, is any form or mixture of gases produced in refineries by distillation, cracking, reforming, and other processes. The principal constituents are methane, ethane, ethylene, normal butane, butylene, propane, and propylene.

57. Ethane is a paraffinic hydrocarbon with molecular formula C2H6.

58. Ethylene is an olefinic hydrocarbon with molecular formula C2H4.

59. Propane is a paraffinic hydrocarbon with molecular formula C3H8.

60. Propylene is an olefinic hydrocarbon with molecular formula C3H6.

61. Butane, or n-Butane, is a paraffinic straight-chain hydrocarbon with molecular formula C4H10.

62. Butylene, or n-Butylene, is an olefinic straight-chain hydrocarbon with molecular formula C4H8.

63. Isobutane is a paraffinic branch chain hydrocarbon with molecular formula C4H10.

64. Isobutylene is an olefinic branch chain hydrocarbon with molecular formula C4H8.

65. Pentanes Plus, or C5+, is a mixture of hydrocarbons that is a liquid at ambient temperature and pressure, and consists mostly of pentanes (five carbon chain) and higher carbon number hydrocarbons. Pentanes plus includes, but is not limited to, normal pentane, isopentane, hexanes-plus (natural gasoline), and plant condensate.

66. Miscellaneous Products include all refined petroleum products not defined elsewhere. It includes, but is not limited to, naphtha-type jet fuel (Jet B and JP-4), petrolatum lube refining by-products (aromatic extracts and tars), absorption oils, ram-jet fuel, petroleum rocket fuels, synthetic natural gas feedstocks, waste feedstocks, and specialty oils. It excludes organic waste sludges, tank bottoms, spent catalysts, and sulfuric acid.

67 – 70. Biomass means non-fossilized and biodegradable organic material originating from plants, animals and/or micro-organisms, including products, by-products, residues and waste from agriculture, forestry and related industries as well as the non-fossilized and biodegradable organic fractions of industrial and municipal wastes, including gases and liquids recovered from the decomposition of non-fossilized and biodegradable organic material.

67. Ethanol is an anhydrous alcohol with molecular formula C2H5OH.

68. Biodiesel means a mono-akyl ester derived from biomass and conforming to ASTM D6751-08, Standard Specification for Biodiesel Fuel Blend Stock (B100) for Middle Distillate Fuels.

69. Rendered animal fat, or tallow, means fats extracted from animals which are generally used as a feedstock in making biodiesel.

70. Vegetable Oil means oils extracted from vegetation that are generally used as a feedstock in making biodiesel.

Methods and Assumptions Used to Derive Emission factors

General Methods

All emission factors were derived from the same basic formula: density multiplied by share of carbon in the fuel. Density is expressed as metric tons of product per barrel. Share of carbon is expressed as percentage of total mass. Where density data are gathered in units of API gravity they are converted to specific gravity using the following formula:

Specific Gravity = 141.5 / (API Gravity + 131.5)

Specific Gravity is the ratio of the density of the petroleum product to the density of water at 39 degrees Fahrenheit.

The density of water is 8.33 pounds per gallon. Pounds per gallon of a petroleum product can be calculated by multiplying its specific gravity by 8.33 pounds per gallon.

There are 42 gallons in a U.S. barrel. Metric tons per barrel can be calculated by multiplying pounds per gallon of petroleum product by 42, then dividing by 2204.62, the number of pounds in a metric ton.

Density values reflect products at 60 degrees Fahrenheit and one atmosphere, unless otherwise noted.

We used 44/12 as the factor for converting carbon to carbon dioxide.

Conventional—Summer

The density in the proposed rule was 0.12 tonnes/bbl, from Dickson, Cheryl, *Petroleum Product Surveys*, Northrop Grumman, Motor Gasolines, 2008.

For the final rule, EPA is providing density values for the breakdown of regular, mid-grade, and premium conventional summer gasolines. EPA has determined these values to be 0.1181, 0.1183, and 0.1185 tonnes/bbl, respectively, from Dickson, Cheryl, *Petroleum Product Surveys*, Northrop Grumman, Motor Gasolines, Summer 2008, published April 2009, Table 1, pg 24. "Summary of Values, Motor Gasoline Survey, Summer 2008", average API values for regular and premium. Density and carbon share for midgrade represents the average of regular and premium.

The carbon share in the proposed rule was 86.96 percent and was calculated based on the composition of a regular unleaded gasoline sample sourced from a Marathon Petroleum Material Safety Data Sheet (http://www.marathonpetroleum.com/content/documents/mpc/msds/0127MAR019.pdf).

For the final rule, EPA is providing carbon share values for the breakdown of regular, mid-grade, and premium conventional summer gasolines. EPA has determined these values to be 86.66, 86.63, and 86.61 percent, respectively, based on a compositional analysis from Dickson, Cheryl, *Petroleum Product Surveys*, Northrop Grumman, Motor Gasolines, Summer 2008, Table 1, pg 24.. Based on 95 samples of regular grade gasoline and 95 samples of premium grade gasoline, the values used to determine carbon share are as follows:

	Percent Mass		Carbon share (% mass), based on molecular formula
	Regular	Premium	
Aromatics (assumed toluene)	32.17	32.75	91.25
Olefins ($C_nH_{2n,}$ assumed 2-methyl-2-butene)	8.44	3.99	85.63
Saturated Hydrocarbons ($C_nH_{2n+2,}$ assumed octane)	57.97	62.09	84.12
Benzene	1.41	1.17	92.26

A weighted average of the carbon share of these compounds was calculated to get the percent mass carbon for regular, mid-grade, and premium conventional summer gasolines.

1. **Regular** (Conventional—Summer): Emission factor did not appear in the proposed Mandatory Reporting Rule—see "Conventional—Summer" above for discussion of emission factor developed.

2. **Midgrade** (Conventional—Summer): Emission factor did not appear in the proposed Mandatory Reporting Rule—In the absence of available sample data, density and carbon share for midgrade gasoline was assumed to be the average of density and carbon share for regular and premium grades of conventional summer gasoline .

3. **Premium** (Conventional—Summer): Emission factor did not appear in the proposed Mandatory Reporting Rule—see "Conventional—Summer" above for discussion of emission factor developed.

Conventional—Winter

The density in the proposed rule was 0.12 tonnes/bbl, from Dickson, Cheryl, *Petroleum Product Surveys*, Northrop Grumman, Motor Gasolines, 2008.

For the final rule, EPA is providing density values for the breakdown of regular, mid-grade, and premium conventional winter gasolines. EPA has determined these values to be 0.1155, 0.1161, and 0.1167 tonnes/bbl, respectively, based on a compositional analysis from Dickson, Cheryl, *Petroleum Product Surveys*, Northrop Grumman, Motor Gasolines, Winter 2007-2008, published July 2008, Table 1, pg 24, average API values

for regular and premium. Density and carbon share of midgrade represents average of regular and premium.

The carbon share in the proposed rule was 86.96 percent, based on the same assumptions as "Conventional—Summer"

For the final rule, EPA is providing carbon share values for the breakdown of regular, mid-grade, and premium conventional winter gasolines. EPA has determined these values to be 86.50, 86.55, and 86.59 percent, respectively, based on a compositional analysis from sample data in Dickson, Cheryl, *Petroleum Product Surveys*, Northrop Grumman, Motor Gasolines, for Winter 2007-2008, Table 1, pg. 24. Based on 174 samples of regular grade gasoline and 174 samples of premium grade gasoline, the values used to determine carbon share are as follows:

	Percent Mass		Carbon share % mass), based on molecular formula
	Regular	Premium	
Aromatics (assumed toluene)	29.87	32.45	91.25
Olefins ($C_nH_{2n,}$ assumed 2-methyl-2-butene)	9.73	4.61	85.63
Saturated Hydrocarbons ($C_nH_{2n+2,}$ assumed octane)	59.10	61.89	84.12
Benzene	1.41	1.06	92.26

A weighted average of the carbon share of these compounds (excluding ethanol) was calculated to get the percent mass carbon for regular, mid-grade, and premium conventional winter gasolines.

4. **Regular** (Conventional—Winter): Emission factor did not appear in the proposed Mandatory Reporting Rule—see "Conventional—Winter" above for discussion of emission factor developed.

5. **Midgrade** (Conventional—Winter): Emission factor did not appear in the proposed Mandatory Reporting Rule—In the absence of available sample data, density and carbon share for midgrade gasoline was assumed to be the average of density and carbon share for regular and premium grades of conventional winter gasoline.

6. **Premium** (Conventional—Winter): Emission factor did not appear in the proposed Mandatory Reporting Rule—see "Conventional—Winter" above for discussion of emission factor developed.

Reformulated—Summer

The density in the proposed rule was 0.12 tonnes/bbl, from Dickson, Cheryl, *Petroleum Product Surveys*, Northrop Grumman, Motor Gasolines, 2008.

For the final rule, EPA is providing density values for the breakdown of regular, mid-grade, and premium non-ethanol portion of reformulated-summer gasolines. EPA has determined these values to be 0.1167, 0.1165, and 0.1164 tonnes/bbl, respectively, from Dickson, Cheryl, *Petroleum Product Surveys*, Northrop Grumman, Motor Gasolines, Summer 2008, published April 2009. These values were derived from 165 samples of regular grade reformulated gasoline, and 164 samples of premium grade reformulated gasoline. See Table 5, pg 28, of "Summary of Values, Motor Gasoline Survey, Summer 2008, Reformulated Alcohol Blended Fuels" for average API gravity values for regular and premium. Density and carbon share were adjusted to reflect only the non-ethanol portion of the fuels. Density and carbon share for midgrade equals the average of regular and premium.

The carbon share in the proposed rule was 86.60 and was calculated based on the composition of a sample of regular unleaded gasoline with ethanol sourced from a Marathon Petroleum Material Safety Data Sheet (http://www.marathonpetroleum.com/content/documents/mpc/msds/0130MAR019.pdf).

For the final rule, EPA is providing carbon share values for the breakdown of regular, mid-grade, and premium reformulated-summer gasolines excluding the ethanol portion of the fuel. EPA has determined these values to be 86.13, 86.07, and 86.00 percent, respectively, based on a compositional analysis from sample data in Dickson, Cheryl, *Petroleum Product Surveys*, Northrop Grumman, Motor Gasolines for Summer 2008, Table 5, pg. 28. Based on 165 samples of regular grade gasoline and 164 samples of premium grade gasoline, the values used to determine carbon share of the non-ethanol portion of the fuels are as follows:

	Percent Mass		Carbon share (% mass), based on molecular formula
	Regular	Premium	
Aromatics (assumed toluene)	25.71	24.26	91.25
Olefins ($C_nH_{2n,}$ assumed 2-methyl-2-butene)	6.67	5.93	85.63
Saturated Hydrocarbons ($C_nH_{2n+2,}$ assumed octane)	66.68	69.03	84.12
Benzene	0.91	0.78	92.26

A weighted average of the carbon share of these compounds (excluding ethanol) was calculated to get the percent mass carbon for regular, mid-grade, and premium reformulated summer gasolines.

7. **Regular** (Reformulated—Summer): Emission factor did not appear in the proposed Mandatory Reporting Rule—see "Reformulated—Summer" above for discussion of emission factor developed.

8. **Midgrade** (Reformulated—Summer): Emission factor did not appear in the proposed Mandatory Reporting Rule—In the absence of available sample data, density and carbon share for midgrade gasoline was assumed to be the average of density and carbon share for regular and premium grades of reformulated summer gasoline.

9. **Premium** (Reformulated—Summer): Emission factor did not appear in the proposed Mandatory Reporting Rule—see "Reformulated—Summer" above for discussion of emission factor developed.

Reformulated—Winter

The density in the proposed rule was 0.12 tonnes/bbl, from Dickson, Cheryl, *Petroleum Product Surveys*, Northrop Grumman, Motor Gasolines, 2008.

For the final rule, EPA is providing density values for the breakdown of regular, mid-grade, and premium for the non-ethanol portion of reformulated winter gasolines. EPA has determined these values to be 0.1165, 0.1165, and 0.1166 tonnes/bbl, respectively, from Dickson, Cheryl, *Petroleum Product Surveys*, Northrop Grumman, Motor Gasolines, Winter 2007-2008, published July 2008. See Table 5, pg 28, of "Summary of Values, Motor Gasoline Survey, Winter 2007-2008, Reformulated Alcohol Blended Fuels" for average API gravity values for regular and premium. Density and carbon share were adjusted to reflect only the non-ethanol portion of the fuels. Density and carbon share for midgrade equals the average of regular and premium.

For the proposed rule carbon shares were based on the same assumptions as Reformulated—Summer.

For the final rule, EPA is providing carbon share values for the breakdown of regular, mid-grade, and premium reformulated-winter gasolines excluding the ethanol portion of the fuel. EPA has determined these values to be 86.05, 86.06, and 86.06 percent, respectively, based on a compositional analysis from sample data in Dickson, Cheryl, *Petroleum Product Surveys*, Northrop Grumman, Motor Gasolines Winter 2007-2008. Based on 145 samples of regular grade gasoline and 144 samples of premium grade gasoline, the values used to determine carbon share of the non-ethanol portion of the fuels are as follows:

	Percent Mass		Carbon share (% mass), based on molecular formula
	Regular	Premium	
Aromatics (assumed toluene)	24.66	25.25	91.25

Olefins ($C_nH_{2n,}$ assumed 2-methyl-2-butene)	6.42	6.02	85.63
Saturated Hydrocarbons ($C_nH_{2n+2,}$ assumed octane)	68.00	68.08	84.12
Benzene	0.92	0.65	92.26

Similar to the proposed rule, a weighted average of the carbon share of these compounds (excluding ethanol) was calculated to get the percent mass carbon for regular, mid-grade, and premium reformulated winter gasolines.

10. **Regular** (Reformulated—Winter): Emission factor did not appear in the proposed Mandatory Reporting Rule—see "Reformulated—Winter" above for discussion of emission factor developed.

11. **Midgrade** (Reformulated—Winter): Emission factor did not appear in the proposed Mandatory Reporting Rule—In the absence of available sample data, density and carbon share for midgrade gasoline was assumed to be the average of density and carbon share for regular and premium grades of reformulated winter gasoline.

12. **Premium** (Reformulated—Winter): Emission factor did not appear in the proposed Mandatory Reporting Rule—see "Reformulated—Winter" above for discussion of emission factor developed.

13. **Gasoline —Other**

This product category and associated emissions factor was not in the proposed rule. In absence of available sample data, EPA is assuming that any other type of gasoline can be represented by the finished motor gasoline in Table 1 with the most conservative density and carbon share factors, which is Conventional Summer Premium.

Blendstocks

14 – 19. **CBOB**

In the proposed rule, physical properties for CBOB were assumed equal to the properties of conventional motor gasoline.

For the final rule, EPA is assuming that the density and carbon share of CBOB is equal to the density and carbon share of the relevant grade and seasonal type of conventional motor gasoline.

20 – 25. **RBOB**

Density in the proposed rule was taken from CITGO MSDS:

http://www.msds.com/index.asp?open=/protected_public/loginsuccessful.asp
At 60°F, avg density = 6.0-6.4 lbs/gal (.1143-.1219 tonnes/bbl)

In the proposed rule, carbon share was assumed to equal to the properties of reformulated gasoline.

For the final rule, EPA is assuming that both the density and carbon share of RBOB are equal to the density and carbon share of the relevant grade and seasonal type of reformulated motor gasoline.

26. **Blendstocks - Other**

The density and carbon share in the proposed rule was based on the assumption that other blendstocks could be represented by isooctane. Density for isooctane came from: http://msds.chem.ox.ac.uk/TR/2,2,4-trimethylpentane.html. Carbon share was based on the molecular formula of isooctane (C_8H_{10}).

For the final rule, EPA is assuming that other blendstocks can be represented by the finished motor gasoline with the most conservative density and carbon share factors, which is Conventional Summer Premium.

Oxygenates

27. **Methanol**

The density in the proposed rule was 0.13 tonnes/bbl, from a Material Safety Data Sheet for methanol (http://avogadro.chem.iastate.edu/MSDS/methanol.htm).

For the final rule, EPA is updating the density to 0.1268 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 15: Density of Solvents as a Function of Temperature. Specifically, the handbook provides density values as a function of temperature between 0 and 100°C at intervals of 10°C. The EPA fit these data to a polynomial of order 2 and then used the fit to extrapolate the value of the density at 60°F.

The carbon share in the proposed rule was 37.50%, calculated from the molecular formula for methanol, CH_3OH.

For the final rule, EPA is updating the carbon share to 37.48% based upon more precise values for the atomic weight of the elements in the compound from the periodic table.

28. **GTBA**

The density in the proposed rule was 0.12 tonnes/bbl, from Material Safety Data Sheets for GTBA (http://www.sciencestuff.com/msds/C1403.html and

http://msds.chem.ox.ac.uk/BU/tert-butyl_alcohol.html).

For the final rule, EPA is updating the density to 0.1257 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 3: Physical Constants of Organic Compounds. Density was corrected to 60°F using the API Manual for Petroleum Measurement Standards (MPMS) Chapter 11.1, "Temperature and Pressure Volume Correction Factors for Refined Products".

The carbon share in the proposed rule was 64.90%, calculated from the molecular formula for GTBA, C_4H_9OH.

For the final rule, EPA is updating the carbon share to 64.82% based upon more precise values for the atomic weight of the elements in the compound from the periodic table.

29. **MTBE**

The density in the proposed rule was 0.12 tonnes/bbl, taken from American Petroleum Institute, Alcohols and Ethers: A Technical Assessment of Their Applications as Fuels and Fuel Components, API 4261.

For the final rule, EPA is updating the density to 0.1181 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 3: Physical Constants of Organic Compounds. Density was corrected to 60°F using the API MPMS Chapter 11.1, "Temperature and Pressure Volume Correction Factors for Refined Products".

The carbon share in the proposed rule was 68.20%, calculated from the molecular formula for MTBE, $(CH_3)_3COCH_3$).

For the final rule, EPA is updating the carbon share to 68.13% based upon more precise values for atomic weight of the elements in the compound from the periodic table.

30. **ETBE**

The density in the proposed rule was 0.12 tonnes/bbl, taken from American Petroleum Institute, Alcohols and Ethers: A Technical Assessment of Their Applications as Fuels and Fuel Components, API 4261.

For the final rule, EPA is updating the density to 0.1182 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 3: Physical Constants of Organic Compounds. Density was corrected to 60°F using the API MPMS Chapter 11.1, "Temperature and Pressure Volume Correction Factors for Refined Products".

The carbon share in the proposed rule was 70.50%, calculated from the molecular formula for ETBE, $(CH_3)_3COC_2H_5$.

For the final rule, EPA is updating the carbon share to 70.53% based upon more precise values for atomic weight of the elements in the compound from the periodic table.

31. **TAME**

The density in the proposed rule was 0.12 tonnes/bbl, taken from American Petroleum Institute, Alcohols and Ethers: A Technical Assessment of Their Applications as Fuels and Fuel Components, API 4261.

For the final rule, EPA is updating the density to 0.1229 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 3: Physical Constants of Organic Compounds. Density was corrected to 60°F using the API MPMS Chapter 11.1, "Temperature and Pressure Volume Correction Factors for Refined Products".

The carbon share in the proposed rule was 70.5 percent based on the molecular formula for TAME $(CH_3)_2(C_2H_5)COCH_3$.

For the final rule, EPA is updating the carbon share to 70.53% based upon more precise values for atomic weight of the elements in the compound from the periodic table.

32. **DIPE**

The density in the proposed rule was 0.12 tonnes/bbl, from a Material Safety Data Sheet for DIPE (http://www.coleparmer.com/Catalog/Msds/00803.htm).

For the final rule, EPA is updating the density to 0.1156 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 3: Physical Constants of Organic Compounds. Density was corrected to 60°F using the API MPMS Chapter 11.1, "Temperature and Pressure Volume Correction Factors for Refined Products".

The carbon share in the proposed rule was 70.50%, calculated from the molecular formula for DIPE, $C_6H_{14}O$.

For the final rule, EPA is updating the carbon share to 70.53% based upon more precise values atomic weight of the elements in the compound from the periodic table.

Distillate Fuel Oil

33 - 35. **Distillate Fuel Oil No. 1**

In the proposed rule, EPA included separate categories for Fuel Oil No. 1 and Diesel No. 1. For the final rule, EPA is combining these two product categories under Distillate Fuel Oil No. 1 because EPA believes the products have very similar, if not identical,

characteristics. Values for Ultra Low, Low, and High Sulfur Fuel Oil No. 1 are provided for reporting clarity but, given data constraints, we are assuming the same density and carbon share for each sulfur class.

The density for Fuel Oil No. 1 and Diesel No. 1 in the proposed rule was 0.13 tonnes/bbl, taken from "The Engineering ToolBox" (http://www.engineeringtoolbox.com/fuels-densities-specific-volumes-d_166.html).

For the final rule, EPA is listing the density of Distillate Fuel Oil No. 1 as 0.1346 tonnes/bbl, based upon 4 samples of No. 1 Regular Diesel S15 from the Alliance of Automobile Manufacturers, Diesel Survey - Winter 2008, which EPA believes best represents the characteristics of this product.

The carbon share for both products was 86.40 percent in the proposed rule and remains the same in the final rule, drawn from the carbon share for Fuel Oil No. 1 in Perry's Chemical Engineer's Handbook, 1997 ed., pg. 27-10, Table 27-6.

36 - 38. **Distillate Fuel Oil No. 2**

In the proposed rule EPA included separate categories for Fuel Oil No. 2 and Diesel No. 2. For the final rule EPA is combining these two product categories under Distillate Fuel Oil No. 2 because EPA believes the products have very similar, if not identical, characteristics. Values for Ultra Low, Low, and High Sulfur Fuel Oil No. 2 are provided for reporting clarity but, given data constraints, we are assuming the same density and carbon share for each sulfur class.

The density for Fuel Oil No. 2 and Diesel No. 2 in the proposed rule was drawn from Dickson, Cheryl, *Petroleum Product Surveys*, Northrop Grumman, Diesel Fuel Oils, 2007, pg. 13, Table 2.

For the final rule, EPA has assumed that Distillate Fuel Oil No.2 is most widely represented by Ultra-low Sulfur No. 2 Diesel Fuel. Based upon 144 samples of No. 2 Regular Diesel S15 from the Alliance of Automobile Manufacturers, Diesel Survey - Winter 2008, EPA found a density of 0.1342 tonnes/bbl.

In the proposed rule, the carbon share for Fuel Oil No. 2 was taken from Perry's Chemical Engineer's Handbook, 1997 ed., pg. 27-10, Table 27-6. Carbon share for Diesel No. 2 was based on EIA's Documentation for Emissions of Greenhouse Gases in the United States, October 2008, pg. 191: "If one knows nothing about the composition of a particular petroleum product, assuming that it is 85.7 percent carbon by mass is not an unreasonable first approximation."

In the final rule, EPA adopts a carbon share for Distillate Fuel Oil No. 2 of 87.3 percent from Perry's Chemical Engineer's Handbook, 8th ed., 2008, Table 24-6, pg. 24-9.

39. **Distillate Fuel Oil No. 4**

In the proposed rule, EPA included separate categories for Fuel Oil No. 4 and Diesel No. 4. For the final rule, EPA is combining these two product categories under Distillate Fuel Oil No. 4 because EPA believes the products have very similar, if not identical, characteristics.

The density for Fuel Oil No. 4 and Diesel No. 4 in the proposed rule was 0.15 tonnes/bbl, taken from "The Engineering ToolBox" (http://www.engineeringtoolbox.com/fuels-densities-specific-volumes-d_166.html).

For the final rule, EPA has updated this density to 0.1452 tonnes/bbl from Perry's Chemical Engineer's Handbook, 8th ed., 2008, pg. 24-9, Table 24-6.

In the proposed rule, the carbon share for both products was 86.47 percent, taken from the carbon share for Fuel Oil No. 4 in Perry's Chemical Engineer's Handbook, 8th ed., 2008, pg. 24-9, Table 24-6. This carbon share remains unchanged in the final rule.

40. **Residual Fuel Oil No. 5 (Navy Special)**

The density in the proposed rule was 0.14 tonnes/bbl, taken from Wauquier, J.-P., ed. Petroleum Refining, Crude Oil, Petroleum Products and Process Flowsheets (Editions Technip - Paris, 1995) pg. 225, Table 5.16.

In the final rule the density was updated to four significant digits.

In the proposed rule, the carbon share was assumed to be 85.7% based on from EIA's Documentation for Emissions of Greenhouse Gases in the United States, October 2008, pg. 191: "If one knows nothing about the composition of a particular petroleum product, assuming that it is 85.7 percent carbon by mass is not an unreasonable first approximation.

For the final rule, EPA has used a carbon share of 85.67%, the average of 12 ultimate analyses of residual oil samples gathered by EIA in 1994, from Science Applications International Corporation, *Carbon Emissions Coefficients for U.S. Fuels,* prepared for U.S. Energy Information Administration, October 31, 1994.

41. **Residual Fuel Oil No. 6 (a.k.a. Bunker C)**

The density in the proposed rule was 0.16 tonnes/bbl, taken from Perry's Chemical Engineer's Handbook, 1997 ed., Table 27-6, pg. 27-10.

For the final rule, EPA is updating the density to 0.1528 tonnes/bbl from Perry's Chemical Engineer's Handbook, 8th ed., 2008, Table 24-6, pg. 24-9.

The carbon share in the proposed rule was 85.68% taken from Perry's Chemical Engineer's Handbook, 1997 ed., Table 27-6, pg. 27-10.

For the final rule, EPA is updating the carbon share to 84.67% from Perry's Chemical Engineer's Handbook, 8th ed., 2008, Table 24-6, pg. 24-9.

42. **Kerosene-Type Jet Fuel**

For both the proposed rule and final rule, the density and carbon share of kerosene-based jet fuels was based on the average composition of 39 fuel samples taken by Boeing Corporation in 1989. Data was drawn from O.J. Hadaller and A.M. Momenthy, *The Characteristics of Future Fuels,* Part 1, "Conventional Heat Fuels" (Seattle, WA: Boeing Corp., September 1990), pp. 46-50. In the final rule, the density was updated to four significant digits.

The data sources are the same as those in EIA's Documentation for Emissions of Greenhouse Gases in the United States, October 2008..

43. **Kerosene**

The density and carbon share in the proposed rule reflect the average of five ultimate analyses of No. 1 fuel oil samples, taken from EIA's Documentation for Emissions of Greenhouse Gases in the United States.

For the final rule, EPA is assuming that the density and carbon share for kerosene are the same as Distillate No. 1 because the physical characteristics of the products are very similar.

44. **Diesel - Other**

This product category and associated emissions factor was not in the proposed rule. EPA is assuming the most conservative density and carbon share factors from Distillate fuel oil Numbers 1, 2, and 4, which are those for No. 4.

Petrochemical Feedstocks

45. **Naphthas (< 401 °F)**

For both the proposed rule and final rule, density is drawn from Meyers, *Handbook of Petroleum Refining Processes*, 3rd ed., (New York, NY: McGraw Hill, 2004), p. 2.10.

For both the proposed rule and final rule, the carbon share of naphthas is estimated based on G.H. Unzelman, "A Sticky Point for Refiners: FCC Gasoline and the Complex Model," *Fuel Reformulation* (July/August 1992), p. 29. The data sources are the same

as those in EIA's Documentation for Emissions of Greenhouse Gases in the United States.

46. **Other Oils (> 401 °F)**

In the proposed rule the density and carbon share were assumed to match Fuel Oil No.2, taken from EIA's Documentation for Emissions of Greenhouse Gases in the United States. Oct. 2007.

For the final rule, EPA is updating the density to 0.1390 tonnes/bbl, the maximum density requirement for Fuel Oil No.2 in ASTM Standard D396-09. EPA is also adopting a carbon share of 87.30 percent from Perry's Chemical Engineer's Handbook, 8th ed., 2008 Table 24-6, pg. 24-9.

Unfinished Oils

47. **Heavy Gas Oils**

Density and carbon share factors did not change from the proposed rule to the final rule, except that the factors were updated to four significant digits. The density and carbon share for heavy gas oils were taken from Shell Oil Company Mars Blend Crude assay page, www.marscrude.com/mars_assays/july99/assay99.xls, January 28, 2009.

48. **Residuum**

Density and carbon share factors did not change from the proposed rule to the final rule, except that the factors were updated to four significant digits.

The density for residuum is drawn from Shell Oil Company Mars Blend Crude assay page, www.marscrude.com/mars_assays/july99/assay99.xls.

Carbon share was assumed to be 85.7% from EIA's Documentation for Emissions of Greenhouse Gases in the United States, October 2008, pg. 191: "If one knows nothing about the composition of a particular petroleum product, assuming that it is 85.7 percent carbon by mass is not an unreasonable first approximation."

Other Petroleum Products and Natural Gas Liquids

49. **Aviation Gasoline (Finished)**

A carbon coefficient for aviation gasoline in both the proposed rule and final rule was calculated on the basis of the EIA standard heat content of 5.048 million Btu per barrel from EIA, *Annual Energy Review*, Appendix A (Washington, D.C., 2008) www.eia.doe.gov/emeu/aer. This heat content correlates to a specific gravity of approximately 0.7057 according to *Thermal Properties of Petroleum Products, Bureau of Standards* No.97 (1929). Based on U.S. EPA, *Inventory of U.S. Greenhouse Gas*

Emissions and Sinks: 1990 -2007, Annex 2, Page A-62. aviation gasoline was assumed to be 87.5% iso-octane, 9.0% toluene, and 3.5% xylene. According to American Society for Testing and Materials, ASTM and Other Specifications for Petroleum Products and Lubricants (Philadelphia, PA, 1985),the maximum allowable sulfur content in aviation gasoline is 0.05 percent, and the maximum allowable lead content is 0.1 percent. These amounts were judged negligible and were excluded for the purposes of this analysis. This composition yielded a carbon share of 85.00 percent.

50. **Special Naphthas**

Density and carbon share factors did not change from the proposed rule to the final rule and are based on an analysis of five types of special napthas in EIA's Documentation for Emissions of Greenhouse Gases in the United States*.* For the final rule the density was updated to four significant digits.

There are five special naphthas: hexane, odorless solvent, Stoddard solvent, high flash point, and mineral spirits. Hexane is a pure paraffin containing 6 carbon atoms and 14 hydrogen atoms. Thus, it is 83.63% carbon. Its density is 0.1043 tonnes/bbl. The other hydrocarbon compounds in special naphthas are assumed to be either paraffinic or aromatic. The portion of aromatics in odorless solvents is estimated at less than 1% with a density of 55 degrees API or 6.32 pounds per gallon and a carbon share of 84.51%. Stoddard solvents have a carbon content of 84.44%, contain 15% aromatics, and have an estimated density of 47.9 degrees API or 6.57 pounds per gallon. High flash point solvents also contain 15% aromatics, have an estimated carbon content of 84.7% and a density of 47.6 degrees API or 6.58 pounds per gallon. High solvency mineral spirits contain 30% aromatics, have an estimated carbon share of 85.83% and a density of 43.6 degrees API or 6.73 pounds per gallon (Boldt and Hall, 1985). The carbon coefficients of the five special naphthas are weighted according to the following formula: approximately 10% of all special naphtha consumed is hexane and the remaining 90% is assumed to be distributed evenly among the four other solvents.

Table 6-9. Characteristics of Non-hexane Special Naphthas

Special Naphtha	Aromatic Content (Percent Volume)	Density (Degrees API)	Carbon Content (Percent Mass)	Carbon Coefficient (MMTC/QBtu)
Odorless Solvent	1	55.0	84.51	19.41
Stoddard Solvent	15	47.9	84.44	20.11
High Flash Point	15	47.6	84.70	20.17
Mineral Spirits	30	43.6	85.83	20.99

Note: All coefficients based on Higher Heating (Gross Calorific) Value and assume 100% combustion.

51. **Lubricants**

Density and carbon share factors did not change from the proposed rule to the final rule, except that the density factor was updated to four significant digits.

The ASTM Petroleum Measurement Tables give the density of lubricants at 25.6 degrees API or 0.1428 tonnes/bbl degrees API (*ASTM and Other Specifications for Petroleum Products and Lubricants,* Philadelphia, PA, 1985).

Ultimate analysis of a single sample of motor oil yielded a carbon content of 85.8%. Standard heat content was adopted from EIA, Annual Energy Review (2008), Appendix A,www.eia.doe.gov/emeu/aer/contents.html.

52. **Waxes**

The density and carbon share of waxes are unchanged in the final rule, except that the factors were updated to four significant digits.

Carbon content of waxes was drawn from EIA's Documentation for Emissions of Greenhouse Gases in the United States. Paraffin waxes are assumed to be composed of 100% paraffinic compounds with a chain of 25 carbon atoms. The resulting carbon share for paraffinic wax is 85.23%. Microcrystalline waxes are assumed to consist of 50% paraffinic and 50% cycloparaffinic compounds with a chain of 40 carbon atoms, yielding a carbon share of 85.56%.

The density of paraffin wax is estimated at 45 degrees API or 0.1273 metric tons per barrel from American Society for Testing and Materials***,*** *ASTM and Other Specifications for Petroleum Products and Lubricants* (Philadelphia, PA, 1985). The density of microcrystalline waxes is estimated at 36.7 degrees API or 0.1335 metric tons per barrel based on 10 samples found in V. Guthrie (ed.), *Petroleum Products Handbook* (New York, NY: McGraw-Hill, 1960).

A weighted average density and carbon coefficient was calculated for petroleum waxes, assuming that wax consumption is 80% paraffin wax and 20% microcrystalline wax. The weighted average carbon content is 85.30%, and the weighted average density is 0.1285 metric tons per barrel.
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53. **Petroleum Coke**

The density in the proposed rule was 0.0698 tonnes/bbl, taken from “The Engineering ToolBox” (http://www.engineeringtoolbox.com/fuels-densities-specific-volumes-d_166.html).

For the final rule, EPA is updating the density to 0.1818 tonnes/bbl, from *ASTM and Other Specifications for Petroleum Products and Lubricants,* Philadelphia, PA, 1985.

The carbon share in the proposed rule was 92.28%, estimated from two samples from S. W. Martin, "Petroleum Coke," in Virgil Guthrie (ed.), *Petroleum Processing Handbook* (New York, NY: McGraw-Hill, 1960), pp. 14-15. This carbon share remains unchanged in the final rule.

54 - 55. **Asphalt and Road Oil**

Density and carbon share factors did not change from the proposed rule to the final rule, except that the density factor was updated to four significant digits.

The ASTM petroleum measurement tables show a density of 5.6 degrees API or 0.1634 tonnes/bbl (*ASTM and Other Specifications for Petroleum Products and Lubricants,* Philadelphia, PA, 1985).

Ultimate analyses of twelve samples of asphalts showed an average carbon content of 83.47% from EIA's Documentation for Emissions of Greenhouse Gases in the United States, October 2008, Chapter 6, pg. 201.

56. **Still Gas**

In the proposed rule, density and carbon share were drawn from EIA data on four samples of still gas. The table below shows the composition of those samples.

Composition for Four Samples of Still Gas

Sample	Hydrogen (percent)	Methane (percent)	Ethane (percent)	Propane (percent)
One	12.7	28.1	17.1	11.9
Two	34.7	20.5	20.5	6.7
Three	72.0	12.8	10.3	3.8
Four	17.0	31.0	16.2	2.4

One still gas sample was drawn from American Gas Association, *Gas Engineer's Handbook,* (New York, NY: Industrial Press, 1974), pg. 3.71, and three still gas samples came from C.R. Guerra, K. Kelton, and D.C. Nielsen, Natural Gas Supplementation with Refinery Gases and Hydrogen," in Institute of Gas Technology, *New Fuels and Advances in Combustion Technologies* (Chicago, IL, June 1979).

In the final rule, density is estimated at 0.1405 metric tons per barrel based on the heat content of still gas as estimated by EIA, 6.0 million Btu per barrel, and the relationship of heat content to density from U.S. Department of Commerce, Bureau of Standards,

Thermal Properties of Petroleum Products, Miscellaneous Publication No.97, November 9, 1929.

Carbon content is assumed to equal 77.7% based on data from the 2006 Intergovernmental Panel on Climate Change Guidelines, Volume 2; Energy Tables 1.2 and 1.3. Background calculations:

Net calorific content of refinery (still) gas is 49.5 TJ/Gg, and carbon content of refinery (still) gas is 15.7 kg C/GJ.

15.7 kg/GJ = 15.7 Mg/TJ = 0.0157 Gg C/TJ

0.0157 Gg C/TJ * 49.5 TJ/Gg still gas = 0.777 Gg C/Gg still gas = 77.7 mass% C in still gas

57. **Ethane**

The density in the proposed rule was 0.592 tonnes/bbl, from V.B. Guthrie (ed.), Characteristics of Compounds, Petroleum Products Handbook, (New York, NY: McGraw Hill, 1960), pg. 3-3.

For the final rule, EPA is updating the density to 0.0866 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 3. Density is at -89ºC / -128ºF. This is the density of liquid ethane; it is a gas at 60°F and 1 atm.

The carbon share in the proposed rule was 80.00%, calculated from the molecular formula for ethane, C_2H_6.

For the final rule, EPA is updating this number to 79.89% based upon more precise values for atomic weights of the elements in the compound from the periodic table.

58. **Ethylene**

The density in the proposed rule was 0.0901 tonnes/bbl, from a Material Safety Data Sheet for ethylene (http://www.rmisonline.com/chemicaldatabase/ViewInfo1.aspx?SID=112).

For the final rule, EPA is updating the density to 0.0903 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 3. Density is at -104ºC / -155ºF. This is the density of liquid ethylene; it is a gas at 60°F and 1 atm.

The carbon share in the proposed rule was 85.71%, calculated from the molecular formula for ethylene, C_2H_4.

For the final rule, EPA is updating this number to 85.63% based upon more precise values for atomic weights of the elements in the compound from the periodic table.

59. **Propane**

The density in the proposed rule was 0.0783 tonnes/bbl, from V.B. Guthrie (ed.), Characteristics of Compounds, Petroleum Products Handbook, (New York, NY: McGraw Hill, 1960), pg. 3-3.

For the final rule, EPA is updating the density to 0.0784 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 3. Density is at -25ºC / -77ºF. This is the density of liquid propane; it is a gas at 60°F and 1 atm.

The carbon share in the proposed rule was 81.80%, calculated from the molecular formula for propane, C_3H_8.

For the final rule, EPA is updating this number to 81.71% based upon more precise values for atomic weights of the elements in the compound from the periodic table.

60. **Propylene**

The density in the proposed rule was 0.0825 tonnes/bbl, from V.B. Guthrie (ed.), *Characteristics of Compounds, Petroleum Products Handbook*, (New York, NY: McGraw Hill, 1960), pg. 3-3.

For the final rule, EPA is updating the density to 0.0803 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 3. Density is at -25ºC / -77ºF. This is the density of liquid propylene; it is a gas at 60°F and 1 atm.

The carbon share in the proposed rule was 85.71%, calculated from the molecular formula for propylene, C_3H_6.

For the final rule, EPA is updating this number to 85.63% based upon more precise values for atomic weights of the elements in the compound from the periodic table.

61. **Butane**

The density in the proposed rule was 0.0927 tonnes/bbl, from V.B. Guthrie (ed.), Characteristics of Compounds, Petroleum Products Handbook, (New York, NY: McGraw Hill, 1960), pg. 3-3.

For the final rule, EPA is updating the density to 0.0911 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 3. Density is at -25ºC / -77ºF. This is the density of liquid butane; it is a gas at 60°F and 1 atm.

The carbon share in the proposed rule was 81.80%, calculated from the molecular formula for butane, C_4H_{10}.

For the final rule, EPA is updating this number to 82.66% based upon more precise values for atomic weights of the elements in the compound from the periodic table.

62. **Butylene**

The density in the proposed rule was 0.1111 tonnes/bbl, from Meyers, *Handbook of Petroleum Refining Processes*, 3rd ed., (New York, NY: McGraw Hill, 2004), p. 1.45

For the final rule, EPA is updating the density to 0.0935 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 3. Density is at -25ºC / -77ºF. This is the density of liquid butylene; it is a gas at 60°F and 1 atm.

The carbon share in the proposed rule was 85.71%, calculated from the molecular formula for butylene, C_4H_8.

For the final rule, EPA is updating this number to 85.63% based upon more precise values for atomic weights of the elements in the compound from the periodic table.

63. **Isobutane**

The density in the proposed rule was 0.0893 tonnes/bbl, from V.B. Guthrie (ed.), Characteristics of Compounds, Petroleum Products Handbook, (New York, NY: McGraw Hill, 1960), p. 3-3.

For the final rule, EPA is updating the density to 0.0876 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 3. Density is at -25ºC / -77ºF. This is the density of liquid isobutane; it is a gas at 60°F and 1 atm.

The carbon share in the proposed rule was 82.80%, calculated from the molecular formula for isobutane, C_4H_{10}.

For the final rule, EPA is updating this number to 82.66% based upon more precise values for atomic weights of the elements in the compound from the periodic table.

64. **Isobutylene**

The density in the proposed rule was 0.0933 tonnes/bbl, from a Material Safety Data Sheet for isobutylene (http://www.siri.org/msds/f2/clc/clcvz.html).

For the final rule, EPA is updating the density to 0.0936 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 3. Density is at -25ºC / -77ºF. This is the density of liquid isobutylene; it is a gas at 60°F and 1 atm.

The carbon share in the proposed rule was 85.71%, calculated from the molecular formula for isobutylene, C_4H_8.

For the final rule, EPA is updating this number to 85.63% based upon more precise values for atomic weights of the elements in the compound from the periodic table.

65. **Pentanes Plus**

Pentanes plus is a mixture of hydrocarbons mostly pentanes and higher, the exact mixture of hydrocarbons is unknown. For the purposes of this rule EPA has chosen to use the characteristics of hexane to represent pentanes plus in order to reflect the large shares of pentanes, while capturing the impact of the increased carbon content of those hydrocarbons in the mix with longer carbon chains.

The density in the proposed rule for hexane, 0.1043 tonnes/bbl, was found at http://www.engineeringtoolbox.com/specific-gravity-liquids-d_336.html.

For the final rule, EPA is updating the density to 0.1055 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 15.

The carbon share in the proposed rule was 83.70%, calculated from the molecular formula for hexane, C_6H_{14}.

For the final rule, EPA is updating the carbon share to 83.63% based upon more precise values for molecular weight.

66. **Miscellaneous Products**

In the proposal and final rule, we rely on the same underlying data sources for density and carbon share and assume that all miscellaneous products have the same density and carbon content as crude oil.

The density and carbon content for crude oil were developed from an equation incorporating density and sulfur content to derive carbon content based on 182 crude oil samples, including 150 samples from U.S. National Research Council, *International Critical Tables of Numerical Data, Physics, Chemistry, and Technology* (New York, NY: McGraw-Hill, 1927).

67. **Ethanol**

The density used in the proposed rule to determine the emission factor for ethanol was 0.12 tonnes/bbl.

For the final rule, EPA is updating the density to 0.1267 tonnes/bbl, from the Handbook of Chemistry and Physics, Section 15: Density of Solvents as a Function of Temperature. Specifically, the handbook provides density values as a function of temperature between 0 and 100ºC at intervals of 10ºC. The EPA fit this data to a polynomial of order 2 and then used the fit to extrapolate the value of the density at 15ºC.

The carbon share in the proposed rule was 52%, calculated from the molecular formula for ethanol, C_2H_5OH.

For the final rule, EPA is updating this number to 52.14% based upon more precise values for molecular weight.

68. **Biodiesel**

Density and carbon share factors did not change from the proposed rule to the final rule.

Density and carbon share for 100% biodiesel were derived from Tables II.E.1-1 and IV.A.3-1 respectively in *A Comprehensive Analysis of Biodiesel Impacts on Exhaust Emissions*, October 2002.

The density factor is based on 31 neat biodiesel samples, 12 of which included a full complement of measured fuel properties and nearly all of which included specific gravity. The carbon content was calculated from measures of H/C ratio and oxygen content for 17 100% biodiesel fuels.

69**. Rendered Animal Fat**

Density and carbon share factors did not change from the proposed rule to the final rule.

Density is from Griffin Industries, Material Safety Data Sheet, Identity: Chicken Fat, March 19, 2007 (http://www.griffinind.com/Griffin%2004%20Site/PDFs/MSDS%20sheets/MSDS%20StabilizedChickenFat.pdf).

Animal fat means fats extracted from animals, with 76.19% carbon by mass, characterized by the composition of fatty acids described in the table below, adapted from Cyberlipid Center, *Lipids of Land Animals*, accessed September 9, 2008, http://www.cyberlipid.org/glycer/glyc0071.htm, estimated by poultry fat.

Composition of Animal Fat and Vegetable Oil

Fatty acid	Carbon share	Animal fat	Vegetable oil
14:0	73.7%	1%	0%
16:0	75.0%	24%	9%
16:1	75.6%	5%	0%
18:0	76.1%	8%	6%

18:1	76.6%	44%	27%
18:2	77.1%	17%	51%
18:3	77.7%	1%	7%

Using the assumptions displayed in the table, the percent mass of carbon for animal fat was calculated using the following equation:

Carbon Share = $\sum [\%C_{FA} \times X_{FA}]$

Where $\%C_{FA}$ is the percent mass of carbon of a fatty acid and X_{FA} is the composition portion of that fatty acid in animal fat or vegetable oil as shown in Table 2.

70**. Vegetable Oil**

Density and carbon share factors did not change from the proposed rule to the final rule.

Density is from Weast, R.C., et al. CRC Handbook of Chemistry and Physics, Boca Raton: CRC Press, 1988-1989: F3. Accessed from http://hypertextbook.com/facts/2000/IngaDorfman.shtml.

Vegetable oil means oils extracted from vegetation, with 76.77% carbon by mass, characterized by the composition of fatty acids described in the table below, adapted from Cyberlipid Center, *Positional distribution of major fatty acids in triglycerides of some plant oils*, accessed August 13, 2009.,http://www.cyberlipid.org//cyberlip/home0001.htm.

Using the assumptions displayed in the table, the percent mass of carbon vegetable oil were calculated using the following equation:

Carbon Share = $\sum [\%C_{FA} \times X_{FA}]$

where $\%C_{FA}$ is the percent mass of carbon of a fatty acid and X_{FA} is the composition portion of that fatty acid in animal fat or vegetable oil as shown in Table 2.

Composition of Animal Fat and Vegetable Oil

Fatty acid	Carbon share	Animal fat	Vegetable oil
14:0	73.7%	1%	0%
16:0	75.0%	24%	9%
16:1	75.6%	5%	0%
18:0	76.1%	8%	6%
18:1	76.6%	44%	27%
18:2	77.1%	17%	51%
18:3	77.7%	1%	7%