LCA Case Studies

Allocation of Energy Use in Petroleum Refineries to Petroleum Products

Implications for Life-Cycle Energy Use and Emission Inventory of Petroleum Transportation Fuels

Michael Wang*, Hanjie Lee and John Molburg

Center for Transportation Research, Energy Systems Division, Argonne National Laboratory, 9700 South Cass Avenue,
Argonne, IL 60439, USA

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* **Corresponding author** (mqwang@anl.gov)

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Abstract

Aim, Scope, and Background. Studies to evaluate the energy and emission impacts of vehicle/fuel systems have to address allocation of the energy use and emissions associated with petroleum refineries to various petroleum products because refineries produce multiple products. The allocation is needed in evaluating energy and emission effects of individual transportation fuels. Allocation methods used so far for petroleum-based fuels (e.g., gasoline, diesel, and liquefied petroleum gas [LPG]) are based primarily on mass, energy content, or market value shares of individual fuels from a given refinery. The aggregate approach at the refinery level is unable to account for the energy use and emission differences associated with producing individual fuels at the next sub-level: individual refining processes within a refinery. The approach ignores the fact that different refinery products go through different processes within a refinery. Allocation at the subprocess level (i.e., the refining process level) instead of at the aggregate process level (i.e., the refinery level) is advocated by the International Standard Organization. In this study, we seek a means of allocating total refinery energy use among various refinery products at the level of individual refinery processes.

Main Features. We present a petroleum refinery-process-based approach to allocating energy use in a petroleum refinery to petroleum refinery products according to mass, energy content, and market value share of final and intermediate petroleum products as they flow through refining processes within a refinery. The approach is based on energy and mass balance among refining processes within a petroleum refinery. By using published energy and mass balance data for a simplified U.S. refinery, we developed a methodology and used it to allocate total energy use within a refinery to various petroleum products. The approach accounts for energy use during individual refining processes by tracking product stream mass and energy use within a refinery. The energy use associated with an individual refining process is then distributed to product streams by using the mass, energy content, or market value share of each product stream as the weighting factors.

Results. The results from this study reveal that product-specific energy use based on the refinery process-level allocation differs considerably from that based on the refinery-level allocation. We calculated well-to-pump total energy use and greenhouse gas (GHG) emissions for gasoline, diesel, LPG, and naphtha with the refinery process-based allocation approach. For gasoline, the efficiency estimated from the refinery-level allocation underestimates gasoline energy use, relative to the process-level-based gasoline efficiency. For diesel fuel, the well-to-pump energy use for the process-level allocations with the mass- and energy-content-based weighting factors is smaller than that predicted with the refinery-level allocations. However, the process-level allocation with the market-value-based weighting factors has results very close to those obtained by using the refinery-level allocations. For LPG, the refinery-level allocation significantly overestimates LPG energy use. For naphtha, the refinery-level allocation overestimates naphtha energy use. The GHG emission patterns for each of the fuels are similar to those of energy use.

Conclusions. We presented a refining-process-level-based method that can be used to allocate energy use of individual refining processes to refinery products. The process-level-based method captures process-dependent characteristics of fuel production within a petroleum refinery. The method starts with the mass and energy flow chart of a refinery, tracks energy use by individual refining processes, and distributes energy use of a given refining process to products from the process. In allocating energy use to refinery products, the allocation method could rely on product mass, product energy contents, or product market values as weighting factors. While the mass- and energy-content-based allocation methods provide an engineering perspective of energy allocation within a refinery, the market-value-based allocation method provides an economic perspective. The results from this study show that energy allocations at the aggregate refinery level and at the refining process level could make a difference in evaluating the energy use and emissions associated with individual petroleum products. Furthermore, for the refining-process-level allocation method, use of mass – energy content – or market value share-based weighting factors could lead to different results for diesel fuels, LPG, and naphtha. We suggest that, when possible, energy use allocations should be made at the lowest subprocess level – a confirmation of the recommendation by the International Standard Organization for life cycle analyses.

Outlook. The allocation of energy use in petroleum refineries at the refining process level in this study follows the recommendation of ISO 14041 that allocations should be accomplished at the subprocess level when possible. We developed a method in this study that can be readily adapted for refineries in which process-level energy and mass balance data are available. The process-level allocation helps reveal some additional energy and emission burdens associated with certain refinery products that are otherwise overlooked with the refinery-level allocation. When possible, process-level allocation should be used in life-cycle analyses.

Keywords: Allocation methods; energy use of petroleum refining; life cycle assessment; petroleum products; petroleum refining; petroleum transportation fuels

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Introduction

Petroleum has been the dominant energy source since overtaking coal in the middle of the last century. The shift from coal to petroleum is generally regarded as environmentally beneficial, but the energy use required for extraction, transport, and refining of petroleum adds significantly to the environmental burden of petroleum use. The petroleum refining industry is energy intensive; it accounts for about 7% of total U.S. energy consumption (Energy Information Administration [EIA] 1997). More than 80% of the refining industry process energy is provided by refinery plant byproducts, including refinery gas, petroleum coke, liquefied petroleum gas (LPG), fuel oil, and other refined products. This study focuses on allocation of the total energy use in petroleum refineries among different petroleum refinery products.

Allocation of petroleum refinery energy use (and the resultant emissions) among different products is needed in fuel-cycle analyses to evaluate various transportation fuels. In such analyses, energy use and emissions from a facility are usually allocated to individual fuels so that fuel-cycle energy use and emissions for producing a given fuel can be evaluated on a full fuel-cycle basis (Wang 1999, Furuholt 1995). The allocation methods used so far for petroleum-based fuels (e.g., gasoline, diesel, and LPG) are based primarily on mass, energy content, or market value share of individual fuels from a given refinery. This aggregate approach, which allocates total energy use and emissions at the refinery plant level, is essentially the one used in Argonne's Greenhouse gases, Regulated Emissions, and Energy use in Transportation (GREET) model, which is a fuel-cycle model that evaluates vehicle/fuel systems from energy feedstock recovery to fuel use in vehicles (http://greet.anl.gov provides the GREET model and associated documents).

Allocation of energy use and emissions at the refinery level (aggregate approach) assumes that equal energy is expended during refining of all fuel product slates. This approach is unable to account for the energy use and emission differences associated with producing individual fuels at the next sub-level: individual refining processes within a refinery. In addition, the aggregate allocation approach ignores the fact that different refinery products go through different processes within a refinery. Consequently, results based on aggregate allocation suffer from their insensitivity to the changes in individual refining processes used to produce a different mix of refinery products – such as increases in diesel fuel production for a possible shift from spark-ignition engine vehicles to diesel engine vehicles. Furuholt (1995) applied an allocation method based on eight general refining processes for Norwegian refineries. He demonstrated that a switch from refinery-level-based allocation to *refining-process-level*-based allocation can have significant effects when calculating the energy use and emissions associated with individual refinery products. Similarly, in this study, we seek a means of allocating total refinery energy use among various refinery products at the level of individual refinery processes. Allocation at the subprocess level (i.e., the refining process level) instead of at the aggregate process level (i.e., the refinery level) is also advocated by the International Standard Organization (ISO 1998).

There are a number of approaches that may be used to allocate the total energy use and emissions of a refinery to its products (General Motors Corporation et al. 2001). For example, individual refineries have data on crude input, electricity and gas use, inputs of other feedstocks, and output data for product slates. If researchers had access to these data at the level of each individual refining process within a refinery, they could calculate the energy use expended and the emissions generated for each individual product. It appears that Furuholt used proprietary data from the Norwegian oil company Statoil. However, such proprietary data are usually not available to researchers outside of refineries.

A second approach to allocation is using openly available U.S. refinery production data and a rule-of-thumb product energy intensity that is accepted in industry. For example, in the case of energy allocation based on mass shares of products, the product slate data for total U.S. petroleum production can be obtained from such open literature as EIA's publications. In 1999, for instance, the total volume of the petroleum products produced by U.S. refineries comprised 46.7% gasoline, 20.0% diesel, and 33.3% other products. The energy use and associated emissions of U.S. refineries could be allocated based on the mass shares of these products. But we know that, on a per-unit basis, some petroleum products require more energy and generate more emissions than do others. To address the issue, a rule-of-thumb adjustment could be applied to the above allocation. For example, 60–65% of the total refinery process energy may be allocated to gasoline production, 18–20% to diesel production, and the remaining 13–22% to the production of other refining products (General Motors Corporation et al. 2001). However, no detailed analysis was done to confirm or disprove the rule-of-thumb allocation adjustment.

An alternative approach is to use a linear programming (LP) model to simulate operation of a typical (or notional) refinery with certain crude quality, product slate, and product quality. Linear programming simulations can provide detailed information that is representative of petroleum refining. This approach might be criticized because a simulated refinery differs from an actual one in terms of configuration, refining technology advancements, crude oil quality, and product quality. Of course, the simulation could be calibrated to an actual refinery or an aggregate of refineries. But such an analysis would be expensive, and the data are proprietary and generally available only through petroleum refining engineering consultants or refinery operators.

For these reasons, we present a methodology that is less compelling theoretically but overcomes the problem of data availability. Our alternative approach is based on energy and mass balances of individual refining processes within a refinery, which appears to be similar to the methodology used in Furoholt (1995). Our approach follows material and energy flows through individual refining processes and allocates energy use in these processes to petroleum products using proper weighting factors. We then determine total energy use for producing a given petroleum product by adding energy use allocated to the product for all the refining processes involved in producing that product. The differences between our study and Furuholt's study lie in the following areas. First, our refining processes are based on the mass and energy flows of a simplified, generic U.S. refinery, while Furuholt's processes were based on a European refinery. Second, we analyzed major refinery products including gasoline, diesel, LPG, residual oil, etc., while Furuholt examined regular gasoline, gasoline with methyl tertiary butyl ether (MTBE), and diesel.

1 Methodology

For our analysis, we developed a refinery process flow chart (**Fig. 1**) that we based on data provided in Brown et al. (1996) to demonstrate our methodology. The chart shows major refining processes that are interconnected by energy and material streams (for presentation purpose, only products and intermediate streams are shown). The Brown et al. study incorporated an appropriate level of detail, was prepared as part of a comprehensive energy analysis, and is available without violating confidentiality of information for a given petroleum refinery.

Fig. 2 shows a refining process with multiple input streams (S_1 and S_2) and output streams (P_1, P_2, and P_3). The input streams might be feedstocks or intermediate products. The output streams might be intermediate or final products. Each stream has two attributes: a weighting factor, *w* (mass-, energy content-, or market value-based) and an embedded energy (H) (in MJ). Embedded energy is simply the cumulative process energy that has to be expended to create the stream. Thus, if the stream in question is a final product stream, H is the cumulative process energy invested in that final stream. The sum of embedded energy over multiple production processes for a fuel product is taken to be the total process en-

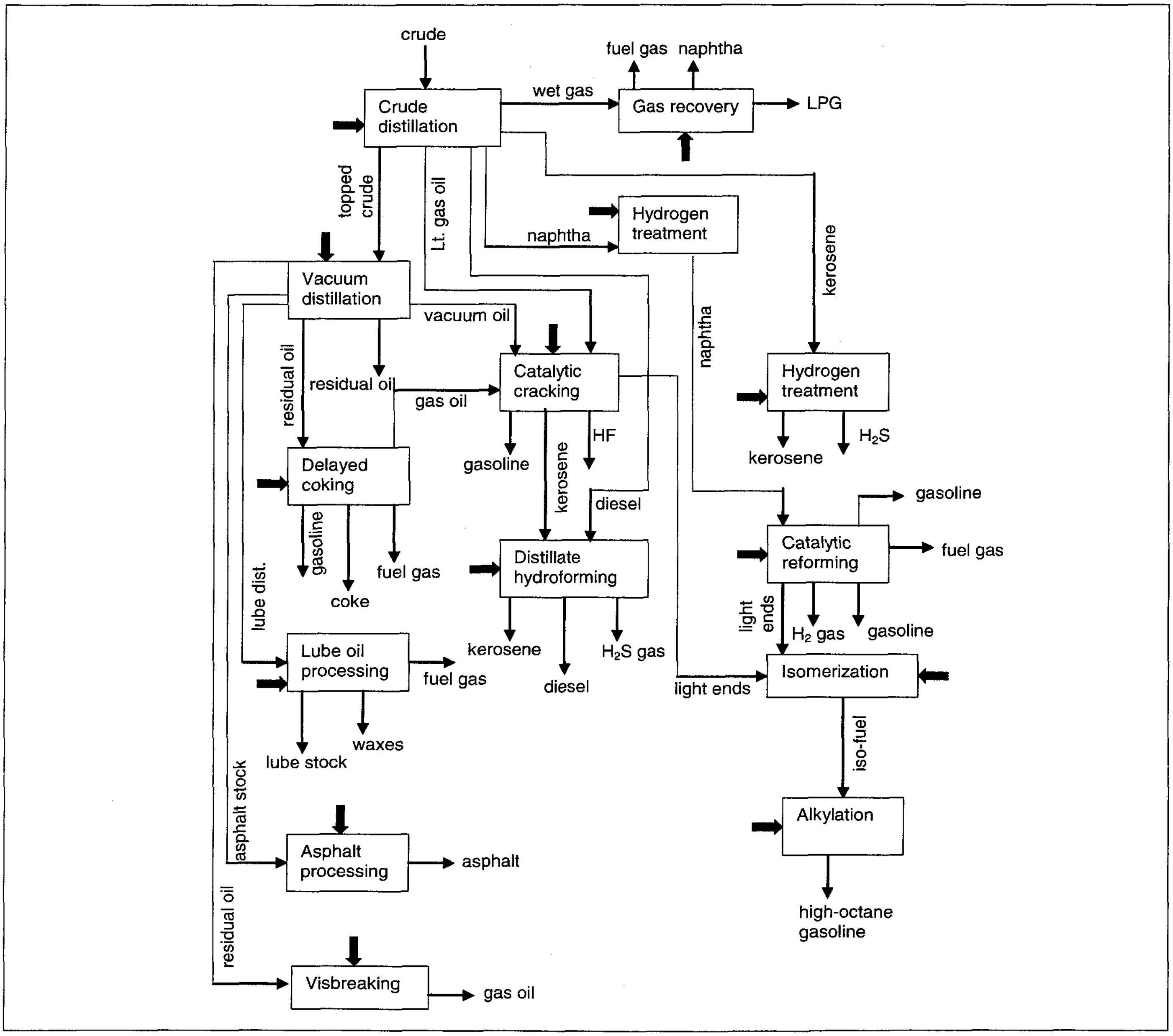

Fig. 1: Process flow in a petroleum refinery (solid block arrows represent unit process energy [process fuels, electricity, and steam])

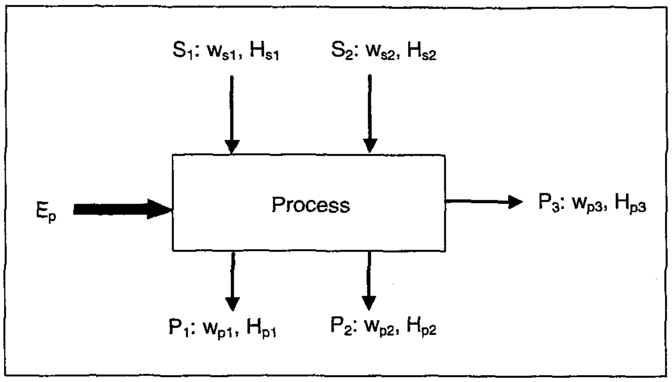

Fig. 2: A schematic flow of a refining process

ergy use for that product. The essence of our approach is to calculate the embedded energy (H) for each product. For any processing unit in this flow chart, an outgoing stream either goes into another unit as a feedstock or it becomes a final product stream. An outgoing stream never becomes a part of process energy for other units.

Process energy (E_p), (in MJ) represented by a solid black arrow, can be in the form of process fuels, steam, or electricity. Some processes consume all three of these energy sources. We must differentiate the three energy sources because they are characterized by different emission profiles.

Energy carried in from the input streams (H_{s1} or H_{s2}) represents the cumulative process energy expended from the very first process (e.g., atmospheric distillation) to the current process. With incoming energy (H_{s1} and H_{s2}) and current process energy use (E_p), the cumulative energy invested so far for stream P_1 can be allocated according to the following equation:

$$E_{p1} = (H_{s1} + H_{s2} + E_p) \times w_{p1} / (w_{p1} + w_{p2} + w_{p3}) \qquad (1)$$

where the quantity W_{p1} (i=1, 2, and 3) is the weight used to distribute the energy. This value is determined on the basis of mass, energy content, or market value share of the three product streams.

This allocation is repeated for all output streams from the refining process under evaluation. After we complete the allocation calculation for all processes in the refinery, we can obtain the product-specific energy use for a final fuel product by summing the energy use of all production processes for that fuel. For example, we obtain the value of energy use for refining gasoline by adding up the H values from all gasoline production processes within the refinery.

If we use a mass-based allocation, stream mass serves as the weighting factor for distributing energy among different streams. This seems to be a rational choice, because in each refining process, energy use is usually proportional to the mass of products processed. Some analysts may favor the energy-content-weighting approach because the primary use of most refinery products is to obtain energy by burning them. In the energy-content-based approach, we calculate the weights by multiplying the mass of each stream by the lower heating value (LHV) of the stream.

Using fuel mass or energy content (heating value) as the weight to distribute process energy provides an engineering perspective for distributing process energy use and the resulting emissions. A third allocation can be carried out using fuel product market values because some of the fuel products can be sold at significantly higher prices than can others, even though their heating values may differ only moderately. For example, gasoline and residual (or heavy) oil have LHVs of 43,540 J/g and 41,310 J/g, respectively, but gasoline can be sold at an average price of \$9.62/10^3 MJ in the U.S. market; residual oil is sold at a much lower average price of \$2.55/10^3 MJ. Because the decision to build a refinery is based on potential economic returns, the market-value-based allocation method could capture economic decisions associated with whether and how to build a refinery. Using a fuel's market value as the allocation weight to distribute process energy can have considerable effects on energy allocations. For the market-value-based allocation, we determine the allocation weight of a given stream by multiplying the stream mass by the product of LHV and the market value (based on LHV) of that stream.

2 Data Sources and Data Processing

2.1 Petroleum refinery flow chart

The flow chart and associated data, adapted from Brown et al. (1996), provided mass and energy balances for a refinery and for each refining process. With a few minor exceptions, we found these mass and energy balances to be internally consistent. However, we were concerned that (1) the refinery data sources are not well documented, and (2) it is unclear whether LHV or higher heating value (HHV) was used in converting process energy from mass units to energy units. We use a fuel's LHV to perform the conversion because the recovery of heat from water vapor in combustion products is not practical in the motor vehicles that we intend to evaluate eventually.

In addition to using a fuel's LHV to convert process energy, we had to make additional assumptions regarding stream compositions in cases where stream labeling is ambiguous. In several processes, one of the output streams was labeled 'fuels.' For these processes, we made the following assumptions:

(1) In the delayed coking process, we changed the stream label 'fuels' to 'gasoline.' Although this stream can be either a naphtha or gasoline fraction, the light cut of this stream is frequently isomerized to improve its octane number, or it is blended directly into finished gasoline; the heavy cut is generally fed into a catalytic reformer and eventually the reformate is blended into gasoline.

(2) In the distillate hydroforming process, the two input streams were labeled kerosene and diesel. Because the primary purpose of this unit is to reduce sulfur content in fuel products, we split the original single output stream labeled 'fuels' into two streams: kerosene and diesel. We prorated the masses of the two split streams according to the incoming stream masses.

(3) In the catalytic reforming process, an output 'fuels' stream was missing in the flow chart, according to the accompanying data sheet. Instead of labeling the stream 'fuels,' as indicated in the data sheet, we labeled it 'gasoline' because more than 85% of the volume yield is reformate.

(4) In the gas recovery process, we assumed that the stream labeled 'fuel products' was naphtha.

(5) We hope to obtain additional process flow data from more recent sources. At the time of this writing, we used the best data source available to us. Updated refinery data can be readily incorporated into the methodology that we developed here.

2.2 Energy contents and market values of petroleum products

As discussed in Section 2, allocation of petroleum refining process energy use and emissions can be based on mass, energy content, or market value share of individual refinery products (streams.) Brown et al. did not provide fuel energy contents (heating values) or market values for intermediate and final fuel products. For petroleum final products, these data can be found in the open literature, but for refinery intermediate streams, these values have to be estimated. For energy content-based allocation, we completed the following data processing steps to obtain the energy contents of products. LHVs are used in our analysis for the reasons mentioned in Section 3.1 and for consistency with the GREET model. When LHVs are available from the GREET model, they are taken from the model. When heat content for an intermediate stream is not available from the GREET model or other literature, but an API (American Petroleum Institute) gravity can be obtained for the stream, both LHV and HHV can be obtained from a heat of combustion chart (Himmelblau 1982) by using the stream's API gravity value. If none of the values (HHV, LHV, or API gravity) is known, a density value is substituted for specific gravity to calculate HHV, using the equation ($Q = 12400 - 2100d^2$ cal/g) (Speight 1991), and 90% of the calculated HHV value is taken to be the LHV for the stream.

Market prices for most product streams are taken from EIA's *State Energy Price and Expenditure Report 1999* (EIA 2001a). These prices are end user prices. Common petroleum products are generally sold to several sectors. Diesel fuels, for example, are sold to residential, commercial, industrial, and transportation sectors. For common fuels for which both sector-specific consumption data and sector-specific price data are available, we take into account sector market price variations by averaging fuel prices across sectors using sector consumption data (EIA 2001b) as weighting factors. Petroleum product prices from EIA's *State Energy Price and Expenditure Report* are given in dollars per unit of energy. Although it is not stated explicitly, we believe that the EIA database uses HHVs to represent energy content. Hence, we have converted EIA's prices to LHV-based prices.

The estimation for fuel (stream) energy content and market value introduces uncertainties into allocation weighting factors, particularly for the market-value-based method, because refinery intermediate streams are generally intended to use internally or as feedstocks for downstream processes, instead of being sold in the marketplace. Nevertheless, the allocation method that employs market values as weighting factors provides an economic perspective for distributing the energy use and emissions of a refinery among refinery products.

3 Results

3.1 Allocation by product mass

The results of process energy allocation among refinery products using product/stream mass as weights are summarized in Table 1. The product mass split (column 2) and energy allocation results (columns 4–7) are for one kg of crude input. As the last row of the second column shows, there is a 1% mass imbalance. For a refined product fuel, each entry in a column represents the energy use of the corresponding energy source (e.g., fuel, electricity, or steam) over all processes refining that fuel. The next four columns show the splits of energy use in different forms. Although the emissions calculation is not reported here, emissions can be estimated on the basis of the energy results in models such as GREET.

For this particular refinery, 46% (by weight) of the final products is gasoline. If we used this product split to allocate energy use at the refinery level, we would allocate 46% of the fuel, steam, and electricity use in the petroleum refinery to gasoline production. However, when we allocate energy use at the refining *process* level, accounting for process-dependent gasoline production, 61.3% of process fuels, 53.5% of electricity, and 27.6% of steam are allocated to gasoline. The difference between the refinery-level- and the refining-process-level-based allocations is substantial. Similar differences in energy allocation can be expected for other fuels when using the two levels of allocation. Furthermore, energy use information for other refining products (e.g., lube oil) can be determined by means of the process-level-based allocation approach. For example, production of lube oil blendstock requires a considerable amount of steam (much more than fuel and electricity), relative to production of other products. This fact has a considerable impact on estimating emissions associated with producing lubricating oils. Without categorizing process energy forms and going one step deeper – into process-level energy allocation – the higher energy levels associated with lube oil production would be difficult to identify.

The last column in **Table 1** shows the relative energy intensity associated with producing individual fuels. The relative energy intensity is defined as the ratio of total energy use share to the mass share of a given fuel. In this way, the energy intensity of a petroleum refinery as a whole is one. As discussed in Section 4.5, the relative energy intensity value is needed to obtain product-specific efficiencies from an overall refinery plant efficiency. By using this approach of calculating product-specific efficiencies from the refinery plant overall efficiency and product-specific relative energy intensities, we implicitly assume that allocations of total refinery energy use among different petroleum products remain the same even as the refinery plant's overall efficiency changes. This is an approximation from real-world refinery operation. Ideally, we would prefer to go through the same steps for a new refinery with a new overall plant efficiency as we have gone through for the simplistic refinery examined in this study.

The relative energy intensity results show that production of lube oil and asphalt is very energy intensive, and therefore could generate considerable emissions. Caution should be taken for these products. Because output shares of these products are so small, a small change in energy use can change the relative energy intensity significantly.

Table 1: Mass-based process energy allocation by final product: 1 kg of crude feed

Final Product	Mass (kg)	Mass Share (%)	Allocated Energy Use (KJ)				Allocated Energy Use Share (%)				Energy Intensity (%)
			Fuel	Electricity	Steam	Total	Fuel	Electricity	Steam	Total	
Residual oil	0.004	3.4	0.1	1.7	5.2	0.4%	0.2%	0.1%	0.3%	0.2%	44.2%
Fuel (still) gas	0.044	65.5	4.5	30.5	100.5	4.4%	3.0%	4.4%	4.7%	3.4%	78.2%
Naphtha	0.001	0.5	0.1	0.9	1.5	0.1%	0.0%	0.1%	0.1%	0.1%	52.4%
Diesel	0.094	146.3	9.3	39.4	195.0	9.3%	6.7%	9.2%	6.1%	6.6%	71.1%
Kerosene	0.137	188.6	11.2	44.5	244.3	13.6%	8.6%	11.2%	6.8%	8.3%	61.1%
Gasoline	0.465	1345.6	53.9	183.5	1583.0	46.0%	61.2%	53.5%	28.2%	53.7%	116.6%
LPG	0.058	31.2	5.8	51.7	88.7	5.7%	1.4%	5.8%	8.0%	3.0%	52.4%
Gas oil	0.045	128.2	2.9	19.1	150.2	4.5%	5.8%	2.9%	2.9%	5.1%	114.3%
Heavy fuel oil	0.040	66.4	3.4	14.4	84.1	4.0%	3.0%	3.4%	2.2%	2.9%	72.1%
Lube stocks	0.070	113.5	5.4	204.9	323.8	6.9%	5.2%	5.4%	31.6%	11.0%	158.5%
Asphalt	0.020	47.8	1.5	23.8	73.1	2.0%	2.2%	1.5%	3.7%	2.5%	125.3%
Waxes	0.009	14.6	0.7	26.3	41.6	0.9%	0.7%	0.7%	4.1%	1.4%	158.5%
Coke	0.005	12.7	0.3	3.7	16.7	0.5%	0.6%	0.3%	0.6%	0.6%	114.2%
H_2 gas	0.005	17.1	0.6	1.1	18.9	0.5%	0.8%	0.6%	0.2%	0.6%	129.3%
H_2S gas	0.013	16.3	0.9	4.1	21.3	1.3%	0.7%	0.9%	0.6%	0.7%	56.1%
Total	1.010	2197.8	100.7	649.4	2947.9	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%

3.2 Allocation by product energy content

For the energy-content-based allocation method, we determined the weighting factor (*w*) for an individual refinery stream to be the product of the stream's mass (g) and its heat content (kJ/g). The allocation results are provided in Table 2, which shows that the allocated energy uses for individual refinery products are quite similar to those obtained by the mass-based allocation method described in Section 4.1. This finding is not surprising because petroleum product heating values generally deviate only moderately from that of crude oil. If all refining products had the same energy content per unit of mass, the two allocation methods would give identical results. We do see, however, that refinery products with energy contents (per unit mass) higher than that of crude (e.g., kerosene, diesel, and LPG) get larger allocations than those with energy contents lower than that of crude (e.g., asphalt and coke). As Table 2 shows, the allocated energy use for diesel, kerosene, fuel gas, and hydrogen increases slightly, while the allocated energy use for others decreases slightly.

Table 2: Energy content-based process energy allocation by final product: 1 kg of crude feed

Final Product	Mass (kg)	Mass Share (%)	Allocated Energy Use				Allocated Energy Use Share (%)				Energy Intensity (%)
			Fuel (kJ)	Electricity (kJ)	Steam (kJ)	Total (%)	Fuel	Electricity	Steam	Total	
Residual oil	0.004	3.1	0.1	1.6	4.8	0.4	0.1	0.1	0.2	0.2	41.3
Fuel (still) gas	0.044	92.9	6.2	42.1	141.2	4.4	4.2	6.1	6.5	4.8	110.0
Naphtha	0.001	0.5	0.1	0.9	1.5	0.1	0.0	0.1	0.1	0.1	50.9
Diesel	0.094	147.6	9.4	39.9	196.9	9.3	6.7	9.3	6.1	6.7	71.8
Kerosene	0.137	192.5	11.5	45.6	249.6	13.6	8.8	11.4	7.0	8.5	62.4
Gasoline	0.465	1334.7	53.6	184.4	1572.6	46.0	60.7	53.2	28.4	53.3	115.9
LPG	0.058	28.4	5.1	44.8	78.3	5.7	1.3	5.0	6.9	2.7	46.2
Gas oil	0.045	126.6	2.9	18.6	148.1	4.5	5.8	2.9	2.9	5.0	112.7
Heavy fuel oil	0.040	58.9	3.1	12.8	74.8	4.0	2.7	3.0	2.0	2.5	64.0
Lube stocks	0.070	111.4	5.3	202.1	318.8	6.9	5.1	5.3	31.1	10.8	156.0
Asphalt	0.020	46.8	1.5	23.5	71.8	2.0	2.1	1.5	3.6	2.4	123.0
Waxes	0.009	14.7	0.7	26.6	42.0	0.9	0.7	0.7	4.1	1.4	160.0
Coke	0.005	12.1	0.3	3.6	16.0	0.5	0.6	0.3	0.6	0.5	109.6
H_2 gas	0.005	21.2	0.8	1.4	23.4	0.5	1.0	0.8	0.2	0.8	160.3
H_2S gas	0.013	6.2	0.3	1.6	8.2	1.3	0.3	0.3	0.2	0.3	21.5
Total	1.010	2197.8	100.7	649.4	2947.9	100.00	100.0	100.0	100.0	100.0	100.0

It is worth pointing out that, because heating values of most refining products deviate only slightly from that of crude, the changes are so small that inaccuracies in product/stream heating values can lead to results that we know intuitively are incorrect. For example, the heating value of gasoline is higher than that of crude; however, the allocated energy use for gasoline calculated by the energy-content-based method decreases slightly. If all heating values used as weighting factors in our allocation method are accurate, allocated energy use for those products with high energy contents should increase. The inaccuracy could be caused by the ambiguity in stream composition and estimates of heating contents for intermediate streams. To gauge the accuracy of our estimates for intermediate stream heating values, we calculated the total energy content of all refinery products. Ideally, this value should be equal to the energy content of one kg of crude. The estimated energy content of the entire slate of refined products is 4.13% more than that of one pound crude. This inaccuracy could be the primary cause for the decreased energy use for gasoline.

3.3 Allocation by product market value

As stated in Section 1, the decision of whether and how to build a refinery is made on the basis of the potential economic returns of the plant. The market-value-based allocation method could reflect that decision making process. **Table 3** summarizes the results of the market-value-based allocation method. The table shows that this approach redistributes the total energy use in the refinery considerably among refinery products. Because diesel, lube oil, and waxes can be sold at much higher market prices than other products, they are allocated more energy use using this method. On the other hand, residual oil and fuel gas, which have lower market values (if the latter were to be sold in the market at all), are allocated less energy use shares. The overall distribution from this allocation method, however, is still similar to that from the mass-based allocation method. The decrease in steam use for production of gasoline is primarily attributable to the increase in steam use for production of lube oil and waxes.

The market-value-based method involves greater uncertainties than either mass- or energy content-based methods. The first uncertainty is with the estimation of market values for intermediate streams (e.g., light ends) that are generally used as plant fuel or feedstock for downstream refining processes and are not intended for sale in the market. In such cases, the price of a refinery product with similar energy content was used (for example, the price of natural gas sold to electric utilities was used to approximate the price of fuel gas because the two contain similar energy and could serve the same purpose).

The second uncertainty is caused by the lack of a physical basis for using market values as weighting factors. The use of mass and energy content as weighting factors is not only consistent with our intuition that energy consumption is tied to the amount of mass processed and to the energy content of that mass, but it is also consistent with conservation of mass and energy during refinery processes. For one kg of crude input, the sum of the mass of all final products should be equal to one kg, and the sum of the energy content of all products should be equal to the energy content in one kg of crude. This mass and energy conservation constraint guarantees that the sum of all relative weighting factors would be equal to unity. However, there is no such constraint for market values, although the market price for a refinery product should have a strong correlation with its energy content, the prices are really determined by the demand and supply balance. The lack of theoretical constraint is directly connected with the fact that the sum of weights (normalized) used in the

Table 3: Market value-based process energy allocation by final product: 1 kg of crude feed

Final Product	Mass (kg)	Mass Share (%)	Allocated Energy Use				Allocated Energy Use Share (%)				Energy Intensity (%)
			Fuel (kJ)	Electricity (kJ)	Steam (kJ)	Total (%)	Fuel	Electricity	Steam	Total	
Residual oil	0.004	2.3	0.0	1.3	3.7	0.4	0.1	0.0	0.2	0.1	31.4
Fuel (still) gas	0.044	31.3	2.5	17.7	51.5	4.4	1.4	2.5	2.7	1.7	40.1
Naphtha	0.001	0.3	0.1	0.7	1.1	0.1	0.0	0.1	0.1	0.0	36.7
Diesel	0.094	181.7	10.8	48.9	241.4	9.3	8.3	10.7	7.5	8.2	88.0
Kerosene	0.137	156.7	8.6	35.5	200.8	13.6	7.1	8.6	5.5	6.8	50.2
Gasoline	0.465	1469.1	60.4	201.2	1730.8	46.0	66.8	60.0	31.0	58.7	127.5
LPG	0.058	26.1	6.4	57.0	89.5	5.7	1.2	6.4	8.8	3.0	52.9
Gas oil	0.045	116.7	2.7	15.4	134.7	4.5	5.3	2.6	2.4	4.6	102.6
Heavy fuel oil	0.040	18.9	1.0	3.9	23.8	4.0	0.9	1.0	0.6	0.8	20.4
Lube stocks	0.070	119.6	5.4	210.4	335.4	6.9	5.4	5.4	32.4	11.4	164.2
Asphalt	0.020	42.5	1.4	22.0	66.0	2.0	1.9	1.4	3.4	2.2	113.0
Waxes	0.009	19.4	0.9	34.0	54.3	0.9	0.9	0.9	5.2	1.8	206.5
Coke	0.005	2.1	0.0	0.6	2.8	0.5	0.1	0.0	0.1	0.1	18.9
H_2 gas	0.005	11.0	0.4	0.8	12.2	0.5	0.5	0.4	0.1	0.4	83.7
H_2S gas	0.013	0.0	0.0	0.0	0.0	1.3	0.0	0.0	0.0	0.0	0.0
Total	1.010	2197.8	100.7	649.4	2947.9	100.0	100.0	100.0	100.0	100.0	100.0%

market-value-based approach is not equal to unity. Finally, because market prices fluctuate over time, the results with the market-value-based method will fluctuate over time.

The fact that similar overall distribution results were obtained for the market-value-based allocation method and the other two allocation methods is partly attributable to assumptions made about the prices of intermediate streams. For example, we assumed that the prices of vacuum oil, a feedstock to visbreaker and delayed coker processes, are the same as that of residual oil, and that the prices of light ends, wet gas, and still gas are the same as that of natural gas sold to electric utilities. The effect of such simplification is to essentially homogenize the weighting factors among products and intermediate streams, leading to allocation results similar to those yielded by the mass-based allocation method.

3.4 Comparisons between refining-process-level-based allocations and refinery-level-based allocations

To see the differences in energy allocation obtained by using the process- vs. the refinery (aggregate)-level allocation approaches, we calculated refinery-level-based energy allocation using EIA's petroleum supply data for 2001 (EIA 2002) for major petroleum fuel products (i.e., gasoline, diesel, LPG, kerosene, and residual oils). For this allocation estimation, the petroleum refinery yield data were from EIA's data; the energy contents and market values of the products were obtained from several sources including EIA. Note that for the process-level-based energy allocation, energy shares for residual oil and heavy fuel oil were combined. For the refinery-level-based allocation, because it is difficult to know the composition of the 'others' category, its energy content and market value were treated the same as that for residual oil.

Table 4 shows significant differences in allocated energy use between the process-level-based and the refinery-level-based allocation approaches. For the refinery-level-based allocation, the mass-based method results in refinery energy shares of 37.5% for gasoline, 19.1% for diesel, and 7.1% for LPG (these are the mass shares of these products). For the process-level-based allocation, the mass-based method results in 52.4%, 6.6%, and 3.3% of the total energy use for gasoline, diesel, and LPG, respectively. The large differences in allocated gasoline and diesel energy use are attributable to (1) the two different levels at which allocations are conducted, and (2) the difference in the output slate between the refinery used in this study and that of current aggregate U.S. refinery output. In particular, while the U.S. refinery industry produces 37.5% gasoline, 19.1% diesel, and 7.1% LPG, respectively, the refinery that we analyzed here had outputs of 46.5%, 9.4%, and 5.8% for gasoline, diesel, and LPG, respectively.

For the same level-based allocation, there are also differences in allocated energy use among the different weighting factor bases. For the refinery-level-based allocation, we observe that energy use allocated to residual oil and diesel increased slightly from the mass-based method to the energy-content-based method and then to the market-value-based method. Energy use allocated to gasoline was considerably increased. Energy use allocated to kerosene and LPG increased from the mass-based method to the energy-content-based method, but decreased from the energy-content-based method to the market-value-based method. Energy use allocated to the 'others' category decreased considerably. For the process-level-based allocation, however, changes in energy shares are relatively small among the three weighting factor bases. The marked differences in energy allocations at the refinery level are primarily caused by using residual oil's energy content and market value as weights for the 'others' category to distribute energy use. Because we do not know the composition of the 'others' category, it is hard to calculate its weighting factor. The approximation of the weighting factors for the 'others' category with residual oil's weighting factors could lead to considerable under-weighting of the 'others' category for energy-content- and market-value-based methods because some products (e.g., naphtha, light ends) in the 'others' category have higher energy contents and some (e.g., lube stock, waxes) have much higher market values than residual oil. Because the total product shares have to be equal to one, a large increase in gasoline share and a small increase in diesel share result from this underestimation. This comparison shows a shortcoming of the refinery-level-based allocation, especially for energy-content- and market-value-based methods. Without detailed knowledge of energy balance at the refining process level, the refinery-level approach could overestimate energy use for some products but underestimate energy use for others.

3.5 Calculated energy efficiencies for individual petroleum products

In fuel-cycle analyses of vehicle/fuel systems, energy efficiencies for transportation fuels are often used to determine which fuels are efficient to produce. Furthermore, efficiency values for individual fuels can be used in fuel-cycle models such as GREET

Table 4: Energy allocation for refinery products at the refinery plant level and at the refining process level

Product	Refinery Plant Level (%)			Refining Process Level (%)		
	Mass	Energy Content	Market Value	Mass	Energy Content	Market Value
Residual oil[a]	5.2	5.3	1.9	3.0	2.7	0.9
Diesel	19.1	19.9	21.2	6.6	6.7	8.2
Kerosene	8.9	9.0	5.3	8.3	8.5	6.8
Gasoline	37.5	41.6	57.6	53.7	53.3	58.7
LPG	7.1	8.8	8.4	3.0	2.7	3.0
Others[b]	22.2	15.4	5.7	25.4	26.2	22.3

[a] For the refining-process-level-based allocation, energy use for residual oil and heavy fuel oil were added together.

[b] The 'others' category includes many refinery products. Here we use residual oil's energy content and market value as weights to allocate energy use to this category.

to simulate total energy use and emissions for a fuel cycle. By using the estimated energy use for individual petroleum refinery products presented in the preceding sections, we can calculate efficiencies for individual petroleum products. Product efficiency is defined as the ratio of energy content in the product to the sum of product energy content and energy use in producing the product, as shown in the following equation:

$$\eta_s = \frac{e_s}{e_s + e_p} \qquad (2)$$

where e_s and e_p are energy content of the product and total energy use (or embedded energy) to produce the product, respectively. Both energy content and energy use in our calculations are based on LHV.

By introducing a product relative energy intensity χ_s (i.e., the ratio of energy use share to production mass share for a given product), we can obtain the energy efficiency η_s for a given refinery product from a refinery's overall efficiency η_o and the product's relative energy intensity:

$$\eta_s = \frac{1}{1 + \chi_s(1/\eta_o - 1)} \qquad (3)$$

Equation (3) provides a relationship among product efficiency, product relative energy intensity, and plant overall efficiency. The equation shows that product efficiency increases if the overall plant efficiency increases, while product energy intensity is kept constant. On the other hand, product efficiency decreases if its relative energy intensity increases, while the plant overall efficiency is constant. The particular refinery evaluated in this study has an overall efficiency of 93.1%. With this plant efficiency and relative energy intensities for petroleum products (as presented in Tables 1–3), we calculated the energy efficiencies of individual refinery products by using Equation (3). The results are shown in **Table 5**.

The plant overall efficiency of 93.1% seems too high for current U.S. refineries. One reason for this is that the refinery evaluated in Brown et al. (1996) could represent a simple refinery, while current U.S. refineries are usually complex, with configurations for high gasoline production. Also, U.S. refineries have been under pressure in the past 10 years to produce better-quality fuels, although the quality of crude input to refineries has been deteriorating. All these factors contribute to increased energy use in U.S. refineries in recent years. The current U.S. refineries are believed to have an overall efficiency of around 87.8% (see General Motors Corporation et al. 2001). Using an overall efficiency of 87.8%, instead of 93.1%, we calculated the so called adjusted product efficiencies (see Table 5).

Table 5 shows that production of gasoline is less efficient than production of other fuels (e.g., diesel, kerosene, and LPG). This finding is consistent with our understanding that refining of a fuel (such as gasoline) that involves more intensive refining processes generally requires more energy. The identical efficiencies (with the mass-based weighting factors) of naphtha and LPG are coincidental. It is interesting to note that production of lube oil stock, waxes, and asphalt is actually more energy intensive than production of gasoline, even though production of the former requires fewer refining processes (see Fig. 1). Tables 1 through 3 reveal that production of these products requires significantly more steam than production of other refinery products, causing their high relative energy intensities.

3.6 Well-to-pump energy use and greenhouse gas emissions of transportation fuels

To illustrate the effects of allocated energy use for petroleum-based transportation fuels on their total energy use and greenhouse gas (GHG) emissions from crude recovery wells to fuels available at pumps of refueling stations (well-

Table 5: Energy efficiencies of individual refinery products

Refinery Product	Product Efficiency for the Evaluated Refinery (%)[a]			Product Efficiency for a Current Typical U.S. Refinery (%)[b]		
	Mass-Based	Energy Content-Based	Market Value-Based	Mass-Based	Energy Content-Based	Market Value-Based
Residual oil	96.8	96.8	97.5	94.1	94.2	94.9
Fuel (still) gas	94.4	93.5	97.3	90.0	88.5	94.5
Naphtha	96.0	96.2	97.3	92.7	93.1	94.5
Diesel	95.0	95.0	94.0	91.0	91.0	88.1
Kerosene	95.7	95.7	96.5	92.2	92.1	92.9
Gasoline	92.3	92.3	93.1	86.4	86.4	86.5
LPG	96.0	96.0	95.6	92.7	92.7	91.1
Gas oil	92.4	92.5	93.2	86.6	86.7	86.7
Heavy fuel oil	95.0	95.3	98.5	91.0	91.5	97.0
Lube stocks	88.6	88.7	88.0	80.5	80.7	77.6
Asphalt	91.4	91.5	92.2	84.9	85.1	84.9
Waxes	88.6	88.8	85.7	80.5	80.8	74.0
Coke	92.2	92.6	98.7	86.3	86.9	97.2
H_2 gas	91.5	89.7	95.0	85.1	82.2	89.9
H_2S gas	96.0	97.2	NE	92.7	94.9	NE

[a] Refinery product efficiencies were estimated from an overall refinery efficiency of 93.1% (for the refinery evaluated in this study) and product relative energy intensities presented in Tables 1–3.

[b] Refinery product efficiencies were estimated from an overall refinery efficiency of 87.8% (for a current U.S. refinery) and product relative energy intensities presented in Tables 1–3.

to-pump [WTP]), we calculated WTP total energy use and GHG emissions for gasoline, diesel, LPG, and naphtha by using the GREET model. Currently, naphtha is a petrochemical feedstock. Some maintain that when fuel-cell vehicles are introduced to the market, naphtha could become a fuel-cell vehicle fuel.

The GREET model contains detailed calculations of energy use and emissions from petroleum recovery, transportation, refining (which we updated through this study), and petroleum product transportation and storage. In GHG emissions calculations, besides emissions from process fuel combustion, we included CO_2 and CH_4 emissions from gas flaring and venting and crude processing in oil fields. For details about GREET's calculations, see Wang (1999) and other reports posted at http://greet.anl.gov.

In GREET simulations, we included five cases for each of the fuels: (1) the energy-content-based allocation at the refinery level; (2) the energy-content-based allocation at the refinery level with rule-of-thumb adjustments; (3) the mass-based allocation at the process level; (4) the energy-content-based allocation at the process level; and (5) the market-value-based allocation at the refinery level. All five cases are for a current U.S. refinery with an overall energy efficiency of 87.8%. For the first case, each of the fuels has an energy efficiency of 87.8% – the overall efficiency of the refinery. For the second case, the efficiencies are 85.5%, 89.0%, 93.5%, and 91.0% for gasoline, diesel, LPG, and naphtha, respectively. These are the efficiencies currently used in the GREET model. For the remaining three cases, energy efficiencies were calculated using equation (2) and are presented in Table 5.

In our analysis (presented in the preceding sections), we were able to determine the amount of process fuels, electricity, and steam required to produce each individual petroleum product. The above analysis was not able to specify the types of fuels for steam and electricity generation. We used GREET's default assumptions for electricity and steam generation for the calculations in this section. In particular, we assumed a U.S. average electricity generation mix under which more than 50% of electricity is generated from coal. We assumed that steam is generated in petroleum refineries with refinery gas and natural gas. For the process fuels consumed in refineries, the majority of them are refinery gas and natural gas.

Fig. 3 presents WTP energy use for the four fuels under the five cases. For gasoline, the GREET efficiency overestimates energy use for gasoline production, while the efficiency from the refinery-level allocation underestimates gasoline energy use. The three cases for process-level-based allocations have similar results. For diesel fuel, the WTP energy use for the process-level allocations with the mass- and energy-content-based weighting factors is smaller than that predicted with the refinery-level allocations. However, the process-level allocation with the market-value-based weighting factors has results very close to those obtained by using the refinery-level allocations. The findings for gasoline and diesel fuel can be explained by looking at the products' relative energy intensities. Table 1 shows that lube stock, asphalt, and waxes are fairly energy intensive. That is, a great deal of energy has to be expended to produce them, which effectively takes away some energy burdens from other products such as gasoline and diesel – leading to smaller energy allocations to these products compared to those that result from refinery-level allocations. On the other hand, for the market-value-based weighting factors, because diesel fuel can be sold at a relatively high price, its allocated energy use increases, causing diesel fuel results similar to those obtained by using the refinery-level allocations.

For LPG, the refinery-level allocation significantly overestimates LPG energy use, while the other four cases have similar results. The slightly large energy use for the process-level allocation with market-value-based weighting factors is attributable to the fact that LPG can be sold at high prices. For naphtha, both the refinery-level allocation and the adjusted refinery-level allocation overestimate naphtha energy use. Naphtha is generally used as a feedstock to petrochemical processes, and not as a combustion fuel. So, estimated energy use for the process-level allocation with the market-value-based weighting factors is smaller than that predicted with the other four cases.

Fig. 4 shows WTP GHG emissions for the four fuels under the five cases. GHG emissions here are CO_2-equivalent emissions of CO_2, CH_4, and N_2O. The GHG emission patterns among the five cases for each of the fuels are similar to those of energy use.

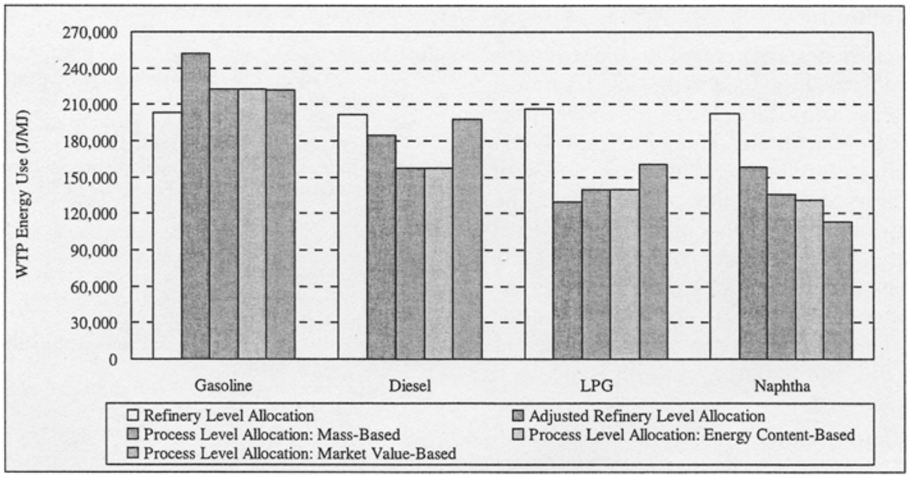

Fig. 3: Well-to-pump energy use for fuel production: joules per MJ of fuel available at fuel pump

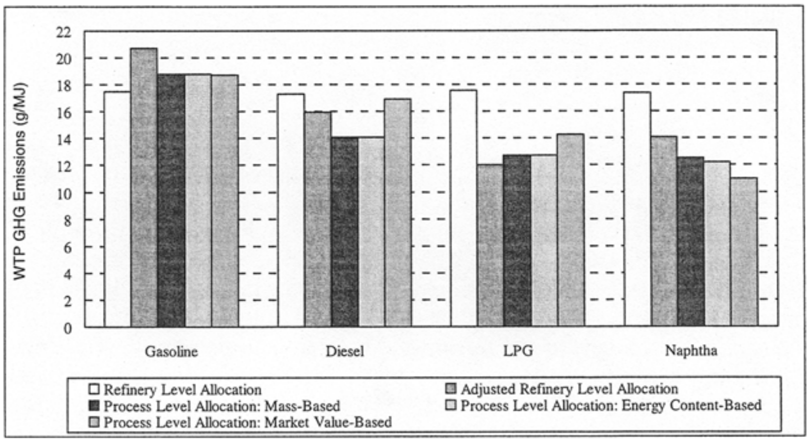

Fig. 4: Well-to-pump greenhouse emissions for fuel production: grams per mj of fuel available at fuel pump

4 Conclusions

We presented a refining-process-level-based method that can be used to allocate energy use of individual refining processes to refinery products. The process-level-based method captures process-dependent characteristics of fuel production within a petroleum refinery. The method starts with the mass and energy flow chart of a refinery, tracks energy use by individual refining processes, and distributes energy use of a given refining process to products from the process. In allocating energy use to refinery products, the allocation method could rely on product mass, product energy contents, or product market values as weighting factors. While the mass- and energy-content-based allocation methods provide an engineering perspective of energy allocation within a refinery, the market-value-based allocation method provides an economic perspective.

The results from this study show that relative energy intensities of individual refinery products, and consequently their energy efficiencies, vary significantly among refinery products. This finding implies that, without detailed energy allocations at the refining process level, researchers using an energy allocation approach at the aggregate refinery level could over-predict energy use for some refinery products but under-predict energy use for others. The new method is intuitively correct and can be easily adapted to future available refinery data. It can also be expanded to include new refining processes, such as a desulfurization unit, to estimate efficiencies for production of a reformulated or low-sulfur fuel.

We applied the energy efficiencies generated in this study for four petroleum-based transportation fuels to the GREET model to estimate WTP energy use and GHG emissions. To compare with the current practice, we estimated energy use and GHG emissions with energy allocations at the refinery level and with adjusted energy allocations at the refining process level. The results show that energy allocations either at the refinery level or at the process level can make a difference in evaluating the energy use and emissions of different fuels. Furthermore, for the process-level allocations, use of mass-, energy-content-, or market-value-based weighting factors can result in different results for diesel fuel, LPG, and naphtha.

5 Recommendations and Outlook

The allocation of energy use in petroleum refineries at the refining process level in this study follows the recommendation of ISO 14041 that allocations should be accomplished at the subprocess level when possible. We developed a method in this study that can be readily adapted for refineries in which process-level energy and mass balance data are available. The process-level allocation can reveal some additional energy and emission burdens associated with certain refinery products that are otherwise overlooked with the refinery-level allocation. When possible, process-level allocation should be used in life-cycle analyses.

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