Updating NAEI Carbon Emission Factors

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Executive summary

Carbon emissions from combustion of fuels comprise about 80% of the UK's estimate of national greenhouse gas inventory (GHGI) emissions, of which almost half are from sectors where rigorous regulation and reporting (e.g. via the European Union Emissions Trading System (EU ETS)) does not occur. While we have a relatively high level of confidence in the carbon content of these fuels, their high contribution to national totals means that there is value in seeking continued improvement to our understanding of emissions from these sources. The last time that a large study of UK carbon factors was conducted was in 2004, so a new carbon factors review was recommended via the UK GHGI improvement programme to look into the non-EU ETS solid and liquid fuels used in the UK.

In this project, we have established:

- When you consider the relative contribution to UK emissions and the likely variability of fuels with time, the season and by end use, that the high priority fuels to investigate for further data were petrol, LPG, petroleum coke, other industry energy use coal and domestic coal;
- While there is a large amount of analysis on petrol and petrol-blending products and there is clearly a strong impact on carbon content depending on the blending agents, but there is not currently sufficient data to provide a robust alternative to the current NAEI method to estimate the carbon content of petrol;
- Petrol specifications are more complicated than just the summer and winter standards; there are intermediate standards which mean that there are a few months each year where petrol characteristics will transition between summer and winter blends and vice versa;
- Coal, petroleum coke and LPG, for the applications in scope of this work, are all primarily from imports, and that some of the key countries that we import fuel from do not conduct country-specific analysis on fuels;
- US and German country-specific analyses of coals indicates a strong relationship between carbon content and calorific value, justifying the current NAEI approach to determining a time-series of carbon factors;
- LPG for energy use has one major supplier;
- The costs of suitable sample analysis techniques and an approach to determining how many samples should be required; and,
- Our recommendations for future improvement based on our expert judgment as inventory compilers informed by the advice of stakeholders.

A few pieces of information were considered commercially confidential, and are not presented in this publically available version of the report.

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1 Introduction

Emissions of carbon dioxide from fuel combustion account for around 80% of total UK greenhouse gas (GHG) emissions in 2015 (Ricardo, 2017a). Approximately 40% of these emissions are calculated using carbon emission factors (CEFs) taken from the 2004 carbon factors review, or other data sources dating from 1989 – 1994, notably petroleum fuels used for transport sources. This project has assessed the status of all of the current CEFs used in the inventory, reviewed literature and consulted stakeholders to update factors, where possible, that are not considered robust. The project has also produced a strategy for developing emission factors where necessary.

To deliver this project, four tasks have been undertaken:

1. Defining the robustness of the CEFs
2. Identifying which CEFs are considered to already be sufficiently robust
3. Identifying which CEFs could be updated using existing information
4. Identifying a strategy for sampling to fill gaps identified in this study.

Tasks 1 to 3 have been documented in interim reports throughout the duration of this project, and for completeness, are also summarised in this report. Some of the details included are in appendices. Task 4 is fully documented here.

1.1 Solid fuels

Solid fuels (or coals) are combustible material, formed from plant remains. This plant material initially builds up as a peat deposit, which is then buried by younger deposits. Over millions of years, the deposits are altered by high temperatures and pressure into coal. The degree of alteration can vary enormously, and coals are typically sub-divided into various categories depending upon the extent of this alteration. Systems of coal classification differ from country to country but one broad classification would be to separate coal into four ranks – lignite, sub-bituminous coal, bituminous coal and anthracite – with the carbon content and calorific value increasing from lignite through to anthracite.

"Higher ranking" coal such as anthracite will typically have been buried deeper, and been subject to greater pressures and temperatures than "lower-ranking" coals such as lignite. Generally, within a small area, the deeper the coal deposit is, the higher its rank. This implies that one can expect coal quality to vary even within a localised area, and large countries like the US have significant deposits of all ranks of coal. Even in a smaller country like the UK, there are deposits both of lignite, for example, in Northern Ireland, and anthracite, for example, in Wales, as well as large deposits of bituminous coal[1]. So, one should not expect the coal of a particular nation or even a particular region to be uniform in terms of rank, or therefore carbon content. Lignite is not extracted or known to be used to any significant extent in the UK and we would expect that coal for domestic and industrial customers would be bituminous or anthracitic. However, these are all very broad categories and the carbon contents of coals cover a very wide range. For example, one system suggests the following figures for carbon content, on a dry, mineral matter-free basis, of bituminous coals alone:

Low volatile bituminous	78-86%
Medium volatile bituminous	69-78%
High volatile bituminous	<69%

UK energy statistics provide separate figures for consumption of anthracite and for steam coal and the Digest of UK Energy Statistics (DUKES) explains that these are classifications used by UK coal producers and coal importers. DUKES also states that steam coal tends to "have calorific values at the lower end of the range", while anthracite "has a high heat content". However, DUKES does not provide any detailed definition of the two types of coal.

In addition to coal and anthracite, the residential sector uses manufactured solid fuels. The Coal Merchant's Federation consider that manufactured solid fuels are the dominant fuels in the residential sector and that the activity data in the UK inventory do not align with their understanding of this market. We have therefore included information on this fuel in our findings below.

[1] Bituminous coal, also called soft coal , the most abundant form of coal, intermediate in rank between sub-bituminous coal and anthracite according to the coal classification used in the United States and Canada. In the UK bituminous coal is commonly called "steam coal".

1.2 Liquid fuels

Liquid fuels are those derived from crude oil. Crude oil is separated out by heating it to a high temperature and condensing in a fractioning column which has a gradient of temperatures. Specific hydrocarbons or groups of hydrocarbons condense at different temperatures, dictated primarily by the length of the hydrocarbon molecules and are collected depending on when they condense. Because of this process crude oil products can have well quantified and specific applications. After separation, products often go through further processes, e.g. cracking, to produce other hydrocarbons.

1.2.1 Petrol

Base gasoline is a light distillate primarily used for burning in road engines. Petrol is relatively volatile, but the level of volatility and other parameters are controlled by EU standards. The base gasoline is often blended with products that control the ‘octane level’, measured in Research Octane Numbers (RON); this determines whether the fuel will combust correctly in standard petrol engines. Historically, petrol was blended with lead-based additives until they was phased out in the 1990s. In reaction other products, mostly oxygenates like methyl tert-butyl ether (MTBE), ethyl tert-butyl ether (ETBE), ethanol and reformate were used to replace the impact that the lead-additives had on fuel. Blends including up to 5% ethanol have become standard for just over a decade.

1.2.2 LPG

Liquid Petroleum Gases (LPG) are petroleum products, consisting primarily of propane and butane, used for heating, as feedstocks for the chemical industry, and as aerosol propellants. These are very volatile hydrocarbons which require pressurised containers to avoid evaporation.

1.2.3 Petroleum coke

The term petroleum coke is used in UK energy statistics and the UK inventory to refer to a number of different products, but within the context of this report, we are referring only to a solid by-product from a refinery process known as coking. Coking is an intense form of thermal cracking, which is used to convert residual oils into more valuable transport fuels, but the process also produces the solid residue which is sold as petroleum coke. Only one UK refinery has a coking process. Many refiners, including the UK site, further process the petroleum coke by driving off volatiles in a calciner to produce anode-grade petroleum coke. This form of petroleum coke is almost pure carbon, and is used in the manufacture of anodes used in steelworks and aluminium smelters. Non-calcined or fuel-grade petroleum coke is used as a low-cost fuel or as a reductant or additive in industrial processes such as chemicals manufacture or brickmaking. The petroleum cokes used in industrial processes and in mineral industry kilns are well characterised, due to the fact that these users are all included in EU ETS. For this project, therefore, we are only interested in fuel-grade coke used as a residential sector fuel, or as a small-scale industrial fuel.

1.2.4 Aviation turbine fuel

Aviation turbine fuel is a middle distillate with similar properties to burning oil, except that the properties of the fuel are rigorously controlled to ensure that it can safely be used for aviation. It is the primary aviation fuel.

1.2.5 Burning oil

Burning oil, often referred to as kerosene, is a middle distillate primarily used for heating.

1.2.6 Aviation spirit

Aviation spirit is an aviation fuel more like petrol that is used in a small number of typically small aircraft.

1.2.7 Gas oil

Gas oil is a middle distillate and used in a wide range of industrial engines. Gas oil is very similar to diesel, the main difference for most gas oil being that gas oil has different tax requirements so is dyed to mark it as a non-road fuel. Some gas oils differ more in characteritics from diesel where the fuel quality standards permit this, e.g. high sulphur gas oil and marine gas oil.

1.2.8 Diesel

Diesel (or DERV in DUKES and the NAEI) is a middle distillate used in road engines. Diesel has a very narrow range of allowable densities in EU specifications and can be blended with biodiesels, with similar properties, without altering the base fuel.

1.2.9 Fuel oil

Fuel oil is a heavy distillate or residual product used in very large engines, e.g. for shipping and small power stations. Fuel oil specifications are much less strict than those of most lighter distillates, so comparatively fuel oil can have a wider range of fuel properties. The properties are wide enough that often fuel oil is specified as ‘light’ ‘medium’ or ‘heavy’ fuel oil. Fuel oil used for marine purposes is additionally referred to as ‘bunkers fuel oil’, which again, can have different properties.

1.2.10 OPG

Other Petroleum Gases (OPG) are products that remain gaseous in the fractioning column. Almost all OPG is either burned by refineries for energy or used as a feedstock for the chemical industry. The small amount of OPG in scope of this work is the OPG used in ’other industries’.

2 Task 1: Defining the robustness of the CEFs

To define the robustness of CEFs used in the NAEI, a quantitative method was developed; this is described in the following section.

2.1 Approach to Assessing Robustness

For each fuel, we have assessed several criteria for each of three key fuel properties that contribute to a carbon emission factor. The fuel parameters are presented in Table A 1 and the criteria are presented in Table A 2. Each criteria and fuel property has a weighting, which when combined with the criteria scorings and the maximum possible points using Equation 1 (below), provides an overall robustness score between 0 and 100%. Where a parameter or criteria is not applicable to a factor, a score is not provided and the parameter does not contribute to the maximum possible points to score against. For example, the IPCC guidance does not provide a confidence interval for oxidation factors or calorific values, so it is not possible to compare the NAEI assumption to the IPCC guidelines. It would therefore be unreasonable to take this into account when rating the factor.

Equation 1: Robustness scoring system

$$Robustness\ Score\ (\%) = \frac{\sum_{c,p} Score_{c,p} * W_c * W_p}{\sum_{c,p} 2 * W_c * W_p} * 100$$

Where:

$Score_{c,p}$ is the score given for a given fuel parameter and criteria, which can have a value of 0, 1, or 2, where 2 is the highest robustness;

W is the weighting. The higher the value the more the overall score is driven by that criteria or parameter; and,

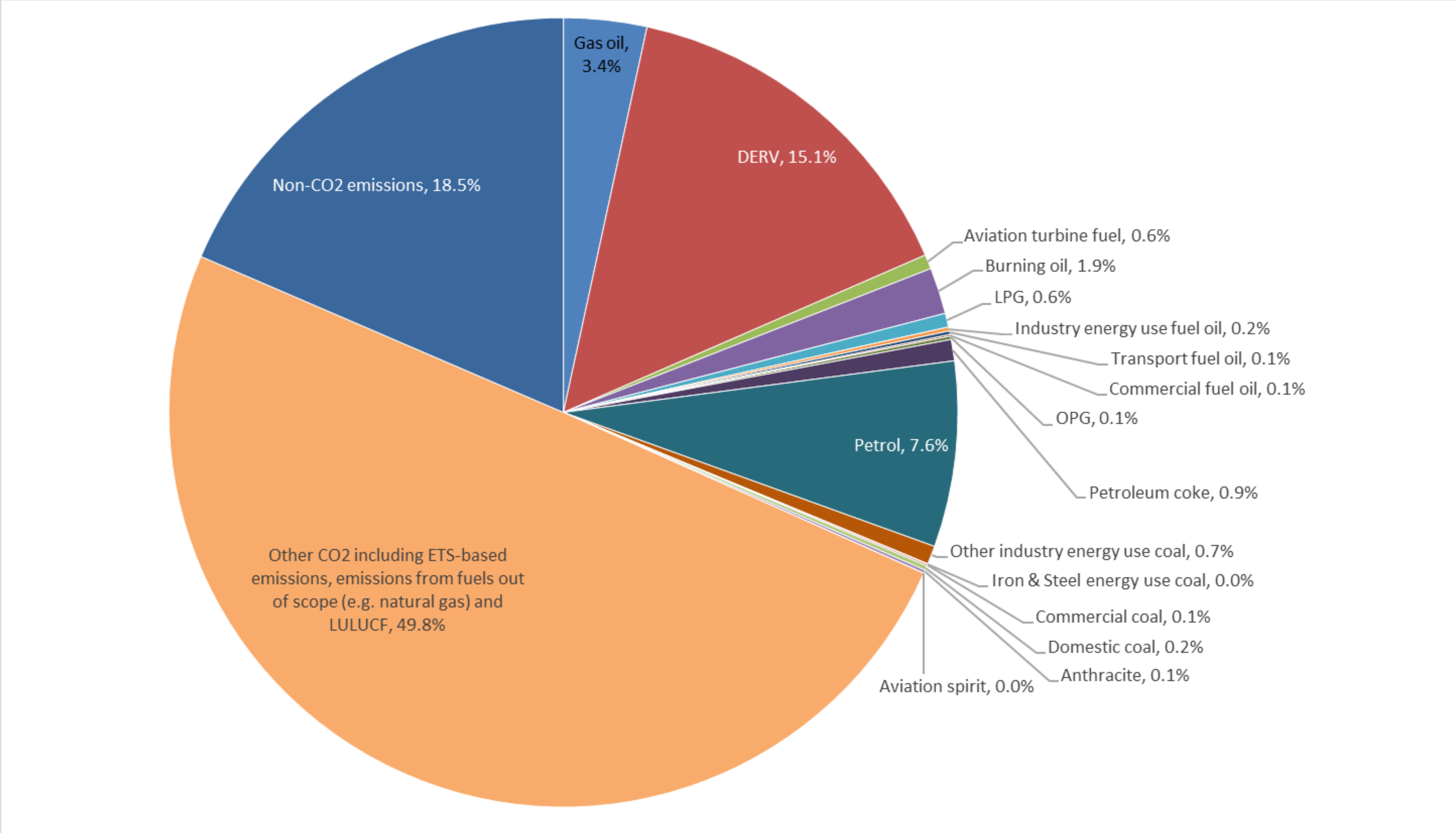
c, p are the specific criteria and fuel parameter, respectively.

The overall score is then compared to a required threshold which is dependent on the relative importance of the source. The thresholds are presented in Table A 3. If the score is more than 5% lower than the threshold then it was considered a high priority for the rest of this project, if the score is within 5% of the threshold we treated the fuel as a lower priority for further work, and if the score is over 5% higher than the threshold then we said it was sufficiently robust that further research is not necessary.

2.2 Approach to Grouping Factors

As the same CEFs can be used for, and are applicable to, multiple sources it is important to group sources so that the significance of a specific CEF can be considered when determining the score that the CEF should have to be considered sufficiently robust. To this end, we have used our judgment to group CEFs by end use where we would expect CEFs to be the same. The groupings can be found in Figure 1, along with the relative contribution of the source groups to the national total.

Figure 1: Summary of the contribution of different source groups to 2015 UK only National Emissions



3 Task 2: Assessing the robustness of CEFs

The results of the assessment of robustness are summarised in Table A 4 in Appendix 2. The results meant that our priorities for the rest of the project were:

- High priority:
    - Petrol
    - LPG
    - Small scale energy use of petroleum coke
    - Other industry energy use coal
    - Domestic coal
- Medium priority:
    - Gas oil
    - Industry energy use fuel oil
    - Transport fuel oil (see paragraph below)
    - Iron & Steel energy use coal
- Low priority:
    - DERV
    - OPG
    - Commercial / institutional coal
    - Anthracite
- Not a focus of this project:
    - Aviation turbine fuel
    - Burning oil
    - Commercial / institutional fuel oil
    - Aviation spirit.

For simplicity, the assessment has only considered emissions from the UK. The impact of including emissions from the UK Overseas Territories (OTs) and Crown Dependencies (CDs) should be considered though, even if the effects on CO_2 emissions are realtively small. The most significant impact of including these territories would be that journeys between the UK and the OTs and CDs would be included in the national total. The CEFs of aviation fuels are safely above the threshold of robustness, so it did not make a difference whether we assessed them for this work, but as transport fuel oil is only a marginal pass, it means that we paid closer attention to this fuel application than otherwise.

4 Task 3: Identifying which CEFs could be updated using existing information

Task 3 was "*Which CEFs could be updated using existing information?*", which involved reviewing literature and consulting stakeholders to identify and understand existing information that was useful for this study. This section also summarises the stakeholder consultation conducted, and the implied recalculation to each carbon factor.

4.1 Literature Review

A review of available literature was conducted. This included key literature sources that were identified in the proposal for this project and other sources that have been identified in literature searches and during stakeholder consultation. Table 1 presents the reports identified and findings of relevance to the project.

Table 1: Literature review findings

Literature source	Findings of interest
A carbon factors review conducted by the German Inventory Agency last year: "CO_2 Emission Factors for Fossil Fuels" UmweltBundesamt (2016)	Demonstrates strong linear correlations between carbon content and calorific values of hard coals, but a much weaker relationship for lignite. This is based on fuel compositional analysis. Analysis of the impact of petrol grade, refinery and year on the carbon content based on fuel composition analysis. These parameters have a combined impact of up to just 3% on the carbon content of fuels and the review shows that paraffin, aromatic and oxygenate contents have a strong relationship with the variations in carbon content. Note that the most recent petrol analysis presented was based on 2002 data, so would precede large scale bio-fuel blending. Demonstrates a very narrow range of carbon contents for diesel by refinery and even the summer and winter blends are within 0.1% of one another.
A 2014 Joint Research Centre (JRC) study: "Well-to-wheels analysis of future automotive fuels and powertrains in the European context. Conversion factors and fuel properties" JRC (2014)	Presents calorific values, densities and carbon contents for a selection of liquid and solid fuel including blending agents (e.g. oxygenates and synthesised fuels) and biofuels. Upon consultation, the CONCAWE team who worked with JRC confirmed that these estimates are based on a chemical composition consistent with the EU specifications (e.g. on aromatics and olefins), and they would not expect much flexibility in those specifications. We have asked for a qualitative indication of how much variation is possible.
A 2013 CONCAWE paper, "Assessment of the impact of ethanol content in gasoline on fuel consumption, including a literature review up to 2006" CONCAWE (2013)	Provides fuel properties for unleaded petrol and gasoline. This is potentially useful for distinguishing the biogenic carbon content of fuel when analysing blended samples.
A 2013 JRC paper, "Effect of oxygenates in gasoline on fuel consumption and emissions in three Euro 4 passenger cars" JRC (2013)	Provides fuel properties for several different blends of petrol including high octane fuel, base fuel, MBTE blended fuel and 5 or 10% biofuels blends. As expected, it demonstrated that biofuel and other oxygenates have a large impact on carbon content. A subtler implication of this data is that the octane number appears to have a strong relationship with carbon content. Given that the octane content of the fossil component needs adjusting depending on the oxygenate (biofuel/MBTE) blend this may be relevant to trends in carbon contents of the fossil component of petrol.
A 2016 report, "Dutch market fuel composition for GHG emissions" TNO (2016)	Presents an analysis of Netherlands road fuel compositions, including the biogenic and fossil blending agent contents and compositional differences with season.
An article in Journal of Energy Engineering, September 2014, "Vapor Pressure and Octane Numbers of Ternary Gasoline–Ethanol–ETBE Blends" Dalli et al., (2014)	Provides information on the octane number, density and the benzene, aromatic and olefin content of blending components and demonstrates the impact of blending agents on vapour pressure and octane number. This highlights the fact that the fossil component of fuel is likely to vary depending on blending agents used.
USGS Analysis, "Chemical Analyses of Coal, Coal-Associated Rocks and Coal Combustion Products Collected for the National Coal Quality Inventory" USGS (2006)	Compositional analysis of a variety of coals extracted from across the US including carbon contents and calorific values. Given the size of the US, it may be that the variation in coal qualities is representative of global coal variations. This has allowed us to assess the relationship between carbon content and calorific values and review the range of possible carbon factors for coal.

The selection criteria applied in Tasks 1 and 2 meant that aviation fuels fell outside the scope of this project, therefore the European Aviation Safety Agency report mentioned in our bid was not consulted.

4.1.1 Factors for shipping fuels

In the recent project "A Review of the NAEI shipping methodology" (Ricardo, 2017b), fuel and gas oil carbon factors for maritime use were revised in the NAEI using International Maritime Organisation (IMO) 2015 data (IMO, 2015). This review found that the carbon content of each marine fuel type is constant and is not affected by engine type, duty cycle or other parameters when looking on a kg CO_2 per tonne fuel basis. The NAEI fuel-based CO_2 emissions factors for main and auxiliary engines at slow, medium and high speeds are the same as assumed in IMO (2015) and are based on MEPC 63/23, Annex 8:

Heavy Fuel Oil (HFO) $EF_{baseline}$ CO_2 = 3,114 kg CO_2/tonne fuel

Marine Diesel Oil (MDO) $EF_{baseline}$ CO_2 = 3,206 kg CO_2/ tonne fuel

Liquefied natural gas (LNG) $EF_{baseline}$ CO_2 = 2,750 kg CO_2/ tonne fuel

CO_2 emissions are unaffected by the sulphur content of the fuel burned.

The CO_2 factors listed above differ from the factors currently used in the NAEI. They are 3.4% lower than in the NAEI for fuel oil and 0.5% higher than in the NAEI for gas oil. The differences are shown in Table 2 below. The differences are quite large for fuel oil, but the newly proposed figures are much closer to the defaults in the 2006 IPCC Guidelines than the existing values used in the current NAEI.

Table 2: Difference between NAEI, IMO and IPCC CEFs

kt C/Mt	Existing carbon factors used in GHGI	Proposed new carbon factors (IMO, 2015)	IPCC 2006 CEF using IPCC NCV
Fuel oil/HFO	879	849	853
Gas oil/MDO	870	874	869

4.2 Other national inventories

In recent years, almost all UK coal has been imported, including both steam coal and anthracite. Hence it was agreed with BEIS that data from countries that we import coal from may give a more representative picture of UK coals used than would be gained by talking to UK manufacturers. Countries that we import the largest amount of fuel from are Russia, USA, Colombia and South Africa.

4.2.1 Russia

The coal mined in each state and region of Russia has its own emission factor for carbon dioxide. The properties of coal can vary significantly between state and region, as perhaps may be expected. The regional emission factors are subsequently used to create a national average, weighted by consumption from each source. The same factor is used for anthracite, and bituminous coal, while sub-bituminous is reported as not applicable and a figure of 101,200 kg CO_2 / TJ net is used for lignite for all years. The data for anthracite/bituminous coal are shown in Table 3 for a selection of years.

Table 3: Russian coal carbon emission factors (kg CO_2/TJ net)

Factor	1990	1995	2000	2005	2010	2015
National average emission factor	93,800	93,700	93,650	93,500	94,100	94,200

4.2.2 Colombia

In the calculation of their greenhouse gas emissions, Colombia uses IPCC default factors for all fuel types and activities. This means that it would not add any value to further analyse Columbia's contribution to UK consumption of imported coal at this stage.

With an understanding of Columbian coal and how the fuel feeds into end-use markets, it may be of value for the UK to determine Columbia-specific factors. Note that the German study (UmweltBundesamt, 2016) analysed come Columbian coal samples, as Columbian coal is a significant proportion of German imports aswell.

4.2.3 South Africa

A net calorific value of 0.0192 TJ per tonne is used in conjunction with an emission factor for sub-bituminous coal of 96,250 kg CO_2 / TJ for stationary coal consumption. It is not clear from the South African NIR what the source of this factor is – in one context it is presented as being from the IPCC 2006 Guidelines but that cannot be so, since the IPCC default is slightly different. The South African

NIR also consistently uses the term 'sub-bituminous' to describe coal and does not mention anthracite, bituminous coal or lignite. We are not sure if this means that all or most South-African coal is sub-bituminous, or that a factor appropriate for sub-bituminous coal was chosen for use in the South African inventory, despite other types of coal being produced. Certainly, the UK has imported significant quantities of anthracite from South Africa in recent years, so South African production is not limited to sub-bituminous coal. However, we assume that sub-bituminous coal is the dominant type and that suggests that South African coal may be relatively low carbon content and, if this is so, then likely to be mostly imported for use at power stations rather than as a domestic or industrial fuel.

4.2.4 USA

Since 1990, coal from the USA has had reasonably constant carbon emission factors, as demonstrated in Table 4. The CEF for anthracite is constant which might indicate that it is not updated regularly or that a constant value has been chosen because variability in the CEF over time is very low.

Table 4: USA weighted average emission factors for coals (kg CO_2 / TJ net)[2]

Fuel	1990	1995	2000	2005	2010	2015
Other bituminous coal	92,509	92,739	93,138	93,135	93,145	93,240
Anthracite	103,445	103,445	103,445	103,445	103,445	103,455
Sub-bituminous coal	96,951	96,953	96,911	96,952	96,946	96,946
Lignite	97,232	97,280	97,352	97,377	97,474	97,474

As the USA does not export lignite or sub-bituminous coal, the emission factors for other bituminous coal and anthracite are the ones of relevance to this report.

In 2013, the United States Geological Survey undertook a chemical analysis of coal across various mines and regions. Some averaged calorific values are presented in Table 5. This demonstrates the variability of coals that could be imported to the UK and therefore the variability in emission factors for coal imported into the UK.

Table 5: Calorific values by region

State	Average Calorific Value (MJ/kg)
Colorado	24.89
Illinois	31.53
Indiana	26.46
Kentucky	24.21
Oklahoma	30.92
Pennsylvania	24.76
Tennessee	30.82
West Virginia	28.85
Wyoming	21.49

4.3 Stakeholder consultation

The stakeholders we have engaged with to date on this project are presented in Table 6, along with a summary of the key findings for this project.

[2] US figures are reported in gross energy terms but have here been converted to a net energy basis assuming a gross to net conversion factor of 0.95 (as used to convert UK figures elsewhere in the report).

Table 6: Summary of key stakeholder engagement

Organisation	Areas of consultation
DUKES team at BEIS	Further understanding of published DUKES, and data underlying DUKES. Overarching understanding of fuel usage in the UK, key sources of data on UK fuel use and contacts with data suppliers and industry experts.
Petrol Retailers Association (PRA)	Industry insight on road fuels from a retailer's perspective.
UK PIA	Overarching understanding of petroleum product supply in the UK, key sources of data on UK petroleum products and contacts with data suppliers and industry experts.
Coal Merchants Federation (CMF)	Overarching understanding of solid fuels supply in the UK, key sources of data on UK solid fuels and contacts with data suppliers and industry experts.
Petroineos	Industry insight on petroleum products from a refiners' perspective.
CONCAWE and JRC	Clarifications on research conducted by CONCAWE and JRC and wider understanding of the European fuels market.
Department for Transport	Support in understanding the Renewable Transport Fuel Obligation (RTFO) and associated data.
Greenergy	Industry insight on road fuels from a non-refinery supplier's perspective.

4.4 Findings

4.4.1 Petrol

The research has indicated that petrol carbon content depends on the octane number, blending agents and whether a winter or summer blend is being produced, among other properties.

Instead of trying to determine a factor for blended fuels, it may be easier to determine the carbon content of each of the products used for blending separately to determine a weighted factor. Unfortunately, while the RTFO provides good data on road fuels and blending agents for recent years, the early years of the RTFO (which started in 2009) present less complete data, and there is no data for before 2009. We have been unable to indentify more complete statistics on road fuel blending agents, so we cannot currently pursue an approach of using blending products to estimate final petrol compositions for most of the historic time-series.

Data on various product characteristics are presented in Table A 5. The current factor used in the NAEI is within the range of the various literature factors identified, which can give us confidence that we are not an outlier, but we would need to do further analysis to understand the finer detail of what the drivers of differences are between the literature factors.

4.4.2 Diesel

As with petrol, diesel is often blended with biofuels, but unlike petrol, the fuel being blended with has little or no bearing on the base fuel. Thus, it should be safe to assume that the base fuel will have a constant carbon content.

The values identified during this study are presented in Table 7. Note that the NAEI carbon content currently used (Netcen, 2004) is marginally higher than the literature value for a base fuel and Netherlands diesels, and higher than all the other potential products for blending in diesel. Given the very small difference, we recommend that the current diesel factor is retained as it is the slightly more conservative of the base diesel factors (in other words CO_2 emissions are very unlikely to be underestimated using this factor).

Table 7: Road diesel characteristics from literature

Product	Source	% C	Density (kg/m^3)	NCV (MJ/kg)
Diesel	Netcen (2004)	86.3	838	43.4
Diesel	JRC (2014)	86.1	832	43.1
Synthetic diesel	JRC (2014)	85.0	780	44.0
Biodiesel (methyl ester)	JRC (2014)	77.3	890	37.2
Biodiesel (ethyl ester)	JRC (2014)	76.5	890	37.9
Hydrotreated vegetable oil (HVO)	JRC (2014)	85.0	780	44.0
Diesel (winter)	TNO (2016)	85.2	835	43.0
Diesel (summer)	TNO (2016)	85.0	834	43.1

4.4.3 Gas Oil

Multiple stakeholders stated that gas oil was indistinguishable from road diesel other than a dye used to flag the different taxes for non-road diesel.

4.4.4 OPG

The only stakeholder we talked to who could discuss OPG with authority was UKPIA. UKPIA informed us that OPG is inherently variable and difficult to monitor. It is unlikely that there is better data available on OPG composition than is currently used in the NAEI.

4.4.5 LPG

We have established that there is one major supplier of LPG for use as a fuel in the UK, but we have been unable to engage with an appropriate contact during this project.

4.4.6 Petroleum Coke

We have established that the petroleum coke within scope of this work is exclusively imported. DUKES does not present import statistics by country of origin for petroleum coke like they do for coal, but we have found alternative statistics (HMRC, 2017) which make it clear that imports are dominated by imports from the United States. There are also significant imports from Venezuela, but as Venezuela uses IPCC defaults to estimate emissions from petroleum coke use, it does not tell us anything about the country-specific fuel properties. The Coal Merchants Federation (CMF) have confirmed that petroleum coke used as a residential sector fuel in the UK, is imported from USA and Venezuela. A summary of the petroleum factors from the US, countries which contribute >1% to UK imports and use country-specific factors (Spain and Norway), the IPCC default and UK factors are presented in Table 8. One complication with petroleum coke, is that the term can refer to calcined or non-calcined coke and that the latter would be expected to have significantly lower carbon content than the former. The high value for Norwegian petroleum coke could be an indication that most or all production is calcined. For this project, we are only interested in non-calcined coke, so further investigation would be needed to establish which of the factors in Table 8 are exclusively for non-calcined coke.

Table 8: International factors for petroleum coke

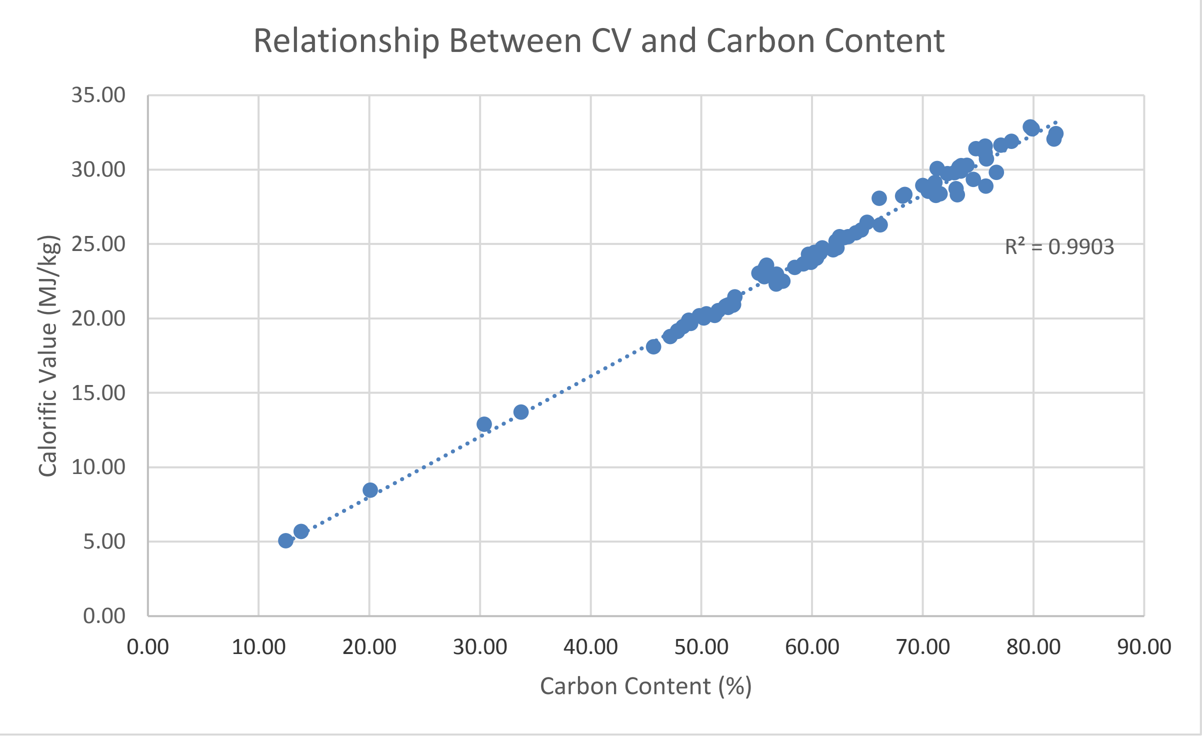
Coal type	CEF, kg CO_2 / TJ net
Spain	98,500
USA	96,780
Norway	102,570
UK – residential sector	96,131
IPCC	97,500

Petroleum coke used as a residential fuel is almost all sold in the form of manufactured solid fuel (MSF) where the pet coke is blended with other components such as anthracite and low volatility coal, and then formed into ovoids for sale. One industry contact estimated pet coke use as being in the region of 150-200 ktonnes per year for manufactured fuels, with maybe another 2 ktonnes sold in lump form as 'pure' pet coke. The use of pet coke in MSF has increased over time and the CMF therefore thinks that the carbon content of MSF may therefore have changed quite significantly over time.

4.4.7 Coal

While the carbon content of coals varies widely, this carbon content should be closely related to the heat content, and so the calorific value of coals is commonly assumed in inventories to be a good guide to carbon content. In Figure 4-1 we use United States Geological Survey (USGS, 2006) data to demonstrate the very strong relationship between calorific value and carbon content in coals; similar analysis in the German study (UmweltBundesamt, 2016) demonstrated similar results for hard coals. We also analysed the standard deviation of the USGS data, which yielded a 95% confidence interval of approximately +/-10% for both the carbon content and the calorific value.

Figure 4-1: Comparison of calorific value against Carbon content in USGS data



For UK coals, estimated average gross calorific values (GCV) are provided in Annex A of DUKES, with figures for 1980, 1990 and 1996-2016 given for coal and anthracite used in various sectors. A summary is given in Table 9, and suggests that different qualities of coal are used for different sectors.

Table 9: DUKES calorific values for coals

Fuel-sector	GCV (GJ per tonne)		
	Minimum	Maximum	Mean
Coal – power stations	25.4	26.3	26.0
Coal – iron & steel industry	28.9	31.3	30.4
Coal – other industries	26.5	27.8	26.9
Coal – domestic	29.7	31.1	30.5
Coal – other users	25.3	30.4	28.0
Anthracite - domestic	33.3	34.7	34.1

The only other data on calorific values we are aware of is from the EU ETS data set, and that data set is only complete for power stations; not all industrial plant will be included in EU ETS. The average GCV for coal used at power stations over the period 2005-2016 is 26.1 GJ per tonne based on the DUKES time-series, whereas the figure based on EU ETS data would be 25.8, so 1.4% lower. The DUKES calorific values are based on data provided by fuel suppliers and the quality of the data is uncertain. The Coal Merchants Federation (CMF) were not able to provide any information on the origin of the figures, but considered the figures for residential fuels reasonable.

The 2006 IPCC Guidelines for National Greenhouse Gas Inventories provides Tier 1 carbon emission factors for coals that are expressed in terms of emissions per unit energy on a net basis. A single value is provided for all uses of bituminous coal, and a slightly higher value is suggested for anthracite. Separate values are also suggested for sub-bituminous coal and lignite as well, although these factors are not considered relevant for the UK, on the basis that all coal consumption is deemed to be bituminous or anthracitic. The approach by the IPCC implies that there is a constant relationship between carbon content and net energy content on a mass basis for all bituminous coals, and that there is a different, constant relationship between carbon emissions and net energy content for all anthracites. This is in line with one aspect of the current UK methodology: where we only have emission factor data for some years, we extrapolate to other years using the calorific values published in DUKES. In other words, the approach suggested by the IPCC is entirely consistent with the approach we use to generate a full time-series of emission factors.

The current UK approach does differ in that the emission factors we use imply a different relationship between carbon content and calorific value than that suggested by the IPCC. We also use different relationships for bituminous coals burnt by different sectors, whereas IPCC suggests that a single figure is appropriate. Table 10 shows the IPCC and UK assumptions to illustrate this.

Table 10: IPCC Default and UK factors for coals

Coal type	Inventory	Consumer Type	CEF, kg CO_2 / TJ net
Lignite	IPCC	All	101,000
Sub-bituminous	IPCC	All	96,100
Bituminous	IPCC	All	94,600
	UK	Domestic	92,000
	UK	Iron & steel	90,400
	UK	Other industry	94,000
	UK	Public & commercial	95,000
Anthracite	IPCC	All	98,300
	UK	Domestic	98,700

It is reasonable for the UK to assume different relationships between bituminous coals consumed by different sectors – the IPCC suggests different figures for the 4 major ranks of coal, so it seems reasonable that there should be some variation within those ranks as well. However, some of the UK relationships are significantly different to the IPCC default, and therefore are liable to be questioned by reviewers The UK approach, for example, implies that coals used in the iron & steel sector have about 5% less carbon per unit of energy content than coals used in the public and commercial sector. One aim of this project or of any subsequent analytical programme should be to establish whether the UK assumptions tabulated above are reasonable, or if different relationships exist, or indeed if the IPCC assumptions are appropriate for the UK. Data on the calorific values of UK coals are therefore of key importance, both for the current GHGI methodology, and for any future alternative method involving either the use of IPCC defaults or extrapolation of emission factor data from one year to another. It is vital that UK coal data covers both calorific values and carbon contents, both to help verify the DUKES GCV time-series, and to help determine what relationship there is between calorific value and carbon content for coals consumed in the UK.

Table 11 presents the average coal CEFs for the countries investigated due to their large contribution to UK coal imports. The table also shows the factor that has been calculated by taking their weighted average in comparison with the relative contribution to UK imports. The analysis shows the current UK CEFs (presented in Table 10) are typically lower than the CEFs for imported coals, but that there are some significant differences in the CEFs used by different countries. The weighted factor of imported coal is quite variable across the time-series analysed, reflecting the fact that different countries have dominated UK imports at different times e.g. South Africa provided 35% of imports in 2005 but only 2% in 2015. Columbian coal is not included in the analysis since we do not have country-specific data and this is a significant gap. Colombia was the source of 52% of imported coal in 2016 and has been a significant source of UK imports since at least 2001.

It should be noted that we have no way of telling whether there is bias in characteristics of fuels likely to be exported by countries compared to the coal they use domestically, and, we have no way of telling how imported coals feed into UK end uses (e.g. if 'Russian' coal is typically used for domestic purposes). The CEFs the NAEI is currently using imply that there is significant variation in coal quality depending on end use, so it is entirely possible that the CEFs of the imported coals appear higher than the current NAEI factors because high CEF coal is used for applications that are out of scope for this project (e.g. power stations or cement). The analysis of other countries' inventory data shows that coal from these countries has quite different CEFs and that these CEFs do change over time, presumably due to changes in the proportion of national production from each deposit within that country. Analysis of CEFs for other countries might be useful, if only to provide more information on the variability of CEFs between countries, which could help to provide further context for the current UK figures. However, we do not believe that the analysis presented here could be used to derive emission factors for the UK inventory – the uncertainties are too great, both in terms of how applicable the countries' factors are, and how appropriate they would be for the coals that are sold to the UK. And, as mentioned above, the absence of country-specific data for Colombia is a serious limitation.

Table 11: Weighted average coal CEFs for countries exporting significant quantities of coal to the UK (t C/TJ net)

Country of origin	1990	1995	2000	2005	2010	2015
Russia	93,800	93,700	93,650	93,500	94,100	94,200
USA	92,509	92.739	93,138	93,135	93,145	93,240
South Africa	96,250	96,250	96,250	96,250	96,250	96,250
Weighted average of above factors depending on their contribution to UK imports			95,393[a]	94,685	94,091	93,805

[a] weighting based on 2001 imports since 2000 data are not available

The CMF provided information on the UK solid fuel market and on the types of fuel used. The key points for this study were:

- The UK solid fuel market seems to be very much dominated by users at opposite ends of the scale in terms of usage per site: there are the large users – power stations, cement & lime kilns and integrated steelworks – and there are the small users that the CMF think of as the residential sector. The CMF don't seem to recognise any significant use of coal except in those two groups.
- Coal for the large users can be a lower quality (e.g. for power stations and cement kilns) than coal for the residential sector.
- Residential fuels for the UK market are sourced from UK coal mines with some imports from Colombia and a small amount imported from Poland. Russia, USA and South Africa do not supply coal for this market.
- Coal for this market is pretty consistent in quality. Typically, fuel suppliers will offer a 'premium' coal with ~2% ash, and a standard product with 4.5 – 5% ash. This is what the market expects and the CMF view was that suppliers would not be able to sustain sales of higher ash / lower carbon coal since their customers would look elsewhere for coal.
- In recent years, this conformity of product has been reinforced by the fact that there are now so few UK coal producers. Coal from any individual mine is likely to be fairly consistent. In the

past, there were more producers and so in theory more variation in coal supplied, and probably regional differences since most UK coal would be sold in the areas close to where it was mined. However, the market would still have expected the same sort of coal as now, and so while coal in the past could have been a bit more variable, it would still be within a relatively narrow band of quality.

- UK fuel producers routinely carry out analyses of fuels and so the UK industry should have data that would allow more robust emission estimates to be made. The suppliers at the REE/CMF meeting did not envisage any problem with supplying data to the GHG inventory team, providing commercial sensitivities were dealt with appropriately. Data would be required from some suppliers not at that meeting (and in one case not even a member of CMF) in order to have a full picture of the UK market.
- Providing data for the past would be much more problematic since the pool of producers/suppliers has contracted significantly over time.

The information from the CMF does raise some questions about the coal consumption data in DUKES and in the GHGI. The CMF see the industrial sector as consisting essentially of just large users such as power stations, cement and lime kilns, and integrated steelworks, and EU ETS returns do support this view. Ignoring those 3 types of process, EU ETS data for 2016 includes just 2 sites (one chemical industry, one brickworks) using more than 1 ktonne of coal and a handful of glass & brick industry sites using less than 1 ktonne per year. Similarly, CMF do not recognise the public and commercial sectors as distinct markets and EU ETS data for 2016 again supports this, with just 3 public sector sites burning coal. The EU ETS and CMF information is hard to reconcile with the DUKES data for 2016 which, for example, indicates that 130 ktonnes of coal was used by the paper and printing sector and 182 ktonnes was used by the 'other industries' sector. EU ETS data does not support this since there are no coal users in either of these sectors in the data for 2016 (although 2 sites used coal until 2009 and 2013 respectively). So, if the quantities of coal given in DUKES are being used by these sectors, then it must be at individual sites where the usage is small, The CMF members do not seem to be aware of widespread use of coal at small industrial sites so either this is not happening, or these sites exist but are not to the fuel suppliers distinguishable from residential users. But as previously stated, the CMF estimates of the residential sector market are consistent with DUKES data for the domestic sector. Taken altogether, the evidence suggests that the allocation of coal to these sectors in DUKES may be significantly too high. Because we have been unable to identify any current coal users in the commercial, public and small industrial sectors apart from the few sites found in EU ETS, it also means that there is no clear path forward for generating better emission estimates. Further discussions with BEIS' DUKES team and the fuel suppliers are probably needed to provide more clarity in this area, so that a solution can be developed.

A few of the sites reporting coal use in EU ETS use Tier 3 emission factors as the basis for their carbon emission estimates. This includes the largest consumer in 2016, which has used Tier 3 or Tier 4 factors since it first reported data in 2005. The EU ETS data for this site and a handful of others could perhaps be used to generate emission factors for the GHGI covering the chemical and paper sectors for at least some years.

4.4.8 Manufactured Solid Fuel (MSF)

The CMF regard MSF as the dominant fuel in the residential sector. While CMF does not have access to actual data on production, the three suppliers present at the REE/CMF meeting consider that they have a good idea of the market, since they dominate sales. Their estimates are significantly different to the numbers in DUKES, with figures of 400-450 ktonnes and perhaps even more suggested by CMF members, compared with a DUKES figure of 236 ktonnes in 2016. The main constituents of MSF are anthracite, low volatility bituminous coal, and petroleum coke. It is possible that DUKES reports these fuels in a slightly different way to the way the CMF see the residential market. For example, DUKES reports much more anthracite sold to the domestic market than the CMF think is reasonable (188 ktonnes in DUKES compared with 100 ktonnes estimated by CMF). The difference might be anthracite that is being used in smokeless fuels. Similarly, DUKES reports pet coke use in 2016 of 95 ktonnes for patent fuel manufacture and 138 ktonnes for non-energy use and the GHGI already assumes that much of the latter is actually used as fuel for the residential sector.

The suppliers have reported that petroleum coke use in manufactured fuels has increased over time, and since petroleum coke has a very high carbon content, this may have led to significant changes in the overall carbon emission factor for MSF over time. In contrast, the GHGI uses a constant carbon emission factors for MSF across all years.

As with coal, the CMF members expressed a willingness to provide data on the composition of fuels (and fuel inputs) but also stressed that it would then be important that any carbon factors derived from these data be applied to appropriate activity data.

5 Task 4: Proposing a strategy for sampling to fill gaps identified in this study

The final task under this project was to identify a strategy for sampling to fill the gaps for those fuels where current literature, research and expert knowledge is unable to identify a robust carbon emission factor.

For factors that have not been considered sufficiently 'robust' and for which existing information is not available to allow an update, a strategy for obtaining a new emission factor has been developed. The fuels that have been identified as a priority are petrol, LPG, pet coke and other industry/domestic coal.

When identifying an effective strategy for sampling of carbon contents of fuels, we have considered the following points:

- The uncertainty in each measurement and therefore how many samples are required to have an acceptable uncertainty;
- The representativeness of the sample; and,
- The cost of analysing samples. Clearly this does not impact the quality of the results, but in conjunction with understanding uncertainties, it allows BEIS to make an informed judgement on the trade-off between costs and robustness.

Different strategies, that consider such factors and the type of fuels, are proposed in Section 5.4.

5.1 Number of samples

The number of samples required to meet a sample period average carbon content target uncertainty can be calculated using Equation 2 (API, 2012).

Equation 2: Number of samples required to achieve a required level of confidence

$$Number\ of\ samples\ = \left(\frac{k_{95\%} \times \sigma / CC_{Average}}{Target\ Percect\ CC_{Uncertainty}} \times 100\right)^2$$

where

$k_{95\%}$ is the 95 % confidence coverage factor

σ is the carbon content standard deviation of the samples

$CC_{Average}$ is the period average carbon content

$Target\ Percect\ CC_{Uncertainty}$ is the target sampling period percent uncertainty

$^{\sigma}/_{CC_{Average}} \times 100$ is the relative standard deviation

Although the standard deviation (σ) and the average carbon content ($CC_{Average}$) are a priori unknown, it is possible to make some assumptions and use the above equation to estimate the minimum number of samples.

The value of $k_{95\%}$ can be estimated from degrees of freedom as described in ISO/IEC Guide 98-3 (ISO 2008) and typically range from 2 (for a normal distribution with infinite degrees of freedom) to 3 (for distributions with very limited degrees of freedom).

For examples, using a conservative estimate for a relative standard deviation of 15% (standard deviation is 15% of the mean), an estimate of $k_{95\%}$ = 3, and if the target carbon content uncertainty is 1 % over the reporting period, then the number of samples required during the period is: 45.

Note that this is assuming your samples are representative, although, if you have a varied market (e.g. petrol with seasonal blends), you may want to take a slightly larger sample to ensure representativeness.

5.2 Representativeness of the sample

Three aspects for obtaining representative results should be considered when planning the fuel sampling strategy: sample size, geographical spread and seasonal variations.

5.3 Cost of analysing samples

Two analytical laboratories, SGS and Intertek, which run testing and analytical services in the UK, have been approached to enquire about cost and turnaround time. The exact cost will depend on the number of samples and the analytical techniques selected that will be different for liquid and solid fuels. Results would be provided in 5-10 days from receiving the samples and the estimated cost is starting from €150/sample for basic elemental carbon only. The sample volume is 200 ml for liquid fuels and 100 g for solid fuels to allow sample preparation and perform different analysis, if required. The additional cost of sample collection should also be considered in final cost estimates.

5.4 Sampling Strategy Required for Determining the Carbon Content

5.4.1 Petrol

In the UK, six major operating refineries supply about 85% of the inland market demand for petroleum products (UKPIA, 2017). To overcome the difficulty of capillary sampling campaign over a large country such as the UK, the ideal solution would be to sample fuel directly at the refineries as this would considerably reduce the logistical effort and costs.

Following the conversation with Greenergy, a large non-refinery supplier of fuel in the UK, it was established that the products at the petrol pump would not vary between brands (with the exception of super or 99 fuels), but upon the terminal that supplies the region the petrol pump was in. Therefore, they recommended that fuel samples are taken from different terminals, rather than collecting samples from filling stations. In the UK, terminals can be divided in three different groups: oil majors, Greenergy, and small independents; we expect UKPIA can advise on how to categorise the UK terminals. Given that the same standards apply to the whole country, no inherent regional differences in petrol are to be expected other than differences in the original sources, which depends ultimately on local terminals. A total of 30 terminals are operating in the UK and it was suggested targeting some terminals in each group to collect representative samples. To consider seasonal changes on the summer, winter and intermediate blends, it is recommended that samples are taken across the year to monitor changes in composition.

5.4.2 LPG

We have not been able to determine whether data or specifications are available to determine LPG carbon contents with a high confidence. We would recommend that any proposed sampling strategy is postponed until this can be determined.

If a sampling strategy is determined to be required, as the UK market is mainly controlled by one supplier, it is recommended to collect samples directly from there. DUKES provides a breakdown of LPG activity by the components of LPG (propane and butane), and as far as we understand propane and butane are typically sold separately, so we would recommend that each of these products are sampled independently.

5.5 Petroleum Coke, Coal, and Manufactured Solid Fuel

Discussions with the Coal Merchants Federation (CMF) have indicated that the solid fuel industry already has significant quantities of data obtained through routine sampling and analysis of their raw materials and fuel products, and that individual fuel producers would be willing to provide data. Further discussions will be needed with those fuel producers to get a better idea of the nature and scope of the data that could be provided, and to agree a procedure for requesting, processing and reporting the data.

However, for the moment we do not see any need for a comprehensive sampling strategy. It is possible that some fuel producers will not be willing to provide data – not all are members of the CMF, and some significant fuel producers within the CMF were not at the REE/CMF meeting and so we do not yet know whether they would also be willing to share their data. If some producers do not supply data, then it may be necessary to obtain samples of their fuels to analyse independently, so that these results can be combined with data from those producers who do provide data. It would be sensible to obtain as much detail as possible from fuel suppliers and so data on calorific values should be sought and data on sulphur contents as well, since these will be useful for improving our understanding of the relationship between carbon and energy content, and for updating the SO_2 emission factors used in the AQPI respectively.

CMF members do not recognise some of the inventory categories as separate markets and would not be able to provide data specifically for those sectors. It therefore seems very likely that there are very few coal users within the public, commercial, and industrial sectors (in the latter case except for very large users such as cement works and steelworks). It is also possible that the few sites that do still use coal, obtain it via routes other than CMF members. EU ETS data for 2016 includes just 5 sites (3 public sector, one chemical industry, one brickworks) using more than 1 ktonne of coal. The largest of these used a Tier 3 emission factors in 2016 (and all earlier years where data where reported), but the rest do not. These sites could perhaps be approached for any data they have on the coal they use – EU ETS suggests they do not measure carbon factors but they may be able to provide other data or even to provide samples for analysis.

5.6 Analytical approach

Determination of carbon content in biofuels, petroleum products, crude oil, and lubricants is usually performed using the ASTM D5291 test method (Carbon-Hydrogen-Nitrogen analysis). Along with carbon content analysis in hydrocarbons, a modified ASTM D5291 method provides hydrogen, nitrogen, and oxygen content data for petroleum among other methods.

The following tests provide additional information that may be necessary to consider how sulphur and oxygen content affect the overall carbon content in fuels. A combined analysis for alkanes (paraffins), alkenes (olefins), naphthenes, oxygenates, and aromatics would replicate the methodology used in the German study (UmweltBundesamt 2016). This extensive evaluation measured concentrations of 113 individual substances in gasoline from all German refineries. The carbon content was calculated using the averages of the individual measurements on hydrocarbons with three to six carbon atoms and aromatics with up to 12 carbon atoms, for three fuel grades: Normal (regular gasoline), Super (premium) and Super Plus (premium plus).

Determination of Net Calorific Value is usually performed using the ASTM D5865 method.

For solid fuels; although analytical methods are available to determine for carbon, hydrogen, nitrogen, oxygen and sulphur (CHNOS) content, the determination of moisture and volatile matter content and ash content are sufficient for the scope of this project. Moisture and volatile matter content can be determined applying the standard ASTM D 3175 method.

Indicative costs are indicated in the Table 12. Depending on the total number of samples, it may be possible to obtain a discount on the price per unit when many samples (greater than 30) are being analysed. A quotation for the methods of analysis of solid fuels, such as ASTM D 3175, has not yet been provided by the analytical laboratories but it should be available soon.

Table 12: Standard sample tests & quoted prices provided[3]

Method	Description	Price per unit
ASTM D5291 Method C	Carbon, Hydrogen and Nitrogen in Petroleum Products and Lubricants	£93.00, £120.00
ASTM D5291 + IP 566	Modified method for CHNO (carbon, hydrogen and nitrogen and oxygen content)	£260.00, £240.00
ASTM D5453 / IP 490	Sulphur Content of Automotive Fuels UVF Method	£100.00

[3] Quotes provided by 2 labs that conduct these tests. One of these labs indicated that the price would be lower if requesting more (e.g. 30) sample analyses.

Method	Description	Price per unit
IP 566	Hydrocarbon Types and Oxygenates in Gasoline by Multi Dimensional GC	£160.00, £550.00
IP 156	Hydrocarbon Types by FIA	£90.00
IP 4 ISO 6245	Ash (Inorganic Content)	£50.00
IP 391	Aromatic Hydrocarbon Types in Middle Distillates by HPLC	£170.00
ASTM D5865	Net Calorific Value Analysis	£220.00, £430.00
ASTM D 3175	Moisture and volatile matter	Not identified

5.7 Developing average carbon content from a future measurement programme

Once the fuels composition is determined from a sampling and measurement programme, the average carbon content could be calculated using the following equations.

The carbon content of a pure component can then be calculated using the following equation:

Equation 3: carbon content of a pure component

$$Wt\%C_{Cj} = \frac{\frac{12\ g\ C}{mole\ C} \times \frac{X\ g\ C}{mole\ C}}{MW_{Cj}\left(\frac{g}{mole\ C}\right)} \times 100\%$$

Where:

$Wt\%C_{Cj}$ is the carbon content of individual hydrocarbon compound on a mass percent basis

J is any hydrocarbon compound CxHyOz

X is the stoichiometric coefficient for carbon (for example X=3 for propane, C_3H_8)

MW_{Cj} is the molecular weight of individual hydrocarbon compound

The carbon content of the fuel mixture can then be calculated using the following equation

Equation 4: carbon content of the fuel mixture

$$Wt\%C_{mixture} = \frac{1}{100} \times \sum_{i=1}^{components} (Wt\%_i \times Wt\%C_i)$$

where

$Wt\%C_{mixture}$ is carbon content of mixture on a mass percent basis

$Wt\%_i$ is weight percent of component i

$Wt\%_i$ is carbon content of component i on a mass percent basis (Equation 3)

An alternative approach to estimate carbon is based on a theoretical approach relating heat of combustion, hence calorific value, to the elemental content of liquid fuels, thus:

Equation 5: Relationship between NCV and chemical composition of solid fuels

NCV (MJ/kg) = 0.339*C+1.256*H-0.109*(O-S)-0.025*(W-9H)

where **C, H, O, S** and **W** are the mass fractions of carbon, hydrogen, oxygen, sulphur and water in the fuel (Ponomarev, 2015).

As part of capacity building work we did with Ukraine, this approach was tested by comparing NCVs derived from the empirically-based equation with values of NCV obtained from the literature for a range of individual hydrocarbons. For the range of hydrocarbons and oxygenates found in motor fuels, the agreement was about 1% for major components (and within ±7% including some ‘problematic’ components present in real motor fuels). The agreement was worse for the small alkynes and diolefins which are not abundant in fuels, but was much better for alkanes, mono-alkenes, aromatics and oxygenates. Relevant correction factors were applied for ‘sensitive’ components to calculate a mixture`s NCV and as result the overall agreement (after correction) was better than 1%.

Based on the current information available, this theoretical approach for liquid fuels derived from the relationship between NCV and fuel properties, it is not applicable due the lack of detailed analysis of component parts.

6 Recommendations

6.1 Petrol

Given the possible variability and likely trends in petrol characteristics identified in this work and the lack of complete statistics of petrol additives we recommend that a fuel sampling project would be the best course of action to improve the UK estimate of current petrol carbon content. Data from the RTFO, combined with data on the composition of blending agents can inform us on the likely biogenic carbon content of fuel.

If possible it may be worth investigating the compositions of blending agents should suitable historic statistics or data are identified for the 1990s and 2000s (e.g. via consultation with Innospec, a major fuel additives supplier). We also recommend that if the UK market shifts again (e.g. if blends with >5% ethanol are mandated by UK parliament), then this analysis should be revisited.

6.2 LPG

We recommend that the one, key supplier of LPG for energy use and/or the UK LPG association (UK LPG) is contacted to understand:

- How accurate it would be to use a stoichiometric analysis for propane and butane
- Whether there are specifications for LPG that mean that there is a narrow range of carbon contents possible
- Whether data are routinely collected on the content or properties of LPGs.

Should there not be sufficient information to make a robust estimate after the above is established, we expect that it would be relatively easy to enact a representative sampling campaign of propane and butane given that only one supplier would need to be contacted for samples to get a representative picture of UK energy use of LPG.

6.3 Coal, Anthracite, Manufactured Solid Fuel & Petroleum Coke

In view of the information provided by the CMF and information available from EU ETS, we recommend that:

- data be requested from solid fuel suppliers, both regarding the carbon content of fuel inputs and fuels, and the quantities sold for each fuel type (bituminous coal, anthracite, MSF). Further discussions will be be needed to establish a procedure for the requesting, processing and reporting of data, including the appropriate treatment of any commercial confidentiality issues. A number of major suppliers have indicated their willingness to provide data but other producers will need to be approached in order to get a full understanding of the solid fuels used in the UK;
- some data have already been received for anthracite from one producer and could, in theory, be incorporated into the version of the GHGI currently being prepared. However, this would probably require a number of assumptions to be made in the absence of data from other producers, and so it might be preferable to wait until a more complete set of data are available;
- since discussions with CMF have established that petroleum coke is little used as a separate fuel for the residential sector, but is used in large quantities in MSF, that the GHGI activity data

be modified to reflect this, so that better carbon factors based on fuel suppliers' data can then be used;

- data could be requested from fuel suppliers for petroleum coke sold as a 'pure' fuel but in view of the low significance of this market, this is a relatively low priority compared with coal, anthracite and MSF;
- data requested should include carbon content but also other data useful for the UK inventory including gross and net calorific value and sulphur content;
- data should extend back across the time-series as far as practicable, although priority should be given to getting data for recent historical years and into the future;
- fuels data given in DUKES need to be re-evaluated and, if necessary, some fuels may need to be re-allocated relative to DUKES (as is already done for other fuels) in order to generate activity data that are consistent both with overall demand figures in DUKES and with data on the solid fuel market from fuel suppliers, and which would also be consistent with data on carbon content provided by the suppliers;
- in particular, consideration needs to be given to activity data for a) manufactured solid fuels for the residential sector; b) anthracite used by the residential sector; c) industrial coal use generally; and,
- EU ETS data for a small number of sites is of a sufficiently high quality that it could be used directly in the UK inventory, although this might require a degree of alignment of the activity data in the EU ETS dataset and that used in the UK inventory, with the need to re-allocate fuel compared with DUKES.

6.4 Gas oil

During the shipping project (Ricardo, 2017b), the carbon factors for gas oil used in shipping were reviewed and an improved factor selected. Due to the similarities in most gas oils and diesel we recommend that any future research for these are done in parallel; if research can confirm that the fuels are indistinguishable a single factor could be used in future.

6.5 Fuel oil

During the shipping project (Ricardo, 2017b), the carbon factors for fuel oil used in shipping were reviewed and an improved factor selected. This application of fuel oil was the only application that was considered a priority for investigation, so we recommend that no further action is required.

6.6 DERV

Given the very small difference between the current NAEI value, the value in the JRC paper (JRC, 2014), the Netherlands data (TNO, 2016) and the default, we recommend that the current diesel factor is retained. The current NAEI values is slightly more conservative than the JRC and Netherlands values, is country-specific and the stakeholder consultation has confirmed that diesel should not vary with time.

6.7 OPG

When discussed with UK PIA it was clear that OPG is a highly variable and difficult to monitor fuel. Given the amount of work that would be required to generate a more robust estimate of carbon emissions from this fuel and the relative insignificance of its use as a fuel in the UK we recommend that it is not worth pursuing further.

7 References

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Appendix 1 – Assessment of Robustness: fuel parameters, criteria, thresholds, and groupings

Table A 1: Fuel parameters and weighting

Fuel Parameter	Weighting	Comment
Carbon content	5	Principal driver of the carbon emission factor, can vary significantly by fuel, or even the market the fuel is intended for.
Oxidation factor	1	The proportion of carbon in a fuel that is assumed to be emitted as a gas rather than remaining as ash. The IPCC default assumption is to assume that 100% is emitted, but it's known that particularly with cruder fuels and in cruder applications (e.g. brown coal burning on a domestic stove) this can be a few percentage points lower. UNFCCC reviewers expect strong evidence to justify using oxidation factors of less than 100%.
Calorific value	3	Used for some fuels to determine a time-series for carbon factors as it's expected that carbon content strongly correlates with carbon content.

Table A 2: Assessment criteria, scoring and weighting

Criteria	Scoring	Weighting
Applicability of factors to different years	2 Points: No time dependence / methodology already accounts for time-series variation 1 Point: Some time dependence unaccounted for 0 Points: Strong time dependence unaccounted for	3
Relevance of the factor to the fuel or application	2 Points: Factor is for the fuel and application used for, or is not expected to vary by application 1 Point: Factor is for the same fuel, but may not be application relevant 0 Points: Factor is for a similar fuel or for a completely different application	3
How the initial data were gathered	2 Points: Strong CS source data 1 Point: Weaker source data or non-CS data (IPCC default) 0 Points: Weak, non-CS data	3
Transparency of the reference	2 Points: Full documentation 1 Point: Weaker documentation 0 Points: Very weak or absent documentation	3
Likely variability of the fuel	2 Points: Well-regulated and/or defined fuel with narrow specification 1 Point: Relatively narrow band of properties to allow the fuel to be applied is specific applications/engines 0 Points: Unregulated, inherently variable fuel that will work regardless of quality	3

Criteria	Scoring	Weighting
Whether the factor is within the IPCC default range	2 Points: Towards the centre of the range 1 Point: Different from the default, but safely within the range 0 Points: Close to the edge of the range or outside	3
Uncertainty parameters assumed and what information these are based on	2 Points: <=2% 1 Point: 2-5% 0 Points: >5%	1

Table A 3: Thresholds for sufficient robustness

Criteria	Score threshold
Very significant fuel (>7.5% of the 2015 inventory)	75%
Significant fuel (1.5-7.5%)	65%
Notable fuel (0.5-1.5%)	55%
Minor fuel (0.1-0.5%)	45%
Insignificant or approaching insignificant fuel (<0.1%)	35%

Appendix 2 – Results Summary of the Assessment of Robustness

Table A 4: Results Summary of the Assessment of Robustness

Category	Data source	Contribution to 2015 emissions	Emission factor uncertainty	Deviation from IPCC default	IPCC 95% confidence interval[4]	Threshold	Score	Assessment	Comments
Gas oil	Carbon Factors Review 2004 (Netcen, 2004)	3.4%	2.0%	1.1%	1.5%	65%	64.7%	Marginal Fail	
DERV	Carbon Factors Review 2004 (Netcen, 2004)	15.1%	2.0%	-0.5%	1.5%	75%	77.3%	Marginal Pass	
Petrol	Carbon Factors Review 2004 (Netcen, 2004)	7.6%	2.0%	1.0%	4.0%	75%	64.7%	Fail	The difference in this result relative to from DERV is that petrol is expected to have more time-series differences (e.g. different blends are used for different seasons). Also, the IPCC confidence interval is wider for petrol than it is for DERV, perhaps linked to seasonal blends and biofuel content.
Aviation turbine fuel	Carbon Factors Review 2004 (Netcen, 2004)	0.6%	3.3%	0.3%	3.3%	55%	68.9%	Pass	Note that the contribution to emissions is much higher for other geographical coverages where journeys between the UK and OTs or CDs are included in the national total.

[4] Expressed as a percentage deviation from the default factor

Category	Data source	Contribution to 2015 emissions	Emission factor uncertainty	Deviation from IPCC default	IPCC 95% confidence interval[4]	Threshold	Score	Assessment	Comments
Burning oil	Carbon Factors Review 2004 (Netcen, 2004)	1.9%	2.0%	-0.2%	2.0%	65%	71.0%	Pass	
LPG	UKPIA (1989)	0.6%	2.1%	-5.7%	3.2%	55%	50.0%	Fail	
Industry energy use fuel oil	Carbon Factors Review 2004 (Netcen, 2004)	0.2%	2.1%	2.2%	2.1%	45%	43.7%	Marginal Fail	
Transport fuel oil	Carbon Factors Review 2004 (Netcen, 2004)	0.1%	2.0%	2.2%	2.1%	45%	45.8%	Marginal Pass	Note that the contribution to emissions is much higher for other geographical coverages where journeys between the UK and OTs or CDs are included in the national total.
Commercial / institutional fuel oil	Carbon Factors Review 2004 (Netcen, 2004)	0.1%	2.1%	2.2%	2.1%	35%	43.7%	Pass	
OPG	IPCC 2006 Guidelines	0.1%	15.0%	0.0%	9.8%	45%	47.9%	Marginal Pass	
Petroleum coke	Carbon Factors Review 2004 (Netcen, 2004)	0.9%	10.0%	3.0%	16.5%	55%	46.4%	Fail	
Other industry energy use coal	Based on Fynes & Sage, 1994	0.7%	10.0%	-0.6%	5.4%	55%	38.2%	Fail	

Category	Data source	Contribution to 2015 emissions	Emission factor uncertainty	Deviation from IPCC default	IPCC 95% confidence interval[4]	Threshold	Score	Assessment	Comments
Iron & Steel energy use coal	Based on Fynes & Sage, 1994	0.0%	10.0%	-4.4%	5.4%	35%	31.4%	Marginal Fail	
Commercial / institutional coal	Based on Fynes & Sage, 1994	0.1%	10.0%	-1.1%	5.4%	35%	38.2%	Marginal Pass	
Domestic coal	Based on Fynes & Sage, 1994	0.2%	10.0%	-2.7%	5.4%	45%	32.7%	Fail	
Anthracite	Based on Fynes & Sage, 1994	0.1%	6.0%	0.4%	3.3%	45%	46.4%	Marginal Pass	
Aviation spirit	Carbon Factors Review 2004 (Netcen, 2004)	0.0%	3.3%	-0.8%	3.9%	35%	68.9%	Pass	Note that the contribution to emissions is much higher for other geographical coverages where journeys between the UK and OTs or CDs are included in the national total.

Appendix 3 – Gasoline characteristics derived from the literature

Table A 5: Gasoline characteristics derived from the literature

Product	Source	% C	% H	% O	RON	Density (kg/m^3)	NCV (MJ/kg)
Petrol	A	85.5	NE	NE	NE	730.5	44.79
Base fuel	B	86.3	13.7	-	95.0	735.9	43.52
E10 Match	B	83.3	13.3	3.4	95.4	745.0	41.94
15% ETBE Splash	B	84.0	13.7	2.3	97.1	734.1	42.59
E10 Splash	B	82.9	13.5	3.6	98.5	740.4	41.93
High Octane	B	86.8	13.2	-	98.0	742.3	43.49
E5 Splash	B	84.7	13.5	1.8	96.9	737.9	42.72
Unleaded Gasoline (95RON)	D	86.4	13.6	-	95	745	43.2
Ethanol	D	52.2	13.0	34.8	>100	794	21.3
Base Gasoline	E	NE	NE	NE	93.4	NE	NE
Reformate	E	NE	NE	NE	100.5	810.0	NE
Base gasoline	E	NE	NE	NE	92.5	720.0	NE
Alkylate	E	NE	NE	NE	94.7	703.3	NE
Dimate	E	NE	NE	NE	95.0	694.5	NE
Isomerate	E	NE	NE	NE	86.4	653.5	NE
Gasoline	C	86.5	NE	NE	NE	745	43.2
Ethanol	C	52.2	NE	NE	NE	794	26.8
MBTE	C	68.2	NE	NE	NE	745	35.1
EBTE	C	70.6	NE	NE	NE	750	36.3
Petrol (winter)	F	83.9	NE	NE	NE	730.4	42.38
Petrol (summer)	F	84.2	NE	NE	NE	745.5	40.96

Where:

A Current NAEI assumptions; carbon content is based on the 2004 Carbon factors review and densities and CVs are based on DUKES

B Effect of oxygenates in gasoline on fuel consumption and emissions in three Euro 4 passenger cars

C Well-to-wheels analysis of future automotive fuels and powertrains in the European context. Conversion factors and fuel properties

D Assessment of the impact of ethanol content in gasoline on fuel consumption, including a literature review up to 2006

E Vapor Pressure and Octane Numbers of Ternary Gasoline–Ethanol–ETBE Blends

F Dutch market fuel composition for GHG emissions

NE Not estimated

RON Research Octane Number

ETBE Ethanol and ethyl-tert-butylether

MTBE Methyl-Tertiary-Butyl Ether

E5/10 Refers to blends of ~5% or 10% biofuel respectively

Splash Refers to a fuel where the base fuel has not been adjusted when blending with oxygenates

Match Refers to a fuel where the base fuel is adjusted to retain the same RON when blended with oxygenates

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